Computation Aided Investigation of Radical Amination and Hydroxylation via Co(II)-Based Metalloradical Catalysis

By

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Abstract

Recent advancements have witnessed the deployment of radical chemistry for the construction of diverse vital molecular structures. Among these advances, metalloradical catalysis (MRC) has been continuously demonstrated as a practical and unique approach whereby open-shell metal-centered catalysts are exploited to initiate and regulate homolytic radical processes. As stable 15e-metalloradicals, Co(II) porphyrin complexes have been proven effective in activating multifarious precursors to forge unprecedented metal-stabilized organic radicals and are capable of conducting various homolytic processes with well-confined reactivity and selectivity thanks to the support of D_2-symmetric chiral porphyrin ligands. Nevertheless, the detailed mechanistic studies of the metalloradical activation of precursors, H atom abstraction (HAA), radical addition, and asymmetric induction have been largely underdeveloped. Therefore, this dissertation mainly focuses on the mechanistic investigations of radical amination and hydroxylation reactions via Co(II)-based MRC with routine experimental methods and powerful computational tools.

- **Chapter 1: Developments on Asymmetric *N*-Heterobicyclization Reactions of Alkenes via Enantioselective Transition Metal Catalysis.** We have viewed recent developments of asymmetric *N*-heterobicyclization of alkenes rendered by

enantioselective transition metal catalysis incorporating first-row, second-row, and third-row transition metals.

- **Chapter 2: Enantioselective Radical *N*-Heterobicyclization with A New Mode of Asymmetric Induction.** We have developed asymmetric radical *N*-heterobicyclization of allyl sulfamoyl azides with the support of a D_2-symmetric chiral bridged amidoporphyrin HuPhyrin ligand. We also revealed a new mode of asymmetric induction that the chirality of a kinetically stable chiral radical center directs the enantioselectivity of the resulting aziridines. The stable chiral radical center was formed from highly challenging enantiofacial selective radical addition and underwent subsequent stereospecific ring closure.
- **Chapter 3: Catalytic Radical *N*-Heterocyclization by Metalloradical C–H Amination involving 1,7-Hydrogen Atom Abstraction.** We have examined intramolecular HAA reaction and pushed its boundary from well-explored 1,5-HAA and 1,6-HAA to unusual 1,7-HAA executed by α-Co(III)-aminyl radicals, which led to the discovery of 1,7-C–H amination and 1,7-HAA triggered indirect 1,5-C–H amination with sulfamoyl azides.
- **Chapter 4: Metalloradical Activation of Alkyl Hydroperoxides for Catalytic Radical C−H Hydroxylation.** We have presented comprehensive studies on the metalloradical activation of oxidants, especially cumene hydroperoxide. We have identified ∞-Co(III)-hydroxide cumyloxyl radical species and utilized it for the development of radical C–H hydroxylation with cumyl alcohol as the byproduct.

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LIST OF ABBREVIATIONS

MRC: metalloradical catalysis

Por: porphyrin

TPP: tetraphenyl porphyrin

RA: radical addition

HAA: hydrogen atom abstraction

RS: radical substitution

TS: transition state

M: molar or metal

L: ligand

Me: methyl

MeO: methoxy

Mes: mesityl

Et: ethyl

iPr: isopropyl

^{t}Bu: tert-butyl

Ar: aryl

Ph: phenyl

Bn: benzyl

Bz: benzoyl

SO_2: sulfonyl

Ts: tosyl

CF_3: trifluoromethyl

BOX: bisoxazolines

PF_6: hexafluorophosphate

acac: acetylacetonate

Boc: *tert*-butoxycarbonyl

TBS: *tert*-butyldimethylsilyl

Ac: acetyl

His: histidine

Phe: phenylalanine

ee: enantiomeric excess

er: enantiomeric ratio

de: diastereomeric excess

dr: diastereomeric ratio

conv: conversion

equiv: equivalent(s)

rt: room temperature

DFT: density functional theory

NCI: non-covalent interaction

HPLC: high performance liquid

chromatography

HRMS: high resolution mass spectrometry

UV-Vis: Ultraviolet–visible spectroscopy

Å: angstrom

C: coulomb

e^-: electron

IR: infrared spectroscopy

NMR: nuclear magnetic resonance

ESI: electrospray ionization

DART: direct analysis in real time

EPR: electron paramagnetic resonance

SiO_2: silica gel

Al_2O_3: aluminium oxide

MS: molecular sieves

TEMPO: (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl

DMPO: 5,5-dimethyl-1-pyrroline *N*-oxide

PBN: *N*-*tert*-Butyl-α-phenylnitrone

$PhCH_3$: toluene

PhH: benzene

PhCl: chlorobenzene

DCM: dichloromethane

THF: tetrahydrofuran

Et_2O: diethyl ether

MeOH: methanol

EtOH: ethanol

TBME: *tert*-butyl methyl ether

MeCN: acetonitrile

DMSO: dimethyl sulfoxide

CCl_4: carbon tetrachloride

DBU: 1,8-diazabicyclo[5.4.0]undec- 7-ene

NMP: *N*-methylpyrrolidone

TMSOTf: trimethylsilyl trifluoromethanesulfonate

Et_3N: triethyl amine

Ph_3N: triphenylamine

DIPA: *N,N*-diisopropylethylamine

PPh_3: triphenylphosphine

K_2CO_3: potassium carbonate

PhIO: iodosobenzene

$PhI(OAc)_2$: (diacetoxyiodo)benzene

$AgClO_4$: silver perchlorate

CHP: cumene hydroperoxide

aq: aqueous

DEDICATION

I dedicate this dissertation to my family: Yi-Ge Wang (my wife), who has been an enduring source of unlimited support and encouragement during the challenges of graduate school and life; and my parents, Chuan-You Xu (my father), Fu-Ling Sun (my mother), whose unconditional love and support throughout my whole life has always given me the strength to move forward, and whose good examples have taught me to work hard for what I aspire to achieve. I am genuinely thankful for having all of you in my life.

Also, I want to dedicate this dissertation to the people that I met in my Master's program at Southern Methodist University: my professors, Professor Peng Tao, Professor Dieter Cremer, and Professor Elfi Kraka, who have made me a guide in computational chemistry, an interdisciplinary field of computational science and life science; my colleagues and friends, Li Shen, Dr. Yun-Wen Tao, Dr. Hong-Yu Zhou, Dr. Feng Wang, Dr. Qin Huang, Dr. Cao Jian, Dr. Stephen Budy and Dr. Caleb Bunton, who gave me tremendous help in research and life.

Lastly, I would like to dedicate this dissertation to world peace, which allows me to commit to my Ph.D. research.

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I thank my fellow lab mates, all the former and current Zhang group members for stimulating discussions, training on wet lab techniques, and all the fun we have had in the past several years. Also, I appreciate the help from my friends, Dr. Zhe-Hui(Zee) Li and Alexander Kaminsky. It is a great pleasure to interact with you people.

Last but not least, I would like to thank all the faculty members and supporting staff in the Department of Chemistry at Boston College.

CHAPTER 1 – DEVELOPMENTS ON ASYMMETRIC *N*-HETEROBICYCLIZATION OF ALKENES VIA ENANTIOSELECTIVE TRANSITION METAL CATALYSIS

1.1 INTRODUCTION

Enantioselective transition metal catalysis is a field certainly at the forefront of modern synthetic research.[1] Consequently, the growth of approaches that facilitate the practical synthesis of enantiopure compounds is of undeniable importance to the diverse domains of central science. Great amounts of efforts have been made on ligand scaffold design or catalyst engineering to leverage repulsive steric interactions between chiral ligands and substrates to disfavor one of the diastereomeric transition states kinetically and accommodate the attractive noncovalent interactions between the ligands and substrates to direct enantioselectivity.[2]

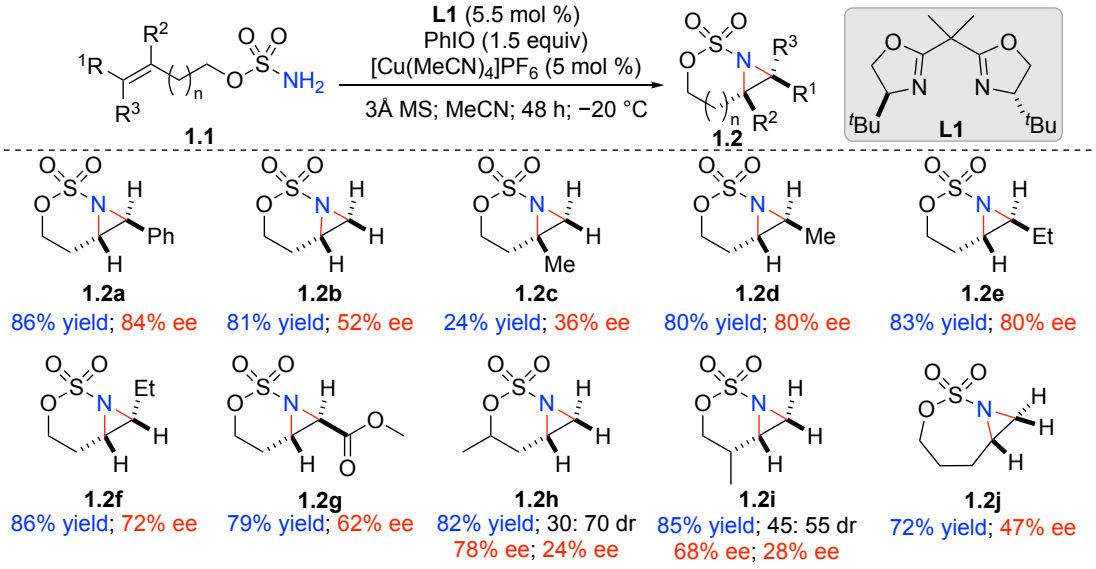
N-Heterobicyclization of alkenes (also known as intramolecular aziridination) is a robust synthetic approach to preparing valuable nitrogen-containing structural motifs. While the first aziridination was demonstrated nearly 60 years ago,[3] asymmetric *N*-heterobicyclization of alkenes rendered by transition metal catalysts has been slow to emerge. However, the recent ten years have witnessed the continuous deployment of first-row, second-row, and third-row transition metal catalysts to asymmetric *N*-

heterobicyclization of alkenes. Therefore, this chapter primarily covers the recent developments in asymmetric *N*-heterobicyclization of alkenes via enantioselective transition metal catalysis.

1.2 COPPER-CATALYZED ASYMMETRIC *N*-HETEROBICYCLIZATION OF ALKENES

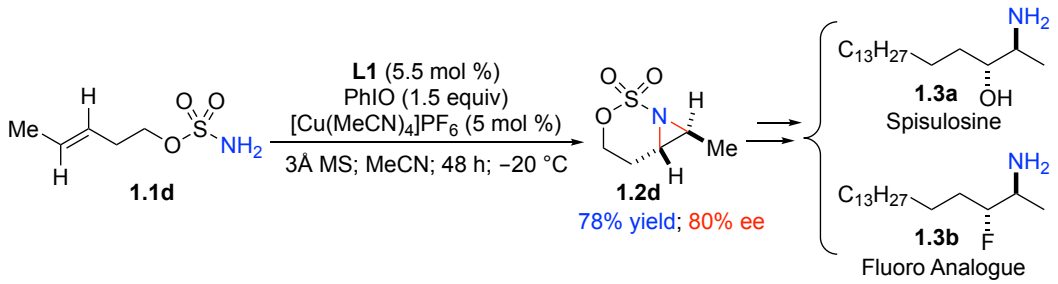
In 2007, the Dauban group reported copper-catalyzed enantioselective *N*-heterobicyclization of unsaturated sulfamates **1.1**, affording [4.1.0]-bicyclic aziridines **1.2a** – **1.2i** and [5.1.0]-bicyclic aziridine **1.2j** in good yields of up to 86% and up to 84% ee in the presence of PhIO (1.5 equiv) with the C_2-symmetric chiral bisoxazolines (BOX) ligand **L1** (Scheme 1.1).[4] As 8 of 10 reported examples (**1.2b** – **1.2f**, **1.2h** – **1.2j**) in this work were aliphatic alkenes-based sulfamates, it can be viewed as the first example of the catalytic asymmetric nitrene transfer to aliphatic alkenes (Scheme 1.1).[4]

Scheme 1.1 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfamate



In 2011, the Dauban group further demonstrated a series of synthetic applications utilizing these bicyclic aziridines to produce various chiral functionalized amines through ring-opening reactions, and applied this asymmetric *N*-heterobicyclization methodology to the total synthesis of chiral Spisulosine and its fluoro analogue (Scheme 1.2).[5]

Scheme 1.2 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfamates and Its Application to the Synthesis of Spisulosine and Its Fluoro Analogue

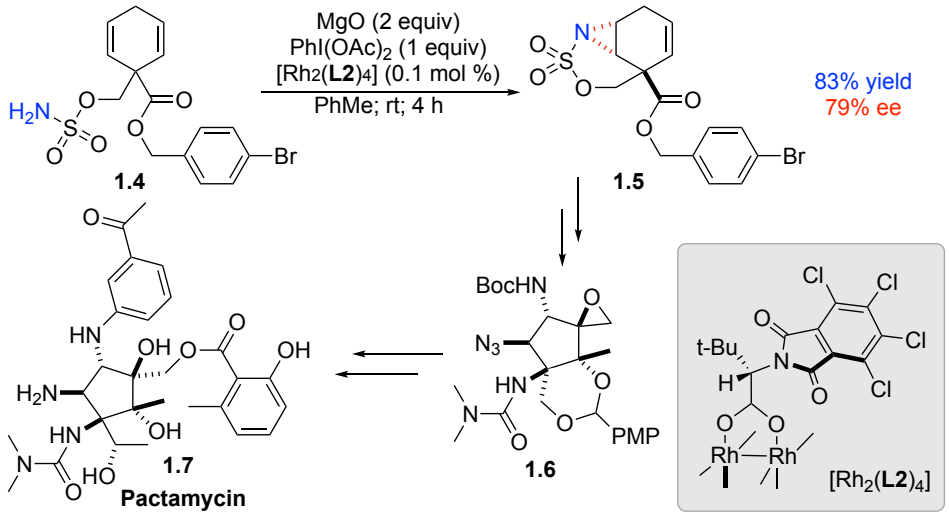


1.3 RHODIUM-CATALYZED ASYMMETRIC *N*-HETEROBICYCLIZATION OF ALKENES

1.3.1 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfamates

In 2017, the Kan group reported the racemic synthesis of the cyclopentane core framework of Pactamycin, which involved $Rh_2(OAc)_4$-mediated catalytic *N*-heterobicyclization of unsaturated sulfamates with oxidant $PhI(OAc)_2$, responsible for the in-situ generation of nitrene from sulfamtes.[6] In 2020, the same group discovered that Rh nitride-mediated *N*-heterobicyclization is applicable for the asymmetric induction with the support of ligand **L2** (**L2** = *S*-TCPTTL). $[Rh_2(\mathbf{L2})_4]$-catalyzed *N*-heterobicyclization of the unsaturated sulfamate **1.4** afforded the enantiopure aziridine **1.5** in 83 % yield and with 79 % ee in the presence of $PhI(OAc)_2$ and MgO (Scheme 1.3).[7] And they further applied this asymmetric *N*-heterobicyclization methodology to the synthesis of chiral cyclopentane core framework of Pactamycin.

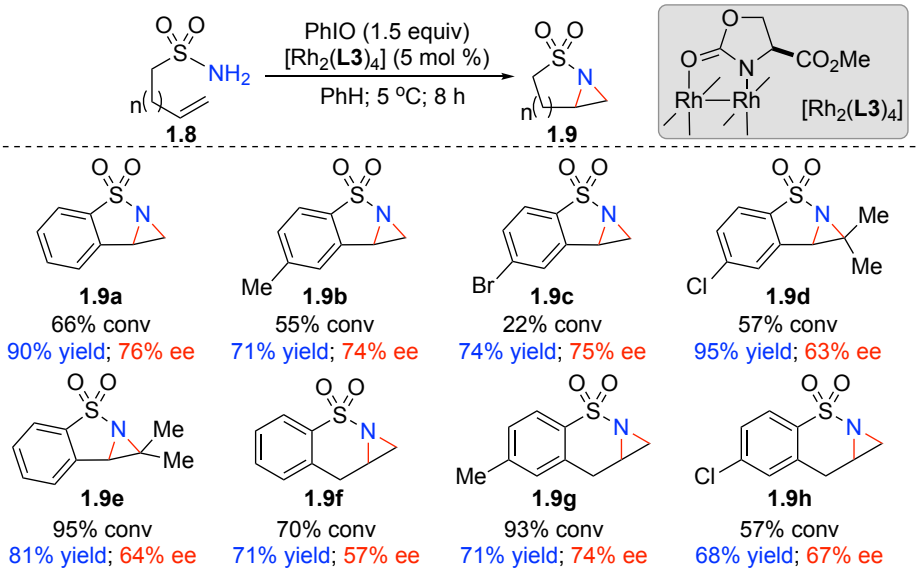
Scheme 1.3 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfamates and Its Application to the Synthesis of the Cyclopentane Core Framework of Pactamycin



1.3.2 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfonamides

In 2003, the Che group reported the asymmetric *N*-heterobicyclization of unsaturated phenyl group containing acyclic sulfonamides **1.8** catalyzed by chiral dirhodium (II,II) complex [Rh_2(**L3**)$_4$] (**L3** = 4*S*-MEOX) in the presence of oxidant PhIO, affording fused cyclic aziridines **1.9** in up to 95% yields based on recovered starting material, along with moderate enantioselectivity (up to 76% ee) (Scheme 1.4).[8]

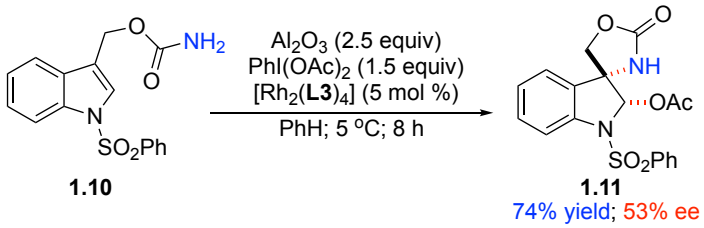
Scheme 1.4 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfonamides



1.3.3 Asymmetric *N*-Heterobicyclization of Unsaturated Carbamates

In 2003, the Che group also reported one example of the asymmetric *N*-heterobicyclization of unsaturated indole carbamate **1.10** catalyzed by several chiral dirhodium(II,II) complexes in the presence of $PhI(OAc)_2$ and Al_2O_3, obtaining the oxazolidinone product **1.11** after in-situ nucleophilic ring-opening. The catalyst $[Rh_2(\mathbf{L3})_4]$ gave the highest enantioselectivity of 53% ee in 74% yield based on recovered starting material. Oxazolidinones can serve as valuable precursors of various medicinally vital vicinal amino alcohols (Scheme 1.5).[8]

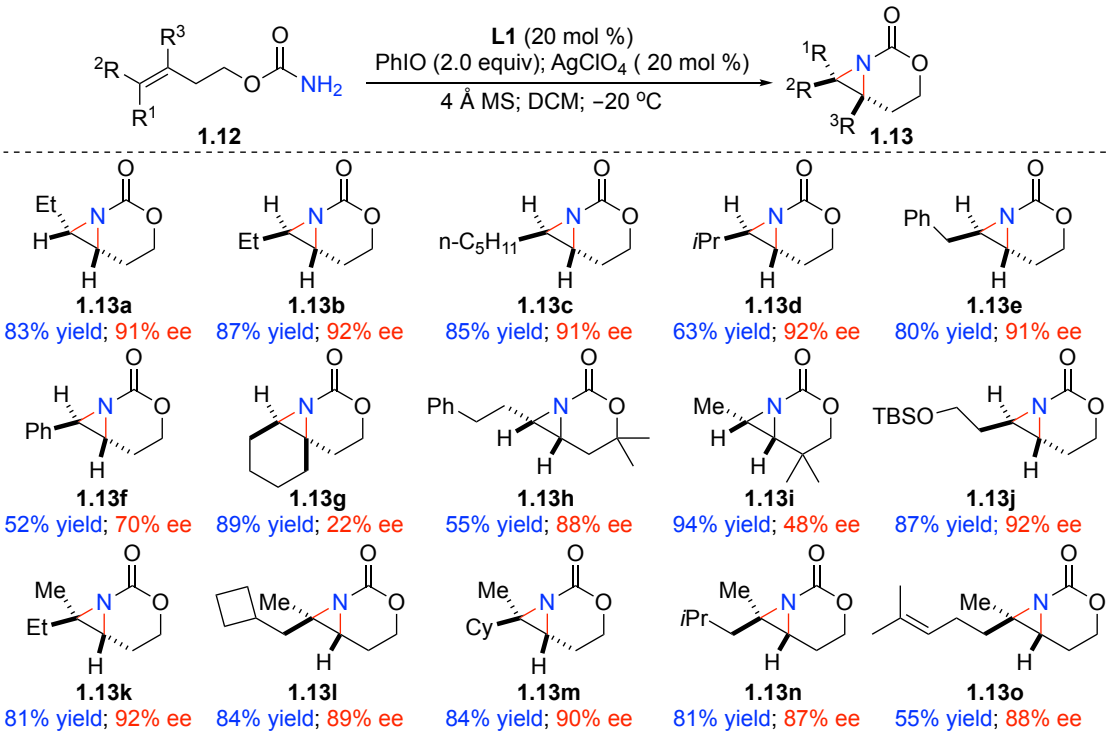
Scheme 1.5 Concomitant *N*-Heterobicyclization of Unsaturated Carbamate and Nucleophilic Ring Opening



1.4 SILVER-CATALYZED ASYMMETRIC *N*-HETEROBICYCLIZATION OF ALKENES

In 2017, the Schomaker group reported chemo- and enantioselective *N*-heterobicyclization of unsaturated carbamate **1.12** via nitrene transfers catalyzed by silver(I) complexes supported by chiral BOX ligand **L1** in the presence of PhIO as oxidant, affording [4.1.0]-bicyclic aziridines **1.13** up to 94% yield and 92% ee (Scheme 1.6).[9] This work presented asymmetric *N*-heterobicyclization of 14 non-activated aliphatic alkenes (**1.12a** – **1.12e**, **1.12g** – **1.12o**), affording the corresponding [4.1.0]-bicyclic aziridines (**1.13a** – **1.13e**, **1.13g** – **1.13o**). Therefore, this work can be highlighted for its successful implementation of asymmetric *N*-heterobicyclization of non-activated aliphatic alkenes. Additionally, this work should be underlined for the implementation of highly challenging *N*-heterobicyclization for trisubstituted alkenes (**1.12g**, **1.12k** – **1.12o**).

Scheme 1.6 Asymmetric *N*-Heterobicyclization of Unsaturated Carbamates



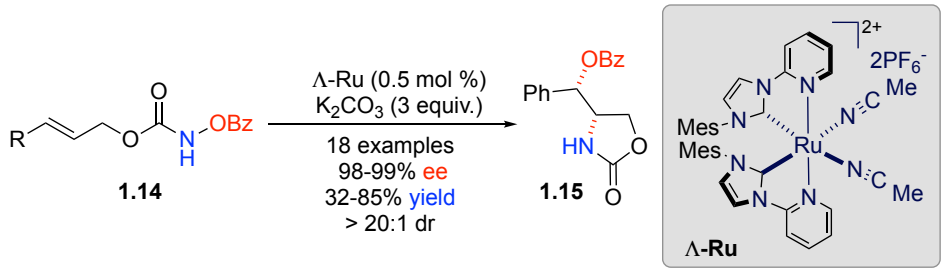
1.5 RUTHENIUM-CATALYZED ASYMMETRIC *N*-HETEROBICYCLIZATION OF ALKENES

1.5.1 Asymmetric *N*-Heterobicyclization of Unsaturated Carbamates

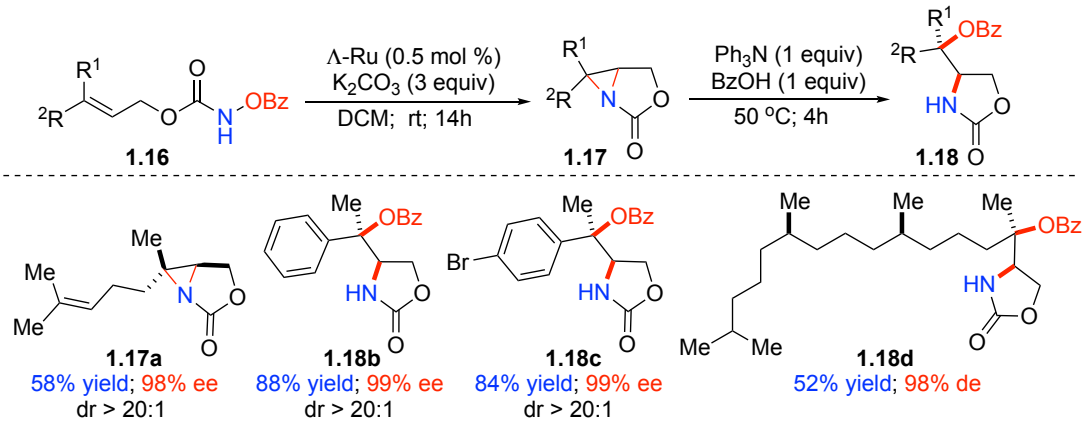
In 2020, the Meggers group reported an asymmetric ring-closing aminooxygenation of alkenes with *N*-benzoyloxycarbamates catalyzed by Λ–Ru, which went through the formation of *N*-heterobicyclization in certain cases.[10] While the 1,2-disubstituted alkenes **1.14** were proposed to directly undergo an aminooxygenation to produce the mono-cyclic carbamates (Scheme 1.7), the trisubstituted alkenes **1.16** were uncovered to stop at the

stage of the aziridination and then execute subsequent ring-opening of the resulting aziridines **1.17** with benzoic acid under harsh conditions, affording the monocyclic carbamates **1.18** over two steps(Scheme 1.8).

Scheme 1.7 Asymmetric Direct Aminooxygenation of Unsaturated Carbamates



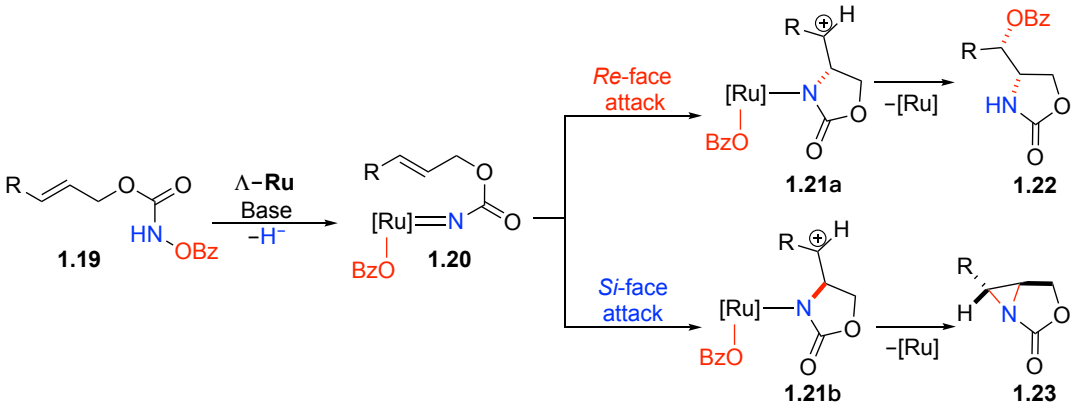
Scheme 1.8 Asymmetric Indirect Aminooxygenation of Unsaturated Carbamates via *N*-Heterobicyclization



The ruthenium catalyst was proposed to activate the *N*-benzoyloxycarbamate substrates to deliver a ruthenium nitrenoid intermediate **1.20** and release a benzoate group, coordinating with the ruthenium (Scheme 1.9). The subsequent addition of the ruthenium nitrenoid (nitrene) to the *Re*-face of the alkene produced the intermediate carbocation **1.21a** at the newly formed carbon stereocenter. The benzoate was then transferred from the ruthenium center to the carbocation, producing mono-cyclic carbamates **1.22**. In contrast,

a nitrene addition from the ruthenium nitrenoid intermediate to the *Si*-face of the alkene could forge an opposite absolute configuration at the newly formed stereogenic center of the carbocation intermediate **1.21b**. From the steric perspective, intermediate **1.21b** favors the formation of an aziridine **1.23** rather than a benzoate transfer. Thus, these two proposed pathways can justify the opposite configurations observed for the direct aminooxygenation products compared to the indirect aminooxygenation products and aziridines (Scheme 1.9).[10]

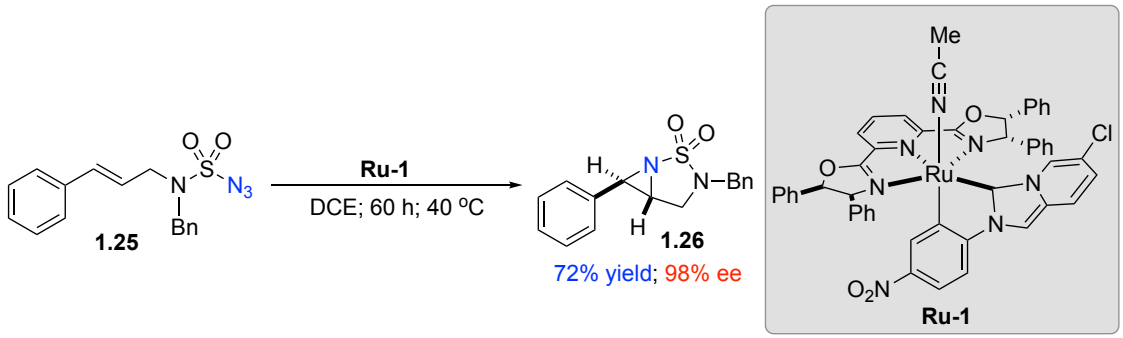
Scheme 1.9 Proposed Mechanism of Aminooxygenation of Carbamates



1.5.2 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfamoyl Azide

In 2021, the Meggers group reported an Ruthenium pybox-catalyzed enantioselective Intramolecular C−H amination of sulfamoyl azides through hydrogen atom abstraction by triplet nitrene and followed by radical rebound.[11] To support this proposed mechanism, they carried out an asymmetric *N*-heterobicylization reaction with sulfamoyl azide **1.24**. The generation of [3.1.0]-bicyclic sulfamoyl aziridine **1.25** could be proposed through radical addition by triplet nitrene and followed by radical rebound.

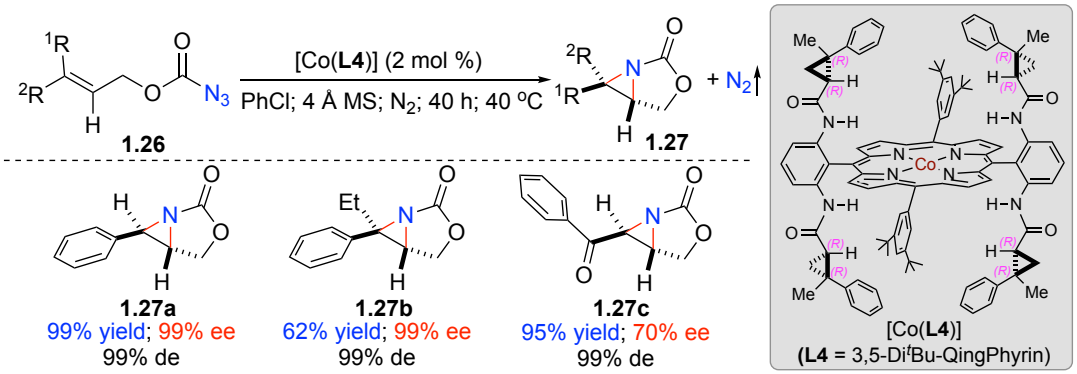
Scheme 1.10 Asymmetric *N*-Heterobicyclization of Unsaturated Sulfamoyl Azide



1.6 COBALT-CATALYZED ASYMMETRIC *N*-HETEROBICYCLIZATION OF ALKENES

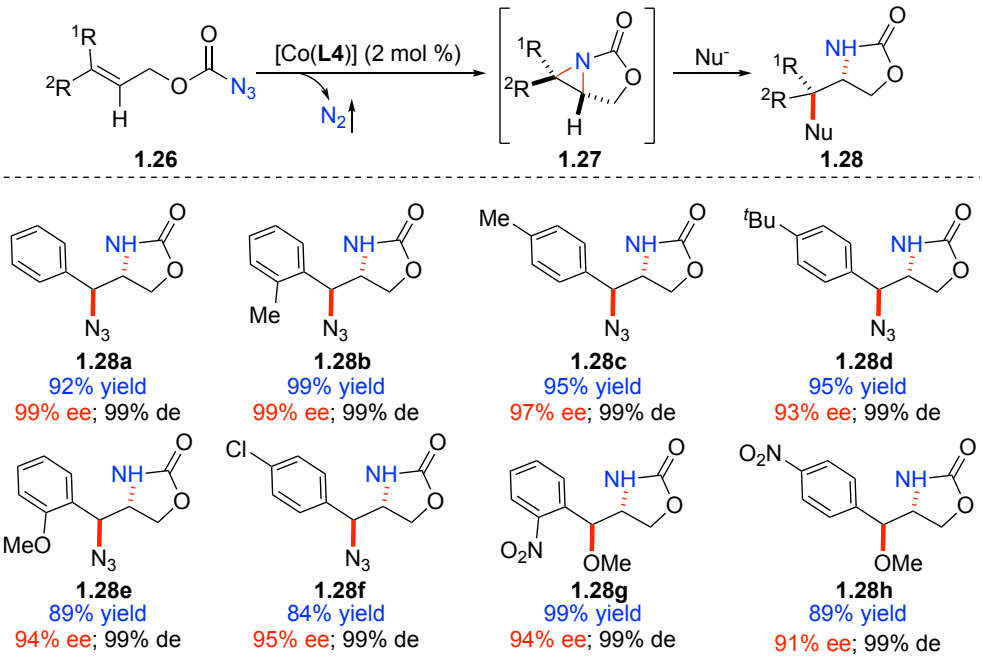
In 2017, the Zhang group reported an asymmetric radical *N*-heterobicyclization of allyl azidoformates **1.26** via metalloradical catalysis (Scheme 1.10), which constructed [3.1.0]-bicyclic aziridines **1.27** through a stepwise radical mechanism.[12] The Co(II)-based porphyrin catalysts were proposed to activate the azidoformates substrates **1.26** to deliver metal supported aminyl radical (α-Co(III)-aminyl radical) intermediate with the release of N_2 as a byproduct. α-Co(III)-aminyl radical could undergo radical addition followed by radical substitution, forming the aziridines **1.27**. The catalyst [Co(**L4**)] (**L4** = 3,5-Di^{t}Bu-QingPhyrin) served as the effective catalyst for *N*-heterobicyclization of allyl azidoformates **1.26**, affording aziridines **1.27** in great yields (up to 99%) with excellent enantioselectivities (up to 99% ee) and diastereoselectivities (up to 99% de).

Scheme 1.11 Asymmetric *N*-Heterobicyclization of Allyl Azidoformates



Due to the poor stability of some resulting aziridines **1.27** from *N*-heterobicyclization of disubstituted allyl azidoformates and inherent difficulty of isolation, these aziridines **1.27** were in situ treated with nucleophiles and transformed into various oxazolidinones **1.28** (Scheme 1.11).

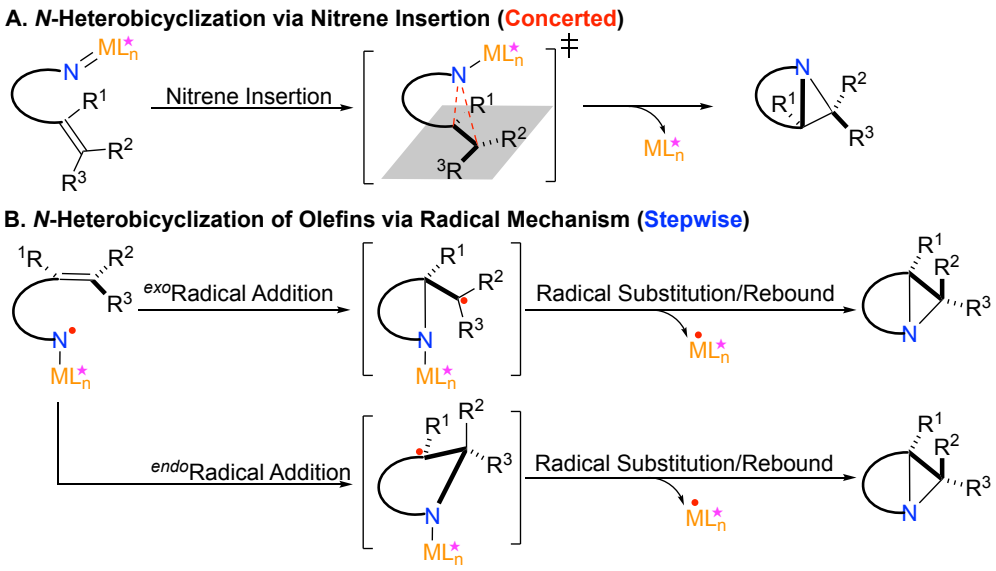
Scheme 1.12 Asymmetric *N*-Heterobicyclization of Allyl Azidoformates and in-situ Ring Opening



1.7 SUMMARY AND OUTLOOK

In this chapter, we have viewed recent developments in asymmetric *N*-heterobicyclization of alkenes via enantioselective transition metal catalysis. In terms of transition metals, there are Cu-, Ru-, Rh-, Ag-, and Co-catalyzed asymmetric *N*-heterobicyclization of unsaturated amides and azides. Regarding the reaction mechanism, there are two classical mechanisms, concerted nitrene transfer mechanism via Cu-, Ru-, Rh-, and Ag-supported catalysts (Scheme 1.12 A) and stepwise radical mechanism (radical addition and subsequent radical substitution/rebound) via Co- and Ru-supported catalysts (Scheme 1.12 B). In terms of the synthetic application of these methodologies, the chiral aziridines formed from asymmetric *N*-heterobicyclization of alkenes could serve as precursors for 1,2-amino alcohols and 1,3-amino alcohols.

Scheme 1.13 Two Classical Mechanisms for Metal-catalyzed Asymmetric *N*-Heterobicyclization



While these asymmetric *N*-heterobicyclization methodologies are very practical and synthetically useful, the asymmetric induction of these works remains underdeveloped due to lack of significant investigations. Thus, there is ample space for future chemists to uncover the mystery of the asymmetric induction in *N*-heterobicyclization with experimental and computational methods. Meanwhile, in addition to the current scope of the resulting aziridines from *N*-heterobicyclization reactions, chiral 1,2-diamine or 1,3-diamine derivates would be an excellent option to explore.

1.8 REFERENCES

1. (a) Cherney, A. H.; Kadunce, N. T.; Reisman, S. E. Enantioselective and Enantiospecific Transition-Metal-Catalyzed Cross-Coupling Reactions of Organometallic Reagents To Construct C–C Bonds. *Chem. Rev.* **2015,** *115*, 9587-9652. (b) Saint-Denis, T. G.; Zhu, R.-Y.; Chen, G.; Wu, Q.-F.; Yu, J.-Q. Enantioselective C(sp3)–H Bond Activation by Chiral Transition Metal Catalysts. *Science* **2018,** *359*, eaao4798. (c) Ye, X.; Tan, C.-H. Enantioselective Transition Metal Catalysis Directed by Chiral Cations. *Chem. Sci.* **2021,** *12*, 533-539. (d) Zhang, Q.; Wu, L.-S.; Shi, B.-F. Forging C−Heteroatom Bonds by Transition-Metal-Catalyzed Enantioselective C–H Functionalization. *Chem* **2022,** *8*, 384-413.

2. Fanourakis, A.; Docherty, P. J.; Chuentragool, P.; Phipps, R. J. Recent Developments in Enantioselective Transition Metal Catalysis Featuring Attractive Noncovalent Interactions between Ligand and Substrate. *ACS Catal.* **2020,** *10*, 10672-10714.

3. Kwart, H.; Khan, A. A. Copper-Catalyzed Decomposition of Benzenesulfonyl Azide in Cyclohexene Solution. *J. Am. Chem. Soc.* **1967,** *89*, 1951-1953.

4. Estéoule, A.; Durán, F.; Retailleau, P.; Dodd, R. H.; Dauban, P. Enantioselective Intramolecular Copper-Catalyzed Aziridination of Sulfamates. *Synthesis* **2007,** *2007*, 1251-1260.

5. Malik, G.; Estéoule, A.; Retailleau, P.; Dauban, P. Aziridines from Intramolecular Alkene Aziridination of Sulfamates: Reactivity toward Carbon Nucleophiles. Application to the Synthesis of Spisulosine and Its Fluoro Analogue. *J. Org. Chem.* **2011,** *76*, 7438-7448.

6. Goto, A.; Yoshimura, S.; Nakao, Y.; Inai, M.; Asakawa, T.; Egi, M.; Hamashima, Y.; Kondo, M.; Kan, T. Synthetic Study on Pactamycin: Stereoselective Synthesis of the Cyclopentane Core Framework. *Org. Lett.* **2017,** *19*, 3358-3361.

7. Ohmi, K.; Miura, Y.; Nakao, Y.; Goto, A.; Yoshimura, S.; Ouchi, H.; Inai, M.; Asakawa, T.; Yoshimura, F.; Kondo, M.; Kan, T. Pactamycin and Its Derivatives: Improved Synthesis Route. *Eur. J. Org. Chem.* **2020,** *2020*, 488-491.

8. Liang, J.-L.; Yuan, S.-X.; Chan, P. W. H.; Che, C.-M. Chiral Rhodium(II,II) Dimers Catalyzed Enantioselective Intramolecular Aziridination of Sulfonamides and Carbamates. *Tetrahedron Lett.* **2003,** *44*, 5917-5920.

9. Ju, M.; Weatherly, C. D.; Guzei, I. A.; Schomaker, J. M. Chemo- and Enantioselective Intramolecular Silver-Catalyzed Aziridinations. *Angew. Chem., Int .Ed.* **2017,** *56*, 9944-9948.

10. Tan, Y.; Han, F.; Hemming, M.; Wang, J.; Harms, K.; Xie, X.; Meggers, E. Asymmetric Ring-Closing Aminooxygenation of Alkenes en Route to 2-Amino-1,3-Diols with Vicinal Stereocenters. *Org. Lett.* **2020,** *22*, 6653-6656.

11. Nie, X.; Yan, Z.; Ivlev, S.; Meggers, E. Ruthenium Pybox-Catalyzed Enantioselective Intramolecular C–H Amination of Sulfamoyl Azides en Route to Chiral Vicinal Diamines. *J. Org. Chem.* **2021,** *86*, 750-761.

12. Jiang, H.; Lang, K.; Lu, H.; Wojtas, L.; Zhang, X. P. Asymmetric Radical Bicyclization of Allyl Azidoformates via Cobalt(II)-Based Metalloradical Catalysis. *J. Am. Chem. Soc.* **2017,** *139*, 9164-9167.

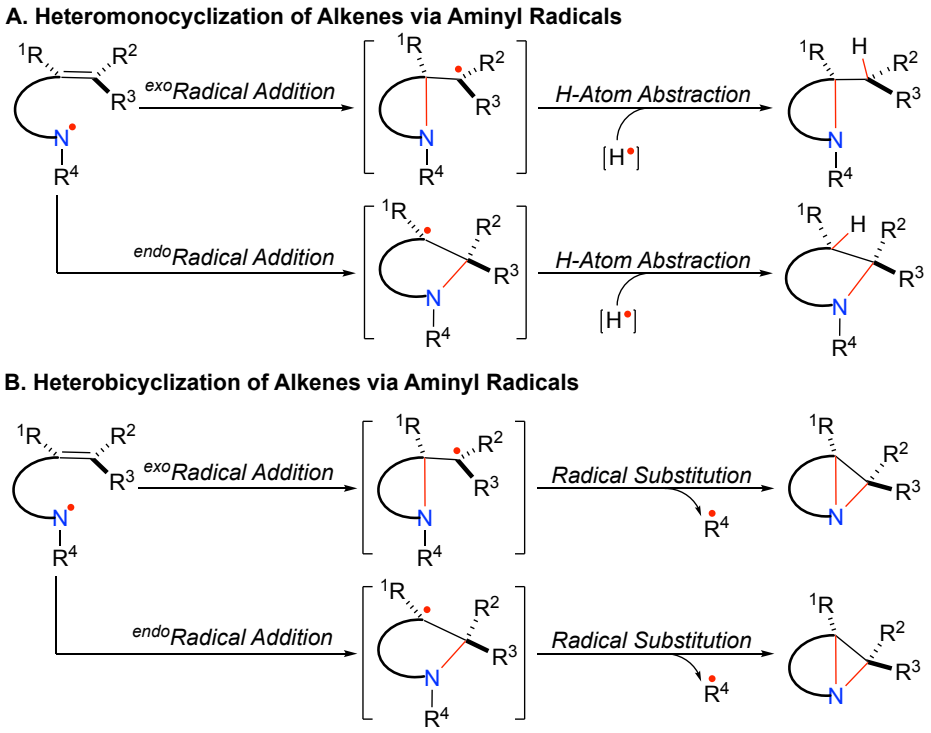
CHAPTER 2 - ENANTIOSELECTIVE RADICAL *N*-HETEROBICYCLIZATION WITH A NEW MODE OF ASYMMETRIC INDUCTION

2.1 INTRODUCTION

Great efforts have been dedicated to employing aminyl radicals as key intermediates for the molecular construction of nitrogen-containing compounds.[1] Among these valuable efforts, aminyl radicals have been established to engage in radical heterocyclization to construct *N*-heterocyclic structures via intramolecular addition to unsaturated π-bonds. Despite numerous demonstrations on radical *N*-heterocyclization of free aminyl radicals, these transformations mainly start with an intramolecular radical addition (RA) to an alkene unit and is followed by subsequent intermolecular radical reactions, such as H-atom abstraction (HAA) (Scheme 2.1.A).[2] In contrast to the well-documented *N*-heteromonocyclization established on the RA-HAA pathway,[2a] it is conceivable that the aminyl radicals might also proceed with radical *N*-heterobicyclization through radical addition and followed by intramolecular radical substitution (RS) at the nitrogen center, generating *N*-heterobicyclic structures (Scheme 2.1.B). However, the RA-RS pathway has not been established as a potential *N*-heterobicyclization process, possibly because it

requires inaccessibly high activation energy to conduct the homolytic radical substitution at the tertiary nitrogen center, involving the cleavage of an existing C–N bond.[3]

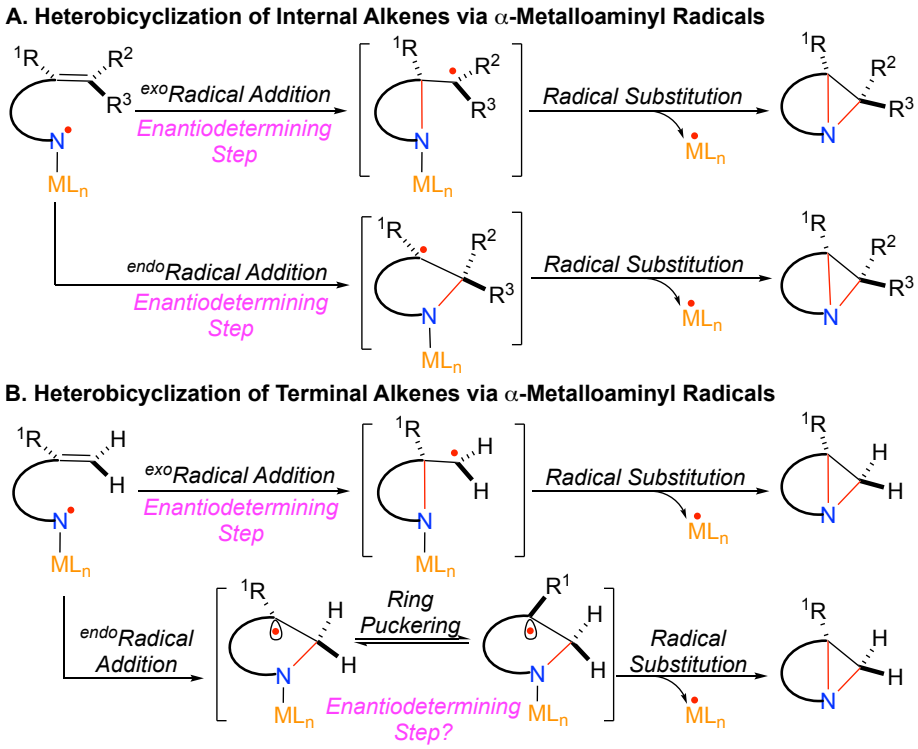
Scheme 2.1 Radical Monocyclization and Bicyclization of Alkenes via Aminyl Radicals



To address this challenge, a potential solution would be to substitute the free aminyl radicals R(R^4)N• with metal-supported aminyl radicals, termed α-metalloaminyl radicals R(LnM)N•, where the alkyl group R^4 is replaced by metal complex LnM (Scheme 2.2). As M–N bond is generally much weaker than the C–N bond,[4] the challenging radical substitution process is then rendered facile. If nitrogen-containing compounds can be accessed by an open-shell metal catalyst (metalloradicals *LnM•) to generate α-metalloaminyl radicals, then a *N*-heterobicyclization process based on the RA-RS pathway could be conducted in a catalytic manner. In addition to its catalytic nature, the further

deployment of chiral metalloradicals *LnM• could facilitate the asymmetric induction into the synthesis of *N*-heterobicyclic structures.

Scheme 2.2 Enantioselective Metalloradical Bicyclization of Alkenes via Metal-supported Aminyl Radicals



Regarding the enantioselective Metalloradical *N*-heterobicyclization of alkenes, asymmetric induction is known to occur in different scenarios. For the enantioselective *N*-heterobicyclization of internal alkenes, the radical addition step would be the enantiodetermining step with the formation of a stereogenic center (when the radical addition step is irreversible), regardless of whether the α-metalloaminyl radical undergoes radical addition to the alkene unit in the *endo*- or *exo*- fashion (Scheme 2.2.A). For the enantioselective *N*-heterobicyclization of terminal alkenes, the radical addition step would still be the enantiodetermining step when occurring in an exo-addition manner to terminal

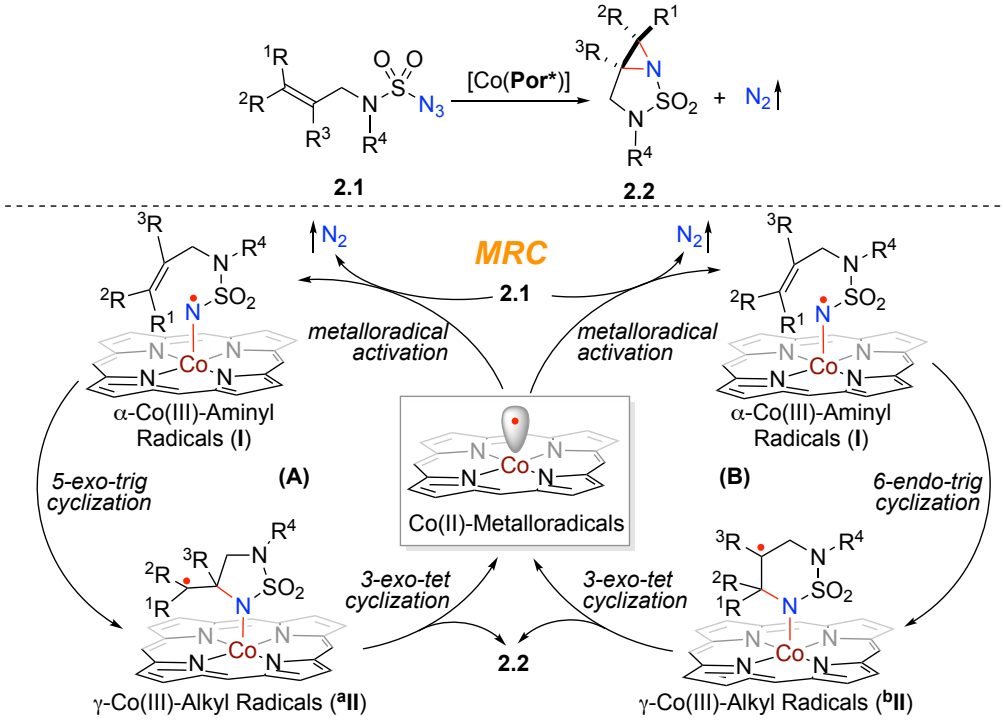
alkenes (when the radical addition step is irreversible). However, it is questionable if the radical addition step could continue to govern asymmetric induction occurring in an *endo*-addition manner to terminal alkenes (when the radical addition step is irreversible), presumably relying on the conformational and kinetic stability of the newly generated chiral radical center on the ring as illustrated in Scheme 2.2.B.

While radical chemistry has been increasingly established in modern synthesis,[5] the ongoing endeavor has encountered some inherent challenges, especially regulating enantioselectivity.[6] Among recent progress in unraveling these challenges,[7] metalloradical catalysis (MRC) presents a conceptually different approach based on catalytic generation of metal-stabilized organic radicals from metalloradical activation of radical precursors and further precise deployment of these reactive radicals in the controllable subsequent radical reactions.[8] As stable 15*e*-metalloradicals, Co(II)-based porphyrins have a unique ability to homolytically activate organic azides to produce α-Co(III)-aminyl radicals, which can function as kinetically competent intermediates in catalytic amination reactions.[9] With the deployment of D_2-symmetric chiral amidoporphyrins as an adaptable ligand platform, Co(II)-based MRC has recently established asymmetric construction of *N*-heteromonocyclic sulfamides through enantioselective intramolecular C–H amination.[10]

While we documented the synthesis of *N*-heterobicyclic sulfamides through *N*-heterobicyclization of allylic sulfamoyl azides via Co(II)-MRC, our previous catalytic system afforded a limited substrate scope and failed to achieve asymmetric induction.[11] Given the recent development of new-generation D_2-symmetric chiral amidoporphyrins,[12] we hoped to enable an asymmetric variant of the metalloradical *N*-heterobicyclization of

allylic sulfamoyl azides **2.1** to produce highly-strained chiral [3.1.0]-aziridines **2.2** (Scheme 2.3).

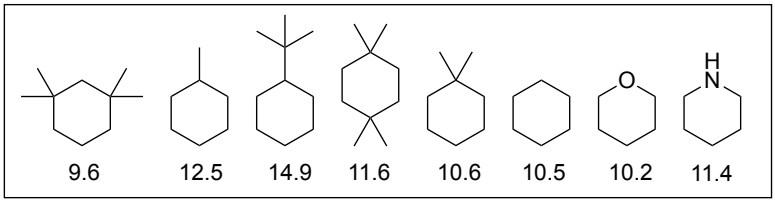
Scheme 2.3 Enantioselective Metalloradical *N*-Heterobicyclization of Allylic Sulfamoyl Azides



Mechanistically, there are two possible catalytic pathways for radical *N*-heterobicyclization at the support of the newly generated α-Co(III)-aminyl radical intermediate **I** from the metalloradical activation of allylic sulfamoyl azides **2.1** (Scheme 2.3). When intermediate **I** undergoes radical addition by 5-*exo-trig* cyclization (Scheme 2.3 A), 5-membered γ-Co(III)-alkyl radical intermediate **^{a}II** is then produced with a stable stereogenic center (when the radical addition step is irreversible). When intermediate **I** undergoes 6-*endo-trig* cyclization (Scheme 2.3 B), 6-membered γ-Co(III)-alkyl radical intermediate **^{b}II** is then formed with a stable stereogenic center (for internal alkenes) or a

chiral radical center (for terminal alkenes) (when the radical addition step is irreversible). Intermediate **II** can further engage in radical substitution via 3-*exo-tet* cyclization to produce bicyclic aziridines **2.2**.

Table 2.1 The Chair-to-Chair Conformational Interconversion Barrier of Free 6-Membered Ring Structures[a]



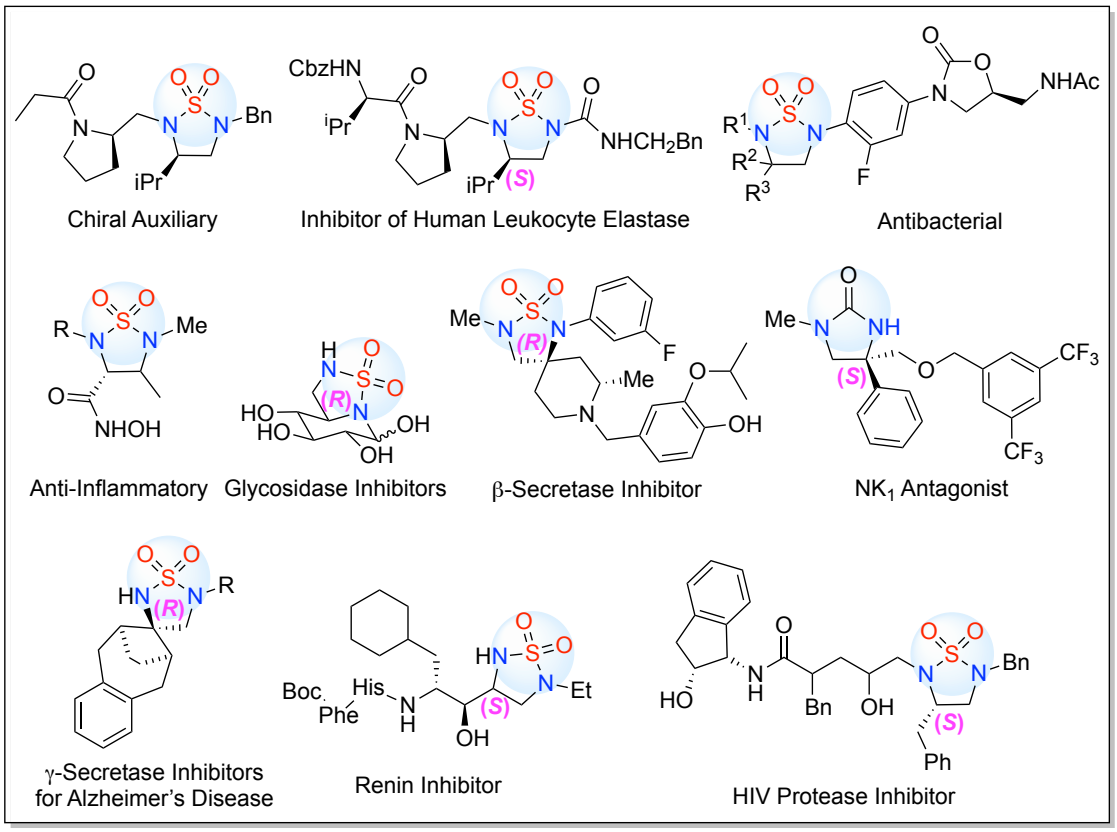
[a]Energy unit: kcal/mol.

Certainly, the regioselectivity of the radical addition step may alter the manner of asymmetric induction and further influence the governance of enantioselectivity (when the radical addition step is irreversible). The enantiodetermining step in catalytic pathway **A** is 5-*exo-trig* radical cyclization regardless of internal alkenes or terminal alkenes (when the radical addition step is irreversible), as **[a]II** is produced with a stable stereogenic center (Scheme 2.3). However, the enantiodetermining step in catalytic pathway **B** for terminal alkenes (R^1 = H, R^2 = H) is uncertain (either 6-*endo-trig* radical cyclization or 3-*exo-tet* cyclization), relying on the conformational and kinetic stability of the chiral radical center on the 6-membered ring of intermediate **[a]II** (when the radical addition step is irreversible) (Scheme 2.3). The inversion of the chirality of this alkyl radical center requires the ring conformation change through ring puckering process, which typically takes around 10-15 kcal/mol for free 6-membered ring structures (Table 2.1).[13] In this case, the chirality of the chiral radical center would be kinetically stable as the subsequent 3-*exo-tet* cyclization

process is very facile. Therefore, the enantioface-selectivity in 6-*endo*-*trig* radical cyclization is expected to determine the enantioselectivity of the product. However, to our knowledge, this fundamental mode of asymmetric induction has not yet been established.

It was necessary to explore whether this *N*-heterobicyclization could realize high enantioselectivity via this mode of asymmetric induction. We anticipated the prospect of addressing this issue by adapting the D_2-symmetric chiral amidoporphyrin ligand platform to embrace a proper steric, electronic, and chiral environment to control the asymmetric metalloradical *N*-heterobicyclization process. If accomplished, it would be beneficial as the resultant *N*-heterobicyclic structures can serve as synthons for the synthesis of functionalized vicinal diamines, which are typical motifs in medicinally essential compounds (Scheme 2.4).[14]

Scheme 2.4 Selected Examples of Biologically Important Molecules Containing Chiral Five-Membered Cyclic Sulfamide and Vicinal Diamine Motifs



2.2 RESULTS AND DISCUSSION

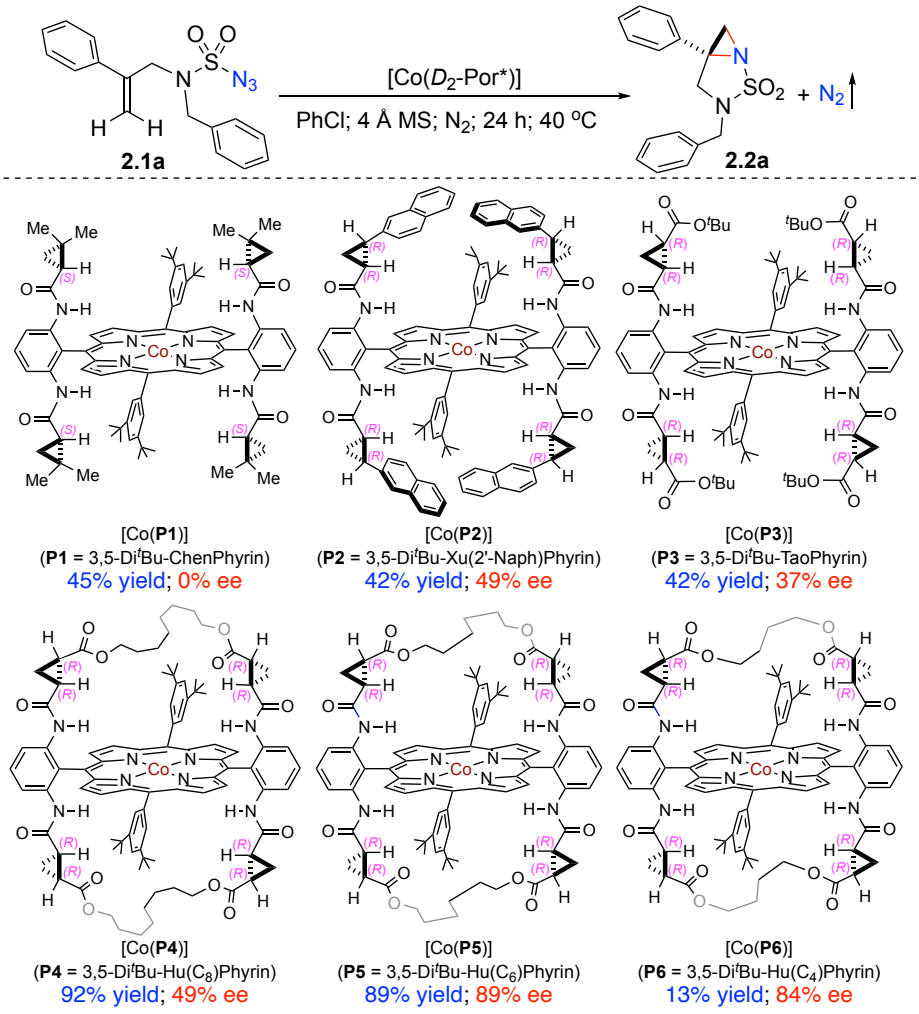
2.2.1 Condition Optimization for Asymmetric Radical *N*-Heterobicyclization of Allylic Sulfamoyl Azides

At the outset of our effort, *N*-benzyl-*N*-allylsulfamoyl azide **2.1a** was selected as a model substrate to explore the proposed asymmetric radical *N*-heterobicyclization by Co(II)-based metalloradical catalysis (Table 2.2). The ligand effects for asymmetric metalloradical *N*-heterobicyclization reaction were examined in chlorobenzene in the presence of 4 Å molecular sieves for 24 h, at 40 °C and under the protection of N_2.

When the first-generation of metalloradical catalyst [Co(**P1**)] (**P1** = 3,5-Di^{t}Bu-ChenPhyrin)[15] was deployed, the catalyzed system achieved the *N*-heterobicyclization reaction of azide **2.1a**, producing the desired [3.1.0]-bicyclic aziridine **2.2a** in a moderate yield of 45%, but failed to realize any notable asymmetric induction. When the second-generation metalloradical catalyst [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-Xu(2'-Naph)Phyrin)[16] bearing 2-naphthyl substituents was employed, a significant increase in the enantioselectivity (49% ee) was achieved along with a slight decrease on the yield (42%). The significant improvement of the enantioselectivity was proposed to be attributed to a more rigid chiral environment, resulting from the existence of multiple intermolecular and intramolecular non-covalent interactions involving the 2-naphthyl substituents. To test this hypothesis, the metalloradical catalyst [Co(**P3**)] (**P3** = 3,5-Di^{t}Bu-Tao(^{t}Bu)Phyrin)[12] bearing chiral amide units with flexible ester groups was examined, causing a decrease in the enantioselectivity of **2.2a** to 37% ee for the *N*-heterobicyclization reaction with the

same yield of 42%. This observation is consistent with our hypothesis, as [Co(**P3**)] has less intermolecular and intramolecular non-covalent interactions formed on the chiral amide units than [Co(**P2**)] but more than [Co(**P1**)] (Scheme 2.5).

Table 2.2 Ligand Effects[a]



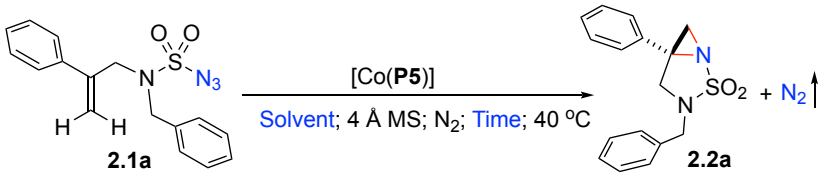
[a]Performed in PhCl at 40 °C for 24 h using [Co(**Por***)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1a**] = 0.2 M; NMR yields; Enantiomeric excess (ee) determined by chiral HPLC.

Continuous efforts in the improvement of the enantioselectivity of the catalytic transformation were made by employing new-generation metalloradical catalysts [Co(HuPhyrin)], Co(II)-based bridged D_2-symmetric chiral amidoporphyrins. The [Co(HuPhyrin)] catalysts are derived from [Co(**P3**)] with alkyl linkages joining two chiral amide units and possess more rigid cavity-like chiral environments for effective asymmetric induction. When [Co(**P4**)] (**P4** = 3,5-Di^{t}Bu-Hu(C_8)Phyrin) with C_8-bridged alkyl linkage was tested, aziridine **2.2a** was produced with higher enantioselectivity than [Co(**P3**)] (49% ee vs 37% ee) along with an exact excellent yield of 92%. The enantioselectivity of **2.2a** was proposed to be depended on the length of the alkyl bridge on HuPhyrin ligand. Therefore, [Co(**P5**)] (**P5** = 3,5-Di^{t}Bu-Hu(C_6)Phyrin) assembled with a shorter C_6-alkyl linkage was tested, giving a dramatic enhancement of enantioselectivity from 49% ee to 90% ee for the production of aziridine **2.2a** along with the slight decrease in the yield from 92% to 89%. When the alkyl linkage of the HuPhyrin ligand was further decreased to a C_4-bridge, it led to a dramatic drop in reactivity as well as a noticeable reduction in enantioselectivity, as demonstrated by [Co(**P6**)] (**P6** = 3,5-Di^{t}Bu-Hu(C_4)Phyrin), delivering aziridine **2.2a** in 13% yield and with 84% ee. This boomeranged result of catalyst [Co(**P6**)] is presumably attributed to the highly constrained cavity due to the short C4-alkyl linkage. Overall, these results established an pronounced ligand effect on the reactivity and enantioselectivity of asymmetric metalloradical bicyclization reaction (Table 2.2). Overall, [Co(**P5**)] was determined as the best catalyst under all screening conditions.

The solvent effects and reaction time were explored with [Co(**P5**)] (Table 2.3). In terms of yield, toluene gave the best yield of 99%. In terms of enantioselectivity, methyl

tert-butyl ether, trifluorotoluene and toluene all gave great ee of 90%. Therefore, toluene was determined as the effective solvent for this metalloradical bicyclization. When the reaction time was changed from 24 h to 14 h, this catalytic system was still effective for producing **2.2a** in 99% yield. Thus, 14 h was chosen as the effective reaction time at these reaction conditions.

Table 2.3 Solvent and Reaction Time Optimization[a]



Entry	Time	Solvent	Yield	ee
1	24 h	Chlorobenzene	89%	89%
2	24 h	Methyl tert-butyl ether	78%	90%
3	24 h	Cyclohexane	86%	62%
4	24 h	Benzene	79%	86%
5	24 h	Dioxane	0%	/
6	24 h	Trifluorotoluene	93%	90%
8	24 h	Toluene	99%	90%
9	14 h	Toluene	99%	90%

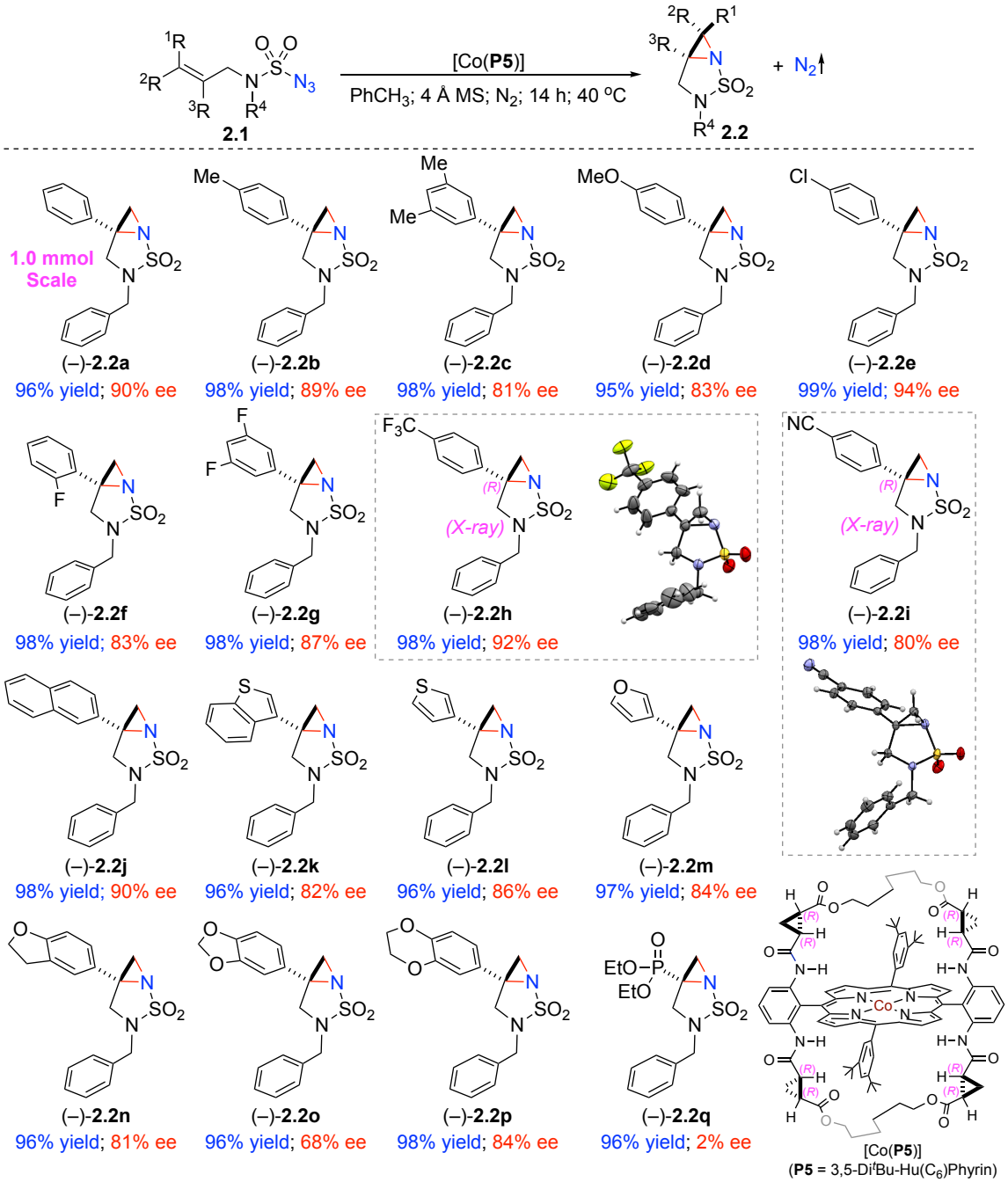
[a]Performed at 40 ºC using [Co(**P5**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1a**] = 0.2 M; NMR yields; Enantiomeric excess (ee) was determined by chiral HPLC.

2.2.2 Asymmetric Radical *N*-Heterobicyclization of Activated Terminal Alkenes

Under the optimized conditions, the generality and versatility of the metalloradical asymmetric *N*-heterobicyclization system catalyzed by [Co(**P5**)] were evaluated with various sulfamoyl azides **2.1** bearing activated terminal alkene units (Table 2.4).

Like *N*-benzyl-*N*-allylsulfamoyl azide **2.1a**, the alkene units of its derivatives possessing substituents with different electronic and steric properties, including 4-Me (**2.1b**), 3,5-di-Me (**2.1c**), 4-MeO (**2.1d**), 4-Cl (**2.1e**), 2-F (**2.1f**), 3,5-di-F (**2.1g**), 4-CF_3 (**2.1h**), and 4-CN (**2.1i**), could be effectively catalyzed by [Co(**P5**)], forming the desired [3.1.0]-sulfamoyl aziridines **2.2b**–**2.2i** with high enantioselectivities in excellent yields (Table 2.3). The absolute configuration of the major enantiomers of both **2.2h** and **2.2i** were established as (*R*) by X-ray crystallography. Significantly, this catalytic metalloradical *N*-heterobicyclization reaction could be scaled up, producing the desired enantioenriched [3.1.0]-sulfamoyl aziridine (–)-**2.2a** in 96% yield with 90% ee on 1.0 mmol scale (Table 2.4).

Table 2.4 Asymmetric Radical *N*-Heterobicyclization of Activated Terminal Alkenes[a]



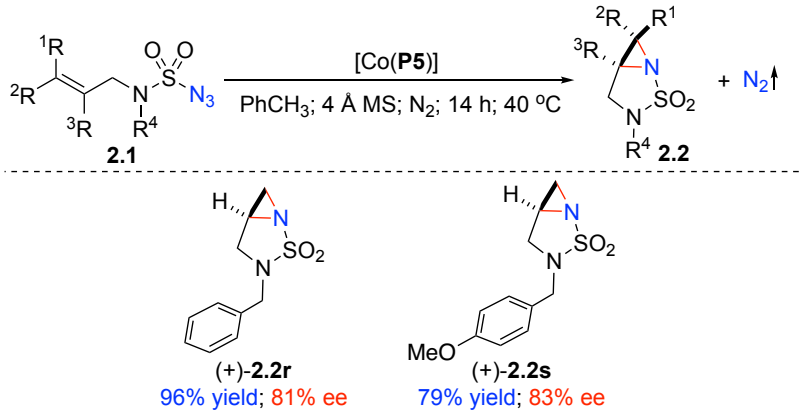
[a]Performed in toluene at 40 ºC for 14 h using [Co(**P5**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1**] = 0.2 M; Isolated yields; Enantiomeric excess (ee) determined by chiral HPLC; Absolute configuration determined by X-ray crystallography.

In addition, the [Co(**P5**)]-catalyzed *N*-heterobicyclization system tolerates various alkenes containing extended arenes and heteroarenes, such as naphthalene (**2.1j**), benzothiophene (**2.1k**), thiophene (**2.1l**), furan (**2.1m**), 2,3-dihydrobenzofuran (**2.1n**), 1,3-benzodioxole (**2.1o**) and 1,4-benzodioxan (**2.1p**), allowing for the construction of chiral [3.1.0]-bicyclic sulfamoyl aziridines **2.2j**–**2.2p** in exceptional yields along with high enantioselectivities (Table 2.4). Moreover, [Co(**P5**)] could perform the *N*-heterobicyclization reaction of substrate **2.1q** possessing a large phosphonate substituent on the alkene unit, giving **2.2q** in high yield, albeit with ineffective asymmetric induction (Table 2.4).

2.2.3 Asymmetric Radical *N*-Heterobicyclization of Non-Activated Terminal Alkenes

Under the optimized conditions, the generality and versatility of metalloradical asymmetric *N*-heterobicyclization system catalyzed by [Co(**P5**)] were evaluated with various sulfamoyl azides **2.1** bearing non-activated terminal alkene units with alkyl substituents (Table 2.5). The catalytic system is effective for asymmetric *N*-heterobicyclization of *N*-allylsulfamoyl azides with nonactivated monosubstituted aliphatic alkenes, such as **2.1r** and **2.1s**, leading to successful construction of [3.1.0]-bicyclic sulfamoyl aziridines **2.2r** and **2.2s** in good to excellent yields with moderate to good enantioselectivities (Table 2.5).

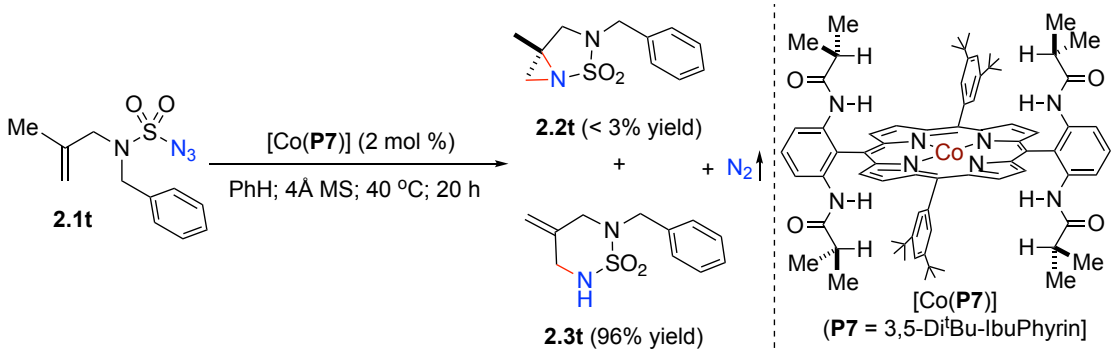
Table 2.5 Asymmetric Radical *N*-Heterobicyclization of Monosubstituted Aliphatic Alkenes[a]



[a]Performed in toluene at 40 ºC for 14 h using [Co(**P5**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1**] = 0.2 M; Isolated yields; Enantiomeric excess (ee) determined by chiral HPLC.

In the asymmetric heterobicyclization of *N*-allylsulfamoyl azides with nonactivated disubstituted aliphatic alkenes, such as olefins carrying various alkyl groups, we noted that the intramolecular amination of allylic C–H bonds would be a potential issue. As demonstrated example of **2.1t**, Co(**P7**)-based system was reported to afford C–H amination product **2.3t** in 96% yield along with the trace amount of *N*-heterobicyclization product **2.2t** (Table 2.6).[17]

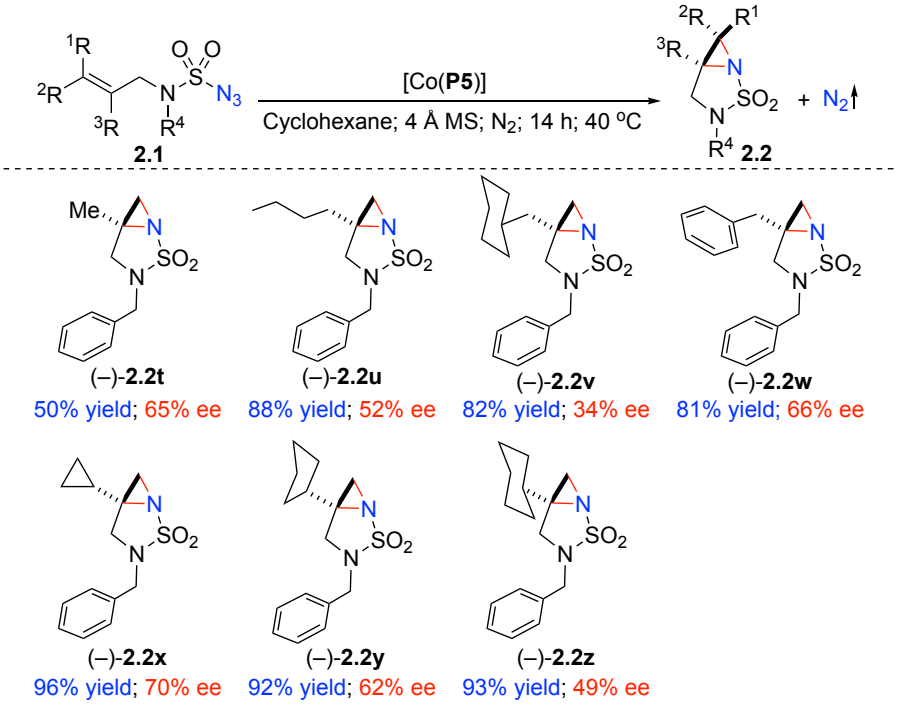
Table 2.6 The Chemoselectivity between *N*-Heterobicyclization and C–H Amination of Disubstituted Aliphatic Alkene[a]



[a]Performed in toluene at 40 ºC for 20 h using [Co(**P7**)] (2 mol %) under N_2 in the presence of 4 Å MS; [**2.1t**] = 0.1 M; NMR yields.

While the intramolecular amination of allylic C–H bonds is preferred over *N*-heterobicyclization in [Co(**P7**)]-based metalloradical system, [Co(**P5**)]-based system could achieve an effective chemoselective reaction with C=C bonds without impacting the allylic C–H bonds as illustrated by the construction of [3.1.0]-bicyclic sulfamoyl aziridines **2.2t**–**2.2z** in good yields with moderate enantioselectivities (Table 2.7).

Table 2.7 Asymmetric Radical *N*-Heterobicyclization of Disubstituted Aliphatic Alkenes[a]



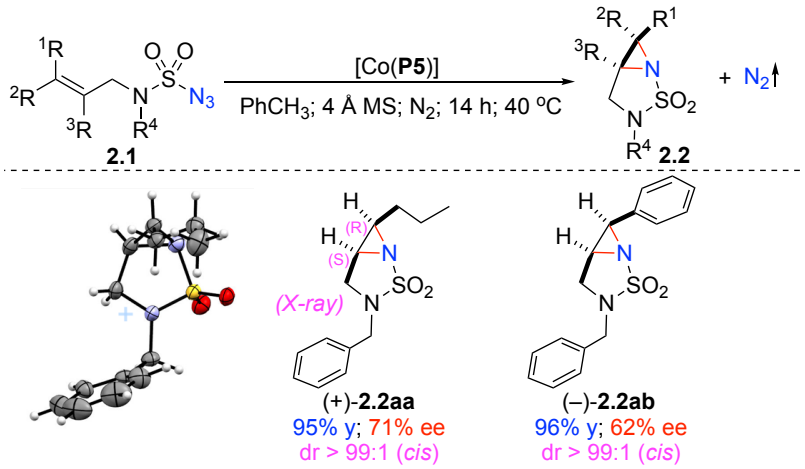
[a]Performed in cyclohexane at 40 ºC for 14 h using [Co(**P5**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1**] = 0.2 M; Isolated yields; Enantiomeric excess (ee) determined by chiral HPLC.

2.2.4 Asymmetric Radical *N*-Heterobicyclization of Internal Alkenes

Under the optimized conditions, the generality and versatility of metalloradical asymmetric *N*-heterobicyclization system catalyzed by [Co(**P5**)] were further evaluated with various sulfamoyl azides **2.1** containing internal alkene units (Table 2.8). This [Co(**P5**)]-based asymmetric *N*-heterobicyclization tolerates *N*-allylsulfamoyl azides possessing internal alkenes as presented by the *N*-heterobicyclization of *cis*-**2.1aa** and *cis*-

2.1ab, producing the corresponding *cis*-**2.2aa** and *cis*-**2.2ab** in excellent yields with reasonable enantioselectivities, as well as retaining the initial *cis*-stereochemistry of the alkene units. The absolute configuration of the major enantiomer of *cis*-**2.2aa** was determined as (*5S,6R*).

Table 2.8 Asymmetric Radical *N*-Heterobicyclization of Internal Alkenes[a]



[a]Performed in toluene at 40 ºC for 14 h using [Co(**P5**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1**] = 0.2 M; Isolated yields; Enantiomeric excess (ee) determined by chiral HPLC; Absolute configuration determined by X-ray crystallography; From corresponding *cis*-olefins.

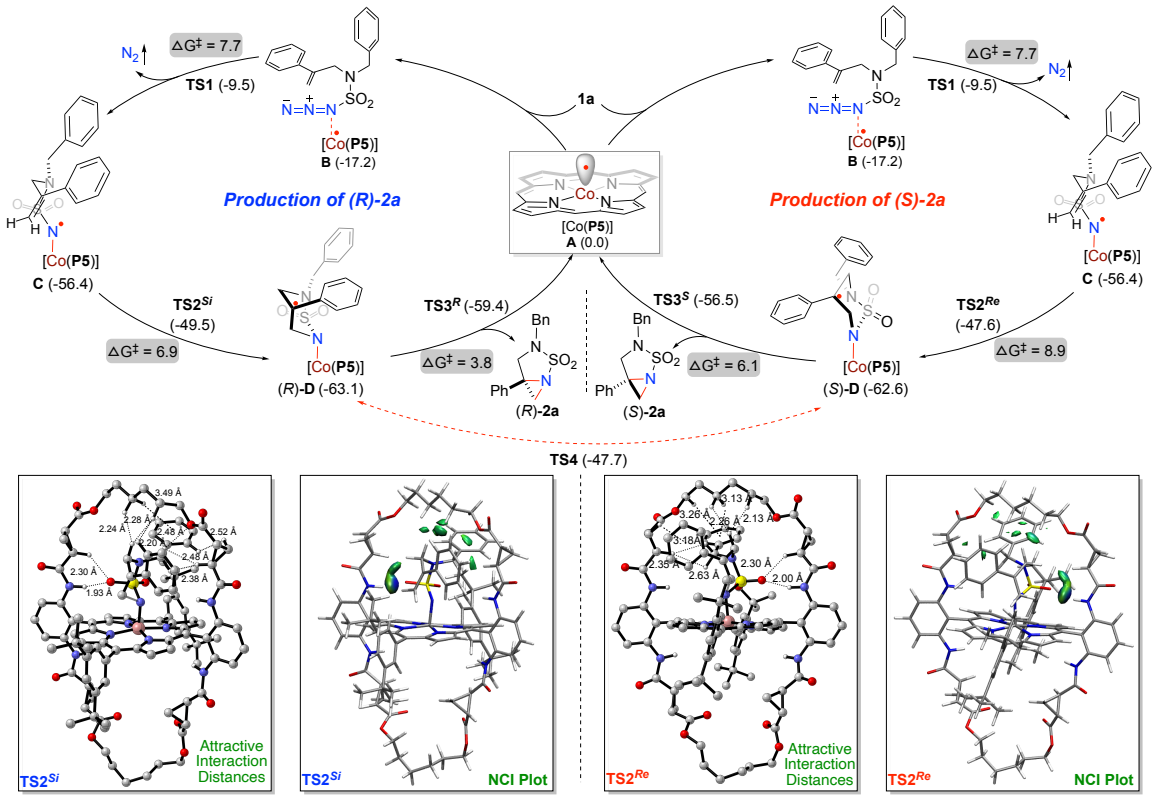
2.2.5 Mechanistic Studies

Computational and experimental investigations were performed to elucidate the proposed stepwise radical mechanism of the Co(II)-based asymmetric *N*-heterobicyclization along with the origin of regioselectivity and enantioselectivity. First, density functional theory (DFT) calculations were conducted to explore the energy profiles

of the pathway and authenticate the origin of the asymmetric induction in the [Co(**P5**)]-catalyzed asymmetric radical bicyclization process of *N*-benzyl-*N*-allylsulfamoyl azide **2.1a** (Scheme 2.5; see Section 2.4.8 for energy diagrams, structures and other details). Experiments were designed to probe and trap radical intermediates in the *N*-heterobicyclization reaction process.

The DFT calculations display strong binding of azide **2.1a** with catalyst [Co(**P5**)] via multiple H-bonding and other noncovalent interactions to assemble the initial substrate complex **B**. The formation of complex **B** is an exergonic process with a release of Gibbs free energy of 17.2 kcal/mol. The optimized structure of complex **B** presents that the internal nitrogen atom of sulfamoyl azide **2.1a** is arranged close to the Co(II)-metalloradical center of [Co(**P5**)] (N---Co: 2.129 Å). The subsequent metalloradical activation (MRA) process is highly exergonic by 39.2 kcal/mol, forging α-Co(III)-aminyl radical intermediate **C** and releasing dinitrogen. In addition, it is accompanied by an accessible activation barrier ($\Delta G^{\ddagger}_{TS1}$ = 7.7 kcal/mol). For the regioselectivity of radical addition, DFT calculations reveal that radical intermediate **C** favors 6-*endo*-*trig* cyclization through the 6-membered T.S. over 5-*exo*-*trig* cyclization through the strained 5-membered T.S. by 8.7 kcal/mol (See Scheme 2.12 for the energy diagram for the regioselectivity and more details in Section 2.4.8).

Scheme 2.5 Computational Investigation of [Co(P5)]-Catalyzed Asymmetric Radical *N*-Heterobicyclization via *endo*-Radical Addition



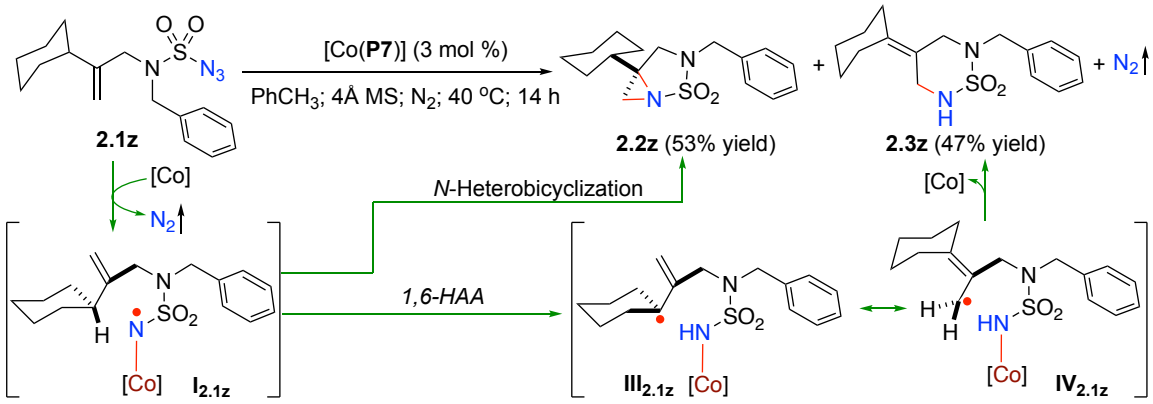
[a]Applied bp86/6-311G(d)/def2-svp level of theory for the geometry optimization and the energy calculations (kcal/mol) at 40 ºC along with Grimme's dispersion correction; Energy unit: kcal/mol.

To justify the origin of the enantioselectivity, the energetics of 6-*endo*-*trig* cyclization was computed to reveal the preference between *Re*- and *Si*-faces of the terminal alkene unit of intermediate **C**, forming γ-Co(III)-alkyl radical intermediate (*S*)-**D** with pro-(*R*) chirality and γ-Co(III)-alkyl radical intermediate (*R*)-**D** with pro-(*S*) chirality, respectively (Scheme 2.5). In radical addition stage, intermediate **C** favorably undergoes pro-(*S*) T.S. **TS2*Si*** over pro-(*R*) T.S. **TS2*Re*** both kinetically ($\Delta G^{\ddagger}_{TS2^{Si}}$ = 6.9

kcal/mol; $\Delta G^{\ddagger}_{\mathbf{TS2}^{Re}}$ = 8.9 kcal/mol) and thermodynamically ($\Delta G^{o}_{(R)\text{-}\mathbf{D}}$ = –6.7 kcal/mol; $\Delta G^{o}_{(S)\text{-}\mathbf{D}}$ = –6.2 kcal/mol). The DFT-optimized structures of $\mathbf{TS2}^{Si}$ and $\mathbf{TS2}^{Re}$ present two hydrogen bonding interactions (N–H•••O=S and C–H•••O=S) between one cyclopropane-carboxyamide unit of the catalyst and the sulfonyl group of the substrate, along with additional noncovalent attractive interactions such as C.H.–π interactions and Van der Waals attraction between the alkyl linkage of the catalyst and the substrate. And the corresponding non-covalent interaction (NCI) plots display more Vander Waals interactions and stronger H-bonding in $\mathbf{TS2}^{Si}$ than $\mathbf{TS2}^{Re}$ (as indicated by the distances in Scheme 2.5), contributing to the energy difference between the two activation barriers. In the 3-*exo*-*tet* cyclization step, both intermediates (*S*)-**D** and (*R*)-**D** proceed with the ring annulation readily through the low activation barriers ($\Delta G^{\ddagger}_{\mathbf{TS3}^{R}}$ = 3.8 kcal/mol; $\Delta G^{\ddagger}_{\mathbf{TS3}^{S}}$ = 6.1 kcal/mol), yielding two enantiomers of the final product [3.1.0]-bicyclic sulfamoyl aziridine, (*R*)-**2.2a** and (*S*)-**2.2a**. In comparison to the activation barrier of 3-*exo*-*tet* cyclization, the interconversion between intermediates (*S*)-**D** and (*R*)-**D** underwent a much higher activation barrier ($\Delta G^{\ddagger}_{\mathbf{TS4}} \approx$ 15 kcal/mol) through chair flipping (ring puckering). Because in addition to the ring puckering of the 6-membered ring, intermediate **D** requires additional energies to shatter multiple noncovalent attractive interactions (such as H-bonding and π-stacking interactions) in the interconversion of two intermediates. Accordingly, intermediates (*S*)-**D** and (*R*)-**D** are predicted to directly undergo the facile 3-*exo*-*tet* cyclization without the interconversion, instantly delivering the respective enantiomer of **2.2a**. Hence, the radical addition step through 6-*endo*-*trig* cyclization is determined as the enantiodetermining step, transforming α-Co(III)-aminyl radical intermediate **C** to γ-Co(III)-alkyl radical intermediate **D** with the formation

of a 6-membered chiral radical center. And the newly formed 6-membered chiral radical center is proven to be kinetically configurationally stable under the reaction condition, not epimerizing before undergoing the subsequent ring annulation in a stereospecific manner. Quantitatively, the energy difference ($\Delta\Delta G^{\ddagger}_{TS2}$ = 2.0 kcal/mol) between **TS2**^{Re} and **TS2**^{Si} matches superbly with the obtained enantioselectivity (90% ee) of [3.1.0]-bicyclic sulfamoyl aziridine **2.2a**. Thus, it further supports that the step of radical addition determines asymmetric induction.

Scheme 2.6 Probing α-Co(III)-Aminyl Radical Intermediate via the Chemoselectivity between *N*-Heterobicyclization and C–H Amination



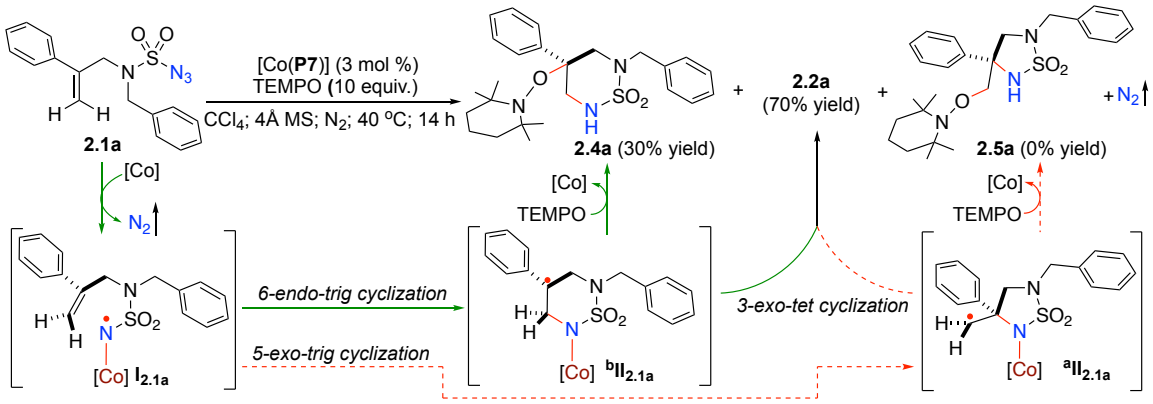
[a]Performed in toluene at 40 ºC for 14 h using [Co(**P7**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1z**] = 0.2 M; NMR yields.

The metalloradical amination reactions of **2.1z** carrying allylic C–H bonds was taken to probe α-Co(III)-aminyl radical and to demonstrate stepwise mechanism. The achiral catalyst [Co(**P7**)] (**P7** = 3,5-Di^{t}Bu-IbuPhyrin)[9a] produces a mixture of the bicyclization product **2.2z** and C–H amination product **2.3z** under standard conditions in 53% and 47% yield, respectively (Scheme 2.6). The production of **2.3z** indicates α-Co(III)-aminyl

radical intermediate $\mathbf{I_{2.1z}}$ was formed through the metalloradical activation and sequentially undergoes 1,6-HAA to deliver ζ-Co(III)-allylic radical intermediate in two resonance structures, 3°-allylic radical $\mathbf{III_{2.1z}}$ and 1°-allylic radical $\mathbf{IV_{2.1z}}$. The radical substitution step favors the less sterically hindered 1°-radical form $\mathbf{IV_{2.1z}}$, producing 6-membered cyclic sulfamide **2.3z**.

TEMPO (2,2,6,6,-tetramethyl-1-piperidinyloxy) radical was proposed to recognize the two potential catalytic pathways, 5-*exo-trig* cyclization pathway by trapping 5-membered γ-Co(III)-alkyl radical intermediate $^{a}\mathbf{II}$, and 6-*endo-trig* cyclization pathway by trapping 6-membered γ-Co(III)-alkyl radical intermediate $^{b}\mathbf{II}$. To this end, the *N*-heterobicyclization reaction of *N*-allylsulfamoyl azide **2.1a** was executed with [Co(**P7**)] in the presense of TEMPO (10.0 equiv) (Scheme 2.7). In addition to the formation of aziridine **2.2a** in 70% yield, 6-membered cyclic sulfamide **2.4a** was generated in 30% yield as a TEMPO-trapped product. The production of **2.4a** rather than 5-membered cyclic sulfamide **2.5a** supports the formation of γ-Co(III)-alkyl radical intermediate $^{b}\mathbf{II_{2.1a}}$ and denies the involvement of γ-Co(III)-alkyl radical intermediate $^{a}\mathbf{II_{2.1a}}$ (Scheme 2.7). Accordingly, the 6-*endo-trig* cyclization was experimentally demonstrated to be favored over the 5-*exo-trig* cyclization by α-Co(III)-aminyl radical intermediate $\mathbf{I_{2.1a}}$, which is consistent with computational investigations.

Scheme 2.7 Trapping of γ-Co(III)-Alkyl Radical Intermediate via TEMPO Radical[a]

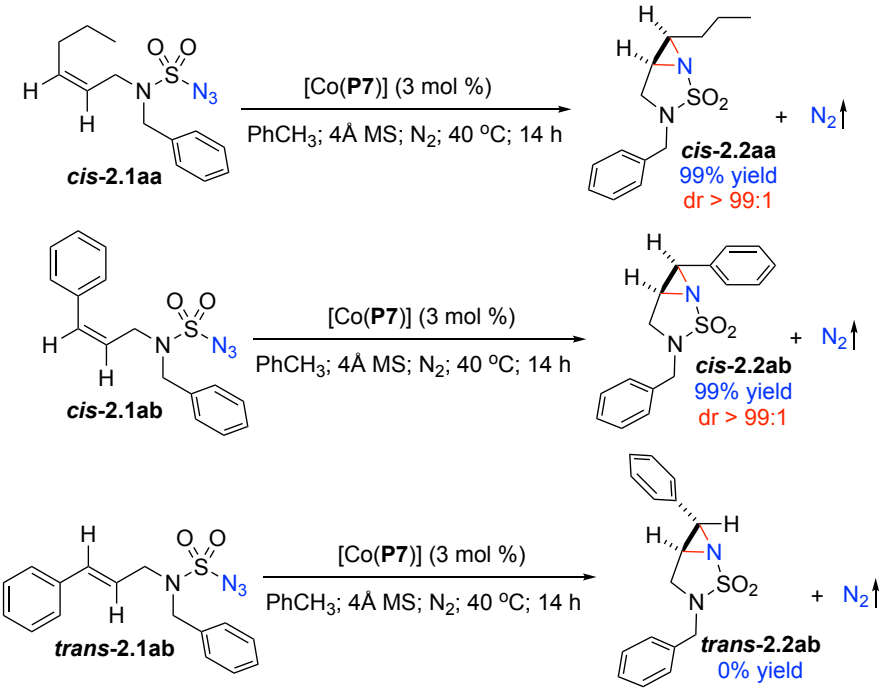


[a]Performed in carbon tetrachloride with TEMPO (10.0 equiv) at 40 ºC for 14 h using [Co(**P7**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1a**] = 0.2 M; NMR yields.

Previously, [Co(**P5**)]-catalyzed *N*-heterobicyclization of *N*-allylsulfamoyl azides *cis*-**2.1aa** and *cis*-**2.1ab** containing *cis*-alkene units afforded the corresponding aziridines *cis*-**2.2aa** and *cis*-**2.2ab**, respectively, with complete conservation of the original *cis*-stereochemistry, revealing the kinetic stereo-stability of the chiral radical center of γ-Co(III)-alkyl radical intermediates ^{b}**II**. To further explore the potential ligand effect on the diastereospecificity, *N*-heterobicyclization reactions of both *cis*-**2.1aa** and *cis*-**2.1ab** were conducted with [Co(**P7**)] under standard conditions. Incredibly, *cis*-**2.2aa** and *cis*-**2.2ab** were yielded exclusively (99%) without the *trans*-isomers, showing the inherent difficulty of the interconversion between intermediates (*R*)-**D** and (*S*)-**D** even with more flexible achiral ligand **P7**. Additionally, *trans*-**2.1ab** didn't perform *N*-heterobicyclization with [Co(**P7**)] under standard conditions and resulted in the full recovery of starting material. These experimental results, along with the findings from the computational studies, validate a novel mode of asymmetric induction in radical chemistry that a

kinetically stereo-stable chiral radical can be formed on a rigid six-membered ring from 6-*endo-trig* cyclization and subsequently execute a facile stereospecific transformation.

Scheme 2.8 Examining Stability of Chiral Radical Center in γ-Co(III)-Alkyl Radical Intermediates through *cis*-Olefins[a]

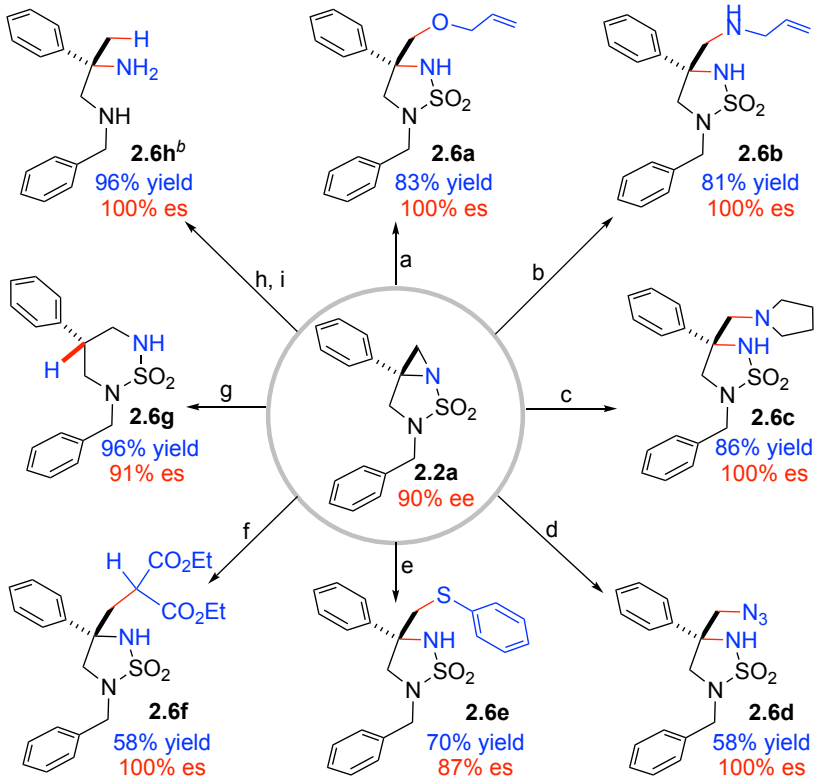


[a]Performed in toluene at 40 ºC for 14 h using [Co(**P7**)] (3 mol %) under N_2 in the presence of 4 Å MS; [**2.1**] = 0.2 M; NMR yields.

2.2.6 Further Transformation

By utilizing the highly strained ring structure of the resulting [3.1.0]-bicyclic sulfamoyl aziridines **2.2**, the synthetic applications of this heterobicyclization were presented with diverse stereospecific ring-opening reactions employing enantioenriched aziridine **2.2a** having 90% ee for demonstration (Scheme 2.9).

Scheme 2.9 Stereospecific Ring-Opening Reactions of Enantioenriched [3.1.0]-Bicyclic Sulfamoyl Aziridine[a]

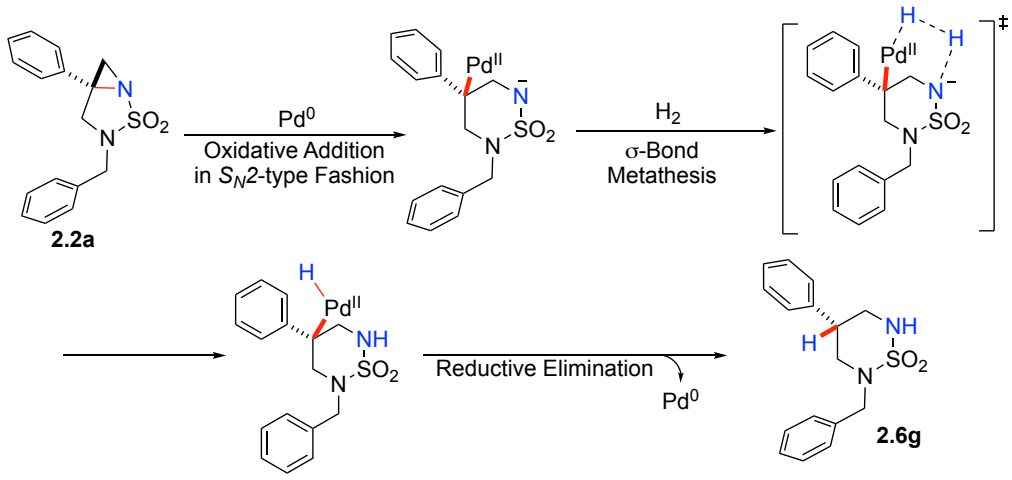


[a](a) 2-Propen-1-ol (10.0 equiv); Sodium Hydride (10.0 equiv); THF/DMSO (1/1); 0 ºC; 12 h. (b) 2-Propenamine (5.0 equiv); THF/DMSO (1/1); 40 ºC; 12 h. (c) Pyrrolidine; THF/DMSO (1/1); 40 ºC; 12 h. (d) Trimethylsilyl Azide (2.0 equiv); Tetrabutylammonium Fluoride (2.0 equiv); THF; rt; 12 h. (e) Thiophenol (5.0 equiv); Sodium Hydride (5.0 equiv); THF/DMSO (1/1) ; 0 ºC; 12 h. (f) Diethyl Malonate (4.0 equiv); Sodium Hydride (2.0 equiv); THF/DMSO (1/1); 40 ºC; 12 h. (g) Pd/C (0.1 equiv); H_2; Diisopropylamine (5.0 equiv); EtOH; rt; 3 h. (h) Lithium Aluminum Hydride (5.0 equiv); THF; 90 ºC; 12 h. (i) 1,1'-Carbonyldiimidazole (1.2 equiv); DCM; rt; 12 h. [b]ee measured with its further transformation product **2.6i** (see 2.4.6 Further Transformations for details).

We established that the aziridine ring of **2.2a** could be regioselectively opened at the *exo*-position by *O*-, *N*-, *S*-, and *C*-based nucleophiles. For instance, when **2.2a** was treated with allylic alcohol under the basic condition, the regioselective ring opening was achieved by the *O*-based nucleophile to deliver 1,2,3-diamino alcohol derivative **2.6a** in 83% yield with retention of the original enantiopurity. As additional examples, the regioselective ring-opening of **2.2a** could be realized with *N*-based nucleophiles such as primary allylic amine, secondary pyrrolidine, and trimethylsilyl azide, producing optically active 1,2,3-triamine derivatives **2.6b**–**2.6d** in yields of 58-86% with full enantiospecificities under mild conditions. As another example, thiophenol could serve as an effective *S*-based nucleophile for **2.2a** to deliver the ring-opening product **2.6e** in 70% yield with 87% es under the basic condition. Similarly, the ring-opening reaction could also be conducted using diethyl malonate as a *C*-based nucleophile, furnishing the product **2.6f** in 58% yield with 100% es in the presence of NaH.

In addition to the stereospecific ring-opening transformations, [3.1.0]-bicyclic sulfamoyl aziridines **2.2** could also be transformed into unprotected diamines, potentially serving as functional building blocks for valuable chiral diamines.[18] To ascertain this synthetic application, **2.2a** was converted to 1,3-diamine derivative **2.6g** in 96% yield with 91% es when the aziridine ring was reduced by H_2 under Pd/C in the presence of diisopropylamine and correspondingly opened at *endo*-position. The Pd^0 could undergo oxidative addition in S_N2-type fashion and largely from the front side due to the steric effects,[19] and subsequently undergo σ-bond metathesis with H_2 to generate Pd^{II}–H species.[20] Lastly, Pd^{II}–H species could undergo reductive elimination to deliver **2.6g**.

Scheme 2.10 Proposed Mechanism for the Generation of 2.6g



Additionally, when **2.2a** was treated with $LiAlH_4$ in THF, the selective ring-opening at the *exo*-position was executed by the hydride, and subsequent removal of the sulfonyl group occurred through the workup, directly delivering unprotected 1,2-diamine **2.6h** in 96% yield with 100% es. Furthermore, **2.6h** could be transformed to imidazolidinone **2.6i** in 74% yield with the original enantiopurity by reacting with carbonyldiimidazole.

2.3 CONCLUSIONS

The first catalytic system for asymmetric radical *N*-heterobicyclization of *N*-allylsulfamoyl azides **2.1** was developed via Co(II)-based metalloradical catalysis (MRC). Given the support of the D_2-symmetric chiral bridged amidoporphyrin 3,5-Di^{t}Bu-Hu(C_6)Phyrin as the effective ligand, the Co(II)-based metalloradical system can activate allyl sulfamoyl azides in a homolytic manner under mild conditions without oxidants or any additives, stereoselectively constructing [3.1.0]-bicyclic sulfamoyl aziridines **2.2** in excellent yields along with great diastereoselectivities and enantioselectivities. It should be emphasized that the [Co(**P5**)]-catalyzed *N*-heterobicyclization system is not limited to *N*-allylsulfamoyl azides containing activated alkenes (**2.1a**–**2.1q**). Notably, the catalytic system proved to be similarly effective for asymmetric heterobicyclization of *N*-allylsulfamoyl azides with nonactivated aliphatic alkenes, such as monosubstituted olefins (**2.1r** and **2.1s)** and disubstituted olefins carrying various alkyl groups (**2.1t**–**2.1z**). This [Co(**P5**)]-based asymmetric *N*-heterobicyclization tolerates *N*-allylsulfamoyl azides possessing internal alkenes as presented by the *N*-heterobicyclization of *cis*-**2.1aa** and *cis*-**2.1ab**, producing the corresponding *cis*-**2.2aa** and *cis*-**2.2ab** stereospecifically in excellent yields with reasonable enantioselectivities. Furthermore, a series of enantiospecific transformations of the enantioenriched [3.1.0]-bicyclic sulfamoyl aziridines were showcased to prepare valuable chiral 1,2-diamine and 1,3-diamine motifs **2.6**. We believe that this Co(II)-based metalloradical system for asymmetric radical *N*-heterobicyclization process may find practical synthetic applications.

Fundamentally, we have revealed a new mode of asymmetric induction that the chirality of radical center on rigid structure can be kinetically stable and directs the enantioselectivity of final product. In this *N*-heterobicyclization system, γ-Co(III)-alkyl radical intermediate **^{b}II** possessing a kinetically stable chiral radical center on a rigid six-membered ring is formed from *6-endo-trig* addition of initially formed α-Co(III)-aminyl radical intermediate **I** to a terminal olefin unit, and can readily undergo stereospecific radical substitution reaction to produce product **2.2** without racemization. The challenging enantioface selectivity in the *6-endo-trig* addition was realized from the fine-tuning of D_2-symmetric chiral bridged amidoporphyrin HuPhyrin ligands to accommodate the weak interactions between substrates and catalysts.

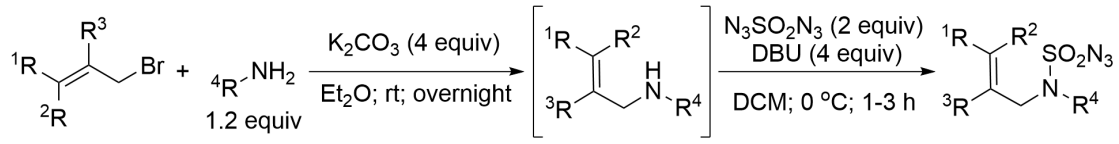
2.4 EXPERIMENTAL SECTION

2.4.1 General Considerations

All bicyclization reactions were performed under a nitrogen atmosphere in an oven-dried glassware following standard Schlenk techniques. 4 Å molecular sieves were dried in a vacuum oven prior to use. Gas tight syringes were used to transfer liquid reagents and solvents in catalytic reactions. Anhydrous solvents were purchased from Sigma-Aldrich and used without further purification. Thin layer chromatography was performed on Merck TLC plates (silica gel 60 F254). Flash column chromatography was performed with silica gel (60 Å, 230-4mesh, 32-63 μm). ^{1}H NMR and ^{13}C NMR were recorded on Varian/Agilent 400, Varian/Agilent 500, Varian/Agilent 600, and Bruker 5instruments with chemical shifts reported relative to residual solvent, and data is reported as: s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, sext. = sextet, sept. = septet, m = multiplet. Infrared spectra were measured with a Nicolet Avatar 320 spectrometer with a Smart Miracle accessory. HRMS data was obtained on an Agilent 11LC/MS/TOF mass spectrometer. HPLC measurements were carried out on a Shimadzu HPLC system with Chiralcel IC, IA and OD-H columns. Optical rotations were recorded on the Rudolph Research Analytical, Autopol® IV, Automatic Polarimeter.

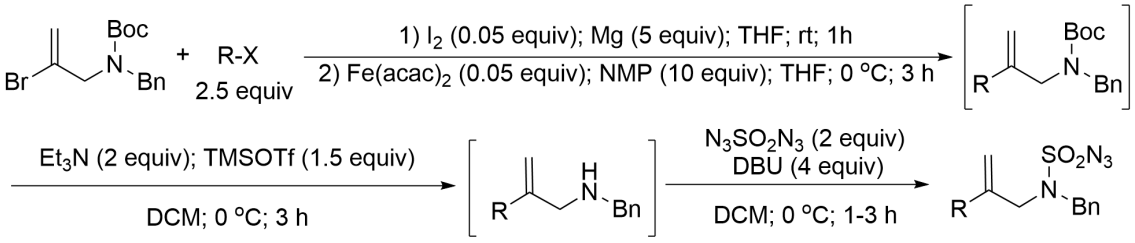
2.4.2 Preparation and Characterization of Allyl Sulfamoyl Azides

Synthetic Method I of Allyl Sulfamoyl Azides



To a solution of amine (1.2 equiv) and K_2CO_3 (4 equiv) in Et_2O was added the solution of bromide (1 equiv) in Et_2O dropwise during 2 h and the reaction was stirred overnight at room temperature. The reaction was wash with water 3 times and the solvent was removed directly under reduced pressure after dried over Na_2SO_4. The crude product (secondary amine) was used directly for next step without any further treatment. According to the reported procedure of the synthesis sulfamoyl azide from secondary amine,[4] a mixture of crude secondary amine from the previous step and DBU (4 equiv) in DCM was added dropwise to a solution of $N_3SO_2N_3$ (2 equiv, 0.3 M in DCM) at 0 °C. After the reaction was completed based on TLC (1~3 h), the majority of the solvent was removed under reduced pressure at room temperature. Purification of this mixture by silica gel column chromatography afforded the allyl sulfamoyl azide. Note: Some azides could be explosive and should be handled carefully.

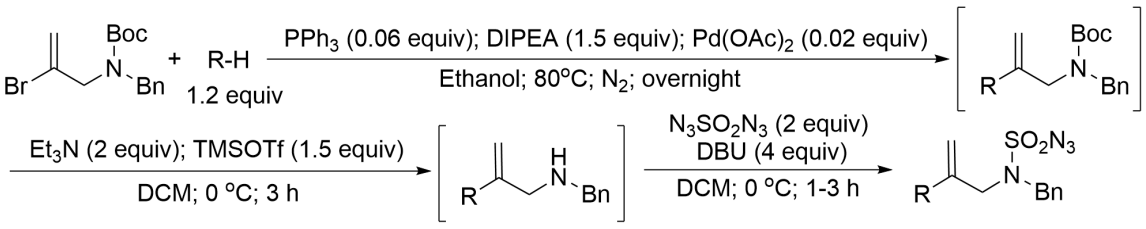
Synthetic Method II of Allyl Sulfamoyl Azides



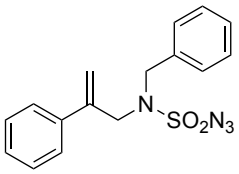
Under stirring, bromide (5 equiv) was added to magnesium (5 equiv) in anhydrous THF (20 mL) dropwise under N_2 at room temperature. Then, a solution of I_2 (0.05 equiv) in anhydrous THF (2 mL) was added dropwise and the solution was turned to dark purple. If the color didn't disappear in 10 mins, the reaction was heat up with heat gun. Stirring was continued for 1 h at room temperature. The organic magnesium bromide was obtained. A well-dried round bottom flask equipped with a magnetic stir bar was charged with a solution of *tert*-butyl benzyl(2-bromoallyl)carbamate and $Fe(acac)_2$ (0.05 equiv) in anhydrous THF (10 mL) under nitrogen atmosphere, and the mixture was cooled to 0 ºC. To the solution *N*-methylpyrrolidone (10 equiv) and freshly made organic magnesium bromide (2.5 equiv) were slowly added. After being stirred for 1 h, aq. 1 M HCl was added. The mixture was extracted with EtOAc (30 mL×3). The combined organic phase was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was directly used for next step without any further treatment.[21]

To a mixture of crude amide from the previous step and Et_3N (2 equiv) in DCM, and TMSOTf (1.5 equiv) was added dropwise at 0 ºC. After stirring for another 3h at 0 ºC, the reaction mixture was washed with $NaHCO_3$ solution, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product (secondary amine) was directly used for next step without any further treatment. The allyl sulfamoyl azide was synthesized with the crude secondary amine from the previous step through same procedure as method **I**.

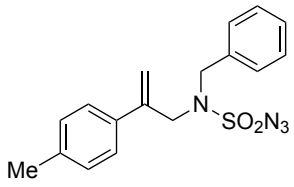
Synthetic Method III of Allyl Sulfamoyl Azides



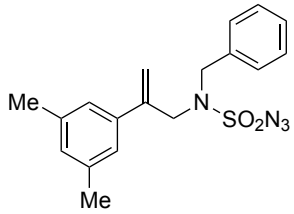
To a 1ml flask charged with $Pd(OAc)_2$ (0.02 equiv) and PPh_3 (0.06 equiv), ethanol, *tert*-butyl benzyl(2-bromoallyl)carbamate (1 equiv), diisopropyl ethyl amine (1.5 equiv), and diethyl phosphite (1.2 equiv) were added. The reaction mixture was heated to reflux overnight. After completion of the reaction, the solution was diluted with ethyl acetate and washed with brine. The organic fraction was dried over Na_2SO_4 and concentrated under reduced pressure. The residue (amide) was directly used for next step without any further treatment.[22] The allyl sulfamoyl azide was synthesized with the crude amide from the previous step through same procedures as method **II**.



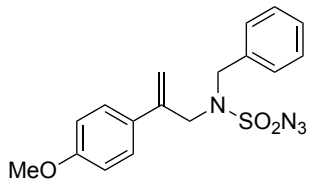
(((Azidosulfonyl)(2-phenylallyl)amino)methyl)benzene 2.1a. Colorless oil. Yield: 81% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^1H NMR (5MHz, $CDCl_3$) δ 7.38 – 7.21 (m, 10H), 5.53 (s, 1H), 5.33 (s, 1H), 4.40 (s, 2H), 4.31 (s, 2H). 13C NMR (126 MHz, CDCl3) δ 142.20, 138.19, 134.35, 128.88, 128.82, 128.63, 128.45, 128.42, 126.59, 117.79, 51.72, 51.70.IR (neat, cm^{-1}): 2127.73, 1381.11, 1167.35. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{16}H_{17}N_4O_2S$: 329.10667, found 329.10615. This is a known compound.[11]



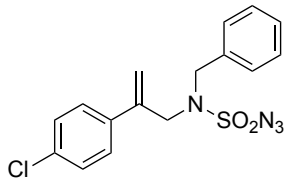
1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-4-methylbenzene 2.1b. White solid. Yield: 60% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.24 (m, 7H), 7.21 – 7.13 (m, 2H), 5.50 (s, 1H), 5.28 (s, 1H), 4.40 (s, 2H), 4.30 (d, *J* = 1.2 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.03, 138.41, 135.32, 134.44, 129.36, 128.96, 128.86, 128.45, 126.51, 117.08, 77.41, 77.15, 76.90, 51.71, 51.65, 21.28. IR (neat, cm^{-1}): 2124.74, 1379.06, 1165.66, 733.80. HRMS (DART$^+$) ([M+H]$^+$): Calcd. For $C_{17}H_{19}N_4O_2S$: 343.12232, found 343.12210.



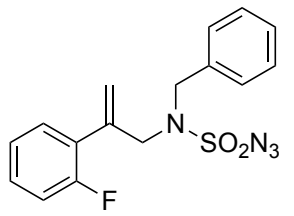
1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-3,5-dimethylbenzene 2.1c. Colorless oil. Yield: 58% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.58 – 7.17 (m, 5H), 7.09-6.90 (d, *J* = 10.4 Hz, 3H), 5.51 (s, 1H), 5.31 (s, 1H), 4.42 (s, 2H), 4.30 (s, 2H), 2.34 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.46, 138.28, 138.12, 134.48, 130.11, 128.92, 128.82, 128.41, 124.50, 117.31, 51.72, 51.67, 21.41. IR (neat, cm^{-1}): 2123.81, 1379.09, 1165.60, 733.54. HRMS (DART$^+$) ([M+H]$^+$): Calcd. For $C_{18}H_{21}N_4O_2S$: 357.13797, found 357.13763.



1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-4-methoxybenzene 2.1d. White oil. Yield: 62% (Method II). R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.45-7.20 (m, 7H), 6.95 – 6.85 (m, 2H), 5.47 (s, 1H), 5.24 (s, 1H), 4.40 (s, 2H), 4.30 (s, 2H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.89, 141.48, 134.44, 130.49, 128.94, 128.83, 128.42, 127.82, 116.40, 114.03, 55.42, 51.87, 51.60. IR (neat, cm^{-1}): 2126.95, 1513.69, 1378.34, 1249.60, 1166.40, 736.88. HRMS ($DART^+$) ($[M+H]^+$): Calcd. For $C_{17}H_{19}N_4O_3S$: 359.11724, found 359.11613.

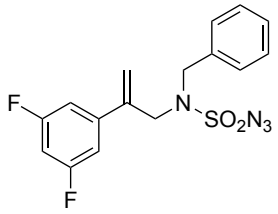


1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-4-chlorobenzene 2.1e. White solid. Yield: 63% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.38 – 7.29 (m, 5H), 7.29 – 7.21 (m, 4H), 5.50 (s, 1H), 5.33 (s, 1H), 4.38 (s, 2H), 4.29 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.20, 136.48, 134.41, 134.20, 128.94, 128.89, 128.82, 128.53, 127.95, 118.37, 51.90, 51.88. IR (neat, cm^{-1}): 2126.71, 1379.59, 1166.15, 734.15. HRMS ($DART^+$) ($[M+NH_4]^+$): Calcd. for $C_{16}H_{19}N_5O_2SCl$: 380.09425, found 380.09399.

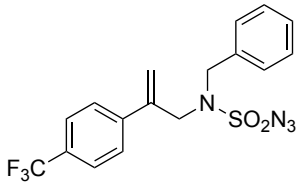


1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2-fluorobenzene 2.1f. Colorless oil. Yield: 65% (Method II). R_f = 0.6 (16:1

Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.39 – 7.27 (m, 6H), 7.24 (m, 1H), 7.14 (m, 1H), 7.07 (m, 1H), 5.48 (s, 1H), 5.45 (s, 1H), 4.42 (s, 2H), 4.25 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.06, 159.09, 138.45, 134.36, 130.40 (d, *J* = 3.8 Hz), 130.07 (d, *J* = 8.2 Hz), 128.91 (d, *J* = 2.7 Hz), 128.52, 126.64 (d, *J* = 14.3 Hz), 124.47 (d, *J* = 3.4 Hz), 121.04, 115.96 (d, *J* = 22.4 Hz), 52.15 (d, *J* = 4.3 Hz), 51.97. ^{19}F NMR (470 MHz, CDCl3) δ -114.70 (m, 1F). IR (neat, cm^{-1}): 2126.59, 1381.29, 1167.32. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{16}H_{16}N_4O_2FS$: 347.09725, found 347.09698.

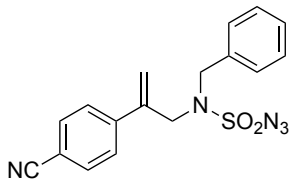


1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-3,5-difluorobenzene 2.1g. Colorless oil. Yield: 73% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.43 – 7.25 (m, 5H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.72 (t, *J* = 8.8 Hz, 1H), 5.47 (s, 1H), 5.34 (s, 1H), 3.81 (s, 2H), 3.60 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.03 (d, *J* = 13.1 Hz, 1C), 162.06 (d, *J* = 13.1 Hz, 1C), 144.50, 143.42 (t, *J* = 9.4 Hz, 1C), 140.09, 128.32 (d, *J* = 30.0 Hz, 1C), 127.08, 115.50, 109.58 – 108.59 (m, 1C), 102.82 (t, *J* = 25.5 Hz, 1C), 53.08, 52.54. ^{19}F NMR (564 MHz, $CDCl_3$) δ -110.22 (m, 2F). IR (neat, cm^{-1}): 2125.87, 1378.60, 1165.00, 1118.60, 733.13. HRMS ($DART^+$) ($[M+NH_4]^+$): Calcd. for $C_{16}H_{18}N_5O_2F_2S$: 382.11438, found 382.11524.

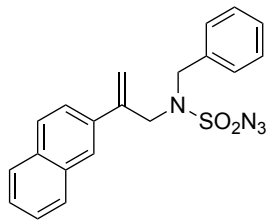


1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-4-(trifluoromethyl)benzene 2.1h. White solid. Yield: 62% (Method II). R_f = 0.6 (16:1

Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.33 (dd, *J* = 4.8, 1.9 Hz, 3H), 7.29 – 7.23 (m, 2H), 5.58 (s, 1H), 5.43 (s, 1H), 4.40 (s, 2H), 4.35 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.59, 141.28, 134.12, 130.35 (q, *J* = 32.6 Hz), 128.89, 128.86, 128.53, 126.97, 125.54 (q, *J* = 3.8 Hz), 124.16 (q, *J* = 272.2 Hz), 119.65, 52.10, 51.99. ^{19}F NMR (564 MHz, $CDCl_3$) δ -62.71 (s, 1F). IR (neat, cm^{-1}): 2128.95, 1326.33, 1166.77, 1119.53, 1066.84. HRMS (DART$^+$) ([M+NH_4]$^+$): Calcd. for $C_{16}H_{15}FN_2O_2S$: 414.12061, found 414.12055.

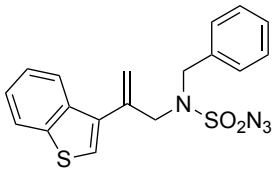


1-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-4-cyanobenzene 2.1i. Colorless oil. Yield: 50% (Method II). R_f = 0.3 (5:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.26 (m, 3H), 7.21 (m, 2H), 5.56 (s, 1H), 5.43 (s, 1H), 4.36 (s, 2H), 4.31 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.45, 141.07, 134.02, 132.42, 128.97, 128.93, 128.64, 127.30, 120.50, 118.70, 112.10, 52.28, 51.99. IR (neat, cm^{-1}): 2129.54, 1381.38, 1167.63. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{15}N_5O_2S$: 354.10192, found 354.10171.

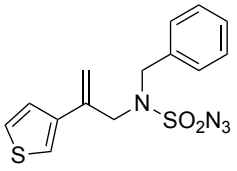


2-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)naphthalene 2.1j. White solid. Yield: 60% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.90 – 7.77 (m, 4H), 7.56 – 7.48 (m, 3H), 7.38 – 7.27 (m, 5H), 5.69 (s, 1H), 5.44 (s, 1H), 4.45 (s, 2H), 4.44 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.05,

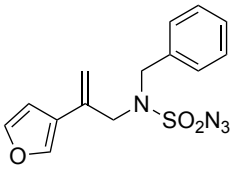
135.40, 134.37, 133.31, 133.26, 128.96, 128.88, 128.86, 128.48, 128.41, 128.33, 127.71, 127.70, 126.54, 126.49, 125.68, 124.54, 118.27, 51.85, 51.80. IR (neat, cm^{-1}): 2127.28, 1381.22, 1167.57. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{20}H_{19}N_4O_2S$: 379.12232, found 379.12190.



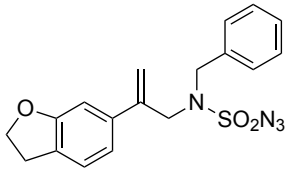
3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)benzo[*b*]thiophene 2.1k. Colorless oil. Yield: 43% (Method II). R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.93 – 7.86 (m, 1H), 7.85 – 7.78 (m, 1H), 7.42 – 7.36 (m, 2H), 7.35-7.29 (m, 4H), 7.28 – 7.23 (m, 2H), 5.61 (s, 1H), 5.60 (s, 1H), 4.42 (s, 2H), 4.30 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.63, 137.71, 136.88, 134.38, 134.24, 128.95, 128.90, 128.59, 124.78, 124.65, 123.12, 122.83, 119.31, 52.95, 52.05. IR (neat, cm^{-1}): 2124.92, 1378.76, 1165.01, 739.52, 608.56. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{18}H_{17}N_4O_2S_2$: 385.07874, found 385.07872.



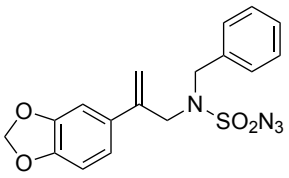
3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)thiophene 2.1l. Colorless oil. Yield: 57% (Method II). R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 4H), 7.29 (m, 3H), 7.18 (dd, *J* = 5.1, 1.4 Hz, 1H), 5.60 (s, 1H), 5.27 (s, 1H), 4.44 (s, 2H), 4.26 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.16, 136.45, 134.45, 129.02, 128.89, 128.52, 126.13, 125.94, 122.19, 116.35, 52.17, 51.79. IR (neat, cm^{-1}): 2129.30, 1166.43, 735.75. HRMS (DART$^+$) ([M+NH_4]$^+$): Calcd. for $C_{14}H_{18}N_5O_2S_2$: 352.08964, found 352.08885.



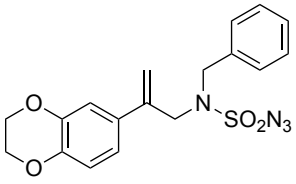
3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)furan 2.1m. Colorless oil. Yield: 68% (Method II). R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.40 (m, 1H), 7.44 – 7.39 (m, 1H), 7.38 – 7.24 (m, 5H), 6.52 (m, 1H), 5.51 (s, 1H), 5.21 (s, 1H), 4.47 (s, 2H), 4.16 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.54, 139.93, 134.31, 133.15, 129.11, 128.87, 128.54, 123.74, 115.45, 108.29, 51.65. IR (neat, cm^{-1}): 2127.80, 1379.13, 1165.54. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{14}H_{15}N_4O_3S$: 319.08594, found 319.08838.



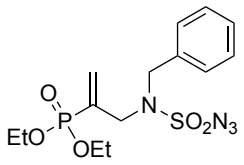
5-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2,3-dihydrobenzofuran 2.1n. Colorless oil. Yield: 67% (Method II). R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.36 – 7.28 (m, 4H), 7.31 – 7.25 (m, 1H), 7.21 – 7.18 (m, 1H), 7.15 – 7.10 (m, 1H), 6.75 (d, *J* = 8.2 Hz, 1H), 5.41 (s, 1H), 5.20 (s, 0H), 4.58 (t, *J* = 8.7 Hz, 2H), 4.39 (s, 2H), 4.27 (s, 1H), 3.20 (t, *J* = 8.7 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.53, 141.93, 134.50, 130.64, 128.94, 128.81, 128.40, 127.52, 126.70, 123.37, 116.12, 109.30, 71.64, 52.03, 51.64, 29.72. IR (neat, cm^{-1}): 2125.71, 1494.09, 1378.73, 1233.15, 1164.39, 608.49. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{18}H_{19}N_4O_3S$: 371.11724, found 371.11735.



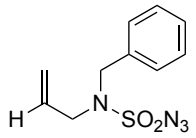
5-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)benzo[*d*][1,3]dioxole 2.1o. Colorless oil. Yield: 45% (Method II). R_f = 0.4 (5:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.39 – 7.32 (m, 3H), 7.31 – 7.27 (m, 2H), 6.88 – 6.82 (m, 2H), 6.81 – 6.77 (s, 1H), 5.98 (s, 1H), 5.43 (s, 1H), 5.24 (s, 1H), 4.40 (s, 2H), 4.25 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.54, 150.45, 144.22, 136.95, 134.80, 131.49, 131.39, 131.01, 122.87, 119.49,110.88, 109.70, 103.91, 54.49, 54.26. IR (neat, cm^{-1}): 2126.79, 1491.39, 1378.81, 1230.57, 1165.84, 1038.61, 609.03. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{17}H_{17}N_4O_4S$: 373.09650, found 373.09618.



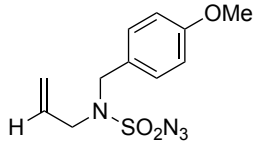
6-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2,3-dihydrobenzo[*b*][1,4]dioxine 2.1p. Colorless oil. Yield: 41% (Method II). R_f = 0.4 (5:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.38 – 7.24 (m, 5H), 6.91 – 6.82 (m, 3H), 5.45 (s, 1H), 5.22 (s, 1H), 4.40 (s, 2H), 4.26 (s, 4H), 4.24 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.98, 143.66, 141.36, 134.50, 131.61, 128.96, 128.85, 128.45, 119.83, 117.38, 116.68, 115.60, 64.56, 64.45, 51.68. IR (neat, cm^{-1}): 2127.96, 1166.31, 904.22, 724.25, 649.33, 608.23. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{18}H_{19}N_4O_4S$: 387.11215, found 387.11117.



Diethyl (3-((azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)phosphonate 2.1q. Light yellow oil. Yield: 72% (Method III). R_f = 0.25 (2:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.44 – 7.17 (m, 5H), 6.23 (d, *J* = 22.2 Hz, 1H), 6.05 (d, *J* = 45.6 Hz, 1H), 4.52 (s, 2H), 4.13 – 4.03 (m, 4H), 4.02 (d, *J* = 8.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 134.40, 134.16, 133.23, 132.15 (d, *J* = 7.5 Hz, 1C), 129.16 (d, *J* = 19.8 Hz, 1C), 128.86, 62.49 (d, *J* = 5.9 Hz, 1C), 52.76, 48.78 (d, *J* = 17.8 Hz, 1C), 16.45 (d, *J* = 6.2 Hz, 1C). ^{31}P NMR (243 MHz, $CDCl_3$) δ 13.13. IR (neat, cm^{-1}): 2124.92, 1378.76, 1165.01, 739.52, 608.56. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{14}H_{22}N_4O_5PS$: 389.10430, found 389.10531.

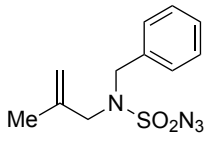


((Allyl(azidosulfonyl)amino)methyl)benzene 2.1r. Light yellow oil. Yield: 65% (Method I). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 5H), 5.87 (ddt, *J* = 16.8, 10.0, 6.7 Hz, 1H), 5.34 (d, *J* = 10.1 Hz, 1H), 5.31 – 5.23 (m, 1H), 4.46 (s, 2H), 3.83 (d, *J* = 6.7 Hz, 2H). IR (neat, cm^{-1}): 2126.34, 1380.53, 1168.09. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{10}H_{13}N_4O_2S$: 253.07537, found 253.07588. This is a known compound.[11]

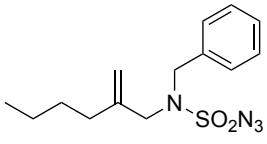


1-((Allyl(azidosulfonyl)amino)methyl)-4-methoxybenzene 2.1s. Light yellow oil. Yield: 75% (Method I). R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR

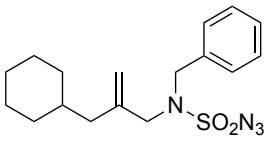
(5MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 8.2 Hz, 2H), 5.85 (ddt, *J* = 16.8, 10.2, 6.7 Hz, 1H), 5.33 (d, *J* = 10.1 Hz, 1H), 5.27 (d, *J* = 17.1 Hz, 1H), 4.40 (s, 2H), 3.85 – 3.78 (m, 5H). IR (neat, cm^{-1}): 2127.40, 1513.68, 1380.93, 1248.38, 1168.51. HRMS ($DART^+$) ($[M+NH_4]^+$): Calcd. for $C_{11}H_{14}N_4O_3S$: 300.11249, found 300.11261. This is a known compound.[11]



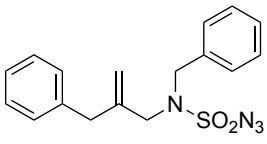
(((Azidosulfonyl)(2-methylallyl)amino)methyl)benzene 2.1t. Light yellow oil. Yield: 61% (Method I). R_f = 0.6 (16:1 Hexanes/EtOAc). ^1H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.31 (m, 1H), 5.05 (s, 1H), 4.97 (s, 1H), 4.46 (s, 2H), 3.80 (s, 2H), 1.76 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.91, 134.44, 129.06, 128.86, 128.50, 116.04, 53.93, 51.53, 19.93. IR (neat, cm^{-1}): 2125.47, 1379.55, 1166.72. HRMS ($DART^+$) ($[M+NH_4]^+$): Calcd. for $C_{11}H_{18}N_5O_2S$: 284.11757, found 284.11741. This is a known compound.[17]



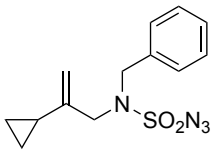
(((Azidosulfonyl)(2-methylenehexyl)amino)methyl) benzene 2.1u. Colorless oil. Yield: 74% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^1H NMR (5MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 5H), 5.06 (s, 1H), 5.03 (s, 1H), 4.46 (s, 2H), 3.84 (s, 2H), 2.04 (t, *J* = 7.7 Hz, 2H), 1.43 (dt, *J* = 15.2, 7.7 Hz, 2H), 1.38 – 1.28 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.98, 134.48, 129.09, 128.83, 128.48, 114.70, 52.81, 51.55, 32.85, 29.56, 22.42, 13.96. IR (neat, cm^{-1}): 2122.58, 1378.23, 1164.79, 698.46, 597.84. HRMS ($DART^+$) ($[M+NH_4]^+$): Calcd. for $C_{14}H_{24}N_5O_2S$: 326.16452, found 321.16459.



(((Azidosulfonyl)(2-(cyclohexylmethyl)allyl)amino)methyl) benzene 2.1v. Colorless oil. Yield: 52% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 5H), 5.05 (s, 1H), 5.02 (s, 1H), 4.45 (s, 2H), 3.78 (s, 2H), 1.93 (d, *J* = 7.1 Hz, 2H), 1.74 – 1.60 (m, 5H), 1.44 – 1.34 (m, 1H), 1.26 – 1.09 (m, 3H), 0.93 – 0.79 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.08, 134.45, 129.07, 128.83, 128.48, 115.90, 52.49, 51.56, 41.34, 35.38, 33.24, 26.55, 26.27. IR (neat, cm^{-1}): 2123.68, 1381.74, 1166.28, 607.70. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{25}N_4O_2S$: 349.16927, found 349.16969.

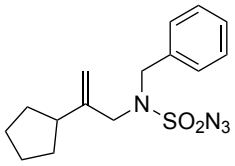


(((Azidosulfonyl)(2-benzylallyl)amino)methyl)benzene 2.1w. Colorless oil. Yield: 54% (Method I). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.37 – 7.26 (m, 5H), 7.25 – 7.18 (m, 3H), 7.16 – 7.11 (m, 2H), 5.12 (s, 1H), 5.03 (s, 1H), 4.40 (s, 2H), 3.78 (s, 2H), 3.34 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.37, 138.25, 134.43, 129.25, 128.94, 128.72, 128.60, 126.74, 116.60, 52.29, 52.02, 40.31. IR (neat, cm^{-1}): 2125.56, 1380.20, 1166.19, 699.37, 608.63. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{19}N_4O_2S$: 343.12232, found 343.12121.



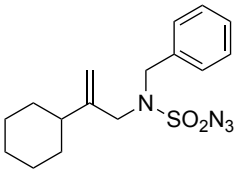
(((Azidosulfonyl)(2-cyclopropylallyl)amino)methyl)benzene 2.1x. Colorless oil. Yield: 50% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.44 – 7.27 (m, 5H), 4.89 (s, 1H), 4.86 (s, 1H), 4.49 (s, 2H), 3.90 (s, 2H),

1.36 – 1.28 (m, 1H), 0.77 – 0.69 (m, 2H), 0.53 – 0.42 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.58, 134.54, 129.08, 128.89, 128.51, 111.25, 53.34, 51.62, 13.67, 6.98. IR (neat, cm^{-1}): 2123.19, 1377.54, 1163.46, 736.27,697.96, 603.96. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{13}H_{17}N_4O_2S$: 293.10667, found 293.10726.



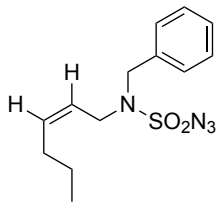
(((Azidosulfonyl)(2-cyclopentylallyl)amino)methyl)benzene

2.1y. Colorless oil. Yield: 67% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.45 – 7.30 (m, 5H), 5.10 (s, 1H), 5.01 (s, 1H), 4.47 (s, 2H), 3.87 (s, 2H), 2.37 (p, *J* = 8.6 Hz, 1H), 1.91 – 1.78 (m, 2H), 1.76 – 1.56 (m, 2H), 1.64 – 1.53 (m, 2H), 1.43 – 1.26 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.29, 134.51, 129.16, 128.85, 128.50, 111.89, 52.96, 51.69, 42.92, 31.49, 24.90. IR (neat, cm^{-1}): 2122.02, 1379.17, 1164.50, 605.14, 595.18. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{15}H_{21}N_4O_2S$: 321.13797, found 321.13803.



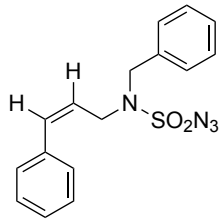
(((Azidosulfonyl)(2-cyclohexylallyl)amino)methyl)benzene

2.1z. Colorless oil. Yield: 69% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.29 (m, 5H), 5.04 (s, 1H), 5.(s, 1H), 4.45 (s, 2H), 3.87 (s, 2H), 1.86 (t, *J* = 11.7 Hz, 1H), 1.81 – 1.66 (m, 5H), 1.33 – 1.21 (m, 2H), 1.21 – 1.05 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.10, 134.60, 129.13, 128.86, 128.50, 112.63, 52.17, 51.72, 40.79, 32.27, 26.73, 26.34. IR (neat, cm^{-1}): 2122.41, 1378.88, 1164.49, 606.36, 586.81. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{16}H_{23}N_4O_2S$: 335.15362, found 335.15525.



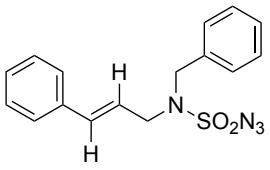
(*cis*-(((Azidosulfonyl)(hex-2-en-1-yl)amino)methyl)benzene

2.1aa. Colorless oil. Yield: 57% (Method I). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.43 – 7.29 (m, 5H), 5.76 – 5.66 (m, 1H), 5.55 – 5.47 (m, 1H), 4.44 (s, 2H), 3.89 (d, *J* = 7.0 Hz, 1H), 1.91 (q, *J* = 7.4 Hz, 2H), 1.36 (h, *J* = 7.4 Hz, 2H), 0.87 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.22, 134.69, 128.89, 128.53, 128.43, 121.94, 51.43, 44.74, 29.30, 22.59, 13.71. IR (neat, cm^{-1}): 2125.75, 1383.27, 1168.15, 606.17. HRMS (DART$^+$) ($[M+NH_4]^+$): Calcd. for $C_{13}H_{22}N_5O_2S$: 312.14887, found 312.14919.



***cis*-(((Azidosulfonyl)(3-phenylallyl)amino)methyl)benzene**

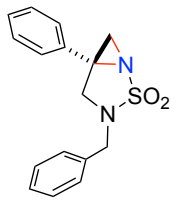
2.1ab. Light yellow oil. Yield: 41% (Method I). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.43 – 7.29 (m, 3H), 7.26 – 7.16 (m, 3H), 7.15 – 7.02 (m, 4H), 6.79 (d, *J* = 12.0 Hz, 1H), 5.88 – 5.69 (m, 1H), 4.37 (s, 2H), 4.13 (d, *J* = 6.9 Hz, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 135.71, 134.46, 134.18, 128.89, 128.83, 128.78, 128.57, 128.41, 127.77, 124.90, 51.76, 45.47. IR (neat, cm^{-1}): 2126.21, 1381.98, 1166.71, 594.09. HRMS (DART$^+$) ($[M+H]^+$): Calcd. for $C_{15}H_{27}N_4O_2S$: 327.18492, found 327.18524.



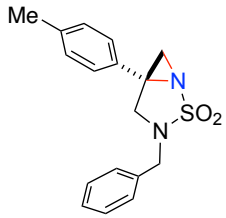
***trans*-(((Azidosulfonyl)(3-phenylallyl)amino)methyl) benzene 2.1ab.** Light yellow oil. Yield: 52% (Method I). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 10H), 6.52 (d, *J* = 15.8 Hz, 1H), 6.17 (dt, *J* = 15.8, 6.9 Hz, 1H), 4.50 (s, 2H), 3.99 (d, *J* = 6.9 Hz, 2H). This is a known compound.[23]

2.4.3 General Procedure for Co(Por)]-Catalyzed Asymmetric Bicyclization and Characterizations of [3.1.0]-Bicyclic Aziridines

An oven dried Schlenk tube was charged with catalyst [Co(**Por**)](3 mol %) and 4Å molecular sieves (50 mg). This reaction vessel was evacuated and backfilled with nitrogen three times. Under nitrogen atmosphere, the allyl sulfamoyl azide substrate (0.1 mmol) was added followed by the addition of 0.5 mL of solvent (toluene for **2.1a – 2.1s**, **2.1aa**, **2.1ab**; cyclohexane for **2.1t – 2.1z**). The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at 40 ºC for 14 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum, and purified by flash column chromatography on silica gel with mixtures of hexane/ethyl acetate in presence of 5% Et_3N. The fractions containing product were collected and concentrated by rotary evaporation to obtain the target compound. All the racemic products (for HPLC) were obtained following the same procedure with achiral catalyst [Co(**P7**)] [Co(3,5-Di^{t}Bu-IbuPhyrin)] and please find the references therein for the synthesis for this catalyst.

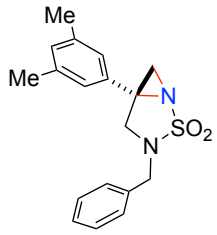


(*R*)-3-Benzyl-5-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2a** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 96%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -165.56 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.64 – 7.16 (m, 10H), 4.51 (d, *J* = 13.8 Hz, 1H), 3.96 (d, *J* = 13.8 Hz, 1H), 3.76 (d, *J* = 9.9 Hz, 1H), 3.35 (d, *J* = 9.9 Hz, 1H), 3.10 (s, 1H), 2.60 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.86, 134.84, 129.09, 129.01, 128.94, 128.71, 128.48, 126.55, 50.27, 49.12, 48.92, 39.32. HPLC analysis: *ee* = 90 %. OD-H (85% hexanes: 15% isopropanol, 1.0 mL/min): t_{major} = 19.854 min, t_{minor} = 22.036 min. IR (neat, cm^{-1}): 1336.50, 1173.43. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{16}H_{17}N_2O_2S$: 301.10052, found 301.09971.

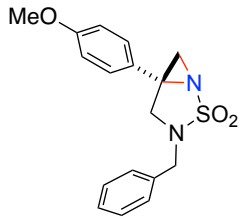


(*R*)-3-Benzyl-5-(*p*-tolyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2b** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 98%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -173.39 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.31 (m, 5H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 4.51 (d, *J* = 13.7 Hz, 1H), 3.92 (d, *J* = 13.7 Hz, 1H), 3.70 (d, *J* = 9.9 Hz, 1H), 3.31 (d, *J* = 9.9 Hz, 1H), 3.08 – 3.04 (m, 1H), 2.58 (s, 1H), 2.33 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.14, 135.00, 131.93, 129.64, 129.06, 128.78, 128.51, 126.55, 50.46, 49.17, 48.99, 39.34, 21.31. HPLC analysis: *ee* = 89%. OD-H (90% hexanes: 10%

isopropanol, 1.0 mL/min): t_{major} = 23.385 min, t_{minor} = 26.843 min. IR (neat, cm^{-1}): 1214.14, 744.30, 688.35. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{17}H_{19}N_2O_2S$: 315.11617, found 315.11578.

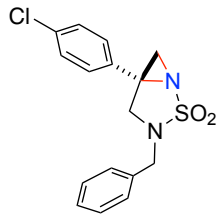


(*R*)-3-Benzyl-5-(3,5-dimethylphenyl)-2-thia-1,3-diazabicyclo [3.1.0]hexane 2,2-dioxide (–)-**2.2c** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 98%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -120.79 (*c* = 1, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.31 (m, 5H), 6.96 (s, 1H), 6.93 (s, 2H), 4.51 (d, *J* = 13.7 Hz, 1H), 3.92 (d, *J* = 13.7 Hz, 1H), 3.69 (d, *J* = 10.0 Hz, 1H), 3.30 (d, *J* = 10.0 Hz, 1H), 3.05 (s, 1H), 2.58 (s, 1H), 2.29 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.78, 135.01, 134.76, 130.76, 129.05, 128.77, 128.50, 124.29, 50.49, 49.33, 48.99, 39.31, 21.30. HPLC analysis: *ee* = 81%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 21.311 min, t_{minor} = 32.745 min. IR (neat, cm^{-1}): 1335.44, 1172.65. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{18}H_{21}N_2O_2S$: 329.13183, found 329.13091.

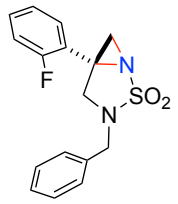


(*R*)-3-Benzyl-5-(4-methoxyphenyl)-2-thia-1,3-diazabicyclo [3.1.0]hexane 2,2-dioxide (–)-**2.2d** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 95%. R_f = 0.3 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -197.56 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.45 – 7.31

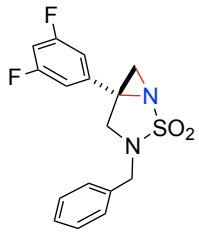
(m, 5H), 7.25 (d, J = 8.8 Hz, 2H), 6.88 (d, J = 8.8 Hz, 2H), 4.52 (d, J = 13.7 Hz, 1H), 3.93 (d, J = 13.7 Hz, 1H), 3.80 (s, 3H), 3.68 (d, J = 10.0 Hz, 1H), 3.31 (d, J = 10.0 Hz, 1H), 3.06 (s, 1H), 2.60 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.25, 135.00, 129.05, 128.77, 128.51, 128.08, 126.86, 114.40, 55.50, 50.62, 49.07, 48.98, 39.22. HPLC analysis: *ee* = 83%. IC (70% hexanes: 30% isopropanol, 1.0 mL/min): t_{major} = 21.014 min, t_{minor} = 38.765 min. IR (neat, cm^{-1}): 1519.22, 1335.66, 1249.81, 1171.05. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{17}H_{19}N_2O_2S$: 331.11109, found 331.11039.



(*R*)-3-Benzyl-5-(4-chlorophenyl)-2-thia-1,3-diazabicyclo [3.1.0]hexane 2,2-dioxide (–)-**2.2e** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 99%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -155.96 (c = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.30 (m, 6H), 7.29 – 7.25 (m, 2H), 7.25 – 7.23 (m, 2H), 4.51 (d, J = 13.7 Hz, 1H), 3.92 (d, J = 13.7 Hz, 1H), 3.71 (d, J = 10.0 Hz, 1H), 3.28 (d, J = 10.0 Hz, 1H), 3.07 (s, 1H), 2.56 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.22, 134.78, 133.48, 129.26, 129.11, 128.77, 128.76, 128.61, 128.03, 50.08, 48.97, 48.45, 39.36. HPLC analysis: *ee* = 94%. OD-H (90% hexanes: 10% isopropanol, 1.0 mL/min): t_{major} = 29.799 min, t_{minor} = 28.344 min. IR (neat, cm^{-1}): 1333.29, 1168.35, 782.31, 726.52, 696.22. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{16}H_{16}N_2O_2SCl$: 335.06155, found 335.06146.

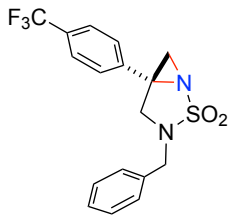


(*R*)-3-Benzyl-5-(2-fluorophenyl)-2-thia-1,3-diazabicyclo [3.1.0]hexane 2,2-dioxide (–)-**2.2f** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 98%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -142.37 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.50 (td, *J* = 7.5, 1.8 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.35 – 7.39 (m, 4H), 7.16 (t, *J* = 7.0 Hz, 1H), 7.07 – 7.01 (m, 1H), 4.49 (d, *J* = 13.9 Hz, 1H), 3.95 (d, *J* = 13.9 Hz, 1H), 3.79 (dd, *J* = 10.1, 2.2 Hz, 1H), 3.26 (d, *J* = 10.1 Hz, 1H), 3.11 (s, 1H), 2.58 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.82, 160.18, 134.82, 131.11 (d, *J* = 8.1 Hz), 129.58 (d, *J* = 3.2 Hz), 128.94 (d, *J* = 47.5 Hz), 128.57, 124.97 (d, *J* = 3.5 Hz), 122.26 (d, *J* = 13.9 Hz), 115.80 (d, *J* = 20.5 Hz), 50.34, 49.07 (d, *J* = 1.7 Hz), 46.14, 38.88. ^{19}F NMR (564 MHz, $CDCl_3$) δ -117.20 – -117.25(m, 1F). HPLC analysis: *ee* = 83%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 19.404 min, t_{minor} = 30.592 min. IR (neat, cm^{-1}): 1339.08, 1174.94, 769.19. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{16}H_{16}N_2O_2FS$: 319.09110, found 319.09078.

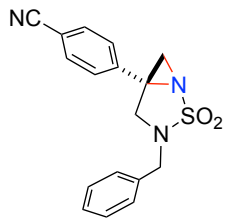


(*R*)-3-Benzyl-5-(3,5-difluorophenyl)-2-thia-1,3-diazabicyclo [3.1.0]hexane 2,2-dioxide (–)-**2.2g** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 98%. R_f = 0.4 (4:1 Hexanes/EtOAc).$[\alpha]_D^{20}$ = -74.19 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.44 – 7.35 (m, 3H), 7.35 – 7.30 (m, 2H), 6.86 (d, *J* = 5.4 Hz, 2H), 6.78 (t, *J* = 8.8 Hz, 1H), 4.51 (d, *J* = 13.7 Hz, 1H), 3.93 (d,

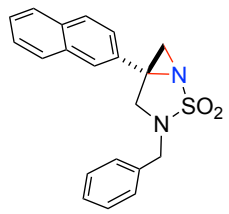
J = 13.7 Hz, 1H), 3.72 (d, J = 9.9 Hz, 1H), 3.28 (d, J = 9.9 Hz, 1H), 3.08 (s, 1H), 2.54 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.38 (d, J = 12.7 Hz, 1C), 162.38 (d, J = 12.7 Hz, 1C), 138.71 (t, J = 9.6 Hz, 1C), 134.60, 128.98 (d, J = 47.8 Hz, 1C), 128.71, 111.15 – 108.45 (m, 1C), 104.79 (t, J = 25.2 Hz, 1C), 77.41, 77.16, 76.91, 49.51, 48.98, 47.86 (t, J = 2.7 Hz, 1C), 39.62. ^{19}F NMR (470 MHz, $CDCl_3$) δ -110.14 – -110.20(m). HPLC analysis: *ee* = 87%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 10.842 min, t_{minor} = 28.979 min. IR (neat, cm^{-1}): 1599.91, 1339.29, 1172.26, 1121.90. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{16}H_{15}N_2O_2F_2S$: 337.08168, found 337.08072.



(*R*)-3-Benzyl-5-(4-(trifluoromethyl)phenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2h** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 98%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -143.36 (c = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.62 (d, J = 7.9 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.42 – 7.23 (m, 5H), 4.52 (d, J = 13.7 Hz, 1H), 3.94 (d, J = 13.7 Hz, 1H), 3.77 (d, J = 9.9 Hz, 1H), 3.32 (d, J = 9.9 Hz, 1H), 3.12 (s, 1H), 2.58 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.93, 134.72, 131.46 (q, J = 33.2 Hz, 1C), 129.19, 128.83, 128.71, 127.11, 127.08, 126.10 (q, J = 3.7 Hz, 1C), 123.86 (q, J = 271.8 Hz, 1C), 49.83, 49.01, 48.37, 39.52. ^{19}F NMR (564 MHz, $CDCl_3$) δ -62.85(s). HPLC analysis: *ee* = 92%. OD-H (90% hexanes: 10% isopropanol, 1.0 mL/min): t_{major} = 31.879 min, t_{minor} = 29.264 min. IR (neat, cm^{-1}): 1324.91, 1172.63, 773.14. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{17}H_{16}N_2O_2F_3S$: 369.08791, found 369.08831.

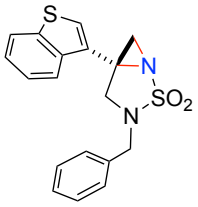


(*R*)-4-(3-Benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0] hexan-5-yl)benzonitrile (–)-**2.2i** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 98%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -190.55 (*c* =1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.41 – 7.35 (m, 3H), 7.35 – 7.30 (m, 2H), 3.94 (d, *J* = 13.7 Hz, 1H), 4.51 (d, *J* = 13.7 Hz, 1H), 3.77 (d, *J* = 9.9 Hz, 1H), 3.30 (d, *J* = 9.9 Hz, 1H), 3.12 (s, 1H), 2.56 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.06, 134.58, 132.88, 129.21, 128.82, 128.76, 127.41, 118.17, 113.25, 49.48, 48.99, 48.12, 39.62. HPLC analysis: *ee* = 80%. OD-H (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} =37.161 min, t_{minor} = 30.478 min. IR (neat, cm^{-1}): 2229.75, 1337.47, 1171.66, 788.08. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{17}H_{16}N_3O_2S$: 326.09577, found 326.09474.

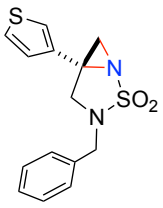


(*R*)-3-Benzyl-5-(naphthalen-2-yl)-2-thia-1,3-diazabicyclo[3.1.0] hexane 2,2-dioxide (–)-**2.2j** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 98%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -210.16 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.85 – 7.76 (m, 4H), 7.54 – 7.46 (m, 2H), 7.43 – 7.37 (m, 3H), 7.37 – 7.31 (m, 3H), 4.54 (d, *J* = 13.8 Hz, 1H), 3.95 (d, *J* = 13.8 Hz, 1H), 3.81 (d, *J* = 9.9 Hz, 1H), 3.42 (d, *J* = 9.9 Hz, 1H), 3.15 (s, 1H), 2.68 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.99, 133.46, 133.09, 132.24, 129.14, 129.10, 128.83, 128.61,

128.11, 127.96, 127.01, 126.98, 126.19, 123.70, 50.40, 49.41, 49.06, 39.57. HPLC analysis: *ee* = 90%. OD-H (90% hexanes: 10% isopropanol, 1.0 mL/min): t_{major} = 32.567 min, t_{minor} = 45.128 min. IR (neat, cm^{-1}): 1337.36, 1219.42, 1174.00, 772.60. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{20}H_{19}N_2O_2S$: 351.11617, found 351.11582.

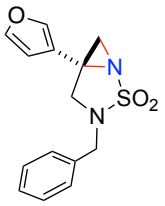


(*R*)-5-(Benzo[*b*]thiophen-3-yl)-3-benzyl-2-thia-1,3-diazabicyclo [3.1.0]hexane 2,2-dioxide (–)-**2.2k** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 96%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -28.99 (*c* = 1.0, $CHCl_3$). ^1H NMR (4MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.29 (m, 8H), 4.54 (d, *J* = 13.7 Hz, 1H), 3.96 (d, *J* = 13.7 Hz, 1H), 3.68 (d, *J* = 10.3 Hz, 1H), 3.46 (d, *J* = 10.3 Hz, 1H), 3.16 (s, 1H), 2.76 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.71, 136.93, 134.82, 129.73, 129.09, 128.81, 128.58, 127.07, 125.24, 125.14, 123.16, 122.44, 50.19, 49.04, 46.28, 37.72. HPLC analysis: *ee* = 82%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 16.812 min, t_{minor} = 25.159 min. IR (neat, cm^{-1}): 1334.90, 1169.72, 761.77, 736.68. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{18}H_{17}N_2O_2S_2$: 357.07260, found 357.07221.

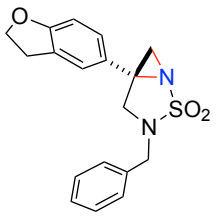


(*R*)-3-Benzyl-5-(thiophen-3-yl)-2-thia-1,3-diazabicyclo[3.1.0] hexane 2,2-dioxide (–)-**2.2l** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 96%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -

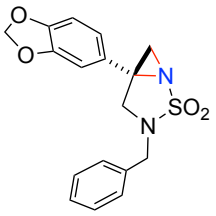
149.97 (c = 1.0, $CHCl_3$). ^1H NMR (6MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2H), 7.36 – 7.34 (m, 2H), 7.33 – 7.30 (m, 2H), 7.27 (d, J = 1.3 Hz, 1H), 7.01 (dd, J = 5.0, 1.3 Hz, 1H), 4.51 (d, J = 13.7 Hz, 1H), 3.93 (d, J = 13.7 Hz, 1H), 3.69 (d, J = 9.9 Hz, 1H), 3.39 (d, J = 9.9 Hz, 1H), 3.07 (s, 1H), 2.66 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.92, 134.94, 129.52, 128.75, 128.60, 127.39, 125.66, 123.82, 49.77, 49.01, 46.18, 39.48. HPLC analysis: *ee* = 86%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 23.071min, t_{minor} = 39.947min. IR (neat, cm^{-1}): 1335.32, 1172.36. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{14}H_{15}N_2O_2S$: 307.05695, found 307.05656.



(*R*)-3-Benzyl-5-(furan-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2m** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 97%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -128.57 (c = 1.0, $CHCl_3$). ^1H NMR (6MHz, $CDCl_3$) δ 7.45 (s, 1H), 7.42 – 7.36 (m, 3H), 7.36 – 7.30 (m, 3H), 6.34 (d, J = 1.9 Hz, 1H), 4.50 (d, J = 13.8 Hz, 1H), 3.92 (d, J = 13.8 Hz, 1H), 3.62 (d, J = 9.9 Hz, 1H), 3.34 (d, J = 9.9 Hz, 1H), 3.04 (s, 1H), 2.64 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) ^{13}C NMR (151 MHz, cdcl$_3$) δ 144.27, 141.14, 134.90, 129.12, 128.77, 128.61, 120.76, 108.73, 49.31, 48.96, 43.51, 38.76. HPLC analysis: *ee* = 84%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 21.001min, t_{minor} = 37.439 min. IR (neat, cm^{-1}): 1333.04, 1173.24. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{14}H_{15}N_2O_3S$: 291.07979, found 291.07930.

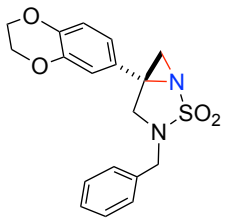


(*R*)-3-Benzyl-5-(2,3-dihydrobenzofuran-5-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2n** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 96%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -158.16 (*c* = 1, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.41 – 7.30 (m, 5H), 7.03 (d, *J* = 8.3 Hz, 1H), 6.72 (d, *J* = 8.3 Hz, 1H), 4.56 (t, *J* = 8.7 Hz, 2H), 4.50 (d, *J* = 13.7 Hz, 1H), 3.92 (d, *J* = 13.7 Hz, 1H), 3.65 (d, *J* = 10.0 Hz, 1H), 3.29 (d, *J* = 10.0 Hz, 1H), 3.17 (t, *J* = 8.7 Hz, 2H), 3.04 (s, 1H), 2.59 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.91, 135.02, 129.08, 128.81, 128.54, 128.19, 126.88, 126.81, 123.77, 109.53, 71.72, 50.90, 49.46, 49.00, 39.24, 29.59. HPLC analysis: *ee* = 81%. IC (70% hexanes: 30% isopropanol, 1.0 mL/min): t_{major} = 32.433 min, t_{minor} = 51.357 min. IR (neat, cm^{-1}): 1334.27, 1171.66. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{18}H_{19}N_4O_3S$: 343.11109, found 343.11107.

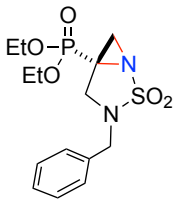


(*R*)-5-(Benzo[*d*][1,3]dioxol-5-yl)-3-benzyl-2-thia-1,3-diaza bicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2o** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 96%. R_f = 0.3 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -150.36 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.41 – 7.30 (m, 5H), 6.82 – 6.73 (m, 3H), 5.95 (s, 2H), 4.50 (d, *J* = 13.7 Hz, 1H), 3.91 (d, *J* = 13.7 Hz, 1H), 3.65 (d, *J* = 10.0 Hz, 1H), 3.27 (d, *J* = 10.0 Hz, 1H), 3.03 (s, 1H), 2.56 (s, 1H). ^{13}C NMR (151 MHz,

$CDCl_3$) δ 148.28, 134.94, 129.11, 128.81, 128.67, 128.58, 120.44, 108.66, 107.29, 101.61, 50.60, 49.14, 49.00, 39.38. HPLC analysis: *ee* = 68%. IC (70% hexanes: 30% isopropanol, 1.0 mL/min): t_{major} = 23.285 min, t_{minor} = 43.094 min. IR (neat, cm^{-1}): 1336.65, 1173.51. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{17}H_{17}N_2O_4S$: 345.09035, found 345.08979.

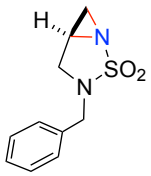


(*R*)-3-Benzyl-5-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2p** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. White solid. Yield: 98%. R_f = 0.3 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -141.36 (*c* = 1.0, $CHCl_3$). ^1H NMR (6MHz, $CDCl_3$) δ 7.42 – 7.36 (m, 2H), 7.36 – 7.29 (m, 3H), 6.86 – 6.80 (m, 2H), 6.80 – 6.76 (m, 1H), 4.50 (d, *J* = 13.7 Hz, 1H), 4.23 (m, 4H), 3.91 (d, *J* = 13.7 Hz, 1H), 3.64 (d, *J* = 10.0 Hz, 1H), 3.29 (d, *J* = 10.0 Hz, 1H), 3.03 (s, 1H), 2.57 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.37, 143.93, 135.01, 129.10, 128.84, 128.56, 128.00, 119.69, 117.89, 115.88, 64.54, 64.47, 50.46, 49.03, 48.89, 39.39. HPLC analysis: *ee* = 84%. IC (70% hexanes: 30% isopropanol, 1.0 mL/min): t_{major} = 24.258 min, t_{minor} = 44.365 min. IR (neat, cm^{-1}): 1336.70, 1173.00. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{18}H_{18}N_2O_4S$: 359.10600, found 359.10649.

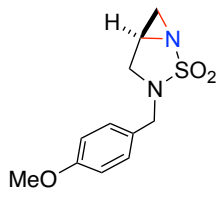


Diethyl (*S*)-(3-benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)phosphonate (–)-**2.2q** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow oil. Yield: 96%. R_f = 0.4 (1:2

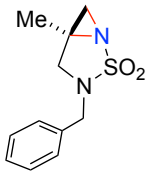
Hexanes/EtOAc). $[\alpha]_D^{20}$ = - 0.20 (*c* = 0.5, $CHCl_3$). ^1H NMR (6MHz, $CDCl_3$) δ 7.42 – 7.32 (m, 3H), 7.31 – 7.27 (m, 2H), 4.44 (d, *J* = 13.8 Hz, 1H), 4.33 – 4.22 (m, 2H), 4.22 – 4.13 (m, 2H), 3.90 (d, *J* = 13.8 Hz, 1H), 3.46 (d, *J* = 10.2 Hz, 1H), 3.36 – 3.31 (m, 1H), 2.78 (d, *J* = 7.0 Hz, 1H), 2.73 (d, *J* = 7.0 Hz, 1H), 1.34 (dt, *J* = 19.2, 7.1 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 134.56, 129.17, 128.75, 128.71, 64.84 (d, *J* = 6.1 Hz, 1C), 63.84 (d, *J* = 6.4 Hz, 1C), 49.14, 45.77 (d, *J* = 12.2 Hz, 1C), 40.85, 39.46, 34.64, 16.53 (t, *J* = 5.3 Hz, 1C). ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.95. HPLC analysis: *ee* = 2%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 99.628 min, t_{minor} = 60.062 min. IR (neat, cm^{-1}): 1344.35, 1262.61, 1178.40, 1019.58. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{14}H_{22}N_2O_5PS$: 361. 09816, found 361.09820.



(*R*)-3-Benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (+)-**2.2r** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow oil. Yield: 96%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = 19.79 (*c* = 1.0, $CHCl_3$). ^1H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.32 (m, 3H), 7.32 – 7.27 (m, 2H), 4.43 (d, *J* = 14.9 Hz, 1H), 3.87 (d, *J* = 14.9 Hz, 1H), 3.42 (dd, *J* = 10.0, 2.6 Hz, 1H), 3.28 (dt, *J* = 10.0, 3.2 Hz, 1H), 3.12 (p, *J* = 4.0 Hz, 1H), 2.64 (s, 1H), 2.43 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.93, 129.01, 128.69, 128.48, 48.83, 45.64, 37.03, 31.92. HPLC analysis: *ee* = 81%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 60.571 min, t_{minor} = 51.630 min. IR (neat, cm^{-1}): 1329.17, 1172.20. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{10}H_{13}N_2O_2S$: 225.06922, found 225.06899.

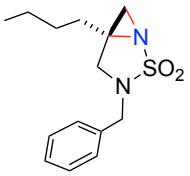


(*R*)-3-(4-Methoxybenzyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (+)-**2.2s** was obtained with catalyst **[Co(P5)]** in toluene through the general procedure. Light yellow solid. Yield: 79%. R_f = 0.3 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = 17.59 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.7 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 1H), 4.37 (d, *J* = 13.7 Hz, 1H), 3.82 (d, *J* = 13.7 Hz, 1H), 3.81 (s, 2H), 3.39 (d, *J* = 10.1 Hz, 1H), 3.25 (dd, *J* = 10.1, 3.9 Hz, 1H), 3.10 (q, *J* = 4.3 Hz, 1H), 2.61 (d, *J* = 3.4 Hz, 1H), 2.41 (d, *J* = 3.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.80, 130.11, 126.83, 114.39, 55.47, 48.28, 45.49, 36.96, 31.87. HPLC analysis: *ee* = 83%. OD-H (90% hexanes: 10% isopropanol, 1.0 mL/min): t_{major} = 38.195 min, t_{minor} = 43.756 min. IR (neat, cm^{-1}): 1513.79, 1331.02, 1248.41, 1171.95, 749.53. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{11}H_{15}N_2O_3S$: 255.07979, found 255.07940.

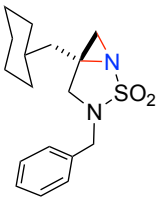


(*R*)-3-Benzyl-5-methyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2t** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 50%. R_f = 0.5 (2:1 Hexanes/EtOAc). (Same R_f as C–H amination product **2.3t**, known compound.[17]) $[\alpha]_D^{20}$ = -9.99 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.40 – 7.35 (m, 3H), 7.31-7.28 (m,, 2H), 4.44 (d, *J* = 13.7 Hz, 1H), 3.86 (d, *J* = 13.8 Hz, 1H), 3.37 (d, *J* = 9.9 Hz, 1H), 3.02 (d, *J* = 9.9 Hz, 1H), 2.76 (s, 1H), 2.33 (s, 1H), 1.47 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.05, 128.99, 128.70, 128.43, 50.45, 48.87, 45.34, 38.59, 18.80. HPLC analysis: *ee* = 65%. OD-H (90% hexanes: 10%

isopropanol, 1.0 mL/min): t_{major} = 18.345 min, t_{minor} = 21.690 min. IR (neat, cm^{-1}): 1328.51, 1170.47, 779.64. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{11}H_{15}N_2O_2S$: 239.08487, found 239.08416.

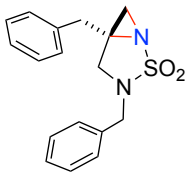


(*R*)-3-Benzyl-5-butyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2u** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 88%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -33.99 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 5H), 4.44 (d, *J* = 13.8 Hz, 1H), 3.85 (d, *J* = 13.8 Hz, 1H), 3.34 (d, *J* = 9.8 Hz, 1H), 3.04 (d, *J* = 9.8 Hz, 1H), 2.72 (s, 1H), 2.35 (s, 1H), δ 1.77 (dt, *J* = 15.0, 7.0 Hz, 1H), 1.66 (dt, *J* = 15.0, 7.0 Hz, 1H), 1.40 – 1.27 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.17, 129.05, 128.73, 128.46, 49.23, 48.99, 48.47, 37.82, 32.22, 26.78, 22.61, 13.96. HPLC analysis: *ee* = 52%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 22.806 min, t_{minor} = 49.290 min. IR (neat, cm^{-1}): 1333.06, 1173.00. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{14}H21N2O2S$: 281.13183, found 281.13211.

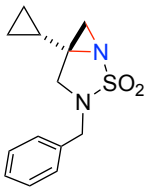


(*R*)-3-Benzyl-5-(cyclohexylmethyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2v** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 82%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -26.39 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.45 – 7.33 (m, 3H), 7.33 – 7.28 (m,

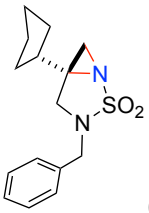
2H), 4.43 (d, J = 13.9 Hz, 1H), 3.86 (d, J = 13.9 Hz, 1H), 3.37 (d, J = 9.9 Hz, 1H), 3.04 (d, J = 9.9 Hz, 1H), 2.75 (s, 2H), 2.33 (s, 1H), 1.83 (dd, J = 14.2, 5.5 Hz, 1H), 1.76 – 1.62 (m, 5H), 1.50 – 1.40 (m, 1H), 1.41 – 1.29 (m, 1H), 1.28 – 1.05 (m, 3H), 1.02 – 0.80 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.14, 128.99, 128.63, 128.39, 49.70, 49.00, 47.33, 40.56, 38.28, 34.30, 33.92, 33.09, 26.21, 26.06, 26.00. HPLC analysis: *ee* = 34%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 24.773 min, t_{minor} = 52.717 min. IR (neat, cm^{-1}): 2922.88, 1333.73, 1173.82, 702.33. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{25}N_2O_2S$: 321.16313, found 321.16288.



(*R*)-3,5-dibenzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2w** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 81%. R_f = 0.5 (2:1 Hexanes/EtOAc). (Same R_f as C–H amination product **2.3w**, known compound.[17]) $[\alpha]_D^{20}$ = -53.39 (c = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.35 – 7.25 (m, 8H), 7.21 – 7.15 (m, 2H), 4.41 (d, J = 13.9 Hz, 1H), 3.81 (d, J = 13.9 Hz, 1H), 3.28 (d, J = 10.0 Hz, 1H), 3.09 (d, J = 14.9 Hz, 1H), 3.05 (d, J = 10.0 Hz, 1H), 2.98 (d, J = 14.9 Hz, 1H), 2.74 (s, 1H), 2.36 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) 135.06, 134.37, 129.46, 128.97, 128.96, 128.59, 128.39, 127.69, 49.04, 48.93, 48.21, 38.83, 37.12. HPLC analysis: *ee* = 66%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 28.193 min, t_{minor} = 40.701 min. IR (neat, cm^{-1}): 1332.62, 1172.01, 702.73. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{19}N_2O_2S$: 315.11617, found 315.11650.

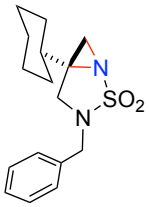


(*R*)-3-Benzyl-5-cyclopropyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2x** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 96%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -56.99 (*c* = 1.0, $CHCl_3$). 1H NMR (6MHz, $CDCl_3$) δ 7.40 – 7.33 (m, 2H), 7.36 – 7.30 (m, 1H), 7.31 – 7.28 (m, 2H), 4.43 (d, *J* = 13.8 Hz, 1H), 3.84 (d, *J* = 13.8 Hz, 1H), 3.43 (d, *J* = 9.8 Hz, 1H), 3.14 (d, *J* = 9.8 Hz, 1H), 2.71 (s, 1H), 2.28 (s, 1H), 1.13 (tt, *J* = 8.1, 5.1 Hz, 1H), 0.63 – 0.55 (m, 1H), 0.52 – 0.43 (m, 2H), 0.40 – 0.31 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.11, 128.99, 128.72, 128.42, 49.94, 48.95, 36.94, 11.43, 2.65, 1.84. HPLC analysis: *ee* = 70%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 20.245 min, t_{minor} = 30.834 min. IR (neat, cm^{-1}): 1333.11, 1170.84. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{13}H_{17}N_2O_2S$: 265.10052, found 265.10066.

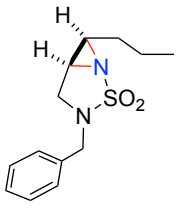


(*R*)-3-Benzyl-5-cyclopentyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2y** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 92%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -44.19 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (5MHz, CDCl3) δ 7.44 – 7.32 (m, 3H), 7.31 – 7.27 (m, 2H), 4.45 (d, *J* = 13.8 Hz, 1H), 3.85 (d, *J* = 13.8 Hz, 1H), 3.33 (d, *J* = 9.8 Hz, 1H), 3.07 (d, *J* = 9.8 Hz, 1H), 2.70 (s, 1H), 2.39 (s, 1H), 2.17 (p, *J* = 8.5, 7.8 Hz, 2H), 1.86 – 1.72 (m, 1H), 1.72 – 1.47 (m, 5H), 1.44 – 1.18 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.20, 128.98, 128.64,

128.38, 50.63, 48.96, 48.80, 40.70, 36.66, 28.13, 28.06, 25.38, 25.33. HPLC analysis: *ee* = 62%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 21.793 min, t_{minor} = 41.204 min. IR (neat, cm^{-1}): 1332.29, 1172.44. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{15}H_{21}N_2O_2S$: 293.13183, found 293.13194.

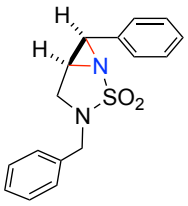


(*R*)-3-Benzyl-5-cyclohexyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2z** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 93%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -40.59(*c* = 1.0, $CHCl_3$). ^1H NMR (6MHz, $CDCl_3$) δ 7.39 – 7.34 (m, 2H), 7.34 – 7.31 (m, 1H), 7.31 – 7.28 (m, 2H), 4.44 (d, *J* = 13.8 Hz, 1H), 3.84 (d, *J* = 13.8 Hz, 1H), 3.29 (d, *J* = 9.7 Hz, 1H), 3.09 (d, *J* = 9.7 Hz, 1H), 2.68 (s, 1H), 2.38 (s, 1H), 1.82 – 1.72 (m, 3H), 1.72 – 1.63 (m, 2H), 1.52 (tt, *J* = 12.2, 3.1 Hz, 1H), 1.25 – 1.15 (m, 2H), 1.14 – 1.05 (m, 2H), 0.95 (qd, *J* = 12.6, 3.5 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.20, 129.02, 128.68, 128.42, 51.50, 49.01, 47.49, 40.19, 36.98, 28.43, 27.92, 26.11, 25.89, 25.87. HPLC analysis: *ee* = 49%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 20.496 min, t_{minor} = 49.134 min. IR (neat, cm^{-1}): 1331.94, 1170.99. HRMS ($DART^+$) ($[M+H]^+$): Calcd. for $C_{16}H_{23}N_2O_2S$: 307.14748, found 307.14777.



(5*S*)-3-Benzyl-6-propyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (+)-**2.2aa** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general

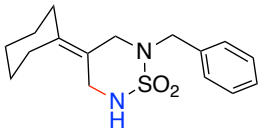
procedure. White solid. Yield: 95% (Calculated based on *cis*-**2.1aa**). R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = 21.39 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 5H), 4.49 (d, *J* = 13.7 Hz, 1H), 3.79 (d, *J* = 13.7 Hz, 1H), 3.40 – 3.29 (m, 2H), 3.20 (t, *J* = 5.3 Hz, 1H), 2.70 – 2.62 (m, 1H), 2.30 – 2.19 (m, 1H), 1.94 – 1.80 (m, 1H), 1.72 – 1.60 (m, 1H), 1.50 – 1.36 (m, 1H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.10, 128.95, 128.70, 128.40, 50.08, 46.86, 45.11, 41.42, 24.71, 21.25, 14.03. HPLC analysis: *ee* = 71%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 54.953 min, t_{minor} = 47.574 min. IR (neat, cm^{-1}): 1328.44, 1168.69. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{13}H_{19}N_2O_2S$: 267.11617, found 267.11559.



(5*S*)-3-Benzyl-6-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide (–)-**2.2ab** was obtained with catalyst **[Co(P5)]** in cyclohexane through the general procedure. White solid. Yield: 96% (Calculated based on *trans*-**2.1ab**). R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -52.79 (*c* =1.0, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.47 – 7.41 (m, 3H), 7.40 – 7.30 (d, *J* = 6.5 Hz, 2H), 7.19 (t, *J* = 8.1 Hz, 1H), 7.11 (t, *J* = 6.7 Hz, 2H), 6.49 (d, *J* = 7.8 Hz, 2H), 4.02 (d, *J* = 13.9 Hz, 1H), 3.95 (d, *J* = 5.4 Hz, 1H), 3.53 (d, *J* = 13.9 Hz, 1H), 3.46 (t, *J* = 4.2 Hz, 1H), 3.42 (dd, *J* = 10.5, 1.8 Hz, 1H), 3.38 – 3.31 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.58, 130.02, 128.69, 128.56, 128.50, 128.39, 128.18, 127.93, 48.92, 47.27, 44.50, 40.69. HPLC analysis: *ee* = 62%. IC (80% hexanes: 20% isopropanol, 1.0 mL/min): t_{major} = 46.237 min, t_{minor} = 51.873 min. IR (neat, cm^{-1}): 1330.03, 1170.11, 729.13. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{16}H_{17}N_2O_2S$: 301.10052, found 301.10052.

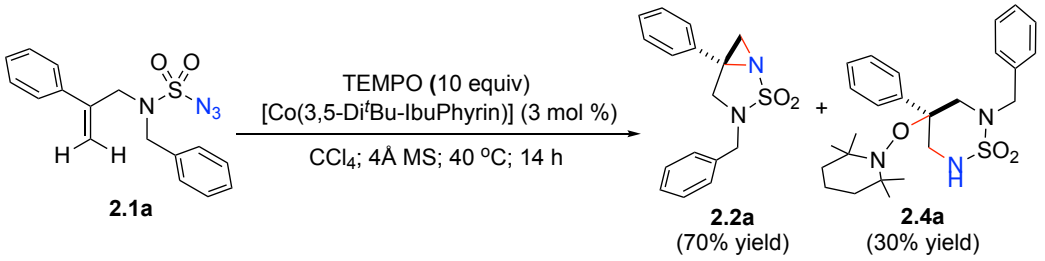
2.4.4 General Procedure for C–H Amination of Sulfamoyl Azides

An oven dried Schlenk tube was charged with catalyst [Co(**P7**)] [Co(3,5-Di^{t}Bu-IbuPhyrin)] (3 mol %) and 4Å molecular sieves (50 mg). This reaction vessel was evacuated and backfilled with nitrogen three times. Under nitrogen atmosphere, the allyl sulfamoyl azide substrate **2.1** (0.1 mmol) was added followed by the addition of 0.5 mL of toluene. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at 40 ºC for 14 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum and afford major products from C–H amination **2.3** and minor products from bicyclization **2.2** in crude. Then purified by flash column chromatography and the fractions containing product were collected.

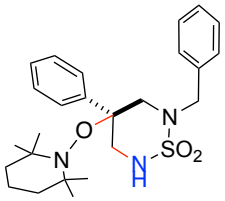


2-Benzyl-4-cyclohexylidene-1,2,6-thiadiazinane 1,1-dioxide 2.3z. White solid. NMR Yield: 47%. R_f = 0.4 (2:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.42 – 7.27 (m, 5H), 4.21 (s, 2H), 4.17 (t, *J* = 7.3 Hz, 1H), 4.06 (d, *J* = 7.3 Hz, 2H), 3.86 (s, 2H), 2.19 (t, *J* = 5.0 Hz, 2H), 1.92 (t, *J* = 6.1 Hz, 2H), 1.59 – 1.54 (m, 4H), 1.50 – 1.43 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.04, 135.90, 128.76, 128.58, 128.04, 115.55, 51.84, 48.59, 45.90, 30.29, 30.20, 28.35, 28.33, 26.55. IR (neat, cm^{-1}): 2926.37, 2309.00, 1333.06, 1168.63,755.60. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for: $C_{16}H_{23}N_2O_2S$: 307.14748, found 307.14749.

2.4.5 General Procedure for TEMPO Trapping Experiment



An oven dried Schlenk tube was charged with catalyst [Co(**P7**)] [Co(3,5-Di^{t}Bu-IbuPhyrin)] (3 mol %) and 4Å molecular sieves (50 mg). This reaction vessel was evacuated and backfilled with nitrogen three times. Under nitrogen atmosphere, the allyl sulfamoyl azide substrate **2.1a** (0.2 mmol) and TEMPO (10 equiv) were added followed by the addition of 1 mL of CCl_4. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at 40 ºC for 14 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum and afford **2.2a** (70% yield) and **2.4a** (30% yield) in crude. Then purified by flash column chromatography and the fractions containing product were collected.

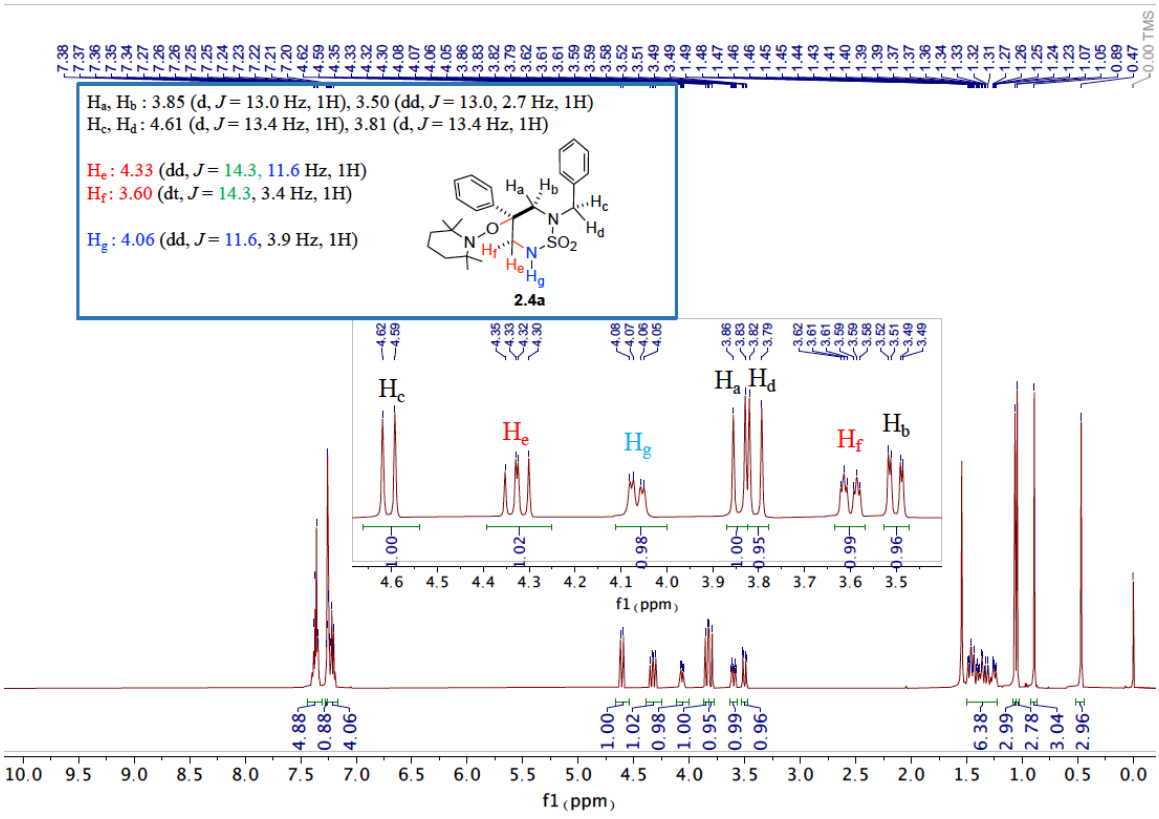


2-Benzyl-4-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-1,2,6-thiadiazinane 1,1-dioxide 2.4a. White solid. NMR Yield: 30%. R_f = 0.4 (2:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.44 – 7.31 (m, 5H), 7.28 – 7.26 (m, 1H), 7.25 – 7.16 (m, 4H), 4.61 (d, *J* = 13.4 Hz, 1H), 4.33 (dd, *J* = 14.3, 11.6 Hz, 1H), 4.06 (dd, *J* = 11.6, 3.9 Hz, 1H), 3.85 (d, *J* = 13.0 Hz, 1H), 3.81 (d, *J* = 13.4 Hz, 1H), 3.60 (dt, *J* = 14.3

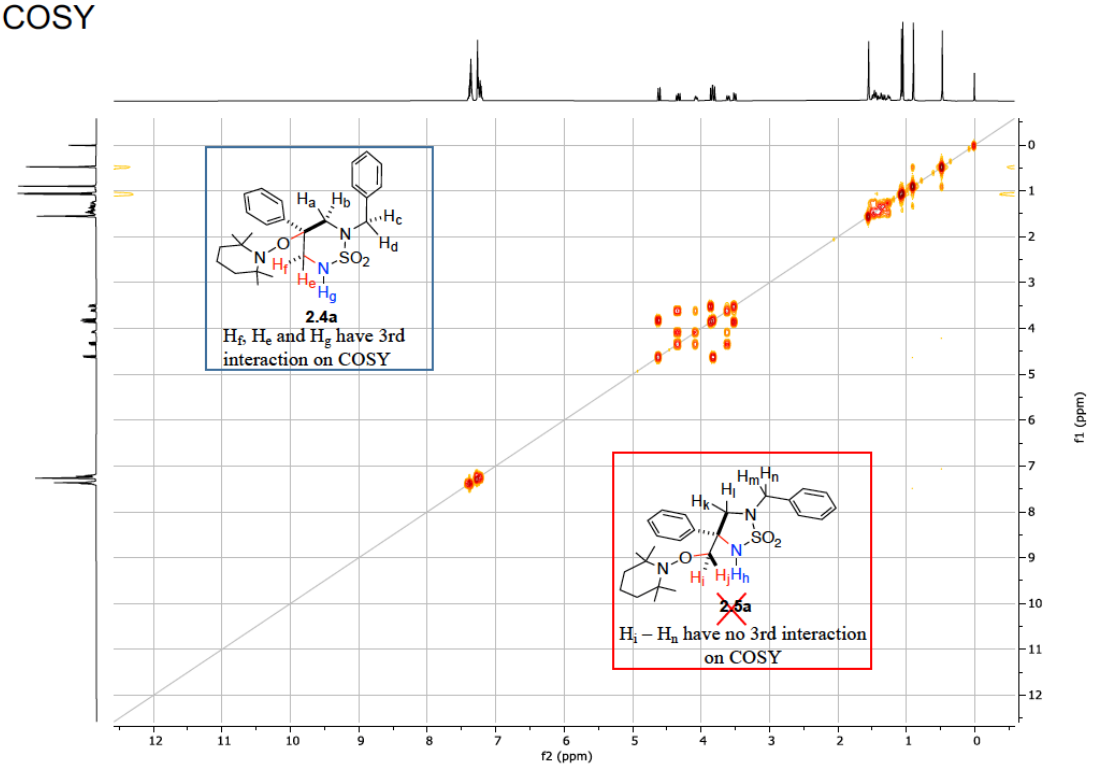
Hz, 3.4 Hz, 1H), 3. 50 (dd, J = 13.0 Hz, 2.7 Hz, 1H), 1.50 – 1.22 (m, 6H), 1.07 (s, 3H), 1.05 (s, 3H), 0.89 (s, 3H), 0.47 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.53, 134.65, 130.02, 128.64, 128.37, 128.17, 128.01, 127.42, 75.22, 60.55, 60.24, 53.91, 52.88, 52.73, 41.07, 40.98, 34.56, 33.86, 20.59, 20.48, 16.92. IR (neat, cm^{-1}): 2930.61, 1449.20, 1332.08, 1163.94, 753.45, 698.98. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{25}H_{36}N_3O_3S$: 458.24719, found 458.24689.

The TEMPO-trapped product **2.4a** was further characterized by the detailed analysis of coupling constants and splitting patterns in ^{1}H-NMR as well as through additional DEPT ^{13}C-NMR, NOSY, COSY, HSQC experiments in the following pages.

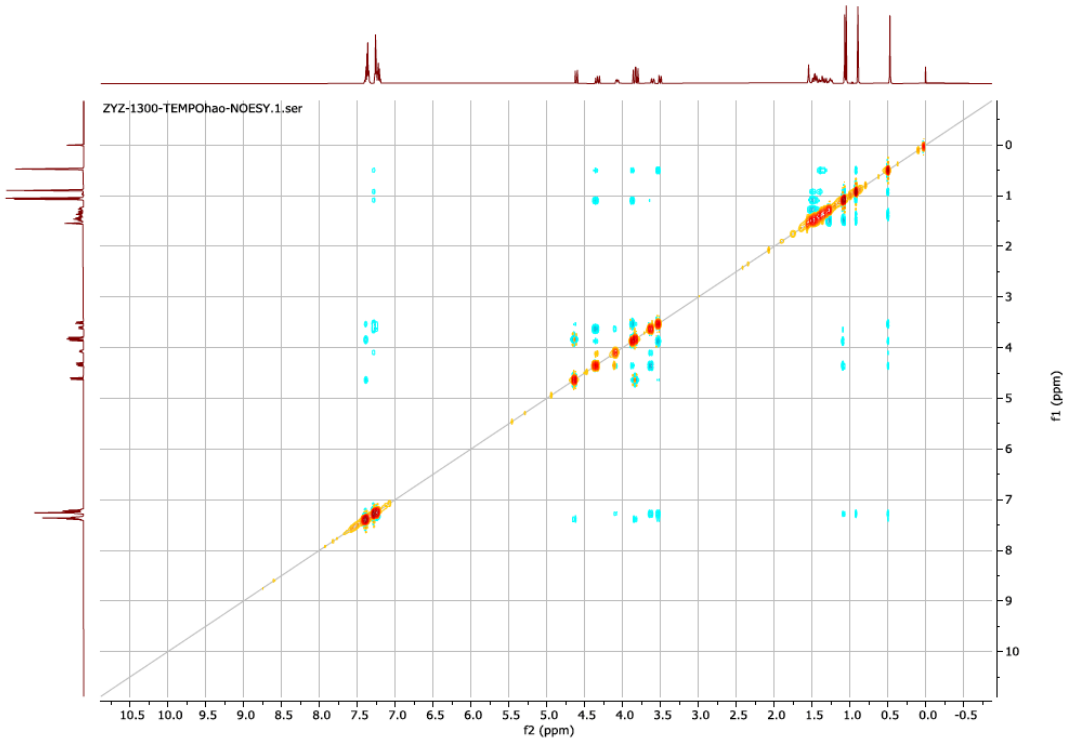
^{1}H NMR 2-Benzyl-4-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-1,2,6-thiadiazinane 1,1-dioxide 2.4a



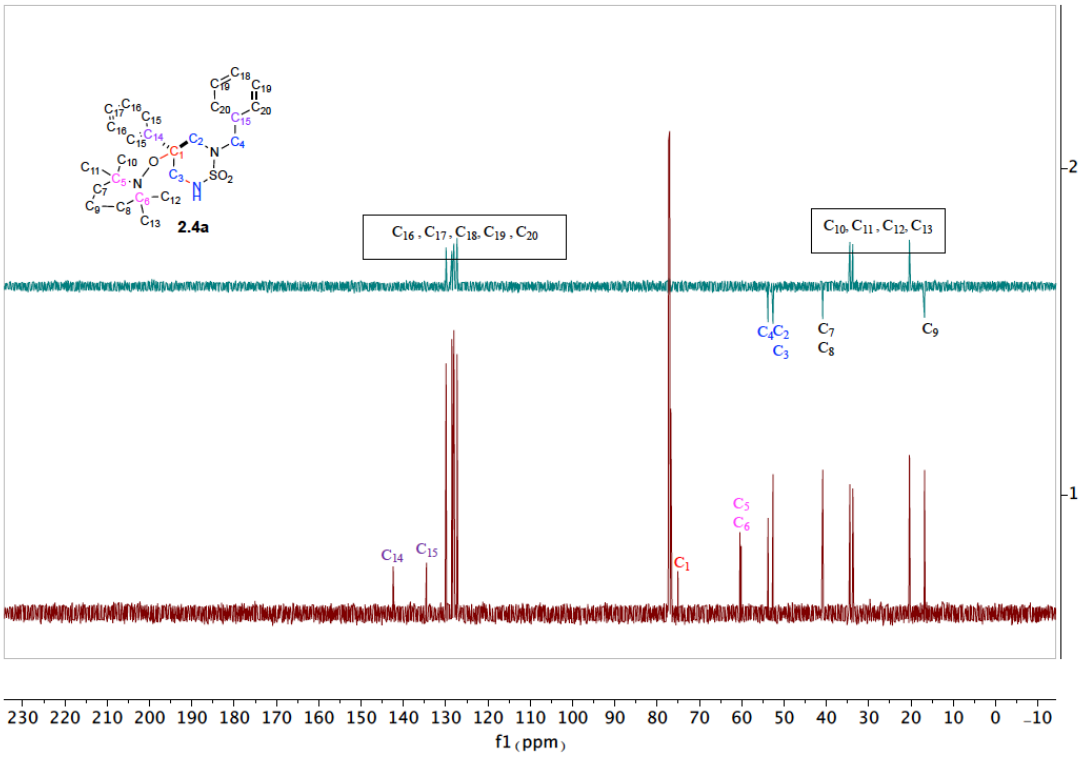
COSY


2.4a
Hf, He and Hg have 3rd interaction on COSY
2.5a
Hi – Hn have no 3rd interaction on COSY
f2 (ppm)
f1 (ppm)

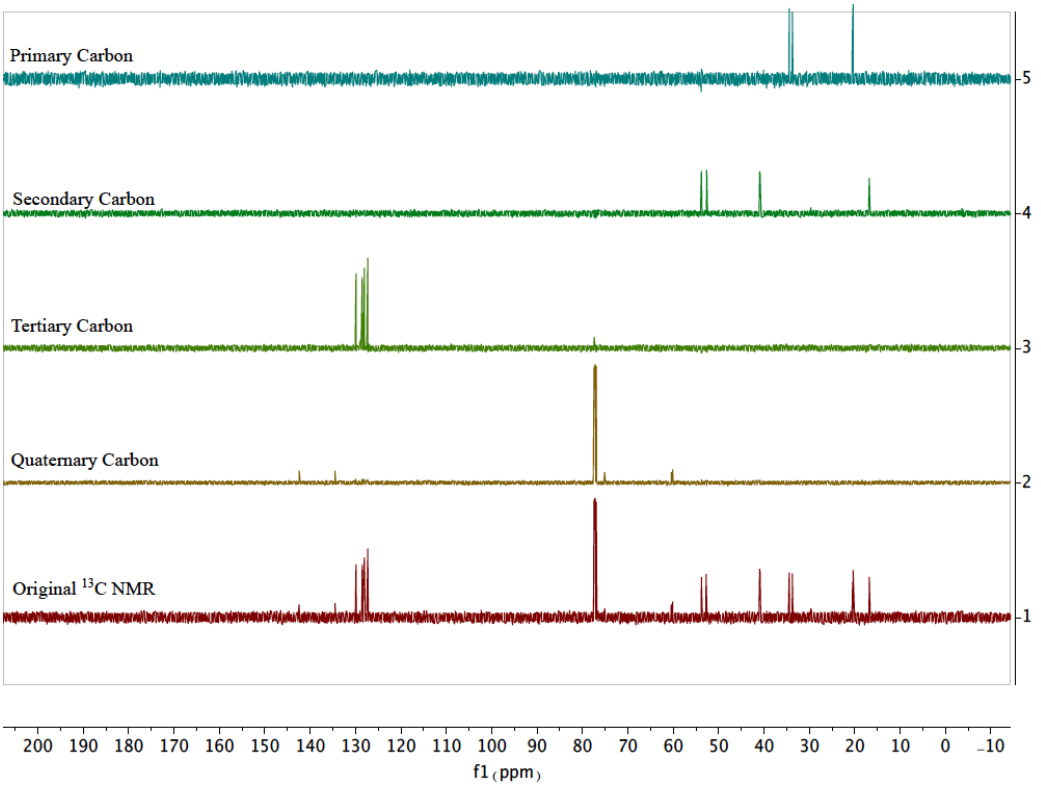
NOESY


ZYZ-1300-TEMPOhao-NOESY.1.ser
f2 (ppm)
f1 (ppm)

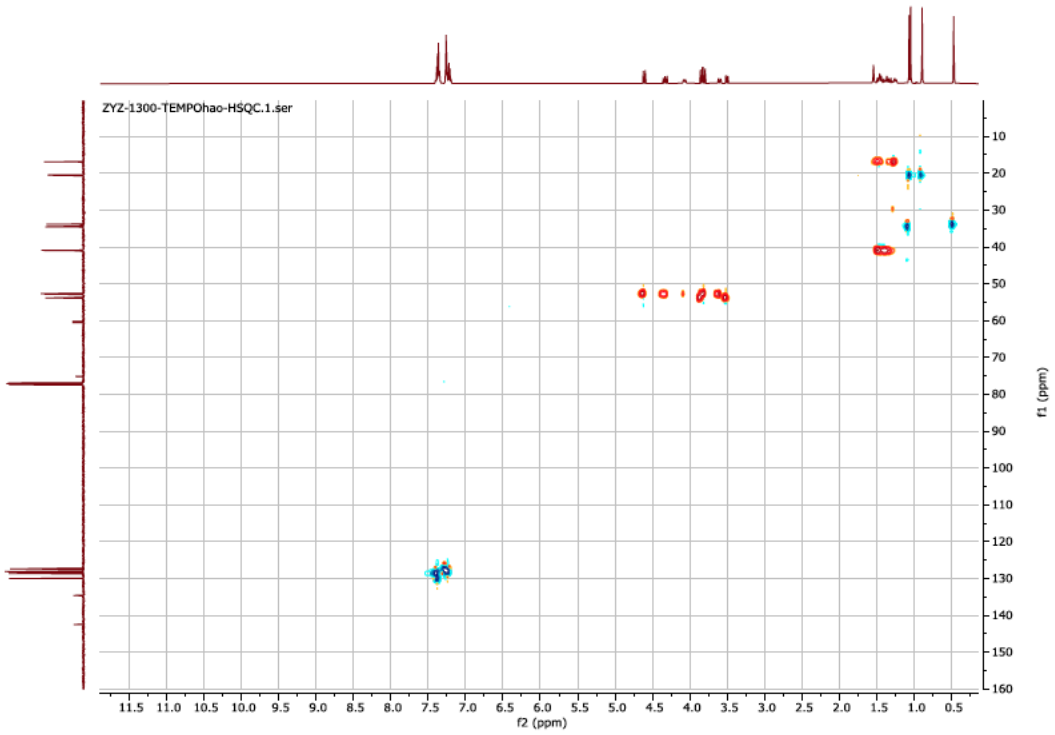
2-Benzyl-4-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-1,2,6-thiadiazinane 1,1-dioxide 2.4a
DEPT - 135°



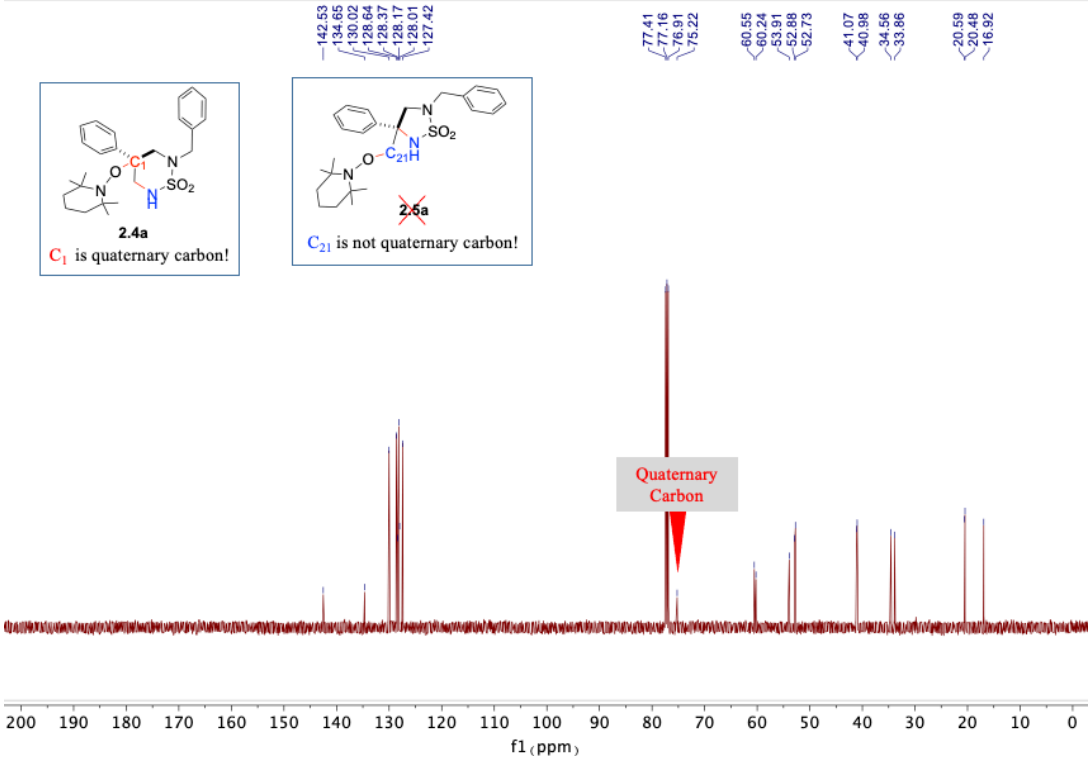
DEPT-Full Edit Mode (by the saturated pattern of carbon)



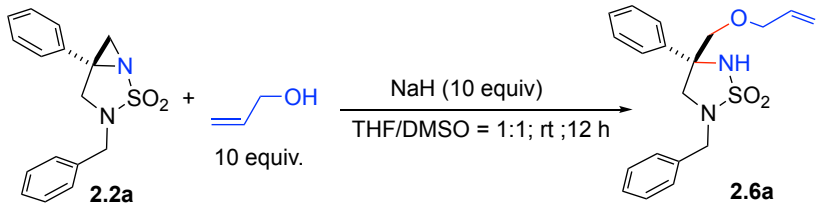
HSQC



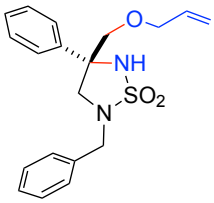
^{13}C NMR 2-Benzyl-4-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-1,2,6-thiadiazinane 1,1-dioxide 2.4a



2.4.6 Further Transformations

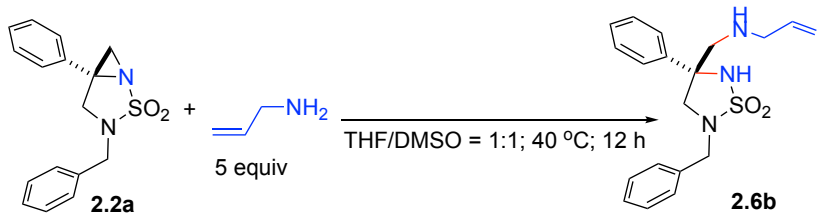


To a solution of **2.2a** (0.1 mmol) and 2-Propen-1-ol (10 equiv) in anhydrous 1:1 THF/DMSO (2 mL), sodium hydride (10 equiv) was added slowly at 0 ºC. The reaction mixture was allowed to warm up to room temperature and continued to stir for 12 h. After the completion of reaction, the reaction was quenched with water at 0 ºC and extracted with EtOAc (10 ml × 3). The combined extract was concentrated under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound **2.6a** as white solid.

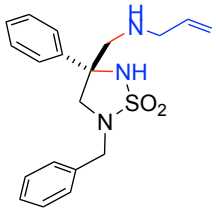


(*S*)-4-((Allyloxy)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide (–)-2.**6a**. White solid. Yield: 83%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -42.79 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (4MHz, $CDCl_3$) δ 7.47 – 7.39 (d, *J* = 6.4 Hz, 2H), 7.39 – 7.27 (m, 8H), 5.79 (ddt, *J* = 16.6, 10.8, 5.7 Hz, 1H), 5.33 – 5.06 (m, 3H), 4.40 (d, *J* = 14.2 Hz, 1H), 3.96 (d, *J* = 5.7 Hz, 2H), 3.77 – 3.68 (m, 1H), 3.66 – 3.57 (m, 2H), 3.26 (d, *J* = 9.8 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.85, 135.29, 133.63, 128.90, 128.83, 128.55, 128.24, 128.23, 125.70, 118.25, 74.30, 72.47, 63.52, 56.68, 50.32. HPLC analysis: *ee* = 93% (Enriched in the purification). IC (70% hexanes: 30%

isopropanol, 1.0 mL/min): t_{major} = 12.016 min, t_{minor} = 13.882 min. IR (neat, cm^{-1}): 1310.24, 1169.75, 699.17. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{19}H_{23}N_2O_3S$: 359.14239, found 359.14289.

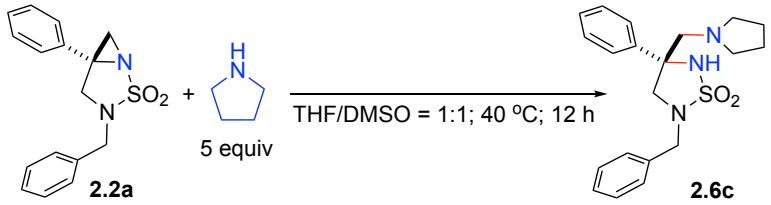


To a solution of **2.2a** (0.1 mmol) in anhydrous 1:1 THF/DMSO (2 mL), 2-propenamine (5 equiv) was added at room temperature. The reaction mixture continued to stir for 12 h at 40 ºC. After the completion of reaction, the solvent was removed under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6b** as white solid.

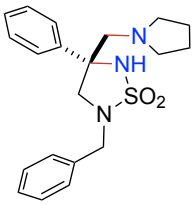


(*R*)-4-((Allylamino)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide (–)-**2.6b**. White solid. Yield: 81%. R_f = 0.2 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$= -57.79 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.42 – 7.26 (m, 10H), 5.76 (td, *J* = 10.7, 5.2 Hz, 1H), 5.12 – 5.01 (m, 2H), 4.50 (d, *J* = 13.6 Hz, 1H), 3.72 (d, *J* = 13.6 Hz, 1H), 3.42 (d, *J* = 9.7 Hz, 1H), 3.18 – 3.13 (m, 2H), 3.13 – 3.08 (m, 2H), 3.07 – 3.02 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.77, 136.09, 135.24, 129.09, 129.01, 128.78, 128.34, 128.11, 125.33, 116.77, 62.46, 57.52, 57.44, 52.07, 50.26. HPLC analysis: *ee* = 92% (Enriched in the purification). IA (70% hexanes: 30% isopropanol, 1.0

mL/min): t_{major} = 6.443 min, t_{minor} = 7.158 min. IR (neat, cm^{-1}): 1167.22, 762.38, 699.99. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{19}H_{24}N_3O_2S$: 358.15837, found 358.15864.

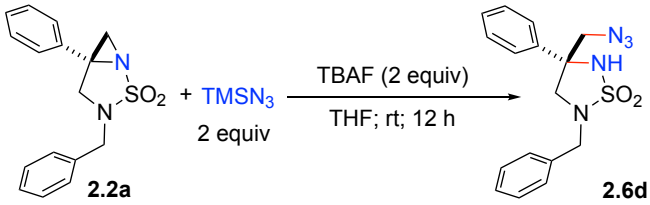


To a solution of **2.2a** (0.1 mmol) in anhydrous 1:1 THF/DMSO (2 mL), Pyrolidine (5 equiv) was added at room temperature. The reaction mixture continued to stir for 12 h at 40 ºC. After the completion of reaction, the solvent was removed under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6c** as colorless crystal.



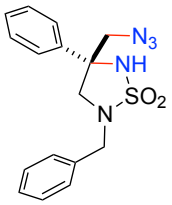
(*R*)-2-Benzyl-4-phenyl-4-(pyrrolidin-1-ylmethyl)-1,2,5-thiadiazolidine 1,1-dioxide (–)-**2.6c**. White solid. Yield: 86%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -53.19 (c = 0.5, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.43 – 7.30 (m, 8H), 7.28 – 7.23 (m, 2H), 4.51 (d, J = 13.5 Hz, 1H), 3.67 (d, J = 13.5 Hz, 1H), 3.34 (d, J = 9.6 Hz, 1H), 3.23 (d, J = 12.4 Hz, 1H), 2.96 (d, J = 9.6 Hz, 1H), 2.85 (d, J = 12.4 Hz, 1H), 2.37 – 2.28 (m, 4H), 1.68 – 1.60 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.50, 135.29, 128.98, 128.86, 128.82, 128.30, 127.73, 124.99, 64.46, 61.75, 58.51, 54.97, 50.27, 23.92. HPLC analysis: *ee* = 99% (Enriched in the purification). ID (90% hexanes: 10% isopropanol, 1.0 mL/min): t_{major} = 21.662 min, t_{minor} = 26.763 min. IR (neat, cm^{-1}): 1164.73,

759.87, 730.01, 697.48. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{20}H_{26}N_3O_2S$: 372.17402, found 372.17414.

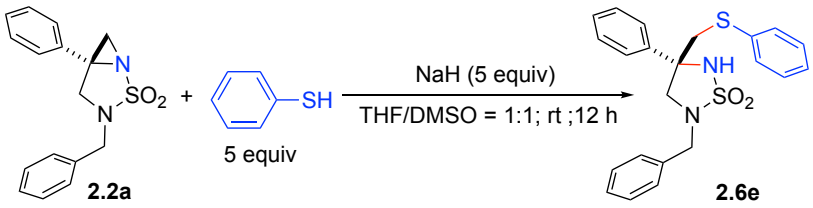


2.2a **2.6d**

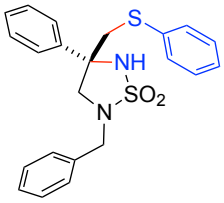
To a solution of **2.2a** (0.1 mmol) in THF (2 mL), $TMSN_3$ (2 equiv) and tetrabutylammonium fluoride (2 equiv) was added sequentially. The reaction mixture was then stirred at room temperature for 12 h. After the completion of reaction, the solvent was removed under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6d** as light-yellow oil.



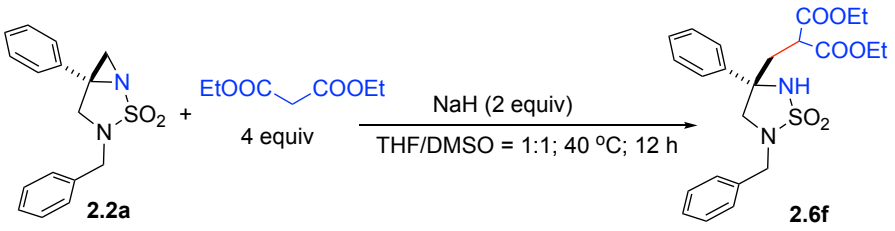
(*R*)-4-(Azidomethyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide (–)-**2.6d**. White solid. Yield: 58%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -49.19 (c = 0.5, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.46 – 7.29 (m, 10H), 5.06 (s, 1H), 4.42 (d, J = 13.8 Hz, 1H), 3.93 (d, J = 13.8 Hz, 1H), 3.87 – 3.73 (m, 2H), 3.51 (d, J = 9.9 Hz, 1H), 3.33 (d, J = 9.9 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.73, 134.78, 129.29, 129.09, 128.92, 128.69, 128.54, 125.47, 62.95, 58.86, 56.42, 50.16. HPLC analysis: *ee* = 90%. IC (70% hexanes: 30% isopropanol, 1.0 mL/min): t_{major} = 9.811 min, t_{minor} = 13.174 min. IR (neat, cm^{-1}): 2104.76, 1295.45, 1163.70, 759.37, 730.18, 696.07. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{16}H_{18}N_5O_2S$: 344.11757, found 344.11637.



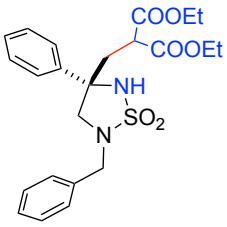
To a solution of **2.2a** (0.1 mmol) and thiophenol (5 equiv) in anhydrous 1:1 THF/DMSO (2 mL), sodium hydride (5 equiv) was added slowly at 0 ºC. The reaction mixture was allowed to warm up to room temperature and continued to stir for 12 h. After the completion of reaction, the reaction was quenched with water at 0 ºC and extracted with EtOAc (10 ml × 3). The combined extract was concentrated under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6e** as light-yellow oil.



(*S*)-2-Benzyl-4-phenyl-4-((phenylthio)methyl)-1,2,5-thiadiazolidine 1,1-dioxide (–)-**2.6e**. Light-yellow oil. Yield: 70%. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -5.99 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.76 – 7.08 (m, 15H), 5.40 (s, 1H), 4.39 (d, *J* = 13.8 Hz, 1H), 3.87 (d, *J* = 13.8 Hz, 1H), 3.76 – 3.51 (m, 3H), 3.32 (d, *J* = 10.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.90, 134.87, 134.50, 131.02, 129.32, 128.95, 128.90, 128.65, 128.37, 128.34, 127.42, 125.44, 63.44, 58.49, 50.11, 46.56. HPLC analysis: *ee* = 78% (*ee* droped). IC (90% hexanes: 10% isopropanol, 0.8 mL/min): t_{major} = 43.898 min, t_{minor} = 47.159 min. IR (neat, cm^{-1}): 1306.41, 1165.21, 735.67, 696.90. HRMS (DART$^+$) ($[M+H]^+$): Calcd. for $C_{22}H_{23}N_2O_2S_2$: 411.11955, found 411.11898.

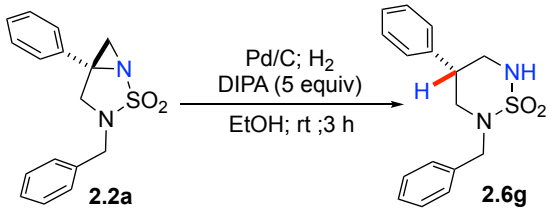


To a solution of **2.2a** (0.1 mmol) and diethyl malonate (4 equiv) in anhydrous 1:1 THF/DMSO (2 mL), sodium hydride (2 equiv) was added slowly at room temperature. The reaction mixture continued to stir for 12 h at 40 ºC. After the completion of reaction, the reaction was quenched with water at 0 ºC and extracted with EtOAc (10 ml × 3). The combined extract was concentrated under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6f** as white solid.

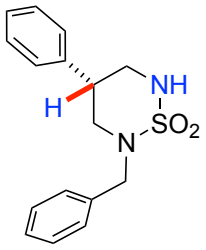


Diethyl (*S*)-2-((5-benzyl-1,1-dioxido-3-phenyl-1,2,5-thiadiazolidin-3-yl)methyl)malonate (–)-**2.6f**. White solid. Yield: 58%. R_f = 0.5 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -34.39 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.40 – 7.35 (m, 4H), 7.34 – 7.28 (m, 4H), 7.26 – 7.23 (m, 2H), 5.78 (s, 1H), 4.36 (d, *J* = 13.8 Hz, 1H), 4.20 (qd, *J* = 7.1, 4.0 Hz, 2H), 4.09 (qd, *J* = 7.1, 5.0 Hz, 2H), 3.84 (d, *J* = 13.7 Hz, 1H), 3.50 (d, *J* = 9.8 Hz, 1H), 3.31 (d, *J* = 9.8 Hz, 1H), 3.30 – 3.27 (m, 1H), 2.68 (dd, *J* = 15.1, 7.2 Hz, 1H), 2.53 (dd, *J* = 15.1, 5.2 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.04, 169.41, 141.68, 135.10, 129.17, 128.98, 128.63, 128.35, 128.31, 125.51, 63.06, 62.55, 62.31, 60.36, 50.33, 48.26, 39.98, 14.10,

14.07. HPLC analysis: *ee* = 90%. IC (80% hexanes: 20% isopropanol, 0.8 mL/min): t_{major} = 35.498 min, t_{minor} = 42.539 min. IR (neat, cm^{-1}): 1727.69, 1301.44, 1167.65. HRMS ($DART^+$) ($[M+H]^+$) Calcd. for $C_{23}H_{29}N_2O_6S$: 461.17408, found 461.17306.

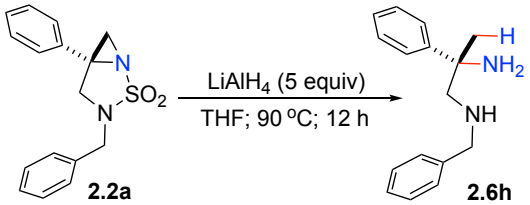


To a solution of **2.2a** (0.1mmol) and 10% Palladium on carbon (50 mg) in EtOH (2 mL), diisopropylamine (5 equiv) was added. The reaction mixture was degassed by bubbling N_2 for 10 mins and then bubbled with H_2 gas for 3h at room temperature. the solvent was removed under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6g** as white solid.

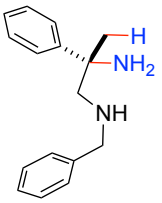


(*R*)-2-Benzyl-4-phenyl-1,2,6-thiadiazinane 1,1-dioxide (–)-**2.6g**. White solid. Yield: 96%. R_f = 0.6 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -82.39 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.47 – 7.33 (m, 4H), 7.33 – 7.22 (m, 4H), 7.21 – 7.12 (m, 2H), 4.68 (dd, *J* = 10.1, 4.6 Hz, 1H), 4.58 (d, *J* = 13.8 Hz, 1H), 4.05 (d, *J* = 13.8 Hz, 1H), 3.89 – 3.76 (m, 1H), 3.58 – 3.47 (m, 2H), 3.27 – 3.17 (m, 1H), 3.11 (tt, *J* = 11.4, 4.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.14, 135.28, 129.05, 128.99, 128.83, 128.17, 127.81, 127.55, 54.05, 52.37, 50.74, 40.34. HPLC analysis: *ee* = 82% (*ee* dropped). IC (90% hexanes: 10% isopropanol, 0.8 mL/min): t_{major} = 39.046 min, t_{minor} = 71.935 min. IR (neat,

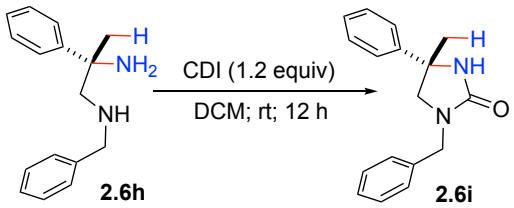
cm^{-1}): 1163.17, 905.60, 755.89, 727.74, 698.54. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{16}H_{19}N_2O_2S$: 303.11617, found 303.11610.



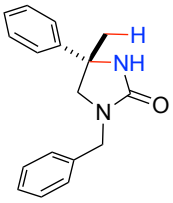
To a solution of **2.2a** (0.2 mmol) in anhydrous THF (2 mL), $LiAlH_4$ (5 equiv) was added slowly at room temperature. The reaction mixture was heat up and stirred for 12 h at 90 ºC. After the completion of reaction, the reaction was quenched with water at 0 ºC and extracted with EtOAc (10 ml × 3). The combined extract was concentrated under vacuum and afforded compound (–)-**2.6h** as light-yellow oil.



(*S*)-*N*^{1}-Benzyl-2-phenylpropane-1,2-diamine (–)-**2.6h**. Light-yellow oil. Yield: 96%. $[\alpha]_D^{20}$ = -8.8 (*c* = 1.0, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.48 – 7.42 (m, 2H), 7.36 – 7.27 (m, 5H), 7.25 – 7.21 (m, 3H), 3.74 (s, 2H), 2.93 (d, *J* = 11.6 Hz, 1H), 2.70 (d, *J* = 11.6 Hz, 1H), 1.96 (s, 3H), 1.45 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.58, 140.58, 128.42, 128.41, 128.07, 126.97, 126.51, 125.48, 61.55, 55.49, 54.25, 29.33. Its *ee* was measured with 3**i**. IR (neat, cm^{-1}): 2924.18, 1494.41, 1453.01, 1215.46, 752.84, 699.27. HRMS (DART$^+$) ([M+H_2]$^+$): Calcd. for $C_{16}H_{21}N_2$: 241.17060, found 241.16993.



To a solution of **2.6h** (0.1 mmol) in anhydrous DCM (2 mL), 1,1'-carbonyldiimidazole (1.2 equiv) was added. The reaction mixture was then stirred at room temperature for 12 h. After the completion of reaction, the solvent was removed under vacuum and purified by flash column chromatography. The fractions containing product were collected and afforded compound (–)-**2.6i** as white solid.

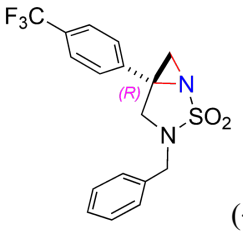


(*S*)-1-Benzyl-4-methyl-4-phenylimidazolidin-2-one (–)-**2.6i**. White solid. Yield: 74%. R_f = 0.4 (1:2 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -11.60 (*c* = 0.5, $CHCl_3$). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.39 – 7.17 (m, 10H), 4.87 (s, 1H), 4.51 (d, *J* = 15.0 Hz, 1H), 4.30 (d, *J* = 15.0 Hz, 1H), 3.37 – 3.27 (m, 2H), 1.65 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.95, 145.68, 137.05, 128.85, 128.79, 128.10, 127.62, 127.51, 124.84, 59.02, 57.37, 47.48, 28.65. HPLC analysis: *ee* = 90%. IC (90% hexanes: 10% isopropanol, 0.8 mL/min): t_{major} = 30.179 min, t_{minor} = 35.072 min. IR (neat, cm^{-1}): 2923.90, 1695.00, 1214.43, 752.61, 688.20. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{19}N_2O$: 267.14919, found 267.14955.

2.4.7 X-Ray Crystallographic Information

The X-ray diffraction data were collected using Bruker-AXS SMART-APEXII CCD

diffractometer (Cu K_α, λ = 1.54178 Å). Indexing was performed using *APEX2*[24] (Difference Vectors method). Data integration and reduction were performed using SaintPlus.[25] Absorption correction was performed by multi-scan method implemented in SADABS.[26] Space group were determined using XPREP implemented in APEX2.[24] The structure was solved using SHELXS-97 (direct methods) and refined using SHELXL97 contained in WinGX v1.70.01program.[27]



(−)-**2.2h**

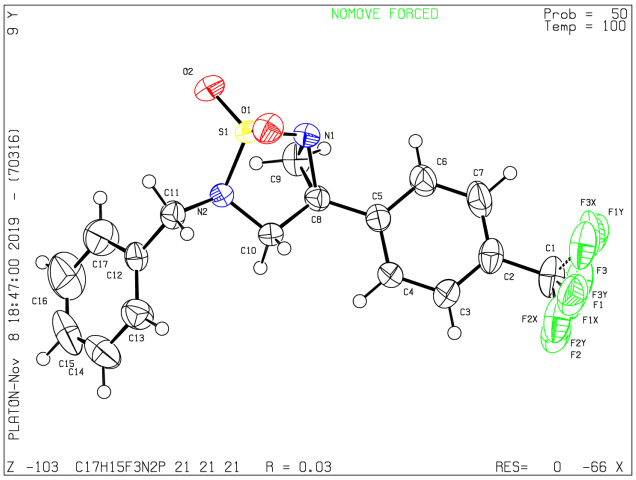
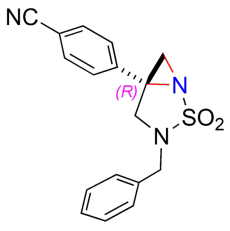


Table 2.9 Crystal Data and Structure Refinement for (−)-2.2h	
Identification code	(−)-**2.2h**
Empirical formula	C17 H15 F3 N2 O2 S
Formula weight	368.37
Temperature	100(2) K

Wavelength	1.54178 ≈	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.8051(4) ≈	α= 90∞.
	b = 13.9494(7) ≈	β= 90∞.
	c = 17.8916(9) ≈	γ = 90∞.
Volume	1698.40(16) ≈^{3}	
Z	4	
Density (calculated)	1.441 Mg/m^3	
Absorption coefficient	2.109 mm^{-1}	
F(000)	760	
Crystal size	0.420 x 0.280 x 0.180 mm^3	
Theta range for data collection	4.018 to 66.497∞.	
Index ranges	-8<=h<=7, -16<=k<=16, -21<=l<=20	
Reflections collected	43308	
Independent reflections	2965 [R(int) = 0.0323]	
Completeness to theta = 66.497∞	99.5 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.7528 and 0.5991
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2965 / 265 / 247
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.0869
R indices (all data)	R1 = 0.0359, wR2 = 0.0889
Absolute structure parameter	-0.006(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.176 and -0.304 e.≈$^{-3}$



(−)-**2.2i**

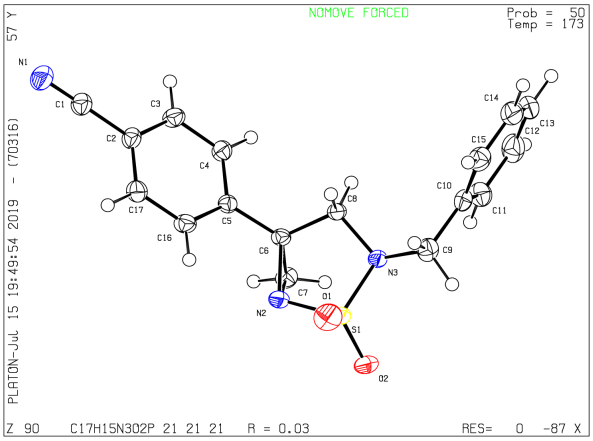
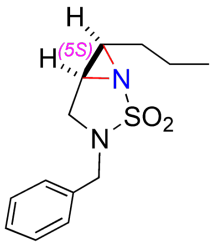


Table 2.10 Crystal Data and Structure Refinement for (−)-**2.2i**		
Identification code	(−)-**2.2i**	
Empirical formula	C17 H15 N3 O2 S	
Formula weight	325.38	
Temperature	173(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.0933(2) ≈	α= 90∞.
	b = 10.7263(4) ≈	β= 90∞.
	c = 23.9103(9) ≈	γ = 90∞.
Volume	1562.74(10) $≈^3$	
Z	4	
Density (calculated)	1.383 Mg/m^3	
Absorption coefficient	0.220 mm^{-1}	
F(000)	680	
Crystal size	0.540 x 0.280 x 0.160 mm^3	
Theta range for data collection	2.081 to 28.287∞.	

Index ranges	-8<=h<=8, -14<=k<=13, -31<=l<=31
Reflections collected	22649
Independent reflections	3880 [R(int) = 0.0581]
Completeness to theta = 25.242∞	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6869
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3880 / 0 / 208
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0757
R indices (all data)	R1 = 0.0389, wR2 = 0.0778
Absolute structure parameter	-0.01(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.211 and -0.322 e.≈$^{-3}$



(+)-**2.2aa**

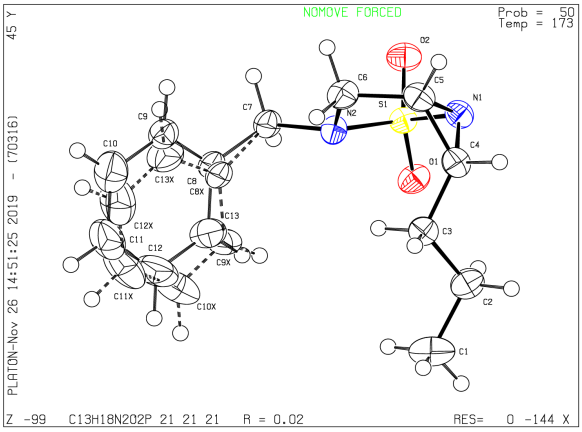


Table 2.11 Crystal Data and Structure Refinement for (+)-**2.2aa**		
Identification code	(+)-**2.2aa**	
Empirical formula	C13 H18 N2 O2 S	
Formula weight	266.35	
Temperature	173(2) K	
Wavelength	1.54178 ≈	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.3956(4) ≈	α= 90∞.
	b = 8.6998(5) ≈	β= 90∞.

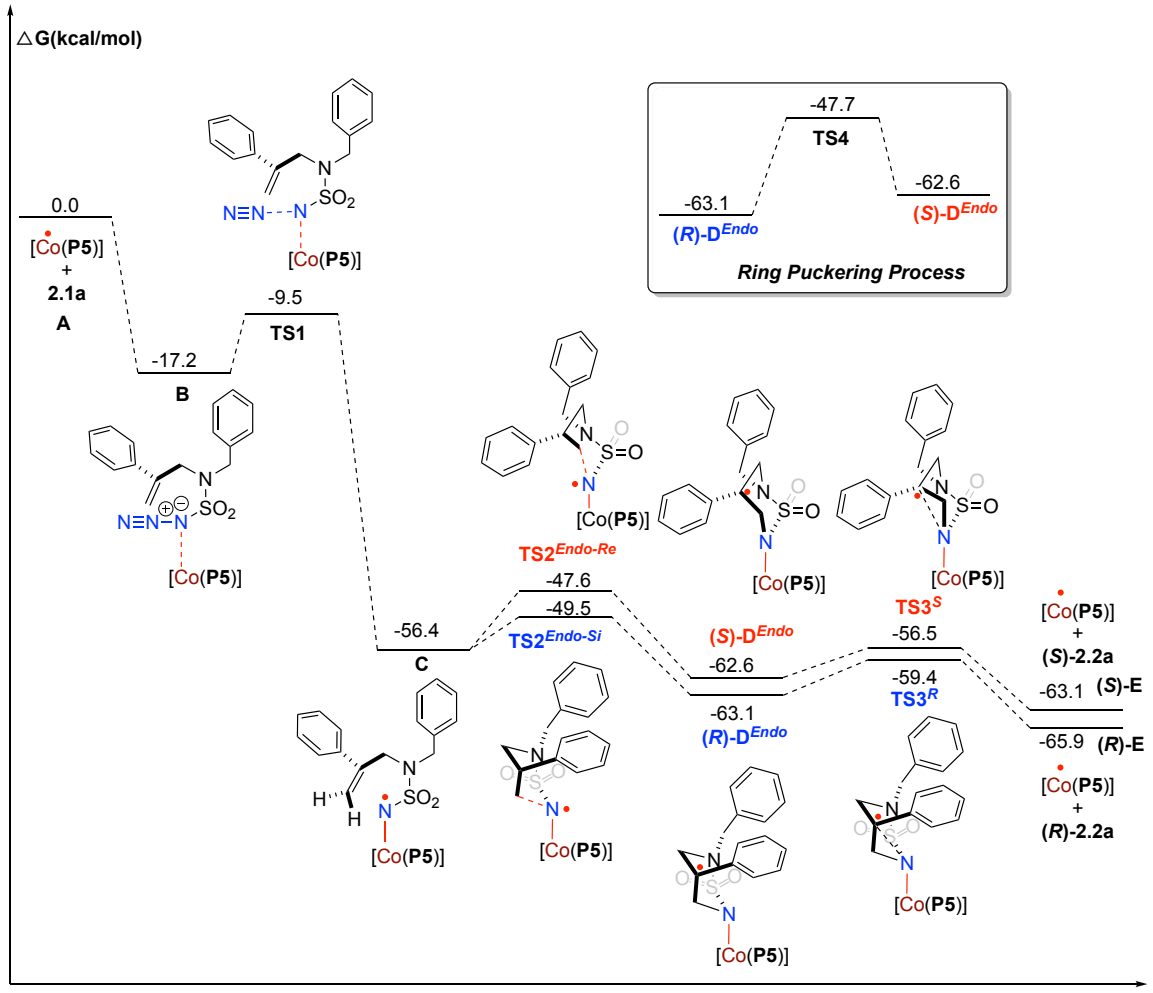
	c = 25.1079(15) ≈ γ = 90∞.
Volume	1397.01(15) ≈^{3}
Z	4
Density (calculated)	1.266 Mg/m^3
Absorption coefficient	2.034 mm^{-1}
F(000)	568
Crystal size	0.380 x 0.260 x 0.150 mm^3
Theta range for data collection	5.381 to 66.393∞.
Index ranges	-7<=h<=7, -10<=k<=10, -29<=l<=29
Reflections collected	25340
Independent reflections	2449 [R(int) = 0.0276]
Completeness to theta = 66.393∞	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6194
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2449 / 265 / 213
Goodness-of-fit on F^2	1.116
Final R indices [I>2sigma(I)]	R1 = 0.0218, wR2 = 0.0580

R indices (all data)	R1 = 0.0219, wR2 = 0.0582
Absolute structure parameter	-0.006(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.116 and -0.254 e.$\approx^{-3}$

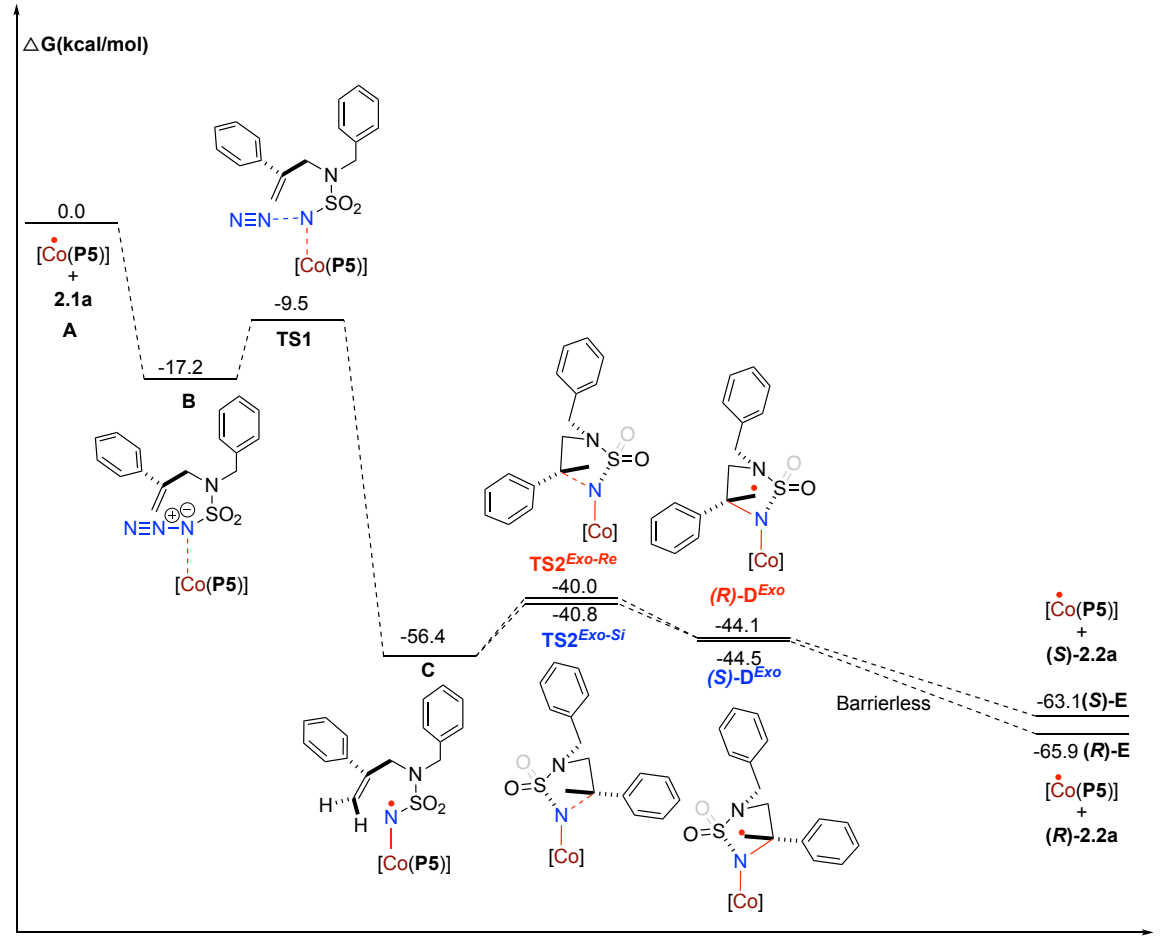
2.4.8 Details on DFT Calculations

In the investigation of the regioselectivity in radical addition step and the asymmetric induction mode, [Co^{II}(**P5**)] was employed for the DFT calculations along with **2.1a** (Scheme 2.10; Scheme 2.11; Scheme 2.12). The geometry optimizations were performed with the Gaussian 16[28] at the BP86[29]/def2-svp[30] level of theory in the gas phase at 40 °C. Gas-phase Hessian matrix calculations were applied to the characterization of all minima (without imaginary frequency) and transition states (with only one imaginary frequency). Thermochemical parameters such as internal energy, enthalpy, entropy, Gibbs free energy and thermal corrections were obtained from these calculations. To better estimate the weak interactions and further improve the accuracy of energies, single point energies were carried out at the BP86 /def2-svp_{Co} // 6-311G*$_{H, C, N, O, S}$ level of theory along with Grimme's dispersion correction[31] (D3-BJ). The structures were displayed by CYLview[32] and VMD[33].

Scheme 2.11 Calculated Energy Diagram for [Co^{II}(P5)] Catalyzed Asymmetric Radical Heterobicyclization of Allyl Sulfamoyl Azides via *6-endo-trig* Cyclization

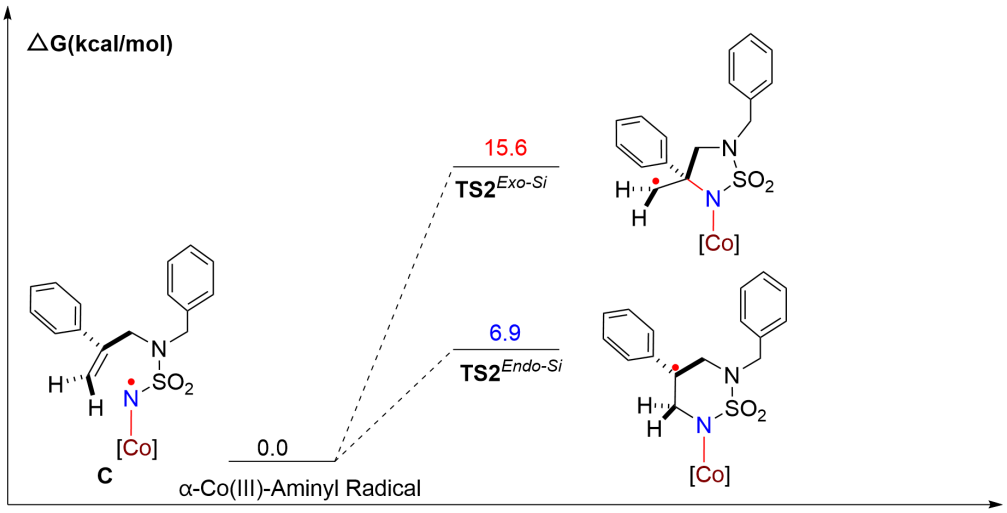


Scheme 2.12 Calculated Energy Diagram for [Co^{II}(P5)] Catalyzed Asymmetric Radical Heterobicyclization of Allyl Sulfamoyl Azides via *5-exo-trig* Cyclization



In Scheme 2.12, it presents the lowest energy transition state of *6-endo-trig* cyclization (**TS2**$^{Endo\text{-}Si}$ in Scheme 2.10) is 6.9 kcal/mol corresponding to Intermediate C and the lowest energy transition state of *5-exo-trig* cyclization **TS2**$^{Exo\text{-}Si}$ in Scheme 2.11) is 15.6 kcal/mol corresponding to Intermediate C. the DFT results favors *6-endo-trig* cyclization by about 8.7 kcal/mol over *5-exo-trig* cyclization, which is consistent with the TEMPO-trapping results.

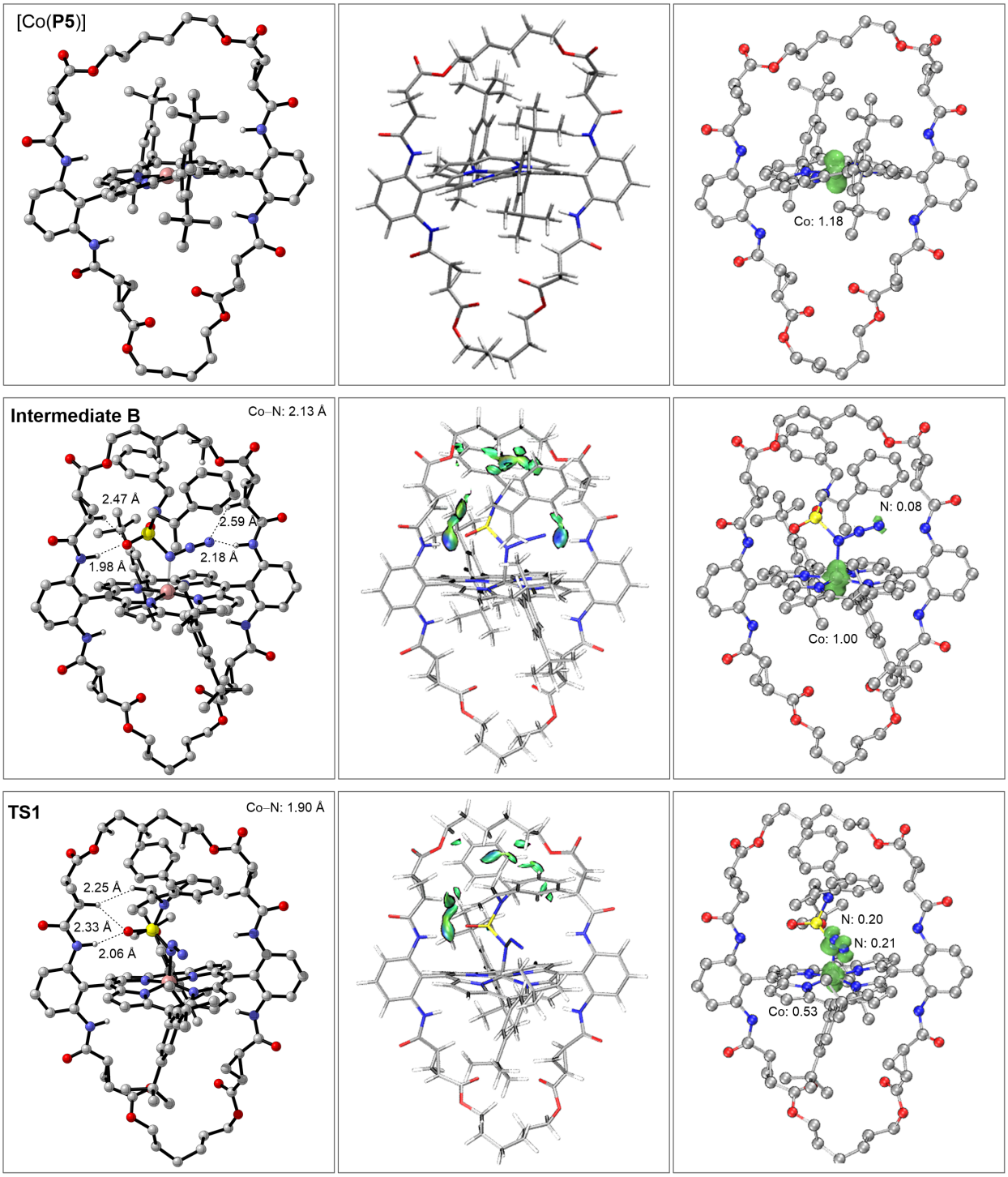
Scheme 2.13 Calculated Energy Diagram for The Regioselectivity in Radical Addition Step.

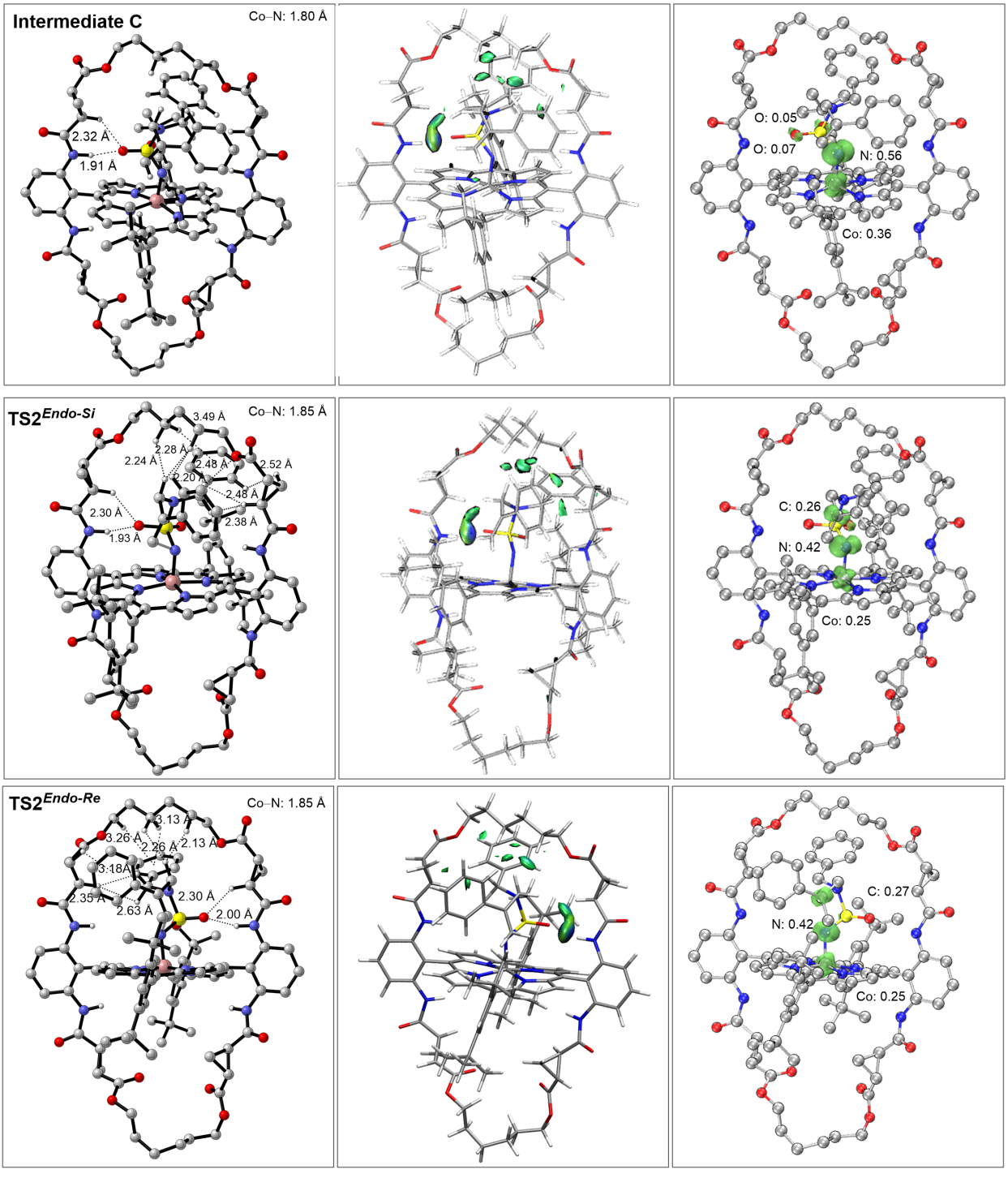


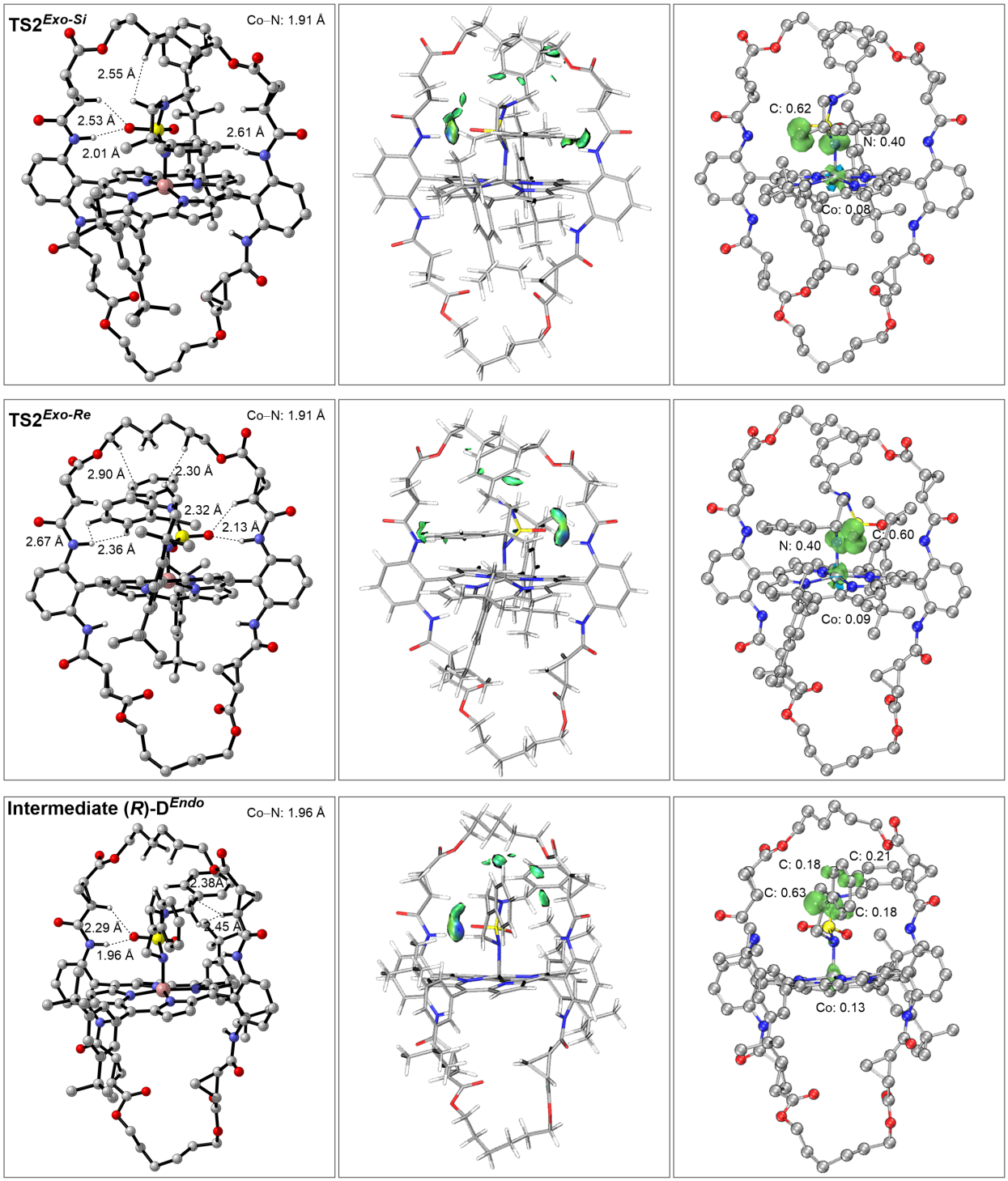
It is known that 6-membered rings can adopt several conformations via ring puckering caused by out-of-plane bending motions associated with the changes in the rotatable ring bonds.[34] The mathematical definition was firstly introduced upon a spherical polar coordinates system, Cremer–Pople puckering coordinates.[35] Recently, a triangular decomposition coordinate system was proposed by Hill and Reilly, which could give a precise definition of ring conformers as a function of triangular planes deviating from a reference plane placed on the monosaccharide ring.[36] In this work, a triangular decomposition coordinate was utilized for the investigation of ring puckering of intermediate D. The operation of the ring puckering was based on Rodrigues' rotation formula.[37] A good sampling along the pathway of the ring puckering was guaranteed by tuning the rotated plane every 0.5 degree for sampling the structures. Then restrained optimization of each structure give the minimal energy pathway of the ring puckering. The structure with the highest energy on this pathway was considered as the transition state.

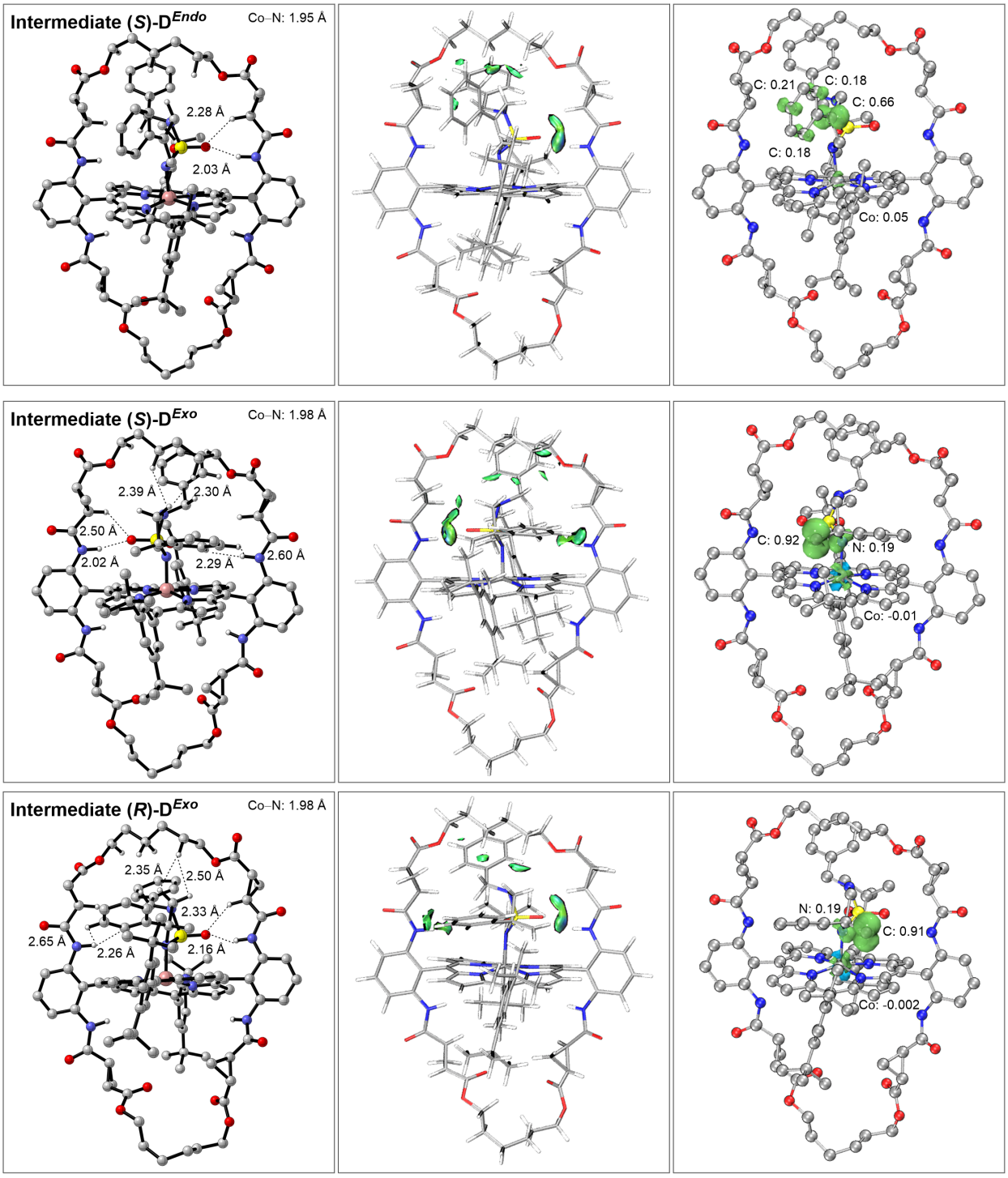
There are 0.5 kcal/mol energy difference between intermediate *(S)*-$\mathbf{D}^{Endo}$ and intermediate *(R)*-$\mathbf{D}^{Endo}$ resulting from various weak interactions. Both of them bear a 6-membered ring with an opposite prochirality in the pocket of catalyst. Moreover, the 6-membered rings are bonded to the catalyst not only via covalent bond (Co-N) but also through H-bonding (O---H-N). The typical barrier of the chair-to-chair conformational inversion on free 6-membered ring structures is around 10-15 kcal/mol (Table 2.1).[13] The interconversion barrier from intermediate *(R)*-$\mathbf{D}^{Endo}$ to intermediate *(S)*-$\mathbf{D}^{Endo}$ is 15.4 kcal/mol, which is slightly higher than the above typical barrier due to the attempt of breaking H-bonding and the steric repulsion from the catalyst in the process of interconversion.

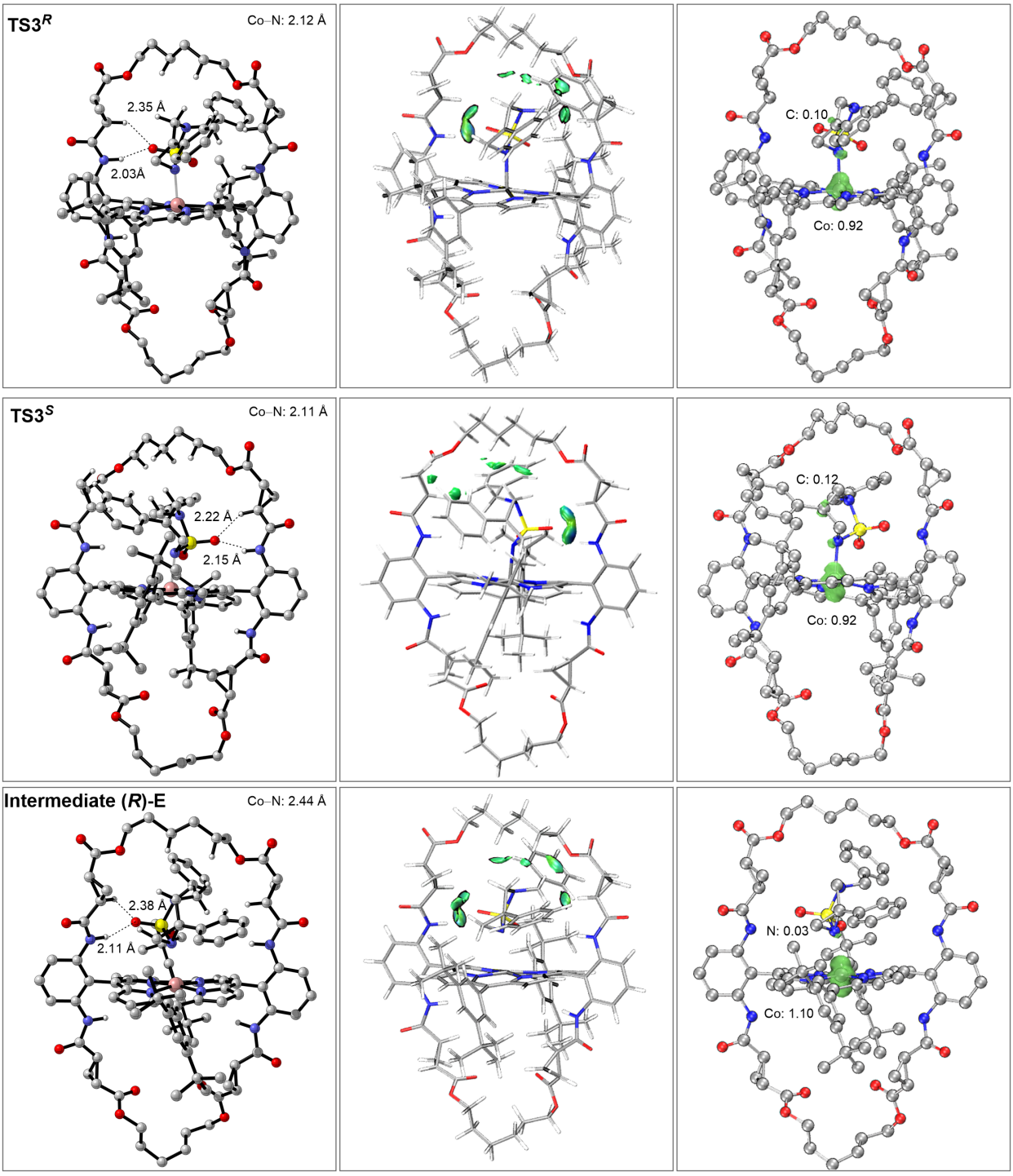
Scheme 2.16 Optimized Structure Models, NCI Plot and Spin Density Representations of Intermediates and Transition States

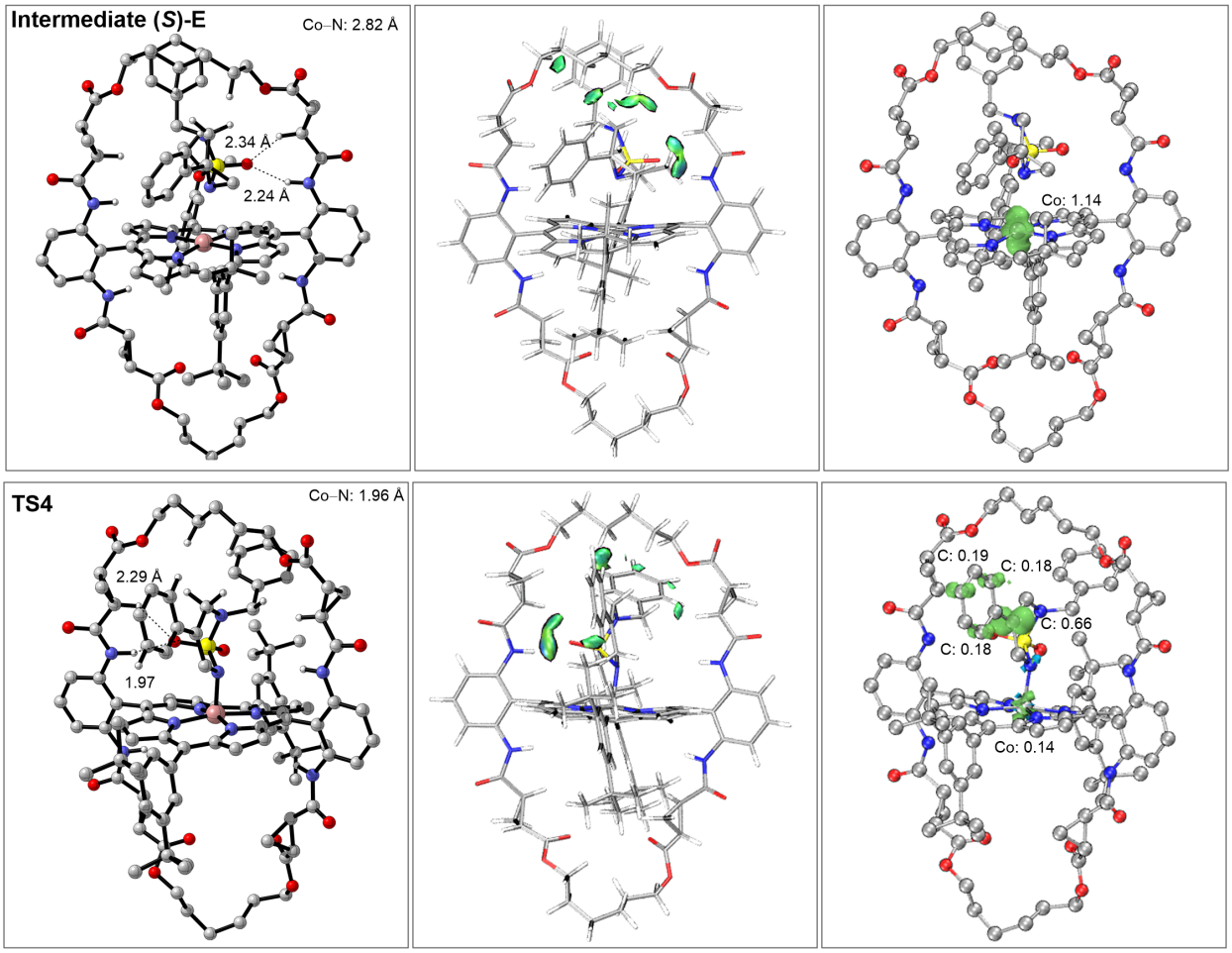



Intermediate C
Co–N: 1.80 Å
2.32 Å
1.91 Å
O: 0.05
O: 0.07
N: 0.56
Co: 0.36
TS2Endo-Si
Co–N: 1.85 Å
3.49 Å
2.28 Å
2.24 Å
2.48 Å
2.52 Å
2.20 Å
2.48 Å
2.30 Å
2.38 Å
1.93 Å
C: 0.26
N: 0.42
Co: 0.25
TS2Endo-Re
Co–N: 1.85 Å
3.13 Å
3.26 Å
2.26 Å
2.13 Å
3.18 Å
2.35 Å
2.30 Å
2.63 Å
2.00 Å
C: 0.27
N: 0.42
Co: 0.25


TS2Exo-Si
Co–N: 1.91 Å
2.55 Å
2.53 Å
2.01 Å
2.61 Å
C: 0.62
N: 0.40
Co: 0.08
TS2Exo-Re
Co–N: 1.91 Å
2.90 Å
2.30 Å
2.32 Å
2.13 Å
2.67 Å
2.36 Å
N: 0.40
C: 0.60
Co: 0.09
Intermediate (R)-DEndo
Co–N: 1.96 Å
2.38Å
2.29 Å
2.45 Å
1.96 Å
C: 0.18
C: 0.21
C: 0.63
C: 0.18
Co: 0.13


Intermediate (S)-D^Endo
Co–N: 1.95 Å
2.28 Å
2.03 Å
C: 0.21
C: 0.18
C: 0.66
C: 0.18
Co: 0.05
Intermediate (S)-D^Exo
Co–N: 1.98 Å
2.39 Å
2.30 Å
2.50 Å
2.02 Å
2.29 Å
2.60 Å
C: 0.92
N: 0.19
Co: -0.01
Intermediate (R)-D^Exo
Co–N: 1.98 Å
2.35 Å
2.50 Å
2.33 Å
2.65 Å
2.26 Å
2.16 Å
N: 0.19
C: 0.91
Co: -0.002


TS3R
Co–N: 2.12 Å
2.35 Å
2.03Å
C: 0.10
Co: 0.92
TS3S
Co–N: 2.11 Å
2.22 Å
2.15 Å
C: 0.12
Co: 0.92
Intermediate (R)-E
Co–N: 2.44 Å
2.38 Å
2.11 Å
N: 0.03
Co: 1.10



Intermediate A

$A_{[Co(II)P5]}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 1.833261 Hartree

G_corr: 1.53387 Hartree

SCF: -6291.334662 Hartree

S: 599.938 Cal/Mol-Kelvin

H: -6289.501401 Hartree

G: -6289.800792 Hartree

Cartesian Coordinates:

C 0.35316200 1.20098600 -2.69294900

N	0.33101600	1.35410500	-1.31016200
H	0.35857800	2.63035200	-4.42872600
C	0.35662000	2.72880900	-1.10332500
C	0.39236400	3.43163700	-2.36464000
H	0.40865500	4.51456300	-2.46767600
C	0.36033600	2.48683000	-3.34963300
C	0.25084000	3.37170500	0.13596100
N	-0.18607100	1.28682500	1.41332200
C	-0.61486700	1.07051400	2.71736100
C	-0.73263900	2.32008800	3.43110200
H	-1.05061600	2.41398400	4.46744400
C	-0.34246300	3.30447800	2.57092600
H	-0.27461100	4.37395300	2.75693700
C	-0.04067200	2.66798300	1.30981300
C	0.46170700	-0.01760200	-3.37766800
H	1.43947000	-4.45379400	-2.50726500
C	1.18012500	-3.40335100	-2.39393100
C	0.93127500	-2.75134900	-1.12882700
H	1.05177800	-2.59200800	-4.44937800
N	0.62113500	-1.40890900	-1.32449000
C	0.65260500	-1.23260100	-2.70337200
C	0.97953100	-2.47068900	-3.37009400
C	-0.82182700	-0.18011300	3.31777400
H	0.32366000	-4.60260100	2.63887200
C	0.11271700	-3.54740800	2.47982600
C	-0.45228100	-2.65732500	3.34780800
H	-0.79894200	-2.82832900	4.36576900
C	-0.47135400	-1.37750000	2.67905500
N	0.02979400	-1.49110500	1.38538100
C	0.38374900	-2.83052200	1.25541000
C	0.87188800	-3.43581200	0.09065300
Co	0.20093100	-0.06422900	0.04255400
C	1.26622600	-4.88160700	0.12117500
C	2.62407500	-5.23661300	0.04353700

C	0.28893400	-5.88886900	0.21117700
C	3.02475800	-6.58433600	0.06274200
H	3.36502000	-4.43679900	-0.02524200
C	0.64710500	-7.24834300	0.22725300
H	-0.76091300	-5.59011900	0.25418000
C	2.01743700	-7.56308800	0.15465400
H	2.31283600	-8.61686600	0.16748200
C	0.36772200	4.86514200	0.18167100
C	-0.77085700	5.66575100	0.38244700
C	1.62293800	5.47409300	0.00911300
C	-0.67553800	7.06793000	0.41656700
H	-1.73768300	5.17113200	0.49949800
C	1.76263400	6.87286700	0.04532700
H	2.49334000	4.83190200	-0.14365000
C	0.60009900	7.63958100	0.24932100
H	0.69153600	8.72990900	0.27768800
C	0.39194800	-0.02746900	-4.87988200
C	1.54986400	0.16299000	-5.67841100
C	-0.85824000	-0.24851100	-5.51760100
C	1.45912900	0.11394300	-7.08355100
C	-0.94497600	-0.29981900	-6.92163300
C	0.21615800	-0.12046000	-7.67607000
H	2.35654900	0.26252400	-7.68022900
H	-1.91010100	-0.48528100	-7.38934800
H	0.15060600	-0.16127800	-8.76769200
C	-1.34951100	-0.19866800	4.72581900
C	-2.74565500	-0.13369100	4.95964500
C	-0.46264600	-0.19443900	5.83630700
C	-3.24402500	-0.00049700	6.26913000
C	-0.96385700	-0.07444700	7.14622200
C	-2.34456000	0.03466800	7.33647600
H	-4.31759600	0.08643300	6.42844300
H	-0.26700800	-0.05866900	7.98232300
H	-2.73164300	0.13907600	8.35469200

C	3.12604600	7.57563100	-0.12467500
C	3.07060400	8.52165600	-1.35046600
H	2.29553600	9.29653800	-1.24005900
H	4.03771000	9.03596100	-1.48330400
H	2.85399800	7.96171700	-2.27499900
C	4.27839500	6.57425900	-0.34404800
H	4.39907700	5.88908700	0.51121200
H	4.13273100	5.96838300	-1.25369400
H	5.22804000	7.12124300	-0.46247700
C	3.44115000	8.40188400	1.14756500
H	4.41294500	8.91387800	1.04298400
H	2.67822500	9.17326400	1.33794600
H	3.49170500	7.75503400	2.03859200
C	-1.90474200	7.97808200	0.62347500
C	-2.06392500	8.91410500	-0.60089600
H	-2.93819800	9.57412500	-0.46903400
H	-1.18154000	9.55715800	-0.74706700
H	-2.21231100	8.33453700	-1.52673400
C	-3.21027300	7.17279000	0.78490700
H	-3.43464500	6.56431800	-0.10670400
H	-3.17955900	6.50265900	1.65972200
H	-4.05673200	7.86336100	0.93154700
C	-1.70428300	8.83278300	1.90015100
H	-0.80879500	9.47093900	1.83441200
H	-2.57281000	9.49415500	2.06001700
H	-1.59524800	8.19474400	2.79238000
C	4.50622900	-7.01074200	-0.00913600
C	-0.39792100	-8.38077300	0.31441900
C	-0.13489000	-9.22819000	1.58454400
H	-0.87068300	-10.04692100	1.65950100
H	0.86830300	-9.68310800	1.57779300
H	-0.21707500	-8.61385500	2.49617400
C	-0.28276900	-9.28506200	-0.93850800
H	0.71427400	-9.74518400	-1.02606000

H	-1.02312400	-10.10181800	-0.89237500
H	-0.46790700	-8.71038300	-1.86071800
C	-1.84154000	-7.84264800	0.38659500
H	-2.00509500	-7.20990900	1.27451900
H	-2.11068600	-7.25634500	-0.50740300
H	-2.54935100	-8.68511500	0.45044500
C	5.45992500	-5.80310600	-0.11328500
H	5.27286900	-5.20384400	-1.01953900
H	5.38145100	-5.13769300	0.76247200
H	6.50266600	-6.15662900	-0.16418500
C	4.87409400	-7.80690800	1.26820800
H	4.26074900	-8.71513100	1.37965900
H	5.93113100	-8.12155000	1.23441300
H	4.73034600	-7.19378500	2.17296400
C	4.72639000	-7.90695200	-1.25364300
H	5.78090400	-8.22528100	-1.31649500
H	4.10641900	-8.81692800	-1.22274900
H	4.47975200	-7.36565400	-2.18164200
N	2.77407600	0.39235000	-5.00781300
H	2.71639700	0.35800300	-3.98988200
N	0.91696200	-0.30701000	5.55887400
H	1.14269000	-0.40590500	4.56925600
N	-3.60716700	-0.25405600	3.84551900
H	-3.18605900	-0.65658400	3.00877600
N	-1.99069500	-0.39199600	-4.68649600
H	-1.81268600	-0.23648900	-3.69449500
C	4.00179500	0.73248200	-5.55137000
C	1.98596200	-0.36258000	6.43828600
C	-4.91363500	0.20027300	3.72348000
C	-3.27719600	-0.77970800	-5.02373900
O	-5.49416000	0.86327900	4.58122000
O	-3.64989800	-1.06239500	-6.16251700
O	1.89804600	-0.25314500	7.66143900
O	4.22378300	0.84665000	-6.75740200

C	-4.20243400	-0.85114400	-3.83761900
H	-3.86897900	-0.43922900	-2.88040400
C	-5.55662200	-0.19957000	2.42049900
H	-5.16714600	-1.08195700	1.90342200
C	-6.13278600	0.87931700	1.52267400
H	-6.06870800	0.71072800	0.44510000
H	-6.04868700	1.91431900	1.86281600
C	-7.06186900	-0.01195000	2.32980600
H	-7.53104900	0.45263800	3.19901700
C	-5.13282500	-2.04089300	-3.75786300
H	-5.07285600	-2.77105400	-4.56757200
H	-5.36223600	-2.42436700	-2.76149300
C	-5.69163600	-0.67799200	-4.12685100
H	-5.96722500	-0.53331500	-5.17267700
C	-7.85997500	-1.04703000	1.61084600
C	-6.52428300	0.00332800	-3.09530200
O	-6.21913500	0.12016800	-1.91760400
O	-7.41536400	-1.91974600	0.88326400
O	-7.69508400	0.43190200	-3.64348900
O	-9.18875200	-0.86642100	1.87177000
C	-8.72436000	0.91496900	-2.72646800
H	-8.34428700	0.81444800	-1.70026800
H	-8.87045900	1.98508800	-2.94712300
C	-9.99517500	0.10299900	-2.96921200
H	-10.36115200	0.30232900	-3.99131600
H	-9.72855700	-0.96774200	-2.94663900
C	-10.10840900	-1.77670100	1.19929000
H	-11.03279800	-1.69185900	1.79060000
H	-9.71353200	-2.80129300	1.28234100
C	-10.33802700	-1.40384700	-0.26589200
H	-9.40669200	-1.60748000	-0.81795300
H	-11.09736900	-2.10366700	-0.66645100
C	-11.12024700	0.38851600	-1.95417000
H	-11.41520200	1.45267000	-2.01721600

H	-12.01160200	-0.18527500	-2.26824500
C	-10.79613200	0.04716900	-0.48402800
H	-10.02558000	0.73286500	-0.09160200
H	-11.69840000	0.24337500	0.12497000
C	5.08403000	0.98177500	-4.53110400
H	4.86665000	0.81208500	-3.47286800
C	3.30460700	-0.59495700	5.74951600
H	3.31473400	-0.69169100	4.66093400
C	4.34597000	-1.38507800	6.50371800
H	4.99891400	-2.03539300	5.91974200
H	4.06182600	-1.73431300	7.49867300
C	6.07315000	2.07666100	-4.86386100
H	6.48273800	2.64747500	-4.02946800
H	5.89962600	2.61863300	-5.79589900
C	6.50895300	0.63594400	-5.00324300
H	6.55732200	0.23688500	-6.01788300
C	4.52818200	0.11236700	6.35650000
H	4.33193700	0.71631100	7.24407700
C	7.51657200	0.03140600	-4.08551600
C	5.59257300	0.66680200	5.47260500
O	7.50680400	0.60366700	-2.84011500
O	5.71571000	-0.05749800	4.31363100
O	6.28397400	1.63021300	5.74913700
O	8.29036300	-0.85036300	-4.41201500
C	8.57270600	0.14883500	-1.95295900
H	8.39544200	-0.91070400	-1.70065000
H	9.52395400	0.20141000	-2.50506900
C	8.57990100	1.04132300	-0.71996400
H	9.52440100	0.85228700	-0.17613100
H	8.62389300	2.09595300	-1.04845300
C	6.77352700	0.36393000	3.40615200
C	7.39246800	0.82681500	0.23001800
H	6.44657800	0.91932500	-0.33322400
H	7.42348800	-0.21426100	0.60346900

C	7.37988900	1.81871600	1.40624900
H	7.20032300	2.83495600	1.01254700
H	8.38367000	1.85829100	1.87276000
C	6.32738800	1.50260300	2.48816000
H	5.36556900	1.23386800	2.01455700
H	6.14309800	2.39272000	3.11078000
H	7.01724700	-0.54959900	2.84404200
H	7.64683700	0.66899900	4.00386000

$A_{2.1a}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 0.316337 Hartree

G_corr: 0.232436 Hartree

SCF: -1387.200835 Hartree

S: 168.125 Cal/Mol-Kelvin

H: -1386.884498 Hartree

G: -1386.968399 Hartree

Cartesian Coordinates:

C	4.45537700	-0.69619500	-1.62617300
C	3.20610200	-0.18012700	-1.26189400
C	2.82818000	-0.08303400	0.09515000
C	3.73930000	-0.54352900	1.07088600
C	4.98648800	-1.05935400	0.70669300
C	5.35152600	-1.13677700	-0.64464100
H	4.72976600	-0.74981700	-2.68423700
H	2.53274400	0.17559300	-2.04736200
H	3.44991400	-0.51741300	2.12586700
H	5.67315000	-1.41408000	1.48172600
H	6.32607900	-1.54399400	-0.93040400
C	1.50875100	0.47997700	0.49333400
C	0.34646100	0.15854500	-0.44290200
H	0.36494600	-0.91602000	-0.70055600
H	0.45175800	0.69845700	-1.39649600

N	-0.99756000	0.44105000	0.07754500
S	-1.83815100	1.77787700	-0.42375700
N	-1.47316300	3.05521400	0.81369400
O	-3.26330800	1.53344600	-0.19917300
O	-1.27822900	2.23261400	-1.70321800
C	-1.56092900	-0.45075300	1.12250200
C	-1.88387800	-1.83140700	0.57956800
H	-2.46578900	0.02949800	1.52014500
H	-0.82986100	-0.51988300	1.94492700
C	-1.16418100	-2.95526900	1.01666700
C	-1.46868300	-4.23304800	0.52563700
C	-2.91625100	-2.00279100	-0.36179400
C	-3.21988200	-3.27674900	-0.85261300
C	-2.49674000	-4.39500000	-0.41028000
H	-2.73693600	-5.39091400	-0.79511500
H	-4.02801100	-3.39984300	-1.58025500
H	-0.35943500	-2.83113100	1.75005300
H	-0.89993700	-5.10056200	0.87429600
H	-3.48395600	-1.13099300	-0.70220200
C	1.35209100	1.22579500	1.60340100
H	2.20304300	1.48750800	2.23739400
H	0.37824800	1.62878500	1.89326200
N	-0.78586800	3.99439400	0.37339600
N	-0.16418300	4.90914200	0.06778900

Intermediate B:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.150848 Hartree

G_corr: 1.801236 Hartree

SCF: -7678.597854 Hartree

S: 700.576 Cal/Mol-Kelvin

H: -7676.447006 Hartree

G: -7676.796618 Hartree

Cartesian Coordinates:

C	6.92780400	-4.49901800	-0.94842300
C	6.06119800	-3.72883100	-0.16414500
C	4.86158100	-3.21755900	-0.70444100
C	4.56871900	-3.48084800	-2.05844800
C	5.44676700	-4.23522000	-2.84697200
C	6.62525900	-4.75179900	-2.29358200
H	7.83778200	-4.91335000	-0.50337400
H	6.29524200	-3.56712100	0.89346200
H	3.64829500	-3.07965600	-2.49233500
H	5.20935600	-4.41708300	-3.89929000
C	3.88082100	-2.51359100	0.17253600
C	4.32830800	-1.32002400	1.01487900
H	5.40109400	-1.37445000	1.25488900
H	3.79125400	-1.33757600	1.97049900
N	4.11721700	0.04291400	0.43712700
S	2.71141200	0.84187500	0.78107900
N	1.42826200	-0.05380600	-0.18619600
O	2.78048300	2.19629800	0.23788900
O	2.29796500	0.54754100	2.15399100
C	5.02655000	0.65824100	-0.56024100
C	5.71770000	1.92605000	-0.08257700
H	4.49645600	0.85747400	-1.50349100
H	5.75894200	-0.12857000	-0.79462900
C	6.07661800	2.90666800	-1.02286200
C	6.75668700	4.06405400	-0.62228600
C	6.04100600	2.13208200	1.26782300
C	6.71066000	3.29343900	1.67347000
C	7.07490400	4.26142100	0.72781100
H	7.59557100	5.17027100	1.04388700
H	6.94520000	3.43798000	2.73233500
H	5.81154800	2.76746100	-2.07614700
H	7.02477300	4.82039900	-1.36638800
H	5.76184900	1.38128300	2.01222800

C	2.62480700	-2.98469500	0.29725900
H	2.29248400	-3.85875200	-0.26972500
H	1.88900900	-2.52093400	0.96026300
C	-0.63919700	-1.04462700	2.84986800
N	-0.79639900	-1.24571000	1.48324100
H	-0.72688600	-2.38525100	4.65257200
C	-1.05800600	-2.60681400	1.35065800
C	-1.07364800	-3.24848700	2.64570600
H	-1.28662300	-4.30177300	2.81306500
C	-0.79203000	-2.28644500	3.57077700
C	-1.26697200	-3.29275700	0.14756100
N	-0.98145600	-1.30784700	-1.32629000
C	-0.94009100	-1.17585400	-2.71120300
C	-1.11185700	-2.45795400	-3.35141400
H	-1.11065900	-2.61800300	-4.42765200
C	-1.27611700	-3.37741600	-2.35661700
H	-1.42687100	-4.45061600	-2.44968000
C	-1.19247700	-2.66423700	-1.10286700
C	-0.47346200	0.19256400	3.48971300
H	-0.68292600	4.71453000	2.55919800
C	-0.63210300	3.63293800	2.45672800
C	-0.68813900	2.92398400	1.19866500
H	-0.42901500	2.84287300	4.51368100
N	-0.63030400	1.54961200	1.40933700
C	-0.51476200	1.40476900	2.78808400
C	-0.50583600	2.69425500	3.43806000
C	-0.80054800	0.02840700	-3.42139000
H	-0.73424800	4.59429900	-2.69463500
C	-0.74286300	3.51679800	-2.54613300
C	-0.72219200	2.53092800	-3.48955900
H	-0.70334500	2.62730100	-4.57391700
C	-0.74201000	1.27340300	-2.77881900
N	-0.76369700	1.48626200	-1.40233100
C	-0.76764500	2.86640300	-1.25550800

C	-0.76263600	3.56587900	-0.04188800
Co	-0.68235200	0.11502400	0.03837800
C	-0.81905400	5.06390600	-0.07995200
C	0.32808400	5.82554700	0.20379900
C	-2.02356200	5.71175400	-0.40529500
C	0.29001300	7.23088400	0.16667700
H	1.25318700	5.29648100	0.44332300
C	-2.10373400	7.11480900	-0.44822700
H	-2.90207900	5.09741600	-0.61534800
C	-0.93445100	7.84376400	-0.16035900
H	-0.97943900	8.93697800	-0.19206400
C	-1.57627800	-4.75989200	0.19236700
C	-2.86096800	-5.21210700	-0.15901200
C	-0.59855200	-5.69300400	0.58183600
C	-3.18699100	-6.57907200	-0.12375800
H	-3.60713500	-4.46985200	-0.45094500
C	-0.88108500	-7.06980000	0.62329200
H	0.39386600	-5.32369400	0.84981000
C	-2.17942900	-7.48051600	0.26759300
H	-2.41647500	-8.54860100	0.29763900
C	-0.44513400	0.21582700	4.99646600
C	0.74950500	0.04801100	5.75037400
C	-1.68086200	0.36932100	5.69029200
C	0.69366400	0.02631300	7.15953800
C	-1.72668600	0.33713400	7.09588900
C	-0.53623400	0.16539600	7.80396300
H	1.61209300	-0.11603000	7.72421300
H	-2.68648700	0.44038600	7.59904700
H	-0.56657100	0.14206100	8.89765500
C	-0.92869500	-0.03103600	-4.92162000
C	-2.24167400	-0.08772400	-5.46567600
C	0.18469900	-0.09101000	-5.80392600
C	-2.44590800	-0.27284900	-6.84354700
C	-0.02735700	-0.26437600	-7.18748700

C	-1.33125500	-0.36691600	-7.67914400
H	-3.46146700	-0.34935200	-7.23012000
H	0.83278500	-0.31518100	-7.85160600
H	-1.48037100	-0.51273100	-8.75339500
C	0.16952800	-8.12248100	1.03599900
C	-0.33959300	-8.90058900	2.27542300
H	-1.28935100	-9.42124700	2.07536300
H	0.39858700	-9.66125900	2.58171800
H	-0.50350100	-8.22331400	3.12952400
C	1.52868000	-7.48783200	1.39429100
H	1.97137300	-6.94715600	0.54171900
H	1.44953100	-6.78811900	2.24251600
H	2.24127600	-8.27654200	1.68596300
C	0.39373300	-9.11213800	-0.13489100
H	1.14124700	-9.87451400	0.14337200
H	-0.53225900	-9.64021700	-0.41220200
H	0.76074900	-8.58777500	-1.03232400
C	-4.59030700	-7.10772500	-0.48838300
C	-5.19527500	-7.84490800	0.73277000
H	-6.20032700	-8.23016000	0.49016800
H	-4.57767600	-8.70172500	1.04548300
H	-5.28980500	-7.16792800	1.59747300
C	-5.55652200	-5.97543400	-0.89212700
H	-5.71070000	-5.25225400	-0.07445900
H	-5.20039700	-5.42401000	-1.77774700
H	-6.54169600	-6.40026700	-1.14486000
C	-4.47790100	-8.09249100	-1.67919200
H	-3.83600100	-8.95580800	-1.44259000
H	-5.47350400	-8.48297100	-1.95043200
H	-4.05530800	-7.59481500	-2.56730500
C	1.52905700	8.10201100	0.46289000
C	-3.41092700	7.86071900	-0.79002800
C	-3.19059500	8.73698500	-2.04866800
H	-4.11580100	9.28056100	-2.30545600

H	-2.39645700	9.48533600	-1.89778600
H	-2.90780300	8.11955200	-2.91696800
C	-3.81271700	8.76612500	0.40141200
H	-3.03891900	9.51623200	0.62962600
H	-4.74623100	9.30880100	0.17439300
H	-3.97943400	8.16968200	1.31322600
C	-4.57986400	6.89578800	-1.07536400
H	-4.37478300	6.23706800	-1.93507600
H	-4.81575300	6.26048500	-0.20606800
H	-5.48793700	7.47285400	-1.31487000
C	2.76781600	7.25626500	0.82094600
H	2.60380300	6.64108000	1.72066000
H	3.06519800	6.58506300	-0.00093200
H	3.62292700	7.92028800	1.02870300
C	1.86901800	8.95301600	-0.78650700
H	1.03853100	9.61846500	-1.07113300
H	2.75195500	9.58595000	-0.59269600
H	2.09455300	8.31059200	-1.65343500
C	1.22681500	9.04239600	1.65663900
H	2.10404900	9.67316300	1.88052600
H	0.37880800	9.71459200	1.45067200
H	0.98347100	8.46556100	2.56388100
N	1.98306300	-0.08869300	5.06075100
H	1.95774700	0.11414600	4.05896600
N	1.48723900	0.02679600	-5.25646600
H	1.53023300	0.05936400	-4.23670200
N	-3.31899400	0.08623100	-4.56922100
H	-3.05993400	0.47447600	-3.66256300
N	-2.84345800	0.56005100	4.90977200
H	-2.67328500	0.63633100	3.90720800
C	3.19406600	-0.52113600	5.57899500
C	2.69095700	0.17158500	-5.92940900
C	-4.63028900	-0.35222800	-4.67928200
C	-4.15849600	0.71831200	5.31468300

O	-5.08492300	-0.96981600	-5.64009500
O	-4.55436100	0.63436400	6.47797100
O	2.81840500	0.12116900	-7.15366000
O	3.38354000	-0.84173100	6.75358200
C	-5.09041800	1.04956400	4.17767600
H	-4.69165700	1.09618600	3.15995400
C	-5.43646500	-0.00800100	-3.45236900
H	-5.10958900	0.84724500	-2.85289700
C	-6.07288400	-1.13817200	-2.66468000
H	-6.09354600	-1.03070400	-1.57775700
H	-5.95205900	-2.15358500	-3.04860800
C	-6.93801100	-0.20251300	-3.49427200
H	-7.35383900	-0.62398600	-4.41159700
C	-6.22614700	1.99395900	4.48797500
H	-6.29021500	2.35489000	5.51634200
H	-6.52835900	2.68096200	3.69521600
C	-6.52880800	0.52311300	4.27739400
H	-6.76976700	-0.06708200	5.16296000
C	-7.77154400	0.79662400	-2.75728700
C	-7.20158500	0.15927200	2.99746400
O	-6.95865500	0.66830200	1.91378900
O	-7.34088800	1.67167700	-2.02476100
O	-8.14846800	-0.80094400	3.20219100
O	-9.09552500	0.57584900	-2.99234700
C	-8.96608900	-1.14532100	2.04137800
H	-8.35095700	-1.03916700	1.13625000
H	-9.22436500	-2.20474900	2.19099000
C	-10.21293500	-0.26286500	1.99592100
H	-10.74259900	-0.36556700	2.95926800
H	-9.89607400	0.79164100	1.92556500
C	-10.02130700	1.46967400	-2.30039200
H	-10.95503400	1.36046400	-2.87276500
H	-9.64931500	2.50122000	-2.39910100
C	-10.22107100	1.10833300	-0.82787900

H	-9.29180200	1.33120500	-0.27968900
H	-10.99019000	1.80315700	-0.43609100
C	-11.18176300	-0.60595300	0.84647600
H	-11.48701100	-1.66618200	0.92968100
H	-12.10631400	-0.01878400	0.99873500
C	-10.66570000	-0.34415600	-0.58430500
H	-9.83426500	-1.02810000	-0.82849300
H	-11.47560900	-0.60436400	-1.29161400
C	4.31334100	-0.64644300	4.56192900
H	4.18002600	-0.15792000	3.59524700
C	3.87977600	0.48548700	-5.04204900
H	3.77093800	0.38016800	-3.96032000
C	4.76712700	1.60554000	-5.54501600
H	5.23433300	2.25054500	-4.79928300
H	4.47363900	2.07839900	-6.48444400
C	5.09355600	-1.95175100	4.60948700
H	5.47197900	-2.35509000	3.66894200
H	4.76519400	-2.68453400	5.34989200
C	5.73957100	-0.70152900	5.13950700
H	5.74657500	-0.57775600	6.22545200
C	5.26169100	0.17461900	-5.63900100
H	5.22622500	-0.27455800	-6.63326300
C	6.91696000	-0.03486800	4.49434200
C	6.45781800	-0.25646000	-4.85105600
O	7.29380300	-0.58125700	3.28468700
O	6.49964200	0.28375000	-3.58933500
O	7.34190400	-0.95825400	-5.30759800
O	7.52748600	0.87849600	5.02015800
C	8.56474300	-0.04413900	2.77488300
H	8.41496700	1.01665200	2.51836000
H	9.29149900	-0.08462400	3.60052200
C	9.05583300	-0.84393700	1.56997000
H	10.09810700	-0.51452100	1.39509900
H	9.11929800	-1.91473300	1.83657300

C	7.76518100	0.12292600	-2.86162800
C	8.24081500	-0.65453700	0.27993300
H	7.24857500	-1.11478400	0.42620800
H	8.06263500	0.42504300	0.13168300
C	8.87105600	-1.26914000	-0.98489300
H	9.14396600	-2.31918600	-0.77722900
H	9.82305800	-0.75393500	-1.21761900
C	7.93948500	-1.25979600	-2.22097600
H	7.30665600	-5.34705700	-2.90852500
H	6.94886400	-1.64816500	-1.92712300
H	8.31452300	-1.95597500	-2.98590000
H	7.71935800	0.92475100	-2.11023300
H	8.58790000	0.33938600	-3.56071200
N	1.86553400	-0.39708700	-1.29723900
N	2.14427200	-0.80609200	-2.33700500

Transition State TS1:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -543.0426 cm-1

H_corr: 2.148161 Hartree

G_corr: 1.799301 Hartree

SCF: -7678.583612 Hartree

S: 699.067 Cal/Mol-Kelvin

H: -7676.435451 Hartree

G: -7676.784311 Hartree

Cartesian Coordinates:

C	5.11824300	-5.81683700	-1.28987200
C	4.93996400	-4.93644300	-0.21764500
C	4.49982400	-3.61081600	-0.42847400
C	4.26205700	-3.19716100	-1.75593800
C	4.43435600	-4.07914600	-2.82861100
C	4.86339300	-5.39296900	-2.60096300
H	5.47011800	-6.83603400	-1.10102200
H	5.17242700	-5.26606000	0.79967900
H	3.90575800	-2.18041100	-1.93819100
H	4.22946300	-3.74052300	-3.84847600
C	4.30195500	-2.69166700	0.72553100
C	4.78377800	-1.24731100	0.61751800
H	5.72742100	-1.23142200	0.05654200
H	5.01485900	-0.86888600	1.62532500
N	3.92025400	-0.28513300	-0.11888600
S	2.52240700	0.30460900	0.65120000
N	1.23130500	-0.45404800	-0.23659700
O	2.38173900	1.73445400	0.32880000
O	2.58267500	-0.13601500	2.06907200
C	4.59832000	0.67244800	-1.01904100
C	5.61970400	1.62069600	-0.39327300
H	3.81748400	1.26344500	-1.52186700
H	5.10065200	0.07404900	-1.79711600

C	6.60986700	2.17372100	-1.22758600
C	7.54563600	3.08840300	-0.72837800
C	5.59447200	2.00200600	0.95756300
C	6.53821700	2.90624100	1.46562600
C	7.51519700	3.45446400	0.62418300
H	8.24914600	4.16187600	1.02187600
H	6.51204000	3.17416900	2.52568400
H	6.64293900	1.88810900	-2.28506300
H	8.30286800	3.51093300	-1.39653700
H	4.83082500	1.60123300	1.62845600
C	3.79397700	-3.14140600	1.89160400
H	3.44687400	-4.17280000	2.00198400
H	3.66454500	-2.48321400	2.75201100
C	-0.72393900	-0.82719600	2.88251900
N	-1.02437600	-1.06567600	1.54577500
H	-0.86780300	-2.04983100	4.76125900
C	-1.55398800	-2.34949400	1.52071900
C	-1.54944100	-2.92437400	2.84511500
H	-1.90454400	-3.92414900	3.08493800
C	-1.02086900	-1.98765400	3.68575700
C	-2.02129400	-3.02450400	0.38603100
N	-1.20740900	-1.31850700	-1.22455500
C	-1.07439900	-1.33716700	-2.60843600
C	-1.64303600	-2.54569800	-3.15405500
H	-1.67603100	-2.79404000	-4.21266100
C	-2.15106300	-3.25529100	-2.10463100
H	-2.67351800	-4.20882400	-2.12752500
C	-1.83636500	-2.51996200	-0.90498500
C	-0.36289900	0.41271600	3.42584300
H	-0.13568900	4.84927300	2.15998600
C	-0.18247800	3.76304200	2.13835700
C	-0.29232200	2.97141600	0.93614700
H	-0.04851600	3.11264800	4.25000800
N	-0.38543900	1.61981000	1.25128700

C	-0.27022300	1.56605200	2.63628200
C	-0.13788200	2.89293600	3.18781800
C	-0.58289700	-0.28565700	-3.39845000
H	0.22482500	4.25327700	-3.06427500
C	0.03477100	3.20931200	-2.82495200
C	0.00163800	2.13609400	-3.67019600
H	0.13829600	2.11832300	-4.75034200
C	-0.30158700	0.97832100	-2.86245700
N	-0.42826000	1.33823100	-1.52578300
C	-0.22341600	2.70885200	-1.49572700
C	-0.23020900	3.51378100	-0.35058300
Co	-0.57036000	0.09896000	0.00539500
C	-0.10174900	4.99644200	-0.51647900
C	1.09109400	5.65029800	-0.15934300
C	-1.17581900	5.73732000	-1.04050300
C	1.22610000	7.04109300	-0.31630000
H	1.91420900	5.04688200	0.22944800
C	-1.08237700	7.13054300	-1.20438400
H	-2.09318600	5.20637000	-1.30496000
C	0.12650100	7.75044700	-0.83597600
H	0.21616000	8.83417600	-0.96038300
C	-2.65661900	-4.36956900	0.56287400
C	-3.93386500	-4.48027500	1.13687000
C	-1.97202300	-5.53298900	0.17228200
C	-4.54489300	-5.73448000	1.31852700
H	-4.45187900	-3.56367600	1.43487300
C	-2.54284500	-6.80656800	0.34640800
H	-0.97267200	-5.42581100	-0.25958000
C	-3.82828900	-6.87817400	0.91713900
H	-4.28599700	-7.85817100	1.05527900
C	-0.34778800	0.55172700	4.92361200
C	0.81769900	0.35598200	5.71342400
C	-1.58200200	0.86644100	5.56559800
C	0.72538700	0.46116300	7.11921900

C	-1.66146600	0.95792000	6.96578000
C	-0.50211500	0.75166900	7.71522200
H	1.61708300	0.30075400	7.71961700
H	-2.61905700	1.18328600	7.43210300
H	-0.55451500	0.82331300	8.80602100
C	-0.63444100	-0.46695600	-4.89107900
C	-1.90052400	-0.33602200	-5.52496500
C	0.49440200	-0.83148000	-5.67142300
C	-2.06203300	-0.65146100	-6.88364900
C	0.32608800	-1.14428900	-7.03634900
C	-0.94518300	-1.06650400	-7.61173800
H	-3.04925700	-0.58047200	-7.33901300
H	1.19176600	-1.44350700	-7.62244800
H	-1.06119500	-1.32198900	-8.66933600
C	-1.75294900	-8.06016900	-0.08493300
C	-2.52320300	-9.36742800	0.19086800
H	-3.47276700	-9.41568100	-0.36737100
H	-1.91433000	-10.22990900	-0.12575000
H	-2.74589400	-9.49950400	1.26262500
C	-0.41354900	-8.11614000	0.69247200
H	0.21544100	-7.23400900	0.49561600
H	-0.58840400	-8.16831800	1.77969500
H	0.16398200	-9.00880600	0.39757700
C	-1.45998000	-7.98266400	-1.60455700
H	-0.89065500	-8.86902000	-1.93253100
H	-2.39540300	-7.94621800	-2.18698300
H	-0.86673100	-7.09206100	-1.86494200
C	-5.95407800	-5.81360100	1.94295500
C	-6.95001200	-5.01311800	1.06644400
H	-7.96274400	-5.05251000	1.50270200
H	-6.66469900	-3.95275400	0.98218300
H	-7.00279600	-5.42793600	0.04647700
C	-6.47114300	-7.26246200	2.05303500
H	-6.54809300	-7.75136800	1.06784500

H	-5.82870000	-7.88459000	2.69774200
H	-7.47922300	-7.26319900	2.49881100
C	-5.91986300	-5.20416200	3.36717900
H	-5.60018000	-4.15025300	3.35870100
H	-6.92188500	-5.24401200	3.82725900
H	-5.22551300	-5.75939500	4.01895700
C	2.52114500	7.79497100	0.05259600
C	-2.24467500	7.98015900	-1.76022300
C	-1.78159900	8.70870500	-3.04692400
H	-2.60056300	9.32510600	-3.45514400
H	-0.92540000	9.37601500	-2.85961400
H	-1.48000000	7.98768300	-3.82432900
C	-2.66654700	9.02899700	-0.70062800
H	-1.83926700	9.70764500	-0.43888700
H	-3.49710800	9.64750600	-1.08139300
H	-3.00466200	8.54025600	0.22765800
C	-3.48046000	7.12644500	-2.11033400
H	-3.25946400	6.37465400	-2.88572100
H	-3.88659800	6.60168100	-1.23022300
H	-4.28099000	7.77461500	-2.50250200
C	3.60415900	6.85557100	0.62058000
H	3.27206300	6.34782700	1.54079800
H	3.90791300	6.08326300	-0.10422500
H	4.50468000	7.43817400	0.87469500
C	3.09259800	8.48270600	-1.21283400
H	2.38296200	9.20502900	-1.64682800
H	4.01820100	9.03091500	-0.96761800
H	3.33354400	7.74087100	-1.99174100
C	2.20573300	8.87021100	1.12262400
H	3.12340200	9.41648500	1.39949500
H	1.47412600	9.61125000	0.76341800
H	1.79571900	8.41142300	2.03720700
N	2.04639300	0.06379200	5.06843500
H	2.04436600	0.08560800	4.04263100

N	1.76766900	-0.85264500	-5.04381900
H	1.76544800	-0.58330300	-4.05900500
N	-2.97471100	0.14280300	-4.74104600
H	-2.70023600	0.62997700	-3.88855200
N	-2.70444500	1.09934900	4.73739200
H	-2.50513300	1.09087600	3.73795200
C	3.24435400	-0.28514900	5.67988400
C	3.00583600	-1.01143900	-5.65167000
C	-4.32159100	-0.18803200	-4.83002600
C	-4.00657700	1.42071400	5.08374700
O	-4.80498100	-0.90791800	-5.69975300
O	-4.44404700	1.46020600	6.23397200
O	3.16220000	-1.33151700	-6.83032900
O	3.40112800	-0.39643000	6.89796500
C	-4.85941600	1.77029500	3.89053500
H	-4.42787300	1.68919800	2.88835400
C	-5.11605100	0.40966400	-3.69659600
H	-4.74061500	1.33280000	-3.24418800
C	-5.81383100	-0.53812100	-2.73766100
H	-5.83242500	-0.24799500	-1.68465200
H	-5.74500700	-1.60846600	-2.94341300
C	-6.62525000	0.29124700	-3.72181000
H	-7.06367300	-0.25098600	-4.56180500
C	-5.87537800	2.87009000	4.08333600
H	-5.92755500	3.31500100	5.07897800
H	-6.06212000	3.52640600	3.23116300
C	-6.35391000	1.43515900	3.96866900
H	-6.69814100	0.95273600	4.88490500
C	-7.40444600	1.43521300	-3.15721200
C	-7.02713700	1.05933200	2.69201700
O	-6.67382100	1.42893000	1.58216200
O	-6.92953900	2.37577200	-2.54203500
O	-8.11217400	0.26892000	2.93113800
O	-8.73592800	1.26599100	-3.39236100

C	-8.93817800	-0.05161600	1.76905300
H	-8.28903200	-0.11386000	0.88389900
H	-9.35365700	-1.04578300	1.99341100
C	-10.04165900	0.99253400	1.60285400
H	-10.59518500	1.06063400	2.55577000
H	-9.57485400	1.97929600	1.44230200
C	-9.61302600	2.29594600	-2.84052200
H	-10.53531300	2.19093800	-3.43187500
H	-9.16108200	3.28043100	-3.03606600
C	-9.88031100	2.11198700	-1.34626900
H	-8.94540500	2.30248600	-0.79495500
H	-10.58593400	2.91355900	-1.05097200
C	-11.03245600	0.67630600	0.46429900
H	-11.47186100	-0.32516300	0.63227900
H	-11.87627100	1.38655100	0.54306100
C	-10.47053500	0.74161800	-0.97137000
H	-9.70868500	-0.04185300	-1.12739500
H	-11.29214500	0.49437000	-1.66980600
C	4.39477700	-0.56634200	4.74021500
H	4.25508700	-0.35705100	3.67789700
C	4.19769400	-0.67802300	-4.77992300
H	4.05256000	-0.56763600	-3.70259500
C	5.21213600	0.24209800	-5.43303600
H	5.73014200	0.95178500	-4.78592500
H	4.98989600	0.58040800	-6.44713000
C	5.29250300	-1.73174100	5.12888700
H	5.74244700	-2.30613300	4.31763600
H	4.99847300	-2.29100400	6.01984800
C	5.79359300	-0.33353800	5.34953800
H	5.73610200	0.05158700	6.37056600
C	5.54598500	-1.22790800	-5.26818200
H	5.47195500	-1.82912200	-6.17638300
C	6.91963900	0.28178200	4.57788000
C	6.69006500	-1.63914400	-4.39470300

O	7.41688900	-0.52342000	3.58591200
O	6.75177300	-0.93626800	-3.21965200
O	7.52379800	-2.45792700	-4.73326300
O	7.38548500	1.37757000	4.84202500
C	8.61495200	0.01061500	2.93235600
H	8.33535400	0.93185100	2.39565000
H	9.33164100	0.28848900	3.72106800
C	9.20078800	-1.02955000	1.98344600
H	10.16250900	-0.61308700	1.62684600
H	9.45271100	-1.94764400	2.54427800
C	7.99014600	-1.08182800	-2.44259900
C	8.30126100	-1.35633300	0.78191700
H	7.42751000	-1.92250000	1.14552300
H	7.90686500	-0.40363300	0.38032000
C	8.97406100	-2.15841900	-0.34739500
H	9.27208800	-3.15117000	0.03385300
H	9.91639000	-1.66181900	-0.65210600
C	8.06163300	-2.34996900	-1.58372700
H	5.00765000	-6.07792100	-3.44169100
H	7.04489500	-2.62679900	-1.25621800
H	8.41579900	-3.18513400	-2.20671500
H	7.99331200	-0.17439200	-1.82176500
H	8.83562300	-1.03614400	-3.14647400
N	1.59942200	-2.00506900	-0.21692300
N	1.03443400	-2.89704100	-0.65540100

Intermediate C

C_{N2}:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

G_corr: -0.014217 Hartree

H_corr: 0.008807 Hartree

SCF: -109.558631 Hartree

S: 46.136 Cal/Mol-Kelvin

H: -109.549824 Hartree

G: -109.572212 Hartree

Cartesian Coordinates:

N	-0.00000000	-0.00000000	0.55383200
N	0.00000000	0.00000000	-0.55383200

$C_{[Co(P5)]}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.138906 Hartree

G_corr: 1.790763 Hartree

SCF: -7569.077659 Hartree

S: 697.629 Cal/Mol-Kelvin

H: -7566.938753 Hartree

G: -7567.286896 Hartree

Cartesian Coordinates:

C	4.58505200	-4.58350300	-2.91182200
C	4.48454400	-4.05137200	-1.62099400
C	3.26855200	-3.51601100	-1.14728700
C	2.15459800	-3.52434600	-2.01131500
C	2.25376900	-4.05691500	-3.30286000
C	3.46840300	-4.58600000	-3.75919400
H	5.53658900	-4.99861600	-3.25637600
H	5.35147200	-4.09961700	-0.95507000
H	1.21374800	-3.09131400	-1.66338300
H	1.37665600	-4.05236400	-3.95661500
C	3.13861000	-3.01715100	0.25043500
C	4.11272800	-1.96705100	0.76998200
H	5.14148600	-2.19414700	0.44734100
H	4.10811800	-1.97684100	1.86832400
N	3.87677800	-0.56294100	0.35220700
S	2.48705400	0.21288200	0.95740000
N	1.32484200	-0.45868900	-0.03111300
O	2.69183000	1.65646500	0.71444100
O	2.37503400	-0.26829800	2.36519200
C	4.35879400	-0.07828800	-0.95311300
C	5.21110500	1.18492300	-0.89346400
H	3.50827900	0.08513900	-1.63913100
H	4.94797600	-0.89722200	-1.39746400
C	5.38319200	1.94221900	-2.06471200

C	6.20291000	3.07758300	-2.07380600
C	5.86190400	1.60037400	0.27798300
C	6.67670500	2.74067600	0.27491200
C	6.85740400	3.48008000	-0.90164300
H	7.49315400	4.37081200	-0.90201500
H	7.16208200	3.06119500	1.20236900
H	4.85722000	1.65033400	-2.97997200
H	6.32107800	3.65562700	-2.99597200
H	5.70451000	1.03962500	1.20298300
C	2.17878300	-3.48815700	1.06900000
H	1.47571200	-4.25484200	0.73184500
H	2.06371000	-3.11720200	2.09061700
C	-0.78739500	-0.88201400	2.97314200
N	-0.95279300	-1.13595200	1.61604700
H	-1.12361000	-2.07144900	4.84533200
C	-1.42455300	-2.44519800	1.55541100
C	-1.56974300	-2.99210800	2.88217000
H	-1.95289900	-3.98613500	3.10053900
C	-1.15385400	-2.03300300	3.75844800
C	-1.74916000	-3.15397900	0.39562100
N	-1.00707800	-1.37528400	-1.17357000
C	-0.88166000	-1.35424100	-2.55566300
C	-1.33826500	-2.59712800	-3.13030100
H	-1.35816000	-2.81704900	-4.19543100
C	-1.74303600	-3.38548300	-2.09302800
H	-2.14340200	-4.39612300	-2.12749100
C	-1.52228600	-2.63229000	-0.88161300
C	-0.45190300	0.34999800	3.54397900
H	0.14158300	4.75702800	2.31514200
C	0.02412100	3.67650100	2.28627500
C	-0.05518300	2.89609200	1.07595900
H	-0.05151100	3.01733500	4.39865800
N	-0.25981400	1.55072500	1.37389400
C	-0.24821000	1.49246400	2.76571600

C	-0.07363000	2.80649200	3.33121600
C	-0.44679100	-0.26864400	-3.32775200
H	0.58922200	4.21270900	-2.88726000
C	0.32344100	3.17988900	-2.67422900
C	0.20005300	2.13569800	-3.54572800
H	0.32857100	2.13244600	-4.62698300
C	-0.15899100	0.97868300	-2.76321000
N	-0.26607200	1.31330800	-1.41565000
C	0.04158100	2.66554100	-1.35635100
C	0.09441100	3.44720600	-0.19773600
Co	-0.40447000	0.03642300	0.10728100
C	0.38443200	4.90956200	-0.32835100
C	1.62829300	5.41347700	0.09283800
C	-0.57533400	5.77722600	-0.87880800
C	1.92916700	6.78114200	-0.03052900
H	2.35801300	4.71004700	0.49932300
C	-0.31311100	7.15211800	-1.01224300
H	-1.53727200	5.36182700	-1.18856300
C	0.94357900	7.62066300	-0.58423200
H	1.16478500	8.68794400	-0.68486100
C	-2.36383800	-4.51689100	0.51920900
C	-3.72848900	-4.68556600	0.22454300
C	-1.59913500	-5.62335200	0.92708400
C	-4.34520600	-5.94383000	0.33868300
H	-4.30332800	-3.81024800	-0.08591300
C	-2.17653600	-6.89995700	1.04843700
H	-0.53956200	-5.47258700	1.14401400
C	-3.54624600	-7.02661700	0.75082200
H	-4.01255700	-8.01200800	0.84565900
C	-0.48541900	0.47268600	5.04196700
C	0.64533700	0.18631000	5.85527400
C	-1.71451500	0.84790400	5.65683900
C	0.52106200	0.25907900	7.26017800
C	-1.82538400	0.91178400	7.05668600

C	-0.70218700	0.61230300	7.83076600
H	1.38298600	0.02137100	7.87907100
H	-2.77870500	1.18615900	7.50491400
H	-0.78140600	0.66007800	8.92126000
C	-0.53161400	-0.41755500	-4.82325200
C	-1.80228800	-0.21405700	-5.42775600
C	0.55836500	-0.84404600	-5.62847700
C	-2.00795000	-0.50379500	-6.78646800
C	0.34410800	-1.13233500	-6.99276500
C	-0.93098100	-0.97271500	-7.54166600
H	-2.99926000	-0.37606100	-7.21960400
H	1.17869700	-1.48266500	-7.59590200
H	-1.08299500	-1.20965900	-8.59904900
C	-1.36967600	-8.13643800	1.49748900
C	-1.97397300	-8.68956100	2.81286900
H	-3.02582400	-8.99220000	2.68874500
H	-1.40970300	-9.57511900	3.15091500
H	-1.93510600	-7.93511800	3.61554800
C	0.11605900	-7.80880600	1.75080100
H	0.61902000	-7.43476500	0.84401900
H	0.24782300	-7.06272500	2.55166100
H	0.64782900	-8.72117900	2.06624200
C	-1.44163100	-9.22887200	0.40126200
H	-0.87338900	-10.12181900	0.71253700
H	-2.47698100	-9.54796900	0.20220000
H	-1.01394500	-8.86793400	-0.54820500
C	-5.84201900	-6.16657600	0.03831400
C	-6.55127300	-6.67908900	1.31688000
H	-7.62440200	-6.84369900	1.12055900
H	-6.12811000	-7.63293900	1.67021600
H	-6.46351300	-5.94981600	2.13868500
C	-6.54807800	-4.87297400	-0.41639400
H	-6.51522400	-4.08893100	0.35792800
H	-6.10858700	-4.46371800	-1.34102000

H	-7.60988400	-5.08319200	-0.62434600
C	-5.99218200	-7.21912100	-1.08890100
H	-5.55071200	-8.18925800	-0.81106800
H	-7.05864500	-7.39185100	-1.31228900
H	-5.50131300	-6.88144600	-2.01626800
C	3.28656700	7.37137900	0.40584800
C	-1.34198400	8.13807600	-1.60374700
C	-0.75602500	8.78199900	-2.88555600
H	-1.47719600	9.49290200	-3.32362600
H	0.17463200	9.33498500	-2.68177000
H	-0.52947200	8.01653700	-3.64587600
C	-1.65209300	9.24781000	-0.56809200
H	-0.75269500	9.82129100	-0.29319600
H	-2.38762500	9.96076200	-0.97804900
H	-2.07206000	8.82074200	0.35714500
C	-2.66979800	7.44710400	-1.97621500
H	-2.53345800	6.66949800	-2.74568000
H	-3.15465700	6.98260200	-1.10196000
H	-3.37366000	8.19050100	-2.38442000
C	4.20467300	6.31218900	1.04897800
H	3.75389500	5.86624500	1.95063500
H	4.45335200	5.49491200	0.35341100
H	5.15358800	6.78252900	1.35513600
C	4.01018200	7.95414500	-0.83418100
H	3.42121800	8.74939200	-1.31886200
H	4.98220700	8.38812800	-0.54356200
H	4.19952100	7.17079600	-1.58605500
C	3.05423900	8.50003100	1.44152800
H	4.01907200	8.92629100	1.76463900
H	2.44918200	9.32452800	1.03238200
H	2.53699300	8.11683700	2.33633800
N	1.87009600	-0.14813100	5.23132200
H	1.91673000	-0.04266500	4.21046200
N	1.83860400	-0.94471800	-5.03118800

H	1.87950900	-0.68728100	-4.04445200
N	-2.83641900	0.30540600	-4.61524400
H	-2.52466600	0.77320200	-3.76488500
N	-2.79823200	1.15953500	4.80290000
H	-2.57374500	1.15004900	3.80875000
C	3.00791200	-0.65519900	5.84559700
C	3.04865900	-1.24066900	-5.65054700
C	-4.20277700	0.06928900	-4.70225100
C	-4.08844400	1.54927700	5.12295200
O	-4.73760500	-0.60701600	-5.57712800
O	-4.54827600	1.60191800	6.26375500
O	3.15192500	-1.64273000	-6.80954500
O	3.09136400	-0.92793200	7.04527700
C	-4.89427800	1.95619100	3.91589900
H	-4.44673600	1.86107200	2.92201000
C	-4.95603100	0.71070900	-3.56456200
H	-4.51072500	1.58916400	-3.08723300
C	-5.75433500	-0.18881900	-2.63875900
H	-5.77152900	0.08355500	-1.58093300
H	-5.77551300	-1.25683500	-2.86638000
C	-6.47040500	0.72484300	-3.62090600
H	-6.93308500	0.23803800	-4.48152400
C	-5.85352500	3.10758300	4.09874800
H	-5.90317100	3.54580200	5.09748600
H	-5.98630900	3.78073500	3.24958500
C	-6.40550200	1.70120500	3.95973200
H	-6.79502700	1.23088700	4.86404600
C	-7.16161800	1.92196100	-3.05247400
C	-7.07151100	1.37529100	2.66596700
O	-6.66824500	1.72657900	1.56700900
O	-6.62740500	2.79540300	-2.38932900
O	-8.21264000	0.65935300	2.87524500
O	-8.49062700	1.88686400	-3.35068600
C	-9.03798200	0.41430800	1.69450100

H	-8.38028500	0.33577600	0.81723500
H	-9.51501700	-0.55858600	1.88727100
C	-10.07194500	1.52897400	1.54052900
H	-10.66203700	1.58391700	2.47200700
H	-9.54105100	2.49220000	1.45223800
C	-9.29497100	2.97491400	-2.79939700
H	-10.18695900	2.98692400	-3.44400900
H	-8.73936600	3.91708400	-2.92218200
C	-9.66399900	2.75180200	-1.33239600
H	-8.74983300	2.83296000	-0.72238700
H	-10.31360600	3.59920100	-1.03669000
C	-11.02649100	1.33607200	0.34483100
H	-11.54446400	0.36350400	0.44402600
H	-11.81961700	2.10283100	0.41978700
C	-10.39023600	1.42333600	-1.05841500
H	-9.69180400	0.58417600	-1.22195600
H	-11.19418800	1.28515700	-1.80576200
C	4.18575300	-0.87505900	4.92308800
H	4.10586700	-0.52707200	3.89159600
C	4.27048400	-0.92700200	-4.82183200
H	4.14543300	-0.72357000	-3.75662800
C	5.33483100	-0.13462200	-5.55963800
H	5.90085000	0.60102200	-4.98622300
H	5.12707000	0.10823000	-6.60368000
C	5.02440400	-2.11053200	5.18758200
H	5.49290500	-2.58847200	4.32559000
H	4.68214700	-2.77197800	5.98673700
C	5.56044600	-0.77023500	5.61770300
H	5.47444600	-0.53475700	6.68055900
C	5.58039400	-1.59904000	-5.24471400
H	5.49370500	-2.29300000	-6.08246100
C	6.73753300	-0.10214200	4.98785700
C	6.67494000	-1.94723200	-4.28694200
O	7.10433700	-0.64526500	3.77853200

O	6.69420500	-1.11619600	-3.19933000
O	7.49953900	-2.82103600	-4.48724000
O	7.34245900	0.81395500	5.51633300
C	8.32786200	-0.07830000	3.21190300
H	8.07536900	0.88957400	2.74545000
H	9.02283900	0.12570100	4.03966700
C	8.92869000	-1.04788700	2.20001700
H	9.92814200	-0.65147100	1.93684000
H	9.10614700	-2.02031800	2.69484800
C	7.88319500	-1.16616900	-2.34600100
C	8.10014100	-1.23838400	0.92163400
H	7.12084800	-1.66910200	1.19625400
H	7.88092400	-0.24609100	0.48835600
C	8.76931200	-2.13784600	-0.13237400
H	8.99469000	-3.12096200	0.31943900
H	9.75103000	-1.71386200	-0.42027500
C	7.90296500	-2.36419700	-1.39135100
H	3.54571700	-4.99533600	-4.77076900
H	6.86468000	-2.57086200	-1.08061600
H	8.24263200	-3.25281100	-1.94507500
H	7.83195200	-0.21074300	-1.80497000
H	8.77182000	-1.16589100	-2.99703500

Transition State TS2$^{Endo\text{-}Si}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -281.6681 cm-1

H_corr: 2.137978 Hartree

G_corr: 1.794694 Hartree

SCF: -7569.070610 Hartree

S: 687.894 Cal/Mol-Kelvin

H: -7566.932632 Hartree

G: -7567.275916 Hartree

Cartesian Coordinates:

C	-4.83015800	4.83373600	-2.48634200
C	-4.58619600	4.07474000	-1.33839700
C	-3.33991500	3.43267100	-1.13177600
C	-2.34787000	3.58580600	-2.13358400
C	-2.59709400	4.33689400	-3.28386200
C	-3.83837900	4.96530400	-3.46828700
H	-5.79979800	5.32224700	-2.61754900
H	-5.35731400	4.02173100	-0.56479100
H	-1.38516200	3.08108400	-2.02001300
H	-1.82041800	4.42330800	-4.04936700
C	-3.07319800	2.68349500	0.10148500
C	-4.13850500	1.81238500	0.74593100
H	-5.15902400	2.08482100	0.44449500
H	-4.08639700	1.87681200	1.84279500
N	-3.97621200	0.37291500	0.39192700
S	-2.50908400	-0.35128000	0.91823200
N	-1.36292200	0.48064200	-0.01006300
O	-2.60380400	-1.76567200	0.50824400
O	-2.45367000	-0.02715200	2.37387200
C	-4.45394400	-0.09336100	-0.92436500
C	-5.30278800	-1.35800200	-0.86876600
H	-3.60677700	-0.24805700	-1.61670200
H	-5.05350200	0.72437100	-1.35806400
C	-5.53383000	-2.07626900	-2.05476100
C	-6.35336000	-3.21171600	-2.05901200
C	-5.89494000	-1.81113600	0.31962800
C	-6.71038600	-2.95133500	0.32002300
C	-6.94946500	-3.65227900	-0.86925800
H	-7.58476600	-4.54336500	-0.86727200
H	-7.15094200	-3.30112200	1.25925400
H	-5.05393700	-1.75361500	-2.98525600
H	-6.51784100	-3.76014900	-2.99212300
H	-5.69007900	-1.27654300	1.25075400
C	-1.80331000	2.54467600	0.62220500

H	-0.95365600	3.05696700	0.17010500
H	-1.66410200	2.21391300	1.65221400
C	0.79643600	0.82011800	2.99593900
N	0.95941200	1.10604400	1.64438600
H	1.13551700	1.96735000	4.89559300
C	1.44931200	2.41003000	1.61587100
C	1.59177100	2.92835800	2.95445400
H	1.97730600	3.91666100	3.19489100
C	1.16718800	1.95226500	3.80817400
C	1.76883400	3.14519600	0.47125000
N	0.98715400	1.41953300	-1.13679000
C	0.83125800	1.44288000	-2.51597600
C	1.28785700	2.69973800	-3.06151800
H	1.28548800	2.95418100	-4.11927400
C	1.72966600	3.44943900	-2.01008500
H	2.14776900	4.45362400	-2.02267500
C	1.52614900	2.66132800	-0.81813800
C	0.47489100	-0.43122000	3.53417100
H	0.00856800	-4.81997900	2.18730600
C	0.09299300	-3.73595200	2.18761300
C	0.14284000	-2.91997900	0.99873100
H	0.14514700	-3.13332000	4.31703500
N	0.30451400	-1.57745900	1.33332900
C	0.29583600	-1.55759500	2.72608100
C	0.16191800	-2.89193400	3.25594800
C	0.37762500	0.38053100	-3.31140400
H	-0.53050900	-4.13844300	-2.99330800
C	-0.29940300	-3.10345900	-2.75203300
C	-0.23049900	-2.02900800	-3.59175700
H	-0.37543200	-1.99834500	-4.67060700
C	0.10747500	-0.88512400	-2.77868000
N	0.24181600	-1.25579600	-1.44382000
C	-0.01119800	-2.61915300	-1.42323900
C	-0.00569500	-3.43773100	-0.28914200

Co	0.41258000	-0.02996000	0.11062500
C	-0.23066200	-4.90779200	-0.46036900
C	-1.44970300	-5.48043300	-0.05559600
C	0.77023200	-5.71481300	-1.02910000
C	-1.68302200	-6.85837300	-0.20977700
H	-2.21332900	-4.82281900	0.36541100
C	0.57559900	-7.09740800	-1.19469400
H	1.71064000	-5.24539200	-1.32712600
C	-0.65666500	-7.63635800	-0.77903200
H	-0.82437900	-8.71078400	-0.90342000
C	2.35152200	4.51945400	0.62795800
C	3.73176900	4.71870900	0.45613000
C	1.52244000	5.61005200	0.94167400
C	4.30152900	5.99683500	0.59737100
H	4.35533600	3.85415200	0.21753900
C	2.05203500	6.90481500	1.08514600
H	0.45202700	5.43150000	1.06696600
C	3.43931500	7.06486300	0.90879500
H	3.86732400	8.06605000	1.01932600
C	0.51621100	-0.58956500	5.02843500
C	-0.61153600	-0.32157600	5.85055200
C	1.74975600	-0.96781500	5.63275100
C	-0.48238000	-0.41316100	7.25357500
C	1.86616400	-1.05066900	7.03117900
C	0.74488800	-0.76777300	7.81452400
H	-1.34222200	-0.18613900	7.87932800
H	2.82320500	-1.32516600	7.47139300
H	0.82925400	-0.83061800	8.90385500
C	0.44428200	0.57175500	-4.80314200
C	1.71231700	0.40989600	-5.42553600
C	-0.66126300	0.99613600	-5.58714900
C	1.89876500	0.74176800	-6.77732000
C	-0.46705100	1.32718000	-6.94469900
C	0.80570100	1.20971300	-7.50939600

H	2.88788300	0.64559000	-7.22354000
H	-1.31430900	1.67642300	-7.53052500
H	0.94252800	1.47806400	-8.56134100
C	1.17301600	8.12798800	1.42049500
C	1.65571500	8.76005300	2.75025300
H	2.70353500	9.09491900	2.69307600
H	1.03906700	9.63910100	3.00341300
H	1.57925600	8.04113200	3.58232900
C	-0.31537800	7.75557600	1.57806800
H	-0.73660700	7.32782100	0.65361500
H	-0.47822800	7.03506700	2.39646200
H	-0.90030900	8.65869200	1.81674900
C	1.29099600	9.17295100	0.28248500
H	0.66992200	10.05673900	0.50684000
H	2.32723500	9.52099400	0.14658500
H	0.95001000	8.75338100	-0.67805500
C	5.81334500	6.25548700	0.42726500
C	6.38600000	6.84191800	1.74223900
H	7.46747500	7.03392500	1.63831500
H	5.90455000	7.79458800	2.01406200
H	6.24389700	6.14359100	2.58310800
C	6.59484500	4.96786500	0.09604500
H	6.50421500	4.21216900	0.89358200
H	6.26024100	4.51275100	-0.85066100
H	7.66620800	5.20199400	-0.01424000
C	6.03671000	7.26586000	-0.72595500
H	5.54142300	8.23038300	-0.53188700
H	7.11357100	7.46583900	-0.85858300
H	5.64441600	6.87418800	-1.67870600
C	-3.00798900	-7.52576700	0.21482600
C	1.65404000	-8.02049600	-1.80030900
C	1.09077100	-8.70767600	-3.06965200
H	1.84890600	-9.37482000	-3.51402400
H	0.20005700	-9.31715100	-2.84953200

H	0.80639100	-7.96280900	-3.83091200
C	2.04612200	-9.10227000	-0.76260900
H	1.18559100	-9.72406700	-0.46892700
H	2.81589000	-9.77396600	-1.17936400
H	2.45485400	-8.64352700	0.15249100
C	2.93018700	-7.25072900	-2.19733900
H	2.73012500	-6.48027300	-2.96006000
H	3.40661400	-6.76105500	-1.33235000
H	3.66785600	-7.94944500	-2.62452800
C	-3.99119000	-6.52236000	0.85094400
H	-3.57555500	-6.05461200	1.75836500
H	-4.27901700	-5.71825800	0.15510900
H	-4.91475600	-7.04676400	1.14653900
C	-3.68801600	-8.14999800	-1.02965100
H	-3.05236400	-8.91153700	-1.50922900
H	-4.63608900	-8.63772900	-0.74535600
H	-3.91523700	-7.37900900	-1.78382300
C	-2.71669000	-8.63891600	1.25252600
H	-3.65610600	-9.12456800	1.56684700
H	-2.05753800	-9.42329500	0.84781800
H	-2.23214300	-8.22550400	2.15218000
N	-1.84196500	0.01286100	5.23687400
H	-1.91154800	-0.13148600	4.22236900
N	-1.93752200	1.05247700	-4.97419100
H	-1.96797400	0.72671100	-4.00742200
N	2.76480000	-0.11225800	-4.63934500
H	2.47167100	-0.61298700	-3.80117200
N	2.83245700	-1.25991300	4.77078400
H	2.60381600	-1.24027000	3.77769600
C	-2.95948800	0.55309700	5.85914200
C	-3.15554100	1.36387100	-5.56841700
C	4.12423500	0.15950600	-4.72994700
C	4.12788100	-1.64057600	5.08002600
O	4.63416700	0.87949100	-5.58464600

O	4.59334700	-1.70456300	6.21805100
O	-3.27293700	1.82241300	-6.70497800
O	-3.01060900	0.86660400	7.05074800
C	4.93367600	-2.01939100	3.86373800
H	4.47868700	-1.91999500	2.87364300
C	4.90342200	-0.50539900	-3.62383400
H	4.48543600	-1.41415200	-3.17979300
C	5.68415000	0.37805900	-2.66811700
H	5.71716200	0.06460900	-1.62212300
H	5.67383200	1.45454600	-2.85264000
C	6.41694300	-0.47587300	-3.69095100
H	6.85987600	0.05708500	-4.53442600
C	5.91603300	-3.15367300	4.02695300
H	5.97956500	-3.60285000	5.02001600
H	6.05720800	-3.81357700	3.16880500
C	6.44036900	-1.73563400	3.90225900
H	6.82545500	-1.26789600	4.80978800
C	7.14347400	-1.67639500	-3.17619200
C	7.09033300	-1.37823500	2.60873800
O	6.69194400	-1.72937600	1.50800600
O	6.63653000	-2.59048000	-2.54718700
O	8.21034400	-0.62992300	2.81923500
O	8.46942800	-1.59364900	-3.47862700
C	9.01177800	-0.33542400	1.63349900
H	8.33752600	-0.23810000	0.77055300
H	9.47700000	0.63808700	1.85068500
C	10.06116300	-1.42651800	1.42404600
H	10.65572500	-1.51440600	2.35021300
H	9.54451400	-2.39251900	1.29287400
C	9.30415400	-2.68415300	-2.97955600
H	10.19524400	-2.64076500	-3.62409400
H	8.77442400	-3.63426700	-3.14753800
C	9.66964100	-2.52210000	-1.50378400
H	8.75757400	-2.65030400	-0.89859100

H	10.33586200	-3.36960200	-1.24796700
C	11.00879800	-1.16258800	0.23672400
H	11.51105000	-0.18725300	0.38034100
H	11.81478700	-1.91870400	0.27327700
C	10.37022600	-1.19434700	-1.16771600
H	9.65546800	-0.36189500	-1.28883300
H	11.16896300	-1.00449900	-1.90931600
C	-4.15667400	0.75211300	4.95821100
H	-4.09973300	0.38228000	3.93256600
C	-4.36755600	1.00185700	-4.74501700
H	-4.23183700	0.74507400	-3.69243500
C	-5.43783700	0.24453100	-5.51017800
H	-5.99817000	-0.51733100	-4.96606300
H	-5.23957600	0.04951900	-6.56600700
C	-4.99600500	1.98686200	5.22158700
H	-5.48822900	2.44780900	4.36375400
H	-4.63880500	2.66166800	6.00276500
C	-5.51571400	0.65126400	5.68534000
H	-5.40876500	0.43320800	6.74991300
C	-5.68148100	1.69226500	-5.12589900
H	-5.59875100	2.42396800	-5.93122400
C	-6.69619700	-0.03519900	5.08328500
C	-6.76776800	1.99838500	-4.14547600
O	-7.07600100	0.48529400	3.86835600
O	-6.77783000	1.12013200	-3.09492100
O	-7.59313900	2.88032800	-4.29991500
O	-7.28871000	-0.94679600	5.63303700
C	-8.28827100	-0.10790700	3.30635000
H	-8.01018700	-1.05644000	2.81541600
H	-8.96602700	-0.35068900	4.13782100
C	-8.92867400	0.86429200	2.32202200
H	-9.91307700	0.43819400	2.04889400
H	-9.14073200	1.81590100	2.84312100
C	-7.95450800	1.14133500	-2.22407300

C	-8.10923800	1.12130100	1.04933100
H	-7.14297100	1.57230700	1.33743500
H	-7.86061200	0.15071100	0.58319600
C	-8.81037100	2.03560400	0.02918200
H	-9.04907100	3.00094600	0.51144800
H	-9.78752500	1.60006900	-0.25698500
C	-7.96707100	2.31137800	-1.23503100
H	-4.03255900	5.54833700	-4.37304300
H	-6.92556900	2.51942500	-0.93540900
H	-8.32356400	3.21227200	-1.75711300
H	-7.89330700	0.17108900	-1.71086100
H	-8.85232200	1.15573700	-2.86220700

Transition State TS2$^{Endo\text{-}Re}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -287.1947 cm-1

H_corr: 2.138143 Hartree

G_corr: 1.795918 Hartree

SCF: -7569.068677 Hartree

S: 685.77 Cal/Mol-Kelvin

H: -7566.930534Hartree

G: -7567.272759 Hartree

Cartesian Coordinates:

C	-4.83794700	-5.35405300	-1.43898700
C	-4.57996100	-4.32705000	-0.52698700
C	-3.34297000	-3.63403300	-0.53198700
C	-2.39396500	-3.99302000	-1.52398700
C	-2.66295100	-5.00702400	-2.44498700
C	-3.88094200	-5.70304000	-2.40198700
H	-5.78993900	-5.89206600	-1.39198700
H	-5.32696400	-4.10106000	0.24001300
H	-1.44397200	-3.45400700	-1.58398700
H	-1.91694800	-5.25401400	-3.20598700

C	-3.02898300	-2.65602900	0.51501300
C	-4.08699600	-1.72804300	1.09001300
H	-4.01699600	-1.67604200	2.18701300
H	-5.10899200	-2.03805700	0.83801300
N	-3.94901500	-0.33704100	0.58001300
S	-2.49402600	0.46797800	0.98501300
N	-1.37001400	-0.41800600	0.07701300
O	-2.37002300	0.27298000	2.46001300
O	-2.64404400	1.83897600	0.46001300
C	-4.52601900	0.00895100	-0.73098700
C	-5.55803500	1.13093700	-0.67898700
H	-3.72902300	0.27696200	-1.44598700
H	-5.00300700	-0.90405600	-1.12798700
C	-6.07304100	1.61593000	0.53201300
C	-7.05505500	2.61691600	0.53601300
C	-6.03504200	1.67193000	-1.88498700
C	-7.01905500	2.66691700	-1.88398700
C	-7.53606200	3.14291000	-0.67098700
H	-8.30207200	3.92390000	-0.66698700
H	-7.38206100	3.06691200	-2.83598700
H	-5.68603600	1.21493500	1.47301300
H	-7.44106000	2.99291100	1.48901300
H	-5.63603700	1.31593600	-2.84198700
C	-1.73498700	-2.41101100	0.93001300
H	-0.89797900	-2.96600000	0.50601300
H	-1.55099300	-1.95200900	1.90201300
C	0.64099900	-1.31797900	-2.58698700
N	0.89799800	-1.30297600	-1.22298700
H	0.96301900	-2.81897500	-4.22998700
C	1.46601500	-2.54296800	-0.95398700
C	1.57102600	-3.32796700	-2.16198700
H	1.98604000	-4.33196100	-2.21198700
C	1.05001600	-2.57197400	-3.17298700
C	1.83302200	-3.02196300	0.30801300

N	1.06699400	-1.00597300	1.55201300
C	0.97699100	-0.73697500	2.91401300
C	1.43000600	-1.86496800	3.68901300
H	1.46700600	-1.89396800	4.77601300
C	1.83801900	-2.81696300	2.80001300
H	2.27403200	-3.79095700	3.00801300
C	1.59101200	-2.29496600	1.47801300
C	0.14998400	-0.24398600	-3.34298700
H	-0.73507700	4.27100200	-2.92598700
C	-0.49106300	3.23400500	-2.70898700
C	-0.13205600	2.73501000	-1.40398700
H	-0.68204800	2.14800300	-4.62898700
N	0.12196200	1.37201400	-1.45198700
C	-0.08803300	1.01601100	-2.78098700
C	-0.47204900	2.16800600	-3.56198700
C	0.65597400	0.50102100	3.48601300
H	0.03691400	4.89501300	2.22401300
C	0.14092900	3.81301400	2.20801300
C	0.28494100	2.95701600	3.26001300
H	0.32593800	3.18501700	4.32401300
C	0.40595900	1.63101800	2.70601300
N	0.33195800	1.66701700	1.31601300
C	0.13894000	3.01101400	1.00901300
C	-0.07406700	3.54101100	-0.26398700
Co	0.39697900	0.13201800	0.07201300
C	-0.31408700	5.01300800	-0.40798700
C	-1.55109500	5.55799100	-0.03898700
C	0.69690100	5.84902200	-0.91998700
C	-1.80211300	6.93998800	-0.16998700
H	-2.32208500	4.87998100	0.33901300
C	0.48788300	7.22901900	-1.05698700
H	1.65290800	5.39903500	-1.19698700
C	-0.77012400	7.74500200	-0.67598700
H	-0.94413900	8.81899900	-0.78098700

C	2.47104000	-4.37495400	0.40501300
C	3.79804200	-4.55093600	-0.00698700
C	1.74605500	-5.47796400	0.90001300
C	4.42806000	-5.81092800	0.07001300
H	4.34603100	-3.68292900	-0.38598700
C	2.33207200	-6.74895600	0.98601300
H	0.70905300	-5.32197800	1.20901300
C	3.67407400	-6.88493800	0.56601300
H	4.14108800	-7.86993200	0.63301300
C	0.13398600	-0.38398600	-4.84198700
C	-1.00100800	-0.83700100	-5.56198700
C	1.32998200	-0.07297000	-5.55198700
C	-0.93200600	-0.97700100	-6.96498700
C	1.39098400	-0.21996900	-6.94898700
C	0.25699000	-0.66898400	-7.62698700
H	-1.80500100	-1.33201200	-7.50598700
H	2.31898100	0.01404400	-7.46798700
H	0.29899100	-0.78398400	-8.71498700
C	0.80497200	0.63102300	4.97501300
C	2.11396900	0.84404100	5.48601300
C	-0.28002500	0.46100800	5.87801300
C	2.36297000	0.81004400	6.86701300
C	-0.01902500	0.43501200	7.26601300
C	1.28897300	0.59203000	7.73201300
H	3.38096800	0.93805800	7.23501300
H	-0.84702300	0.28600100	7.95301300
H	1.46997300	0.55903200	8.81001300
C	1.56808900	-7.98096700	1.51301300
C	1.51710400	-9.06496700	0.40601300
H	2.52310800	-9.39195400	0.10001300
H	0.97411600	-9.95597500	0.76601300
H	0.99809900	-8.69097400	-0.49098700
C	0.12008400	-7.64398600	1.92201300
H	0.08107400	-6.89898700	2.73401300

H	-0.47292100	-7.26199400	1.07501300
H	-0.38290300	-8.55299300	2.29001300
C	2.30109700	-8.54995700	2.75401300
H	1.77110900	-9.43696400	3.14001300
H	3.33410100	-8.85494300	2.52101300
H	2.34708700	-7.80395600	3.56401300
C	5.89606200	-5.95790800	-0.38198700
C	6.41508100	-7.40290100	-0.23798700
H	7.46308200	-7.45588700	-0.57698700
H	6.39208600	-7.74990100	0.80801300
H	5.83709100	-8.11390900	-0.85198700
C	6.02005600	-5.54590600	-1.87098700
H	5.38506500	-6.17891500	-2.51198700
H	5.72504200	-4.49791000	-2.03698700
H	7.06305700	-5.65589200	-2.21498700
C	6.79204900	-5.03489600	0.48201300
H	6.73505300	-5.31089700	1.54801300
H	7.84605000	-5.11788100	0.16501300
H	6.50003500	-3.97690000	0.39401300
C	-3.18212100	7.50296900	0.22801300
C	1.57187000	8.18303300	-1.60098700
C	1.90185500	9.25203800	-0.52998700
H	2.67784600	9.94304800	-0.90198700
H	1.01984700	9.85602600	-0.26298700
H	2.27886200	8.78404300	0.39401300
C	1.04686000	8.88302600	-2.87998700
H	0.13285200	9.46701400	-2.68598700
H	1.80685100	9.57803700	-3.27798700
H	0.81387000	8.14802300	-3.66798700
C	2.87688000	7.44405100	-1.95998700
H	3.32488700	6.94505700	-1.08498700
H	2.72189000	6.68704900	-2.74598700
H	3.61887000	8.16506100	-2.34198700
C	-3.47211600	7.15996500	1.71101300

H	-3.47610200	6.07396500	1.89201300
H	-2.71712200	7.61097500	2.37701300
H	-4.46112200	7.54995200	2.00801300
C	-3.26514200	9.03396800	0.06401300
H	-3.12114600	9.34797000	-0.98298700
H	-4.26114600	9.38695400	0.37601300
H	-2.52214900	9.55897800	0.68801300
C	-4.27011200	6.85895400	-0.66798700
H	-5.26911700	7.23894100	-0.39298700
H	-4.09811500	7.09595700	-1.73098700
H	-4.29209700	5.76295400	-0.56798700
N	-2.18500400	-1.12801700	-4.83898700
H	-2.14400700	-0.93301700	-3.83798700
N	-1.58602400	0.32299100	5.35201300
H	-1.68302400	0.38998900	4.33201300
N	3.14196600	1.11705500	4.55201300
H	2.82496100	1.45705000	3.64501300
N	2.43397600	0.38304500	-4.79698700
H	2.25197400	0.49904300	-3.80098700
C	-3.36199600	-1.68203300	-5.32698700
C	-2.77202200	0.23197500	6.07201300
C	4.49197000	0.80707300	4.63701300
C	3.70997100	0.72106200	-5.21798700
O	5.01997700	0.24908000	5.59601300
O	4.11697200	0.63406800	-6.37598700
O	-2.83802100	0.14397400	7.30001300
O	-3.52899200	-2.02303600	-6.49898700
C	4.57596400	1.24407400	-4.10198700
H	4.17896400	1.25706900	-3.08198700
C	5.23596400	1.20308300	3.38501300
H	4.85295300	2.05507800	2.81401300
C	5.88197900	0.11009200	2.55401300
H	5.86497800	0.24009200	1.46901300
H	5.80999300	-0.91590900	2.92101300

C	6.74396600	1.06210400	3.37201300
H	7.20297200	0.64411000	4.27001300
C	5.54394900	2.35008700	-4.44698700
H	5.55194400	2.68508700	-5.48598700
H	5.73093900	3.10209000	-3.67798700
C	6.07896800	0.95309500	-4.19298700
H	6.41197600	0.38709900	-5.06498700
C	7.51995200	2.09211400	2.61901300
C	6.80597100	0.73710400	-2.90898700
O	6.46096500	1.18910000	-1.82798700
O	7.04294100	2.93010800	1.87101300
O	7.92698100	-0.01088000	-3.11298700
O	8.85495400	1.94713200	2.85601300
C	8.81698300	-0.17286800	-1.96598700
H	8.22398200	-0.07187600	-1.04598700
H	9.19899700	-1.20186300	-2.04898700
C	9.94696900	0.85414700	-2.04198700
H	10.44497100	0.74515400	-3.02198700
H	9.50695500	1.86614100	-2.02998700
C	9.73094200	2.86614400	2.13501300
H	10.66594200	2.83815700	2.71501300
H	9.29692800	3.87613800	2.18701300
C	9.95894800	2.45014700	0.68101300
H	9.01294600	2.57313400	0.13001300
H	10.66993800	3.18215700	0.24901300
C	10.99697100	0.71216100	-0.92198700
H	11.41598500	-0.31083300	-0.94298700
H	11.84196200	1.38317300	-1.16298700
C	10.51496700	1.02615500	0.51001300
H	9.75497700	0.29414400	0.83401300
H	11.37096900	0.88416600	1.19701300
C	-4.46399400	-1.86304800	-4.31298700
H	-4.31199900	-1.50004600	-3.29298700
C	-4.02502300	0.30795800	5.23301300

H	-3.92902300	0.27095900	4.14601300
C	-5.11403500	1.19594300	5.79801300
H	-5.73304300	1.73793400	5.08001300
H	-4.90204200	1.69994600	6.74301300
C	-5.33097700	-3.09506000	-4.48398700
H	-5.72297100	-3.54406500	-3.57198700
H	-5.04396800	-3.77905600	-5.28598700
C	-5.88799500	-1.76406800	-4.90698700
H	-5.87399800	-1.55006800	-5.97798700
C	-5.27801500	-0.31205900	5.87001300
H	-5.11600900	-0.75505700	6.85401300
C	-7.02200500	-1.07708300	-4.21598700
C	-6.37300600	-0.96807400	5.10001300
O	-7.33899700	-1.61708700	-2.99798700
O	-6.47101200	-0.50107600	3.81401300
O	-7.14299500	-1.78308500	5.57701300
O	-7.63601700	-0.15109100	-4.71798700
C	-8.54500500	-1.04310400	-2.39198700
H	-8.32601900	-0.00210100	-2.10698700
H	-9.32900500	-1.02111400	-3.16498700
C	-8.96799400	-1.88110900	-1.19198700
H	-9.96199900	-1.50012300	-0.88598700
H	-9.12698000	-2.92811200	-1.50898700
C	-7.68000700	-0.88109200	3.08801300
C	-8.01099500	-1.81509600	0.00801300
H	-7.06098800	-2.30808400	-0.26798700
H	-7.76000900	-0.75609300	0.19801300
C	-8.56898600	-2.46610400	1.28801300
H	-8.74397100	-3.54210600	1.10701300
H	-9.56699200	-2.04011800	1.51301300
C	-7.65298800	-2.30709200	2.52101300
H	-4.08393100	-6.50504300	-3.11698700
H	-7.73401700	-0.13109300	2.28701300
H	-8.54300900	-0.75010400	3.76101300

H	-6.61398500	-2.55707800	2.24601300
H	-7.93897800	-3.01209600	3.31501300

Transition State TS2$^{Exo\text{-}Si}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -379.2349 cm-1

H_corr: 2.136648 Hartree

G_corr: 1.792452 Hartree

SCF: -7569.054420 Hartree

S: 689.72 Cal/Mol-Kelvin

H: -7566.917772 Hartree

G: -7567.261968 Hartree

Cartesian Coordinates:

C	2.72889400	-2.90788100	-3.23582900
C	2.62240900	-2.08744300	-2.10674600
C	2.56772500	-2.64183500	-0.81598000
C	2.62685900	-4.04522900	-0.69308600
C	2.73289800	-4.86745500	-1.82210000
C	2.78906800	-4.30100100	-3.09969800
H	2.75779100	-2.46040900	-4.23268900
H	2.55813500	-0.99982800	-2.20246600
H	2.62960200	-4.49587400	0.30393700
H	2.78613600	-5.95355400	-1.69755800
C	2.65166000	-1.79342200	0.43421900
C	4.07597600	-1.15003400	0.60590000
H	4.76150800	-1.61601900	-0.11419900
H	4.45019500	-1.37797400	1.61622900
N	4.10035000	0.30082400	0.39345900
S	2.59042200	0.92657400	0.86537700
N	1.65079900	-0.23301100	0.05306400
O	2.45986500	2.27001700	0.26733900
O	2.56745000	0.81325100	2.35111100
C	4.78442900	0.92107300	-0.74779300

C	5.95139000	1.81749800	-0.34096900
H	4.05888000	1.52964700	-1.31632200
H	5.13821800	0.12672600	-1.42672200
C	6.86057100	2.24779500	-1.32481100
C	7.91502800	3.10953100	-0.99751400
C	6.11463000	2.27145100	0.97603100
C	7.17032000	3.13403200	1.30561200
C	8.07410200	3.55568800	0.32203600
H	8.89657100	4.22978000	0.58048400
H	7.28176400	3.48049400	2.33794600
H	6.74153200	1.90195100	-2.35783400
H	8.61452100	3.43300000	-1.77508600
H	5.41180000	1.94008600	1.74499600
C	2.12212500	-2.34530200	1.62486200
H	1.33011100	-3.09325300	1.60383200
H	2.40982900	-1.94773500	2.59797200
C	-0.64768700	-1.07743100	2.83980700
N	-0.71019700	-1.27203200	1.46015400
H	-1.05309700	-2.37275100	4.62568000
C	-1.11571400	-2.59826800	1.30876900
C	-1.33176200	-3.21101200	2.59569000
H	-1.69121900	-4.22677500	2.74357600
C	-1.00987800	-2.28095900	3.54231400
C	-1.27198600	-3.27656500	0.09585600
N	-0.62310900	-1.34850400	-1.33120100
C	-0.49930500	-1.21999500	-2.71041600
C	-0.75971900	-2.47696700	-3.36853600
H	-0.72240500	-2.63099100	-4.44474600
C	-1.06557600	-3.37797800	-2.39294800
H	-1.31797400	-4.43025600	-2.49943300
C	-0.98801000	-2.67652900	-1.13429000
C	-0.43809800	0.14479400	3.48911900
H	-0.40062300	4.65836600	2.53823200
C	-0.37740900	3.57502800	2.44569100

C	-0.35452300	2.86455500	1.19095200
H	-0.34569300	2.78621100	4.51316000
N	-0.36191000	1.48798200	1.40282900
C	-0.35132300	1.34908500	2.78735900
C	-0.34926600	2.63775300	3.43505700
C	-0.26574200	-0.02804900	-3.40989700
H	0.00074200	4.52239400	-2.67182900
C	-0.05618400	3.44581700	-2.52783200
C	-0.02128300	2.45802300	-3.46789000
H	0.05637000	2.55109400	-4.54985500
C	-0.13985900	1.20533900	-2.75909600
N	-0.23978800	1.41911100	-1.38773200
C	-0.19596200	2.80013000	-1.24511700
C	-0.28877800	3.50685800	-0.04476200
Co	-0.24329800	0.03200800	0.05401500
C	-0.25005600	5.00481400	-0.08333200
C	0.95197100	5.67406600	0.20456600
C	-1.40339500	5.73662900	-0.41170100
C	1.01782900	7.07840600	0.16893900
H	1.83079600	5.07170800	0.44444700
C	-1.37788600	7.14240600	-0.45127100
H	-2.32389600	5.18948700	-0.62831700
C	-0.15810000	7.78073400	-0.15770200
H	-0.12209300	8.87441100	-0.18475300
C	-1.76815800	-4.69164700	0.11538200
C	-3.06423100	-4.97984400	-0.33359700
C	-0.95309200	-5.73828600	0.59192800
C	-3.57311300	-6.29485800	-0.31141800
H	-3.68538000	-4.15448700	-0.69404900
C	-1.41902100	-7.06065000	0.62713500
H	0.05851100	-5.49675600	0.92479800
C	-2.73240000	-7.30913700	0.17113000
H	-3.10534600	-8.33551800	0.19639600
C	-0.47196800	0.17051100	4.99085600

C	0.69132600	-0.09360100	5.75811700
C	-1.70551800	0.42006100	5.65716400
C	0.60908700	-0.12568000	7.16507600
C	-1.77907600	0.37295100	7.06088800
C	-0.61874300	0.09884100	7.78867800
H	1.50081200	-0.34740400	7.74680500
H	-2.73657300	0.54395700	7.54955100
H	-0.67301300	0.06615900	8.88114400
C	-0.42412900	-0.05709900	-4.90829000
C	-1.74680900	-0.03891100	-5.43221500
C	0.66860300	-0.14713700	-5.80858300
C	-1.97627800	-0.19422300	-6.81017400
C	0.43443400	-0.28987300	-7.19135100
C	-0.87982500	-0.32834400	-7.66379000
H	-2.99924900	-0.21635500	-7.18338200
H	1.28236600	-0.36985300	-7.86783200
H	-1.05161400	-0.45051400	-8.73748200
C	-0.55653100	-8.23340000	1.13860900
C	-1.26603800	-8.91087400	2.33814700
H	-2.25554400	-9.30838800	2.06273300
H	-0.66249900	-9.75389800	2.71519300
H	-1.41030000	-8.19942900	3.16763300
C	0.83995600	-7.77540800	1.60557200
H	1.41708200	-7.31267600	0.78804700
H	0.78343900	-7.05546500	2.43859800
H	1.41664500	-8.64414500	1.96241300
C	-0.37005300	-9.26910900	0.00127600
H	0.24364000	-10.11712100	0.34982700
H	-1.33208900	-9.67643700	-0.34753000
H	0.13589300	-8.81726300	-0.86760500
C	-5.00998000	-6.56384300	-0.80497100
C	-5.39915400	-8.05281000	-0.70541200
H	-6.43214200	-8.19079700	-1.06406300
H	-4.74999500	-8.69345300	-1.32490800

H	-5.36143400	-8.42289700	0.33246500
C	-6.00789700	-5.74657100	0.05383200
H	-5.94634900	-6.03528300	1.11584200
H	-5.81640400	-4.66379800	-0.00891600
H	-7.04214900	-5.92266200	-0.28762900
C	-5.13312600	-6.13129000	-2.28755400
H	-4.44029700	-6.70299700	-2.92649900
H	-6.15787100	-6.30784900	-2.65609700
H	-4.90948600	-5.06184800	-2.42643200
C	2.31761000	7.85350400	0.47069000
C	-2.62489000	7.98498000	-0.79305500
C	-2.32986200	8.86800200	-2.03152800
H	-3.21285800	9.47819400	-2.28712700
H	-1.48895300	9.55792100	-1.85776200
H	-2.07943900	8.24956900	-2.90902500
C	-2.97513000	8.89342000	0.41239700
H	-2.15078000	9.57897600	0.66531500
H	-3.86298300	9.50822100	0.18595600
H	-3.19755300	8.29268300	1.30941900
C	-3.85525800	7.11062800	-1.10996100
H	-3.68325500	6.44969400	-1.97528700
H	-4.15150200	6.48307500	-0.25358300
H	-4.71523400	7.75478200	-1.35588400
C	3.49575000	6.91452600	0.80004000
H	3.29829100	6.29710000	1.69128000
H	3.73466200	6.23761800	-0.03597800
H	4.39890700	7.51141100	1.00770600
C	2.70841700	8.70402400	-0.76408000
H	1.92681100	9.43389600	-1.02879000
H	3.63589300	9.26724600	-0.56418900
H	2.88261400	8.06527600	-1.64538800
C	2.08896300	8.78791300	1.68534100
H	3.00896600	9.35232200	1.91426800
H	1.28724700	9.52026600	1.49923800

H	1.81335900	8.21059900	2.58301500
N	1.92156800	-0.31058900	5.08630100
H	2.01338000	0.07318700	4.13796900
N	1.97745700	-0.09390100	-5.26844400
H	2.01630200	0.04626000	-4.25831300
N	-2.80432300	0.17729500	-4.52233200
H	-2.52322200	0.54546100	-3.61433800
N	-2.83186100	0.71721200	4.85568700
H	-2.63470900	0.81472500	3.86016100
C	2.99538100	-1.03310400	5.58666300
C	3.18879400	-0.10320900	-5.94701200
C	-4.14660000	-0.15219400	-4.64760500
C	-4.14056700	0.96055100	5.24061800
O	-4.63892100	-0.72307600	-5.61881300
O	-4.56535400	0.86459400	6.39240400
O	3.30022600	-0.21383700	-7.16813700
O	3.00700800	-1.58175300	6.68994100
C	-5.02085000	1.40257700	4.10098500
H	-4.59972500	1.45665000	3.09262100
C	-4.94269900	0.25243300	-3.43469100
H	-4.52729300	1.02833000	-2.78434000
C	-5.77990800	-0.79846600	-2.73074500
H	-5.84074300	-0.73124900	-1.64213000
H	-5.78913200	-1.80408000	-3.15723400
C	-6.45533300	0.28507600	-3.55315300
H	-6.87784900	-0.03541300	-4.50746900
C	-6.08878700	2.41814500	4.42773100
H	-6.14658800	2.74415900	5.46803400
H	-6.32190400	3.15538500	3.65710600
C	-6.49634200	0.98333800	4.15477700
H	-6.80001400	0.38005200	5.01178100
C	-7.16768400	1.37654800	-2.81905900
C	-7.16379600	0.72048600	2.84792200
O	-6.85084200	1.24650700	1.79026400

O	-6.65213500	2.14406500	-2.02372200
O	-8.19047500	-0.16471800	2.99183500
O	-8.48975000	1.38097700	-3.14602400
C	-8.99162000	-0.39919000	1.79215300
H	-8.32857300	-0.35507000	0.91606400
H	-9.37487800	-1.42351900	1.91407900
C	-10.12382400	0.62297800	1.70353700
H	-10.72993400	0.55084700	2.62356100
H	-9.68303700	1.63418700	1.69889600
C	-9.30811900	2.39419700	-2.48242000
H	-10.19898600	2.46042100	-3.12532800
H	-8.76526800	3.35166000	-2.50795900
C	-9.67881300	2.02335800	-1.04628700
H	-8.77099600	2.06501600	-0.42319400
H	-10.34763500	2.82668700	-0.67856200
C	-11.03863200	0.44102100	0.47577900
H	-11.49210900	-0.56779500	0.50027500
H	-11.88254800	1.14794600	0.57886400
C	-10.37913700	0.66104500	-0.90260900
H	-9.65778400	-0.14578100	-1.12054200
H	-11.16488400	0.56647200	-1.67559100
C	4.17117700	-1.15685800	4.64750700
H	4.18660400	-0.53294600	3.75028800
C	4.40296600	0.04907500	-5.06534800
H	4.27215600	0.07382900	-3.98046500
C	5.53880600	0.86676800	-5.63964300
H	6.13210400	1.45704300	-4.93985600
H	5.37554100	1.29798700	-6.62943500
C	4.79980000	-2.53739700	4.57739800
H	5.22340700	-2.85088700	3.62230900
H	4.32768100	-3.31431600	5.18267400
C	5.51958700	-1.44917400	5.33258000
H	5.45292000	-1.48080500	6.42177000
C	5.67735600	-0.64073400	-5.58382800

H	5.55475100	-1.16543600	-6.53291600
C	6.79565800	-0.84858900	4.84210600
C	6.67909400	-1.28094900	-4.68062600
O	7.00226700	-1.06724300	3.50251200
O	6.75213000	-0.66483900	-3.45805300
O	7.38763100	-2.21354200	-5.01100300
O	7.57891300	-0.25667000	5.56243200
C	8.26855200	-0.57253900	2.96267900
H	8.08407600	0.43864300	2.56191300
H	8.98382600	-0.49106200	3.79359300
C	8.75868800	-1.52031900	1.87261600
H	9.76963200	-1.17932700	1.57822300
H	8.88656800	-2.53106700	2.30177600
C	7.83883000	-1.10385300	-2.58102900
C	7.84954500	-1.56967000	0.63663900
H	6.85058800	-1.92032500	0.94737100
H	7.70578200	-0.53682200	0.26808600
C	8.36113500	-2.47299100	-0.49954400
H	8.37329500	-3.52273900	-0.15635800
H	9.41523700	-2.22605800	-0.73373000
C	7.50749500	-2.36840700	-1.78371700
H	2.88116400	-4.93671600	-3.98528500
H	6.43569000	-2.35320800	-1.51476600
H	7.65158100	-3.24842900	-2.42947000
H	7.99407600	-0.23811900	-1.92139500
H	8.73799500	-1.25456600	-3.19796700

Transition State TS2$^{Exo\text{-}Re}$:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -375.5191 cm-1

G_corr: 1.794403 Hartree

H_corr: 2.13678 Hartree

SCF: -7569.055177 Hartree

S: 686.076 Cal/Mol-Kelvin

H: -7566.918397 Hartree

G: -7567.260774 Hartree

Cartesian Coordinates:

C	-2.31001200	-3.60643800	-2.61972100
C	-2.28718800	-2.65004500	-1.59690700
C	-2.27351300	-3.04012200	-0.24827100
C	-2.30671400	-4.41978400	0.04686100
C	-2.34448000	-5.37646700	-0.97513900
C	-2.34378200	-4.97314400	-2.31527400
H	-2.29411100	-3.28378700	-3.66391900
H	-2.24195900	-1.58192000	-1.82256900
H	-2.33173800	-4.74280900	1.09232000
H	-2.38377900	-6.43999700	-0.71921600
C	-2.38372200	-2.06212900	0.90155400
C	-3.85654200	-1.56538100	1.12876600
H	-4.10083800	-1.64265800	2.19826700
H	-4.54224800	-2.22571600	0.58092300
N	-4.10502200	-0.18077000	0.70128200
S	-2.66028100	0.67679100	1.03884400
N	-1.62393800	-0.44153300	0.27973000
O	-2.55638300	0.70394200	2.52325800
O	-2.72380800	1.95809400	0.31236900
C	-4.72058800	0.09970800	-0.60852400
C	-5.80855200	1.16419200	-0.54984900
H	-3.96009700	0.39441700	-1.35485100
H	-5.16242800	-0.84709000	-0.96385900
C	-6.35572600	1.60299000	0.66537600
C	-7.39595000	2.54373200	0.67725000
C	-6.31411700	1.68998400	-1.75181800
C	-7.35802000	2.62295900	-1.74230500
C	-7.90451900	3.05270100	-0.52442300
H	-8.71707200	3.78578200	-0.51399700

H	-7.74294600	3.01243800	-2.68951500
H	-5.94643300	1.21251300	1.60104300
H	-7.80692600	2.88304900	1.63360000
H	-5.88922200	1.37155500	-2.71049500
C	-1.71516800	-2.41910100	2.09561300
H	-0.86447200	-3.10061700	2.09306400
H	-1.97455500	-1.93985800	3.04054400
C	0.43144400	-1.17213100	-2.70713100
N	0.66844700	-1.26971200	-1.33995600
H	0.79748400	-2.52009600	-4.46622200
C	1.25902900	-2.51894600	-1.17558900
C	1.38681500	-3.19578100	-2.44331400
H	1.81222800	-4.18806400	-2.57326200
C	0.87142300	-2.36279300	-3.39196300
C	1.67996100	-3.07334400	0.03603300
N	0.94123500	-1.15361700	1.43751100
C	0.94960300	-0.95303000	2.81740500
C	1.49027200	-2.10292600	3.49565500
H	1.61725900	-2.18238000	4.57310700
C	1.85231200	-2.99869700	2.53062200
H	2.33326800	-3.96614800	2.65585500
C	1.48849800	-2.42342300	1.25981500
C	-0.07791200	-0.05098300	-3.37708300
H	-0.89451000	4.42919600	-2.63362700
C	-0.68870800	3.37091200	-2.48954700
C	-0.32035400	2.77617700	-1.22791900
H	-0.92873200	2.42480200	-4.47545200
N	-0.11509400	1.40878100	-1.36552000
C	-0.33966000	1.15577900	-2.71498300
C	-0.71261000	2.36580100	-3.41031500
C	0.65759600	0.24980100	3.47306900
H	0.04759500	4.71761000	2.49871700
C	0.14101500	3.63705200	2.41694100
C	0.30585900	2.71849100	3.41138200

H	0.38271200	2.88281900	4.48481700
C	0.38289700	1.42590400	2.77504200
N	0.25654600	1.54323400	1.39506500
C	0.08415400	2.90680700	1.17454000
C	-0.17765300	3.51399000	-0.05306000
Co	0.20579700	0.06320700	0.07359100
C	-0.39390100	4.99752900	-0.09518100
C	-1.67890300	5.51486500	0.11079600
C	0.68631700	5.86789500	-0.33534700
C	-1.91139000	6.90630000	0.08448600
H	-2.49633500	4.81101900	0.29193600
C	0.49458900	7.25755000	-0.36878400
H	1.67764500	5.43638300	-0.49234300
C	-0.81294900	7.74692000	-0.15477500
H	-0.97199800	8.82755400	-0.17713500
C	2.37720900	-4.40092800	0.02034000
C	3.68672500	-4.48934200	-0.47165400
C	1.73630800	-5.56085900	0.49967400
C	4.37958500	-5.71739700	-0.49431800
H	4.16993300	-3.57676100	-0.83351000
C	2.39091800	-6.80161500	0.49485000
H	0.70910600	-5.47288100	0.86001600
C	3.71010800	-6.84999500	-0.00712400
H	4.22713900	-7.81215000	-0.01560400
C	-0.07233600	-0.05498700	-4.88369400
C	-1.20297500	-0.41415400	-5.66151200
C	1.13284600	0.31824000	-5.54691800
C	-1.12306900	-0.41001100	-7.06922600
C	1.20704800	0.31416000	-6.95168800
C	0.07689900	-0.05081600	-7.68521100
H	-1.99541800	-0.69533500	-7.65216800
H	2.14084300	0.59607400	-7.43500500
H	0.13080300	-0.05250700	-8.77810800
C	0.86232200	0.29578400	4.95963100

C	2.18171400	0.49891900	5.44373400
C	-0.19331000	0.05958700	5.87994300
C	2.47114100	0.37944500	6.81201200
C	0.10675500	-0.05192200	7.25503900
C	1.42629800	0.09034200	7.69233400
H	3.49658100	0.50003800	7.15993000
H	-0.69843100	-0.25982600	7.95556900
H	1.64022500	-0.00956600	8.76088100
C	1.72376800	-8.09615800	1.00438800
C	1.62791200	-9.11515900	-0.15909700
H	2.61950600	-9.37273100	-0.56368800
H	1.15558800	-10.05062500	0.18611900
H	1.02267700	-8.71366400	-0.98831200
C	0.30159300	-7.84832600	1.54616200
H	0.29968600	-7.14897500	2.39845100
H	-0.37046000	-7.44683800	0.77022500
H	-0.13317300	-8.79747400	1.89949400
C	2.57445800	-8.70247600	2.14883000
H	2.10844200	-9.62967200	2.52329200
H	3.59442500	-8.95462500	1.81864500
H	2.66044900	-8.00077900	2.99454200
C	5.82198600	-5.76907600	-1.03972400
C	6.41949900	-7.19004400	-0.99377700
H	7.44599200	-7.17365200	-1.39481100
H	6.47669600	-7.58299500	0.03473200
H	5.84142200	-7.90296100	-1.60467600
C	5.83127800	-5.28901600	-2.51290400
H	5.20285800	-5.93756400	-3.14516300
H	5.45705500	-4.25819000	-2.61462500
H	6.85702000	-5.31160400	-2.91850300
C	6.72444600	-4.83857800	-0.19082700
H	6.73982300	-5.15565900	0.86472000
H	7.76119400	-4.86094900	-0.56771900
H	6.38171400	-3.79240000	-0.22097900

C	-3.33983300	7.44172100	0.31312400
C	1.64887600	8.24879300	-0.62521900
C	1.79765100	9.19186300	0.59525800
H	2.61714300	9.91146100	0.42773900
H	0.87971800	9.77077900	0.78372800
H	2.02796000	8.62203200	1.51030700
C	1.33557400	9.09000500	-1.88821700
H	0.40422200	9.66788600	-1.77959400
H	2.15101900	9.80690800	-2.08452800
H	1.22814400	8.44616600	-2.77652100
C	2.99754800	7.53431800	-0.84727400
H	3.30271800	6.94075300	0.03005700
H	2.97158500	6.86516500	-1.72310700
H	3.78826000	8.28064500	-1.02817100
C	-3.84929800	6.97024900	1.69848700
H	-3.87511900	5.87246300	1.77691000
H	-3.20523500	7.35093600	2.50836100
H	-4.87325300	7.34081700	1.87630100
C	-3.40631000	8.98187500	0.27449200
H	-3.09342100	9.38686400	-0.70222900
H	-4.44358400	9.31220600	0.44738700
H	-2.78097500	9.44397900	1.05642900
C	-4.27454800	6.88776900	-0.79167000
H	-5.30437100	7.25470800	-0.64257200
H	-3.94052800	7.21133000	-1.79139800
H	-4.31061300	5.78756300	-0.78827900
N	-2.39790300	-0.76542200	-4.98248400
H	-2.37684800	-0.62699300	-3.97172200
N	-1.51422600	-0.05616300	5.37925500
H	-1.65648200	0.20488900	4.39669200
N	3.17893200	0.85223600	4.50340200
H	2.83481900	1.27082100	3.63982400
N	2.23104900	0.68925000	-4.74018700
H	2.04871000	0.67624400	-3.73743900

C	-3.55921100	-1.30434800	-5.52304600
C	-2.66328100	-0.33362100	6.11215400
C	4.52806100	0.52616000	4.52003600
C	3.49450500	1.11804500	-5.11611900
O	5.07331800	-0.12765800	5.40567900
O	3.89538400	1.19814200	-6.27728200
O	-2.67169700	-0.61299600	7.31255200
O	-3.71868300	-1.53797300	-6.72125800
C	4.35183000	1.52033000	-3.94437500
H	3.97204800	1.36481000	-2.93010800
C	5.24739800	1.04465600	3.29881000
H	4.86090100	1.95515400	2.83029800
C	5.86813900	0.04245900	2.34313600
H	5.83449300	0.28886600	1.27912800
H	5.79226300	-1.01687100	2.59866700
C	6.75321300	0.89277600	3.24303500
H	7.22098100	0.37752700	4.08410300
C	5.25065600	2.71907600	-4.13677900
H	5.21896000	3.20238500	-5.11526900
H	5.41119000	3.36056500	-3.26809400
C	5.86500600	1.33277900	-4.09690800
H	6.20869800	0.91968000	-5.04654700
C	7.53044200	1.99054600	2.59458400
C	6.63614300	0.97800100	-2.87051100
O	6.29565800	1.25051400	-1.72919700
O	7.05507700	2.90312400	1.93905300
O	7.79213300	0.33665800	-3.20379000
O	8.86602200	1.81450000	2.80903900
C	8.73633500	0.08319500	-2.11788900
H	8.18503500	0.08692500	-1.16716300
H	9.12998800	-0.92656200	-2.31208800
C	9.84573600	1.13364500	-2.15354900
H	10.30517400	1.11604100	-3.15723700
H	9.39109500	2.13303200	-2.04015200

C	9.74478200	2.79284000	2.17510600
H	10.68267000	2.70394800	2.74410100
H	9.31775200	3.79632100	2.32504800
C	9.95962500	2.51412700	0.68709100
H	9.00734000	2.68807200	0.16069700
H	10.66725500	3.28129900	0.31570900
C	10.94070700	0.91894000	-1.08927600
H	11.36965500	-0.09396600	-1.20799300
H	11.76857500	1.61838400	-1.30824600
C	10.50932600	1.11119000	0.37958900
H	9.76024900	0.35316500	0.66725400
H	11.38758500	0.91473400	1.02297700
C	-4.63808900	-1.63632600	-4.52185300
H	-4.50601400	-1.33992300	-3.47769800
C	-3.94900000	-0.23692700	5.32962500
H	-3.89616600	-0.09124000	4.24873300
C	-5.09594400	0.44394200	6.04691000
H	-5.78492200	1.02467700	5.43123000
H	-4.90029200	0.82117200	7.05284500
C	-5.40018200	-2.92371900	-4.77643100
H	-5.74619100	-3.47135100	-3.89912900
H	-5.07369700	-3.51861400	-5.63210800
C	-6.07145900	-1.61315300	-5.09045100
H	-6.10431200	-1.32077300	-6.14196300
C	-5.11178600	-1.06633500	5.89394700
H	-4.87371900	-1.62768600	6.79921600
C	-7.23446200	-1.08551100	-4.31386500
C	-6.15946600	-1.71490700	5.05548200
O	-7.39369900	-1.69016500	-3.09620400
O	-6.28950500	-1.12486200	3.82478300
O	-6.86213800	-2.63332300	5.43910700
O	-7.98603800	-0.22818900	-4.74399700
C	-8.60174900	-1.28053800	-2.37418700
H	-8.44856800	-0.25267000	-2.00591400

H	-9.43336800	-1.25891100	-3.09464700
C	-8.86721300	-2.25705700	-1.23663300
H	-9.86360000	-1.99785600	-0.83032900
H	-8.96020100	-3.28027100	-1.64395200
C	-7.44742500	-1.53889100	3.03704200
C	-7.83318500	-2.21729400	-0.10170000
H	-6.86309400	-2.58734100	-0.48108100
H	-7.66868800	-1.16186000	0.18343300
C	-8.23658200	-3.04202100	1.13414100
H	-8.29697100	-4.10981500	0.85742100
H	-9.26005500	-2.76023400	1.45033800
C	-7.26784600	-2.88434300	2.32594900
H	-2.36812000	-5.71621100	-3.11805900
H	-7.56765700	-0.71416100	2.32034500
H	-8.32516400	-1.56897400	3.70232700
H	-6.22767100	-2.96653000	1.96689500
H	-7.41190200	-3.69379900	3.05750700

Intermediate (*R*)-D^{Endo}:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.140223 Hartree

G_corr: 1.795815 Hartree

SCF: -7569.093410 Hartree

S: 690.146 Cal/Mol-Kelvin

H: -7566.953187 Hartree

G: -7567.297595 Hartree

Cartesian Coordinates:

C	4.64221300	-4.99837800	-2.46047600
C	4.48417500	-4.04640100	-1.45767700
C	3.22149200	-3.41750200	-1.20906200
C	2.13059000	-3.82693300	-2.04249900
C	2.30157800	-4.77239300	-3.04934300
C	3.55499000	-5.36835200	-3.27020200

H	5.62297700	-5.45655000	-2.61789800
H	5.34175500	-3.81092100	-0.82408100
H	1.14986600	-3.36126200	-1.92704600
H	1.44856700	-5.04111400	-3.67951200
C	3.05719400	-2.44887000	-0.16967700
C	4.19408700	-1.71595000	0.49915700
H	5.18510900	-2.00346300	0.12566700
H	4.18595000	-1.89620800	1.58851200
N	4.08859700	-0.23668500	0.31642700
S	2.58773200	0.38006000	0.89297900
N	1.48197900	-0.55864700	-0.00482500
O	2.52655400	1.78114600	0.46664600
O	2.58797900	0.04486700	2.34389700
C	4.48176500	0.29805800	-1.00540900
C	5.30084200	1.57923700	-0.93251900
H	3.59748200	0.45739200	-1.64922400
H	5.08558600	-0.48226200	-1.49846300
C	5.49927500	2.32490400	-2.10797400
C	6.29321500	3.47798600	-2.10059100
C	5.90120100	2.02026600	0.25637500
C	6.69106600	3.17869900	0.26765800
C	6.89607900	3.90843400	-0.91026600
H	7.51185500	4.81303200	-0.89961300
H	7.13970400	3.51823100	1.20677500
H	5.01434800	2.00825300	-3.03826700
H	6.43336300	4.04753900	-3.02491600
H	5.72506600	1.45966600	1.17791500
C	1.71611300	-2.00804000	0.34340500
H	0.90118600	-2.58020800	-0.10662500
H	1.66406300	-2.16909900	1.43839900
C	-0.68497100	-0.89579000	2.99042200
N	-0.87454500	-1.16374400	1.63908500
H	-0.95462200	-2.08001100	4.88009900
C	-1.35539800	-2.47074000	1.60366100

C	-1.44703200	-3.01641900	2.93675200
H	-1.81576200	-4.01230600	3.17213800
C	-1.01292700	-2.04836000	3.79414000
C	-1.73142800	-3.17391700	0.45564700
N	-0.99228900	-1.41897400	-1.14252000
C	-0.85980300	-1.42623100	-2.52570500
C	-1.36669400	-2.65812300	-3.08146800
H	-1.39123200	-2.89598800	-4.14277300
C	-1.80677600	-3.41441900	-2.03293200
H	-2.25104500	-4.40722100	-2.05388000
C	-1.55103300	-2.65683100	-0.83209900
C	-0.39849900	0.36034200	3.53809300
H	-0.12151300	4.77904500	2.23005400
C	-0.16407400	3.69255700	2.22038300
C	-0.18354300	2.88520700	1.02466100
H	-0.17463600	3.07035600	4.34475500
N	-0.29715500	1.53435500	1.34788600
C	-0.27584700	1.50285900	2.74063700
C	-0.19123200	2.83699600	3.28182000
C	-0.36657400	-0.37227700	-3.30952800
H	0.55787300	4.13695900	-2.94799700
C	0.33778100	3.09733600	-2.71621500
C	0.29030800	2.02852300	-3.56402700
H	0.44282800	2.00810000	-4.64214400
C	-0.05421000	0.87716800	-2.76197200
N	-0.19092800	1.23290200	-1.42338200
C	0.03520800	2.59988800	-1.39413200
C	-0.02491900	3.41404500	-0.25791800
Co	-0.38996700	-0.00117600	0.11316400
C	0.14484900	4.89242300	-0.42122900
C	1.32730300	5.51706000	0.01410000
C	-0.87486000	5.65741700	-1.01437700
C	1.50450700	6.90419900	-0.13187900
H	2.10874500	4.89269600	0.45244000

C	-0.73655700	7.04750700	-1.17309800
H	-1.78616100	5.14857600	-1.33697000
C	0.45973200	7.63876100	-0.72480700
H	0.58339200	8.71991200	-0.84252800
C	-2.31574000	-4.54789400	0.60434100
C	-3.70199600	-4.73722800	0.47403400
C	-1.48318700	-5.64809500	0.87208000
C	-4.27417000	-6.01455900	0.61204800
H	-4.32804600	-3.86521000	0.27181900
C	-2.01547200	-6.94207800	1.01242000
H	-0.40819600	-5.47676600	0.96334500
C	-3.40861100	-7.09206400	0.87839400
H	-3.83879400	-8.09255600	0.98693200
C	-0.43461000	0.50109500	5.03405000
C	0.69796100	0.23100100	5.84779100
C	-1.66928200	0.85859000	5.64919700
C	0.57538400	0.30255700	7.25242400
C	-1.77973400	0.92116400	7.04914700
C	-0.65228300	0.63868600	7.82377000
H	1.43972000	0.07404000	7.87137700
H	-2.73756100	1.17979500	7.49727500
H	-0.73224200	0.68618000	8.91421200
C	-0.44036300	-0.54808900	-4.80235200
C	-1.70558000	-0.36159100	-5.42246300
C	0.65715900	-0.98495100	-5.58999800
C	-1.89852200	-0.68285600	-6.77581900
C	0.45706400	-1.30723700	-6.94845500
C	-0.81426800	-1.16616700	-7.51132000
H	-2.88597300	-0.56689500	-7.22115800
H	1.29819600	-1.66763600	-7.53644600
H	-0.95670100	-1.42750600	-8.56429000
C	-1.13345200	-8.17529000	1.30028600
C	-1.58046900	-8.82921700	2.63188300
H	-2.63122100	-9.15801000	2.59931400

H	-0.96137400	-9.71569800	2.85094500
H	-1.47607000	-8.12602200	3.47427100
C	0.36073500	-7.81265200	1.42146400
H	0.75783600	-7.37160400	0.49262100
H	0.54987000	-7.10639000	2.24663100
H	0.94756100	-8.72226500	1.62885700
C	-1.28985400	-9.19896600	0.14768700
H	-0.66664800	-10.08938400	0.33739700
H	-2.33137500	-9.53990300	0.03640300
H	-0.97567800	-8.76322200	-0.81481500
C	-5.79224200	-6.26219900	0.48760800
C	-6.32561200	-6.86227200	1.81290200
H	-7.41107400	-7.04666000	1.74178500
H	-5.84139800	-7.82109000	2.05686000
H	-6.15196800	-6.17562900	2.65743900
C	-6.57605300	-4.96581600	0.19859600
H	-6.45629000	-4.22180400	1.00320500
H	-6.26841800	-4.49919300	-0.75165900
H	-7.65169200	-5.19261300	0.11867700
C	-6.05931700	-7.25608800	-0.67060200
H	-5.56434600	-8.22610500	-0.50513300
H	-7.14118600	-7.44776900	-0.77079300
H	-5.69553200	-6.85439900	-1.63048300
C	2.78840400	7.62736600	0.32651500
C	-1.83877900	7.92381000	-1.80487100
C	-1.27207400	8.64572400	-3.05320100
H	-2.04809200	9.27875400	-3.51622900
H	-0.41860800	9.29584100	-2.80370000
H	-0.93007300	7.92046800	-3.80967900
C	-2.31066000	8.97862400	-0.77263600
H	-1.48841400	9.63674700	-0.44974500
H	-3.09796800	9.61755600	-1.20780400
H	-2.72454200	8.49457300	0.12697500
C	-3.06546300	7.09833000	-2.24373700

H	-2.80676000	6.34233500	-3.00327200
H	-3.54497300	6.58208500	-1.39614700
H	-3.82143200	7.76468600	-2.69019700
C	3.80062300	6.66530900	0.98081800
H	3.38577400	6.17468700	1.87647800
H	4.13928000	5.87894200	0.28752200
H	4.69304200	7.22853600	1.29976100
C	3.46907500	8.28811500	-0.89862000
H	2.81160900	9.02333400	-1.38966000
H	4.38755200	8.81591200	-0.58968400
H	3.74802400	7.53224400	-1.65071500
C	2.42369800	8.72086900	1.36191100
H	3.33277500	9.24660900	1.70018100
H	1.73938800	9.47679100	0.94501600
H	1.93731300	8.28146900	2.24816200
N	1.92856000	-0.08494600	5.22397800
H	1.99584400	0.08441200	4.21373300
N	1.93240300	-1.05948300	-4.97709300
H	1.96346100	-0.74038600	-4.00799600
N	-2.74885800	0.17316500	-4.63187700
H	-2.44588600	0.67070300	-3.79521200
N	-2.75946500	1.15031400	4.79675800
H	-2.53585500	1.14399600	3.80232200
C	3.04721800	-0.63787400	5.83231200
C	3.14969700	-1.35139500	-5.58014100
C	-4.10921900	-0.09838600	-4.70864900
C	-4.05359200	1.52592500	5.11682000
O	-4.62699900	-0.81862500	-5.55843700
O	-4.51413300	1.57568600	6.25762300
O	3.26884800	-1.79339800	-6.72287100
O	3.09759300	-0.98355400	7.01506100
C	-4.86421100	1.92107500	3.90877300
H	-4.41357200	1.83288500	2.91566700
C	-4.87792300	0.56534600	-3.59453100

H	-4.45571500	1.47323900	-3.15281100
C	-5.64798200	-0.32099500	-2.63284400
H	-5.67130300	-0.00962000	-1.58597200
H	-5.63821400	-1.39705200	-2.81969300
C	-6.39205700	0.53409100	-3.64669800
H	-6.84254600	0.00244100	-4.48697700
C	-5.84042000	3.05790400	4.09077800
H	-5.89779500	3.49442100	5.08984100
H	-5.98206400	3.72957100	3.24189300
C	-6.37169400	1.64374200	3.94994500
H	-6.75576300	1.16638300	4.85288900
C	-7.11618000	1.73079500	-3.12047800
C	-7.02976100	1.30810600	2.65470200
O	-6.63311800	1.66991500	1.55676900
O	-6.60629300	2.64215500	-2.48987700
O	-8.15595500	0.56762800	2.86043900
O	-8.44447400	1.64742200	-3.41348800
C	-8.96742500	0.29945800	1.67532600
H	-8.29972100	0.21003500	0.80648400
H	-9.44027500	-0.67315400	1.87968400
C	-10.00799000	1.40348300	1.49103300
H	-10.59492100	1.48184100	2.42290700
H	-9.48332200	2.36672000	1.37172900
C	-9.27777200	2.73113200	-2.89799700
H	-10.17181100	2.69523800	-3.53893500
H	-8.74937600	3.68361800	-3.05626000
C	-9.63612100	2.54957100	-1.42275200
H	-8.72030900	2.66661400	-0.82087800
H	-10.29840900	3.39520400	-1.15106400
C	-10.96671800	1.16755900	0.30668900
H	-11.47511300	0.19355300	0.43722400
H	-11.76679300	1.92876200	0.36265700
C	-10.33872800	1.21913900	-1.10189600
H	-9.62793200	0.38624000	-1.24169400

H	-11.14381000	1.04398600	-1.84027100
C	4.24780000	-0.80159100	4.92998400
H	4.18788200	-0.41631200	3.91024900
C	4.36087400	-0.98650900	-4.75569500
H	4.22395900	-0.73175000	-3.70274400
C	5.42390900	-0.21916700	-5.51969800
H	5.97986900	0.54457500	-4.97378900
H	5.22233300	-0.02258300	-6.57455100
C	5.11286400	-2.02057300	5.17613500
H	5.61602900	-2.45746500	4.31212300
H	4.77007500	-2.71399800	5.94738100
C	5.60331300	-0.68095200	5.66190900
H	5.49320100	-0.48324900	6.72997000
C	5.67861600	-1.66715500	-5.14120300
H	5.59969400	-2.39686900	-5.94881500
C	6.76451400	0.04154400	5.06710500
C	6.77109100	-1.96488700	-4.16640900
O	7.12431000	-0.42879300	3.82586600
O	6.77508300	-1.08999400	-3.11058400
O	7.60784300	-2.83463000	-4.32577800
O	7.35539300	0.94070600	5.63860800
C	8.30705800	0.20689400	3.25022200
H	7.98689700	1.14179600	2.75836100
H	8.98431700	0.47808900	4.07310100
C	8.97067700	-0.74500000	2.26197000
H	9.93232900	-0.28204400	1.96866800
H	9.22926900	-1.68332100	2.78609700
C	7.96593300	-1.08706500	-2.25962600
C	8.14126400	-1.04590200	1.00538200
H	7.19631400	-1.52941100	1.31134400
H	7.85135200	-0.08940200	0.53292700
C	8.86515500	-1.94472900	-0.01280400
H	9.13759100	-2.89818000	0.47485700
H	9.82584400	-1.48004200	-0.30861900

C	8.02451000	-2.25529900	-1.26990400
H	3.68455700	-6.10726800	-4.06582700
H	6.99330900	-2.49741900	-0.95922700
H	8.40631300	-3.14553100	-1.79214300
H	7.89407700	-0.11808600	-1.74516100
H	8.85301500	-1.08180500	-2.91260100

Intermediate (*S*)-D^{Endo}:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.140424 Hartree

G_corr: 1.796394 Hartree

SCF: -7569.093161 Hartree

S: 689.387 Cal/Mol-Kelvin

H: -7566.952737 Hartree

G: -7567.296767 Hartree

Cartesian Coordinates:

C	-5.07637400	-5.20430000	-1.14482000
C	-4.79375500	-4.00572800	-0.49467200
C	-3.50473600	-3.38647000	-0.58849000
C	-2.53325400	-4.05616900	-1.40107000
C	-2.83407600	-5.24361200	-2.06244600
C	-4.10277800	-5.83559600	-1.93718900
H	-6.06573200	-5.65790000	-1.02932900
H	-5.56450300	-3.56166000	0.14011000
H	-1.54417800	-3.61469600	-1.54667300
H	-2.07084500	-5.71342500	-2.69024100
C	-3.20391300	-2.18233400	0.12480000
C	-4.25392900	-1.29674900	0.75025500
H	-4.24700000	-1.38933300	1.85160000
H	-5.27076100	-1.52904400	0.41081800
N	-4.03208000	0.14083100	0.44152300
S	-2.49020200	0.68998300	0.93510800
N	-1.48942500	-0.34974900	0.03235800

O	-2.44533600	0.41119500	2.39689500
O	-2.36616100	2.06838600	0.44885500
C	-4.48188100	0.62298000	-0.88111900
C	-5.57490400	1.68300800	-0.80328100
H	-3.62556700	1.02510000	-1.44780800
H	-4.85303200	-0.24646300	-1.45115300
C	-6.01516900	2.21741500	0.41615400
C	-7.02050300	3.19612200	0.44060700
C	-6.15341600	2.14724300	-1.99889900
C	-7.15594100	3.12410800	-1.97523800
C	-7.59500000	3.65196900	-0.75222000
H	-8.37795200	4.41638200	-0.73165300
H	-7.59503800	3.46959600	-2.91616000
H	-5.56214300	1.86173000	1.34508400
H	-7.35057400	3.60740500	1.40003100
H	-5.82144100	1.74535100	-2.96293700
C	-1.79617300	-1.76473900	0.45138100
H	-1.06476300	-2.40384100	-0.05003300
H	-1.63811300	-1.89225100	1.54249000
C	0.66506600	-1.36106600	-2.58614400
N	0.86199600	-1.37581500	-1.21022200
H	0.98302700	-2.85535500	-4.23355200
C	1.33289400	-2.65696700	-0.93261700
C	1.45652100	-3.42665500	-2.14757600
H	1.81069300	-4.45401100	-2.19449700
C	1.03464000	-2.62666400	-3.17090800
C	1.55328500	-3.18955200	0.34367700
N	0.89424300	-1.12953000	1.57261200
C	0.77806700	-0.85883800	2.93191700
C	1.06676200	-2.03462600	3.71576000
H	1.05303400	-2.07160500	4.80284600
C	1.40994700	-3.02010700	2.83742400
H	1.73336600	-4.03506500	3.05625100
C	1.28925400	-2.46458500	1.51092300

C	0.23212500	-0.26291000	-3.34281000
H	-0.36984800	4.29542500	-2.91454200
C	-0.20971000	3.24129500	-2.69912200
C	0.11224000	2.71296100	-1.39402500
H	-0.47213300	2.17864200	-4.62366600
N	0.24972500	1.33368400	-1.44148300
C	0.03344400	1.00143900	-2.77497800
C	-0.26942400	2.17989000	-3.55409700
C	0.59869700	0.40941300	3.49874200
H	0.55502400	4.84691200	2.22871900
C	0.52852700	3.75984600	2.21307000
C	0.55288300	2.89488800	3.26775600
H	0.60301500	3.11859600	4.33201400
C	0.51933400	1.56304600	2.71552800
N	0.47801400	1.60433700	1.32337200
C	0.44208900	2.96204100	1.01424000
C	0.26606000	3.51048500	-0.25737800
Co	0.41759700	0.07339400	0.07655300
C	0.17031800	4.99862400	-0.40053200
C	-0.99490600	5.66529000	0.00080700
C	1.24618000	5.72981000	-0.94119000
C	-1.10988100	7.06554600	-0.12518500
H	-1.81965000	5.06917100	0.40181800
C	1.17298700	7.12429000	-1.07489700
H	2.14475600	5.18627700	-1.24217200
C	-0.01583200	7.76404000	-0.65952000
H	-0.08284000	8.84976000	-0.76059900
C	2.06089900	-4.59555700	0.45572300
C	3.38255500	-4.89143600	0.09595500
C	1.21843000	-5.62897300	0.91406900
C	3.88993400	-6.20420800	0.18728100
H	4.02309600	-4.07551300	-0.25230100
C	1.68380000	-6.94803700	1.01814500
H	0.18804700	-5.38042500	1.17806500

C	3.02244500	-7.20597100	0.64852000
H	3.39405400	-8.23020300	0.72633100
C	0.21674100	-0.40346200	-4.84070100
C	-0.92766100	-0.84733600	-5.55204100
C	1.41452200	-0.12008400	-5.55835100
C	-0.86725300	-1.00887500	-6.95177000
C	1.46735700	-0.28828800	-6.95391600
C	0.32431600	-0.73007500	-7.62269700
H	-1.74595700	-1.36302800	-7.48513700
H	2.39694800	-0.07883300	-7.48004700
H	0.36213000	-0.86119500	-8.70843500
C	0.73483400	0.52245800	4.99146500
C	2.04978900	0.61557400	5.52468300
C	-0.37536900	0.45165500	5.87557500
C	2.27085500	0.56282700	6.91000200
C	-0.14205800	0.40595300	7.26815400
C	1.16599600	0.44621200	7.75644900
H	3.28932700	0.59889100	7.29489700
H	-0.99299300	0.33474900	7.94149900
H	1.32538900	0.39950500	8.83817300
C	0.79259200	-8.10641300	1.51264900
C	0.67137100	-9.17405700	0.39609700
H	1.65169800	-9.58954300	0.11364600
H	0.03915600	-10.01284700	0.73364900
H	0.21387900	-8.74777500	-0.51165800
C	-0.62797700	-7.63639600	1.88585600
H	-0.61751600	-6.89214500	2.69912800
H	-1.16076300	-7.19870100	1.02604500
H	-1.22279800	-8.49527900	2.23693100
C	1.43325600	-8.74910600	2.76879000
H	0.80840400	-9.58148100	3.13455300
H	2.43655500	-9.15356700	2.56153400
H	1.53056800	-8.01455900	3.58486800
C	5.35377200	-6.48455000	-0.21213800

C	5.73427800	-7.97058000	-0.05390300
H	6.78484600	-8.11814800	-0.35272200
H	5.63996600	-8.31392400	0.98948800
H	5.11818800	-8.62658400	-0.69085400
C	5.56651700	-6.08704300	-1.69453600
H	4.91270000	-6.67423500	-2.36021100
H	5.35405700	-5.02094300	-1.87181400
H	6.61133700	-6.27223200	-1.99650100
C	6.29904700	-5.64619100	0.68499900
H	6.17227100	-5.90764200	1.74822500
H	7.35193300	-5.83140700	0.41220400
H	6.11370700	-4.56541000	0.58221600
C	-2.41248800	7.76399000	0.31673500
C	2.33381500	7.96527300	-1.64561500
C	2.81089700	8.97637300	-0.57266900
H	3.63955200	9.59069500	-0.96436600
H	2.00521300	9.66151900	-0.26479200
H	3.17095400	8.45573700	0.32968300
C	1.84635900	8.73744600	-2.89744200
H	1.01288800	9.41898200	-2.66505100
H	2.66589100	9.34570700	-3.31667800
H	1.50264400	8.04391400	-3.68235200
C	3.53992600	7.09665200	-2.05750100
H	3.96395800	6.54329600	-1.20363400
H	3.27623100	6.36886900	-2.84260100
H	4.33968700	7.73897500	-2.46095400
C	-2.66757500	7.47368700	1.81722100
H	-2.76476700	6.39545000	2.01815600
H	-1.84478400	7.85988700	2.44140100
H	-3.60126700	7.95925900	2.14859200
C	-2.35640400	9.29325200	0.12605300
H	-2.21511700	9.57480200	-0.93062300
H	-3.30584600	9.74301000	0.45949800
H	-1.54936800	9.75614900	0.71797500

C	-3.59509200	7.21394800	-0.51987400
H	-4.53846800	7.69866700	-0.21563600
H	-3.44437700	7.40929800	-1.59434900
H	-3.72290900	6.12814000	-0.39145200
N	-2.11623900	-1.09929800	-4.82197600
H	-2.09014800	-0.83101400	-3.83750500
N	-1.67904800	0.42836300	5.32737100
H	-1.74964200	0.48578300	4.30512600
N	3.11121100	0.79373000	4.60729500
H	2.83192800	1.12751600	3.68561700
N	2.52916900	0.32836800	-4.81513000
H	2.35148700	0.47492900	-3.82215000
C	-3.27543100	-1.70912400	-5.28257200
C	-2.88076600	0.44951500	6.02453300
C	4.44533200	0.43565200	4.73217100
C	3.81398100	0.61735800	-5.24810600
O	4.93828900	-0.10146000	5.72163000
O	4.21405800	0.48320800	-6.40471900
O	-2.97791100	0.38939000	7.25241500
O	-3.41196100	-2.16013900	-6.42054100
C	4.70047100	1.15322800	-4.15452300
H	4.30324800	1.23164500	-3.13803400
C	5.22546300	0.75537900	3.48190500
H	4.83620100	1.54026000	2.82600900
C	5.95272800	-0.37159500	2.77333300
H	5.96891500	-0.33743300	1.68153600
H	5.91109400	-1.36421200	3.22731200
C	6.73837500	0.68482000	3.53412400
H	7.18353500	0.36167400	4.47723200
C	5.71828700	2.19534600	-4.55051600
H	5.73744500	2.48050800	-5.60421400
H	5.94030500	2.97251600	-3.81668500
C	6.19056100	0.79106100	-4.23124700
H	6.49414800	0.16628300	-5.07277000

C	7.48845800	1.69760600	2.72967600
C	6.90388400	0.60116300	-2.93514600
O	6.60446300	1.15503300	-1.88839700
O	6.98874900	2.47979000	1.93802000
O	7.95266900	-0.25754800	-3.08188400
O	8.82511400	1.60997900	2.97978000
C	8.80810400	-0.43005300	-1.90947300
H	8.19219200	-0.30861100	-1.00688200
H	9.16359700	-1.46954900	-1.97828900
C	9.96755600	0.56419000	-1.95338000
H	10.48866000	0.44291500	-2.91918800
H	9.55616400	1.58798200	-1.94759400
C	9.67218800	2.53731400	2.23307600
H	10.61211700	2.53915500	2.80555300
H	9.21509400	3.53807300	2.27580400
C	9.90059000	2.11245200	0.78170500
H	8.95452100	2.22449900	0.22863900
H	10.60744700	2.84670800	0.34708000
C	10.98293500	0.38937100	-0.80587000
H	11.38643600	-0.64055800	-0.83002200
H	11.84461100	1.05003200	-1.01488000
C	10.46704000	0.69195100	0.61675400
H	9.70267400	-0.04550900	0.91791500
H	11.30698700	0.54717500	1.32197800
C	-4.40270500	-1.79103100	-4.28386700
H	-4.27143800	-1.33408400	-3.29936600
C	-4.10509500	0.61229200	5.15691500
H	-3.99189400	0.53629600	4.07407700
C	-5.12736200	1.60279200	5.67360000
H	-5.68071800	2.17815800	4.92965700
H	-4.89561600	2.10912100	6.61298400
C	-5.28783600	-3.01927900	-4.36218100
H	-5.71122700	-3.37587000	-3.42264400
H	-4.99247700	-3.78016500	-5.08758100

C	-5.80893900	-1.72658400	-4.92469000
H	-5.75640500	-1.61457400	-6.00996300
C	-5.41976300	0.11587500	5.77494100
H	-5.32388600	-0.31579900	6.77274100
C	-6.93852300	-0.94066100	-4.33981500
C	-6.53751200	-0.46700100	4.97994800
O	-7.34375100	-1.38139700	-3.10861500
O	-6.54206900	-0.02862400	3.67953100
O	-7.38979300	-1.20497800	5.44234000
O	-7.47523900	-0.01763000	-4.92892900
C	-8.54715100	-0.71097400	-2.60481200
H	-8.29327100	0.33897400	-2.38645400
H	-9.29578200	-0.71439200	-3.41194500
C	-9.05168200	-1.43848000	-1.36597000
H	-10.03110600	-0.98873500	-1.11443700
H	-9.25439200	-2.49592000	-1.61565200
C	-7.73590900	-0.34350800	2.90169600
C	-8.11571800	-1.33988900	-0.15333900
H	-7.17347800	-1.86190200	-0.39960500
H	-7.84487800	-0.27910200	-0.00186100
C	-8.69779100	-1.93128400	1.14326300
H	-8.91690700	-3.00351500	0.98963100
H	-9.67577400	-1.45912900	1.36006200
C	-7.76807400	-1.78012400	2.36783900
H	-4.32998700	-6.77370600	-2.45140200
H	-7.70065400	0.39133100	2.08495200
H	-8.62065000	-0.14595500	3.52797400
H	-6.74129600	-2.07840700	2.09241700
H	-8.07949500	-2.45358700	3.18063700

Intermediate (*S*)-D^{Exo}

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.793409 Hartree

H_corr: 2.137445 Hartree

SCF: -7569.061379 Hartree

S: 689.401 Cal/Mol-Kelvin

G: -7567.26797 Hartree

H: -7566.923934 Hartree

Cartesian Coordinates:

C	-2.56837400	2.95147700	-3.21015700
C	-2.41704900	2.09324800	-2.11334300
C	-2.45461600	2.58863500	-0.80149700
C	-2.66839900	3.96904900	-0.61678700
C	-2.82847500	4.82807000	-1.71169000
C	-2.77745700	4.32238000	-3.01545600
H	-2.51743100	2.55012200	-4.22569000
H	-2.25378300	1.02070400	-2.25057200
H	-2.74195700	4.37473500	0.39693900
H	-3.00230700	5.89525200	-1.54112800
C	-2.47397100	1.65603000	0.41388600
C	-4.01848900	1.22447700	0.63549200
H	-4.64380800	1.75442700	-0.09242500
H	-4.33251500	1.52627600	1.64531000
N	-4.19993400	-0.21993800	0.47341300
S	-2.67619200	-0.87739700	0.89794800
N	-1.74692900	0.32273100	0.12335500
O	-2.52048200	-2.19105100	0.25379300
O	-2.62496100	-0.81147800	2.38489900
C	-4.82796700	-0.77056700	-0.74196100
C	-5.97166800	-1.73258000	-0.43841100
H	-4.07346500	-1.29873100	-1.35260100
H	-5.19632900	0.06898800	-1.35431500
C	-6.78515900	-2.18046500	-1.49577700
C	-7.82816600	-3.08527400	-1.26324600
C	-6.21930400	-2.21363900	0.85563700
C	-7.26313100	-3.12100400	1.08986000
C	-8.07157900	-3.55923500	0.03368100

H	-8.88524300	-4.26752300	0.21792600
H	-7.44040700	-3.48859800	2.10557100
H	-6.60160200	-1.81172300	-2.51121600
H	-8.45280300	-3.42114600	-2.09724000
H	-5.59169900	-1.86722800	1.68068600
C	-1.98944800	2.30991300	1.64973800
H	-1.31769100	3.16625600	1.62391400
H	-2.18673800	1.84521200	2.61504500
C	0.66927100	1.08777100	2.84190300
N	0.72943700	1.27949800	1.46160700
H	1.10291700	2.37790500	4.62488900
C	1.16437800	2.59633400	1.30811300
C	1.39064000	3.20879600	2.59289600
H	1.76646900	4.21925600	2.73713800
C	1.05608600	2.28539800	3.54171500
C	1.35064100	3.26201900	0.09371800
N	0.67134600	1.34205500	-1.33194900
C	0.58553800	1.20451400	-2.71435500
C	0.92315600	2.44078700	-3.37558300
H	0.92973400	2.58365800	-4.45392800
C	1.22963900	3.34095200	-2.39929800
H	1.53024800	4.38038500	-2.50752600
C	1.08081600	2.65850400	-1.13755800
C	0.43373100	-0.12907800	3.49217000
H	0.28959200	-4.64141800	2.54920000
C	0.28544700	-3.55811500	2.45452100
C	0.25480300	-2.84887900	1.19906700
H	0.30627100	-2.76606900	4.52063900
N	0.30011600	-1.47270500	1.40823800
C	0.31266200	-1.33191700	2.79218200
C	0.29364300	-2.61906900	3.44243900
C	0.29738800	0.02304200	-3.41112000
H	-0.22200200	-4.50053900	-2.65475300
C	-0.11350100	-3.42745700	-2.51497100

C	-0.09654500	-2.44361200	-3.45975900
H	-0.17268300	-2.53826100	-4.54174300
C	0.08267800	-1.19547800	-2.75567200
N	0.15771800	-1.40567100	-1.38200100
C	0.05803400	-2.78344500	-1.23520800
C	0.14506000	-3.49132000	-0.03421200
Co	0.20774600	-0.00936700	0.05709000
C	0.06337300	-4.98686600	-0.06911000
C	-1.13035900	-5.62653000	0.30804600
C	1.17028000	-5.74809100	-0.48163800
C	-1.23395500	-7.02862100	0.27870600
H	-1.97488000	-5.00294900	0.60880800
C	1.10637300	-7.15248000	-0.51835300
H	2.08676900	-5.22472200	-0.76405200
C	-0.10424500	-7.76006700	-0.13530500
H	-0.17058600	-8.85230100	-0.16084400
C	1.87006500	4.66935300	0.11382600
C	3.19784000	4.92850800	-0.25100000
C	1.03761500	5.73654700	0.50567100
C	3.72144600	6.23789700	-0.22835300
H	3.83031800	4.08643300	-0.54748200
C	1.51794300	7.05399200	0.53819700
H	0.00165900	5.51505600	0.77085900
C	2.86294600	7.27442600	0.16811100
H	3.24699500	8.29674100	0.19185000
C	0.47626400	-0.15683200	4.99357100
C	-0.68113600	0.11032900	5.76832800
C	1.71218100	-0.41759900	5.65065600
C	-0.58949400	0.13814300	7.17474600
C	1.79512900	-0.37643400	7.05397500
C	0.64105900	-0.09629700	7.78973100
H	-1.47624100	0.36355700	7.76273500
H	2.75404600	-0.55849600	7.53596200
H	0.70236600	-0.06747500	8.88192700

C	0.47244800	0.03795300	-4.90748300
C	1.79722400	-0.04110700	-5.41847600
C	-0.60678500	0.18035800	-5.81803700
C	2.04751900	0.11324000	-6.79278800
C	-0.35208800	0.32320800	-7.19694200
C	0.96751100	0.30602400	-7.65611500
H	3.07381300	0.09003500	-7.15680600
H	-1.18871100	0.44877400	-7.88070700
H	1.15567900	0.42905500	-8.72693800
C	0.63674800	8.25003100	0.95441000
C	1.27101300	8.95858500	2.17784100
H	2.28099300	9.33899700	1.95816300
H	0.65243200	9.81817200	2.48698700
H	1.35134400	8.27226600	3.03666400
C	-0.79304400	7.81908100	1.33916300
H	-1.31753400	7.33459000	0.49921400
H	-0.80003800	7.12588900	2.19647300
H	-1.38324100	8.70374800	1.62844400
C	0.53894700	9.25072600	-0.22466900
H	-0.08723500	10.11496700	0.05509800
H	1.52690700	9.63795700	-0.51991300
H	0.08754900	8.77582700	-1.11109500
C	5.19143800	6.47786600	-0.63100100
C	5.59364900	7.96379000	-0.53859700
H	6.64876900	8.08130200	-0.83468000
H	4.99334700	8.59863600	-1.21102700
H	5.49592400	8.35683800	0.48685500
C	6.12013500	5.66795300	0.30846300
H	5.99466900	5.98191500	1.35758900
H	5.91823000	4.58645600	0.25749000
H	7.17660500	5.82312500	0.03083000
C	5.40471200	6.01052700	-2.09276800
H	4.76338500	6.57679200	-2.78785700
H	6.45381900	6.16468700	-2.39724000

H	5.17458500	4.94130900	-2.22256100
C	-2.52784000	-7.77112700	0.67354800
C	2.30210900	-8.02595300	-0.95323200
C	1.89632500	-8.88341600	-2.17828200
H	2.74021700	-9.51708000	-2.50025300
H	1.04756100	-9.54904100	-1.95492600
H	1.60654300	-8.24619000	-3.02985200
C	2.70751600	-8.95975700	0.21485300
H	1.88407100	-9.62713400	0.51477000
H	3.56111300	-9.59439600	-0.07845600
H	3.00599800	-8.37746100	1.10188900
C	3.53318400	-7.18312500	-1.34409300
H	3.32419800	-6.51178300	-2.19315500
H	3.90097100	-6.57001800	-0.50516000
H	4.35752400	-7.84842000	-1.64860000
C	-3.64226900	-6.80553100	1.12480600
H	-3.34593900	-6.21437000	2.00660400
H	-3.93469900	-6.10364200	0.32751600
H	-4.54117500	-7.38039000	1.40152800
C	-3.04749100	-8.57676700	-0.54377600
H	-2.31256800	-9.32055100	-0.89096300
H	-3.97161500	-9.11877000	-0.27980300
H	-3.27551700	-7.90987700	-1.39125600
C	-2.22956200	-8.74369800	1.84224600
H	-3.14620000	-9.28337000	2.13514000
H	-1.47284200	-9.49762900	1.57278700
H	-1.85986800	-8.19931100	2.72658900
N	-1.91439000	0.33498300	5.10393600
H	-2.01927900	-0.05872200	4.16135900
N	-1.92215400	0.17494500	-5.29179700
H	-1.97950900	0.00360300	-4.28757600
N	2.83578000	-0.31665100	-4.50184800
H	2.53349400	-0.70356200	-3.60853100
N	2.82958800	-0.71905100	4.83871600

H	2.62547700	-0.79449400	3.84268700
C	-2.98096100	1.06658600	5.60887500
C	-3.12640700	0.26086000	-5.97871000
C	4.18517300	-0.00467200	-4.59790000
C	4.13442500	-0.99913700	5.21115100
O	4.69527500	0.59802900	-5.53979100
O	4.56637400	-0.94097700	6.36271800
O	-3.22167800	0.42484300	-7.19502600
O	-2.98287800	1.61238900	6.71338900
C	4.99826300	-1.43181400	4.05535100
H	4.57288700	-1.44106900	3.04734700
C	4.96125900	-0.47191700	-3.39361200
H	4.54821300	-1.29917400	-2.80826000
C	5.75190400	0.54913800	-2.59706700
H	5.79051600	0.40521300	-1.51481500
H	5.74344600	1.58259900	-2.95074700
C	6.47574400	-0.45690700	-3.47596100
H	6.90906100	-0.06227100	-4.39698900
C	6.03385800	-2.49136200	4.34519800
H	6.08545100	-2.85221100	5.37429100
H	6.24042500	-3.21112100	3.55081400
C	6.48541800	-1.06144100	4.11659500
H	6.81200200	-0.49820900	4.99223900
C	7.20586500	-1.57071300	-2.79658100
C	7.16067600	-0.77927100	2.81777300
O	6.82041300	-1.24700100	1.74116100
O	6.70293800	-2.38902500	-2.04501200
O	8.23086700	0.04646200	2.99415300
O	8.53003500	-1.52978400	-3.11525500
C	9.05567300	0.27328300	1.80930400
H	8.40405100	0.26803000	0.92379200
H	9.47451900	1.28058100	1.95371200
C	10.15143200	-0.78819500	1.72121800
H	10.74996200	-0.74689400	2.64802400

H	9.67526600	-1.78323100	1.70259700
C	9.36871900	-2.54662200	-2.48463300
H	10.25581400	-2.58587400	-3.13495200
H	8.83903000	-3.51067100	-2.52670700
C	9.74263500	-2.19830700	-1.04383600
H	8.83529600	-2.25330100	-0.42085200
H	10.41558300	-3.00379500	-0.68881000
C	11.08430300	-0.62600900	0.50435700
H	11.55625500	0.37421400	0.53336300
H	11.91380600	-1.34827000	0.61767700
C	10.43698300	-0.83510100	-0.88118000
H	9.71501900	-0.02879500	-1.09845200
H	11.22907800	-0.73232700	-1.64664300
C	-4.15664300	1.20501100	4.67225400
H	-4.17548600	0.59227500	3.76757500
C	-4.35133600	0.11497400	-5.11143000
H	-4.22885200	0.04845000	-4.02735700
C	-5.50309100	-0.65252900	-5.72332500
H	-6.11667300	-1.25338400	-5.05058900
H	-5.34333800	-1.05019800	-6.72763500
C	-4.77826800	2.58899100	4.61886700
H	-5.19945800	2.91584400	3.66726300
H	-4.30224400	3.35585400	5.23374200
C	-5.50452600	1.49548600	5.35997400
H	-5.44001300	1.51284100	6.44963000
C	-5.60404900	0.85495800	-5.61081400
H	-5.46486600	1.41315700	-6.53825000
C	-6.78208100	0.90639700	4.85906800
C	-6.59680600	1.47939800	-4.68639200
O	-6.98914200	1.15116200	3.52422500
O	-6.68147800	0.81910300	-3.48814700
O	-7.28991500	2.43458800	-4.98320500
O	-7.56703200	0.30289200	5.56794400
C	-8.25934300	0.67455000	2.97878200

H	-8.09446900	-0.34514300	2.59100800
H	-8.98379300	0.61651100	3.80382200
C	-8.71967300	1.62250100	1.87601500
H	-9.74379400	1.31571000	1.58992600
H	-8.80856500	2.64254400	2.29303100
C	-7.76144700	1.23995900	-2.59429900
C	-7.81538700	1.62476500	0.63523800
H	-6.79387500	1.90663700	0.94321700
H	-7.74086600	0.58903300	0.25534100
C	-8.27842300	2.57401700	-0.48430900
H	-8.25560100	3.61389600	-0.11224100
H	-9.33831800	2.37338400	-0.73583200
C	-7.41535000	2.47786200	-1.76235500
H	-2.90341400	4.98793500	-3.87451300
H	-6.34669300	2.43720300	-1.48367900
H	-7.53672100	3.37465200	-2.38943000
H	-7.92170400	0.35500200	-1.96177100
H	-8.66170000	1.41710600	-3.20279100

Intermediate (*R*)-D^{Exo}

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.794947 Hartree

H_corr: 2.137612 Hartree

SCF: -7569.062205 Hartree

S: 686.654 Cal/Mol-Kelvin

G: -7567.267258 Hartree

H: -7566.924593Hartree

Cartesian Coordinates:

C	2.27410600	-3.51771100	2.69005100
C	2.20252100	-2.54559200	1.68355600
C	2.19834900	-2.90968500	0.33007900
C	2.30207700	-4.27805100	0.00751200
C	2.39149400	-5.25078300	1.01108600

C	2.37144700	-4.87482700	2.35959100
H	2.24891300	-3.21500000	3.74012800
H	2.12283900	-1.48311500	1.92670100
H	2.33880900	-4.58523300	-1.04246800
H	2.48303400	-6.30597200	0.73456700
C	2.25566700	-1.87286900	-0.79510100
C	3.81955900	-1.58001200	-1.09292900
H	4.02486000	-1.75832400	-2.15756800
H	4.43322400	-2.26859100	-0.49980500
N	4.18220600	-0.19668300	-0.76765700
S	2.71992400	0.65809800	-1.07535200
N	1.70423800	-0.50128000	-0.34160900
O	2.59119600	0.70778000	-2.55664200
O	2.73592700	1.92325500	-0.32733800
C	4.79528600	0.10015600	0.54414500
C	5.86564900	1.17974000	0.47185100
H	4.03487900	0.38211300	1.29566900
H	5.25586300	-0.83858500	0.89637100
C	6.42222100	1.59454500	-0.74803900
C	7.45131400	2.54714800	-0.77146700
C	6.35174300	1.74074700	1.66607700
C	7.38528800	2.68496600	1.64483200
C	7.94040500	3.09123200	0.42285500
H	8.74495100	3.83291800	0.40337900
H	7.75553500	3.10177500	2.58625100
H	6.02899900	1.17521700	-1.67802200
H	7.86977700	2.86715800	-1.73121500
H	5.91986100	1.44042500	2.62738500
C	1.63387000	-2.36025000	-2.04560500
H	0.88608200	-3.15219000	-2.04988200
H	1.83314800	-1.83777800	-2.98119700
C	-0.46403700	-1.12968900	2.73103400
N	-0.68542400	-1.25063800	1.36191100
H	-0.87430000	-2.43583900	4.51093100

C	-1.28898400	-2.49658100	1.21495600
C	-1.44307900	-3.14539400	2.49363700
H	-1.88424600	-4.12881900	2.63762200
C	-0.93150700	-2.29912700	3.43284900
C	-1.70323500	-3.06937200	0.00953600
N	-0.95013800	-1.17616600	-1.41857400
C	-0.97460900	-0.98790200	-2.80038900
C	-1.53284200	-2.13958100	-3.46128700
H	-1.67341500	-2.22764600	-4.53639600
C	-1.88889300	-3.02440800	-2.48409900
H	-2.37809800	-3.98958100	-2.59438100
C	-1.50871500	-2.43885300	-1.22321300
C	0.07102100	-0.01079800	3.38473000
H	0.97597700	4.43815500	2.57385900
C	0.75884600	3.38023000	2.44469200
C	0.38496800	2.77100500	1.19140600
H	0.97449600	2.46282000	4.44658700
N	0.16552300	1.40781000	1.34740400
C	0.37411500	1.17513300	2.70280900
C	0.76482400	2.38958800	3.38107400
C	-0.67326900	0.20398500	-3.47146400
H	-0.00043400	4.67466400	-2.55293500
C	-0.10612600	3.59629700	-2.45823900
C	-0.29065200	2.66875800	-3.44083700
H	-0.37529400	2.82222900	-4.51530000
C	-0.37612700	1.38430400	-2.78900400
N	-0.23506900	1.51502100	-1.41206300
C	-0.04553900	2.87867400	-1.20868400
C	0.23777000	3.49653300	0.00914900
Co	-0.18021500	0.04176000	-0.07314200
C	0.46115200	4.97940300	0.03310200
C	1.75135000	5.48965800	-0.15718500
C	-0.62037700	5.85675200	0.24028900
C	1.98773200	6.88074500	-0.14749000

H	2.56951100	4.78110900	-0.31497400
C	-0.42468200	7.24606300	0.25754200
H	-1.61573800	5.43063500	0.38605900
C	0.88811600	7.72819100	0.06003000
H	1.05042600	8.80851500	0.06972700
C	-2.39969000	-4.39734000	0.04122500
C	-3.72073700	-4.47843800	0.50199700
C	-1.74244500	-5.56548700	-0.39347800
C	-4.40957900	-5.70858700	0.53710500
H	-4.21585500	-3.55928600	0.82956700
C	-2.39225600	-6.80864100	-0.37391300
H	-0.70712000	-5.48152000	-0.73088300
C	-3.72362600	-6.85005600	0.09550500
H	-4.23723400	-7.81389100	0.11482600
C	0.06275800	0.01058700	4.89107500
C	1.19470000	-0.33104900	5.67540600
C	-1.14190700	0.39744800	5.54701800
C	1.11465400	-0.30068700	7.08274500
C	-1.21617700	0.41934400	6.95166300
C	-0.08592200	0.06828600	7.69183700
H	1.98792700	-0.57289500	7.67065800
H	-2.14960500	0.71131100	7.42968000
H	-0.13995600	0.08675600	8.78457300
C	-0.88600300	0.23650200	-4.95727800
C	-2.20533700	0.44965200	-5.43689900
C	0.16220400	-0.02047900	-5.88070500
C	-2.50295800	0.31955500	-6.80242600
C	-0.14604900	-0.14200400	-7.25297300
C	-1.46611500	0.01020500	-7.68524000
H	-3.52874800	0.44795700	-7.14650800
H	0.65274400	-0.36779900	-7.95530000
H	-1.68662100	-0.09784100	-8.75164000
C	-1.70738700	-8.11236800	-0.83408900
C	-1.64046500	-9.10325900	0.35539800

H	-2.64192800	-9.35475600	0.73893500
H	-1.15633000	-10.04494300	0.04527500
H	-1.05898500	-8.68035500	1.19092300
C	-0.27149500	-7.87204800	-1.34211200
H	-0.24842700	-7.19453300	-2.21156700
H	0.37727600	-7.44815800	-0.55830900
H	0.17622400	-8.82797500	-1.65918100
C	-2.52451000	-8.74852100	-1.98675500
H	-2.04577700	-9.68276200	-2.32600200
H	-3.55254300	-8.99614200	-1.67883900
H	-2.58891100	-8.06739000	-2.85099300
C	-5.86558700	-5.75288700	1.04571100
C	-6.45568800	-7.17748900	1.02211400
H	-7.49208000	-7.15562300	1.39655300
H	-6.48521100	-7.59750400	0.00318500
H	-5.89018600	-7.87132000	1.66587100
C	-5.91603200	-5.23383100	2.50476600
H	-5.30223600	-5.86241300	3.17066000
H	-5.54871200	-4.19893600	2.58883600
H	-6.95214700	-5.25035700	2.88341100
C	-6.74907300	-4.84977500	0.14860700
H	-6.73463000	-5.19470300	-0.89818100
H	-7.79550600	-4.86746600	0.49798000
H	-6.41187400	-3.80141600	0.16010200
C	3.42152300	7.40863200	-0.35952700
C	-1.57998500	8.24417200	0.48028100
C	-1.70339200	9.17231000	-0.75441500
H	-2.52340600	9.89645800	-0.61082400
H	-0.78034600	9.74607500	-0.93344800
H	-1.91897800	8.59177800	-1.66633000
C	-1.28662900	9.10019900	1.73811900
H	-0.35137300	9.67350000	1.63914100
H	-2.10292100	9.82225900	1.91055400
H	-1.19763000	8.46725700	2.63623600

C	-2.93494700	7.53696000	0.68671700
H	-3.22610800	6.93312800	-0.18837200
H	-2.92738600	6.87905600	1.57136900
H	-3.72626700	8.28806700	0.84350500
C	3.95271900	6.91586800	-1.72923600
H	3.97681000	5.81702100	-1.79151500
H	3.32333000	7.28651500	-2.55513200
H	4.98055600	7.28114900	-1.89511800
C	3.49222800	8.94898200	-0.34173700
H	3.16373700	9.36888500	0.62349800
H	4.53340200	9.27370400	-0.50125900
H	2.88209000	9.40164700	-1.14099700
C	4.33570500	6.86793500	0.76873100
H	5.36909700	7.22943500	0.63168000
H	3.98601800	7.20700000	1.75792300
H	4.36826500	5.76769600	0.78165600
N	2.38998400	-0.69295500	5.00300800
H	2.36650600	-0.58063100	3.98920600
N	1.48535900	-0.14577000	-5.38725400
H	1.64331300	0.14956100	-4.41728100
N	-3.19492200	0.82302500	-4.49595900
H	-2.84389000	1.25123000	-3.63991000
N	-2.23853300	0.75739000	4.73312700
H	-2.05606100	0.72449900	3.73082200
C	3.55699500	-1.21037900	5.55254400
C	2.62053600	-0.48336300	-6.11744800
C	-4.54544900	0.50197400	-4.50132500
C	-3.50037200	1.19807900	5.10069500
O	-5.09655300	-0.16330900	-5.37472900
O	-3.90110400	1.30094400	6.26009400
O	2.60965100	-0.80980200	-7.30571800
O	3.72485400	-1.40702100	6.75618500
C	-4.35554600	1.58285900	3.92154800
H	-3.97716800	1.40509000	2.91041400

C	-5.25864200	1.04154900	-3.28573500
H	-4.86716400	1.95710900	-2.83146400
C	-5.88185400	0.05589100	-2.31457000
H	-5.84583000	0.31766700	-1.25430400
H	-5.81041600	-1.00729600	-2.55493100
C	-6.76508700	0.89627400	-3.22545700
H	-7.23536400	0.37067700	-4.05867700
C	-5.24644200	2.79104900	4.09091800
H	-5.21117100	3.29315800	5.05977200
H	-5.40326700	3.41654600	3.20997400
C	-5.86968300	1.40815900	4.07830000
H	-6.21558200	1.01600300	5.03598100
C	-7.53827700	2.00559200	-2.59232400
C	-6.64429700	1.03522500	2.85953200
O	-6.30222100	1.28229900	1.71289500
O	-7.06022200	2.92451400	-1.94772900
O	-7.80542200	0.41053100	3.20620500
O	-8.87428500	1.83227400	-2.80702600
C	-8.75432600	0.14603700	2.12705900
H	-8.20667900	0.13780000	1.17426700
H	-9.14944800	-0.86063500	2.33397700
C	-9.86106800	1.19950700	2.15563200
H	-10.31964300	1.19127100	3.15982300
H	-9.40382300	2.19675300	2.03403000
C	-9.75052500	2.82063800	-2.18547300
H	-10.68726500	2.73029700	-2.75612600
H	-9.31868400	3.82074400	-2.34385600
C	-9.97023500	2.55672500	-0.69548300
H	-9.01839400	2.73175600	-0.16860900
H	-10.67567600	3.32995000	-0.33263500
C	-10.95739300	0.97964800	1.09382800
H	-11.38951000	-0.03089700	1.22082200
H	-11.78290200	1.68346400	1.30760000
C	-10.52583500	1.15865000	-0.37665500

H	-9.78000600	0.39531000	-0.65858700
H	-11.40507400	0.96083600	-1.01827700
C	4.62942400	-1.56986800	4.55366300
H	4.48860800	-1.30571600	3.50201100
C	3.91508300	-0.39133500	-5.34942600
H	3.87657900	-0.20520600	-4.27416100
C	5.07301200	0.23240700	-6.10064800
H	5.78175000	0.81767400	-5.51228200
H	4.87862200	0.57708900	-7.11844500
C	5.39294900	-2.84957500	4.84061900
H	5.73192500	-3.42316000	3.97727600
H	5.07316000	-3.41858900	5.71620000
C	6.06697900	-1.53032700	5.11012700
H	6.10856600	-1.20705500	6.15226100
C	5.05115700	-1.27095700	-5.89120100
H	4.79143200	-1.85950700	-6.77292800
C	7.22537000	-1.02857500	4.30972200
C	6.08916400	-1.91390800	-5.03607500
O	7.37307900	-1.66768600	3.10801000
O	6.23919600	-1.28440300	-3.82794000
O	6.76858200	-2.86081800	-5.39148700
O	7.98375700	-0.16280300	4.70976400
C	8.57934700	-1.28669400	2.36739600
H	8.43166300	-0.26808100	1.97199100
H	9.41577600	-1.25132400	3.08171900
C	8.83006900	-2.29657900	1.25556900
H	9.82610700	-2.05784300	0.83617800
H	8.91615600	-3.30886700	1.69074300
C	7.39188900	-1.69497700	-3.03131100
C	7.78860400	-2.27838800	0.12709600
H	6.81614400	-2.62081000	0.52564300
H	7.63894900	-1.23035900	-0.19180800
C	8.16623700	-3.14891700	-1.08503100
H	8.20972500	-4.20833200	-0.77505900

H	9.19148300	-2.89614900	-1.41945100
C	7.18787400	-3.00991900	-2.27163300
H	2.43210700	-5.63158400	3.14749100
H	7.53303800	-0.84836400	-2.34460900
H	8.26550100	-1.76754300	-3.69884000
H	6.15022500	-3.05333200	-1.89854300
H	7.30430700	-3.84769500	-2.97569900

Transition state TS3^{R}:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -163.8064 cm-1

H_corr: 2.139424 Hartree

G_corr: 1.797076 Hartree

SCF: -7569.088676 Hartree

S: 686.018 Cal/Mol-Kelvin

H: -7566.949252 Hartree

G: -7567.291600 Hartree

Cartesian Coordinates:

C	-4.41215100	2.80713700	-3.65480300
C	-4.29093500	2.04142800	-2.49546200
C	-3.33846200	2.36530800	-1.48953400
C	-2.50693100	3.49371800	-1.72133700
C	-2.63704600	4.26141400	-2.87784300
C	-3.59059600	3.92714900	-3.85028200
H	-5.15549800	2.53287600	-4.40850200
H	-4.95159600	1.18100400	-2.37126300
H	-1.75384500	3.77978400	-0.98500500
H	-1.98526900	5.12727900	-3.02212000
C	-3.29278500	1.64036900	-0.23071600
C	-4.49694500	0.84134000	0.27486300
H	-5.37260900	0.97324000	-0.37037000
H	-4.77076100	1.23725100	1.26883200
N	-4.27138300	-0.61315000	0.42786900

S	-2.69964700	-0.81663800	1.11992200
N	-1.77875200	0.43787200	0.28833000
O	-2.21002300	-2.13192400	0.71015100
O	-2.84128200	-0.47031900	2.55582200
C	-4.48509500	-1.44139900	-0.78438800
C	-4.95217800	-2.85171100	-0.47096400
H	-3.58846800	-1.47305100	-1.43136000
H	-5.27733700	-0.93336900	-1.36005500
C	-4.59253400	-3.91133300	-1.31951000
C	-5.09915800	-5.19979100	-1.10507400
C	-5.81228700	-3.10699500	0.61012100
C	-6.31120100	-4.39648100	0.83185900
C	-5.96304100	-5.44583800	-0.02957200
H	-6.35382800	-6.45323300	0.14328100
H	-6.97197700	-4.58401000	1.68415100
H	-3.89683900	-3.73114500	-2.14610000
H	-4.80797500	-6.01604200	-1.77355500
H	-6.06069000	-2.29106700	1.29508100
C	-2.20904000	1.77981100	0.76634600
H	-1.42817800	2.51340700	0.55022500
H	-2.50439400	1.83782200	1.82459800
C	0.65328100	1.51250400	2.77762100
N	0.71806600	1.58999800	1.39253000
H	1.00266200	2.97791800	4.44749200
C	1.08122400	2.90677300	1.12419100
C	1.26721200	3.64115100	2.35458900
H	1.59164300	4.67740800	2.41648900
C	0.97144000	2.78708000	3.37680900
C	1.20065900	3.47906900	-0.14909600
N	0.53451300	1.43194500	-1.39881800
C	0.30325300	1.19867900	-2.74891100
C	0.50784200	2.40427100	-3.51510700
H	0.38449700	2.48167500	-4.59337900
C	0.89846300	3.37205500	-2.63504800

H	1.15144400	4.40958000	-2.84249600
C	0.91108800	2.76872200	-1.32328700
C	0.45811600	0.34305300	3.52715000
H	0.82869200	-4.22233400	2.95635800
C	0.69368700	-3.15949900	2.76988300
C	0.62432000	-2.55707700	1.45893600
H	0.51515200	-2.22076200	4.76632300
N	0.48962300	-1.17858600	1.56338700
C	0.44274500	-0.92365600	2.92961900
C	0.53642200	-2.15476200	3.67984300
C	0.05028000	-0.05269900	-3.33840900
H	0.26517600	-4.54109100	-2.26195800
C	0.21846700	-3.45626300	-2.19687500
C	0.00387100	-2.55443400	-3.19803100
H	-0.14219900	-2.74141200	-4.26070500
C	0.05109200	-1.24143800	-2.59269200
N	0.25571400	-1.34076400	-1.22149100
C	0.38137900	-2.70031300	-0.97491200
C	0.61266500	-3.29477000	0.27059600
Co	0.30949000	0.13993800	0.09387500
C	0.80248900	-4.77984300	0.33375200
C	-0.21168200	-5.60569300	0.85047600
C	2.00158400	-5.35098200	-0.12750400
C	-0.04144000	-6.99985400	0.92004100
H	-1.13903000	-5.13558400	1.18470400
C	2.20908700	-6.74060400	-0.07515700
H	2.77628600	-4.68643300	-0.51688000
C	1.17383100	-7.53520100	0.45221000
H	1.32053900	-8.61886600	0.50117700
C	1.62222600	4.91384800	-0.26401500
C	2.88246500	5.23575300	-0.79857500
C	0.76590100	5.94813000	0.15575700
C	3.30321700	6.57214400	-0.91659200
H	3.53467100	4.41747200	-1.11146500

C	1.14536800	7.29782700	0.04984200
H	-0.20872200	5.67936100	0.57011400
C	2.41574100	7.57708200	-0.48779700
H	2.72886800	8.62228600	-0.57352500
C	0.46786900	0.47143500	5.02444000
C	-0.69208700	0.87293400	5.73324300
C	1.68679700	0.28917000	5.74000200
C	-0.62546700	1.11266600	7.11951600
C	1.74590300	0.54044600	7.12265100
C	0.58849800	0.95261400	7.78784500
H	-1.51678700	1.44201300	7.65008300
H	2.69474800	0.42457200	7.64351400
H	0.63468600	1.14711700	8.86371600
C	0.11593400	-0.13032400	-4.84311300
C	1.40454500	-0.11856500	-5.45066700
C	-1.03002100	-0.18236700	-5.67707200
C	1.54214200	-0.08244100	-6.84945600
C	-0.88871700	-0.14926400	-7.07961100
C	0.39002600	-0.08722300	-7.63823800
H	2.53928400	-0.04379700	-7.28596200
H	-1.77877600	-0.17874400	-7.70403100
H	0.48994700	-0.05489800	-8.72748400
C	0.22926000	8.45625300	0.49827000
C	0.93742800	9.27153700	1.60952300
H	1.89158200	9.69923600	1.26336800
H	0.29803100	10.10782700	1.93965700
H	1.15266900	8.64171600	2.48805300
C	-1.11934400	7.95729300	1.05616700
H	-1.69660300	7.39481100	0.30370000
H	-0.98976500	7.31463300	1.94240000
H	-1.73518100	8.81792800	1.36405400
C	-0.06132800	9.38166000	-0.70989300
H	-0.71377500	10.21781200	-0.40594800
H	0.86022100	9.81508700	-1.12947000

H	-0.56952800	8.83093200	-1.51847000
C	4.68504600	6.96085500	-1.48341800
C	5.48366100	7.73469400	-0.40438500
H	6.47568400	8.02197600	-0.79258600
H	4.96913900	8.65728200	-0.09224800
H	5.63621800	7.11653800	0.49530500
C	5.51404100	5.73009100	-1.90346500
H	5.71947100	5.06042600	-1.05215600
H	5.01379700	5.14324100	-2.69122200
H	6.48666100	6.05730800	-2.30573800
C	4.49723500	7.86318900	-2.72885300
H	3.95062400	8.78922600	-2.49007500
H	5.47715800	8.15367700	-3.14425200
H	3.93639300	7.33764200	-3.51904600
C	-1.12997800	-7.94099600	1.47815200
C	3.51564700	-7.40266800	-0.56148900
C	3.19217300	-8.42182600	-1.68275100
H	4.11674600	-8.90702700	-2.03954400
H	2.51253200	-9.21676800	-1.33684100
H	2.71551400	-7.92551500	-2.54397600
C	4.18902300	-8.14042400	0.62303800
H	3.53938700	-8.92433400	1.04389900
H	5.12465900	-8.62388200	0.29354200
H	4.43694900	-7.43903700	1.43630600
C	4.52037900	-6.37576400	-1.12251600
H	4.11390600	-5.82972700	-1.98958800
H	4.82710700	-5.63518600	-0.36627700
H	5.43169100	-6.89608500	-1.46042300
C	-2.37056500	-7.17208800	1.97610500
H	-2.12323900	-6.46935900	2.78854700
H	-2.86087400	-6.60174600	1.17090600
H	-3.11281300	-7.88409600	2.37325100
C	-1.58056200	-8.92024600	0.36520800
H	-0.74522400	-9.53495400	-0.00637200

H	-2.35627100	-9.60638100	0.74647900
H	-2.00194300	-8.37393600	-0.49446500
C	-0.55484400	-8.74902000	2.66854400
H	-1.32234500	-9.42777000	3.07810600
H	0.30945200	-9.36504400	2.37371700
H	-0.22672400	-8.07931000	3.48027100
N	-1.92007000	1.00799500	5.03256100
H	-2.05086500	0.43006900	4.19575400
N	-2.29854700	-0.28430100	-5.05373700
H	-2.27460500	-0.25470900	-4.03345100
N	2.52063700	-0.17589400	-4.59061000
H	2.29465900	-0.37708800	-3.61711000
N	2.81564600	-0.15052600	5.01130300
H	2.62211800	-0.42891900	4.04957000
C	-2.94657200	1.87353600	5.37505700
C	-3.51924500	-0.55647100	-5.64877800
C	3.85724100	0.08199700	-4.85181700
C	4.12512100	-0.30604100	5.43666000
O	4.31116700	0.42142300	-5.94410300
O	4.54993800	0.02625200	6.54387500
O	-3.71137700	-0.61084300	-6.86441700
O	-2.88176500	2.69596400	6.29049700
C	5.00680400	-0.96990200	4.41099600
H	4.56700400	-1.29173600	3.46240100
C	4.71075900	-0.08273200	-3.62305600
H	4.27171700	-0.58111100	-2.75351900
C	5.73786800	0.98240600	-3.30418300
H	5.89398500	1.21959800	-2.24960700
H	5.83181500	1.81148500	-4.00898400
C	6.19300800	-0.37492600	-3.80915400
H	6.56568800	-0.40110400	-4.83491800
C	6.14042700	-1.81284300	4.93911200
H	6.23503500	-1.86630400	6.02538400
H	6.40228000	-2.70392300	4.36548000

C	6.46029000	-0.47481700	4.30664100
H	6.74295000	0.34379500	4.97047200
C	6.80748800	-1.32399100	-2.82905600
C	7.06791700	-0.50704400	2.94516400
O	6.81574300	-1.34620200	2.09384300
O	6.26955400	-1.72599000	-1.80981200
O	7.95396500	0.51505200	2.77688100
O	8.06251700	-1.66857200	-3.22200400
C	8.64122700	0.54385800	1.48669800
H	7.91877100	0.27136800	0.70287600
H	8.93810100	1.59671800	1.36524100
C	9.85132100	-0.38871600	1.49216600
H	10.49321100	-0.12120600	2.34999100
H	9.49746600	-1.41718900	1.67249200
C	8.76842900	-2.63132200	-2.37526500
H	9.62629900	-2.91878400	-3.00156300
H	8.11592000	-3.50707100	-2.23110600
C	9.22666100	-2.07689200	-1.02412100
H	8.36016000	-2.00854300	-0.34866000
H	9.90221500	-2.84174200	-0.59225900
C	10.69035400	-0.33679900	0.19898000
H	11.11868700	0.67591000	0.07756100
H	11.55567200	-1.01135200	0.33582900
C	9.95854600	-0.72692800	-1.10338000
H	9.23844100	0.06113100	-1.38623000
H	10.70128000	-0.75010200	-1.92265700
C	-4.19130900	1.74905600	4.52716300
H	-4.25082300	0.92597500	3.81148300
C	-4.63667800	-0.84752200	-4.67584600
H	-4.44948400	-0.70471300	-3.61031600
C	-5.56434000	-1.98131400	-5.05138500
H	-5.96695200	-2.58581300	-4.23676100
H	-5.35416100	-2.49732500	-5.99038100
C	-4.91694100	3.03564600	4.19213900

H	-5.44003700	3.08667500	3.23573100
H	-4.45874100	3.96073300	4.54919700
C	-5.49594900	2.13504000	5.25552300
H	-5.33964000	2.44623700	6.28992000
C	-6.05747400	-0.55011100	-5.17769900
H	-6.10839600	-0.15945800	-6.19579700
C	-6.74873600	1.35111600	5.06798100
C	-7.16009900	-0.06414300	-4.29945900
O	-7.04640700	1.12706300	3.74162900
O	-6.98108400	-0.42111800	-2.98315700
O	-8.13640100	0.54062300	-4.70150300
O	-7.43955200	0.96194300	5.99154900
C	-8.25413700	0.34673000	3.48702000
H	-7.93336700	-0.69275400	3.29785300
H	-8.86621300	0.35722100	4.39993200
C	-9.00621000	0.92022400	2.29056200
H	-9.94976400	0.34878500	2.19922500
H	-9.29815100	1.96292700	2.51179700
C	-8.12400700	-0.20650700	-2.09310200
C	-8.22996300	0.85360800	0.96766100
H	-7.31845400	1.46903600	1.06197100
H	-7.88056700	-0.18561900	0.81751600
C	-9.03125600	1.32682000	-0.25802500
H	-9.34294900	2.37525800	-0.10426300
H	-9.97112400	0.74730100	-0.34065100
C	-8.24283900	1.23346500	-1.58279700
H	-3.69045300	4.53106100	-4.75671300
H	-7.23080600	1.65156100	-1.43196600
H	-8.71432900	1.84900300	-2.36425300
H	-7.93910100	-0.91923800	-1.27638300
H	-9.03708300	-0.50814100	-2.62869900

Transition State TS3^{S}:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -179.2102 cm-1

H_corr: 2.139315 Hartree

G_corr: 1.796714 Hartree

SCF: -7569.083772 Hartree

S: 686.527 Cal/Mol-Kelvin

H: -7566.944457 Hartree

G: -7567.287058 Hartree

Cartesian Coordinates:

C	-3.73897700	-4.45771200	-2.79991500
C	-3.80051200	-3.49893600	-1.78873100
C	-2.73436000	-3.33008700	-0.86248600
C	-1.59809900	-4.16835200	-1.02523100
C	-1.53987800	-5.12384000	-2.03780900
C	-2.61123800	-5.28051300	-2.92892300
H	-4.57565800	-4.56316700	-3.49512300
H	-4.69485000	-2.87515700	-1.71743000
H	-0.74513300	-4.07095300	-0.35221000
H	-0.64863800	-5.74999900	-2.13205800
C	-2.83862800	-2.41155800	0.25970100
C	-4.18382900	-1.85487200	0.73183300
H	-4.31693900	-2.14605100	1.78894400
H	-5.02449400	-2.28648500	0.17774200
N	-4.31216300	-0.38415000	0.65985300
S	-2.81076200	0.30820000	1.15495700
N	-1.65085300	-0.81993800	0.45852800
O	-2.77257000	0.20435800	2.63365300
O	-2.69348200	1.60650800	0.49206000
C	-4.86037800	0.19196800	-0.58823100
C	-5.71802300	1.42600400	-0.35251500
H	-4.06946100	0.41748800	-1.32724400
H	-5.49796700	-0.59234200	-1.03168000
C	-6.29952600	1.69254000	0.89759100
C	-7.15683500	2.78955000	1.06116400

C	-6.00329700	2.27850800	-1.43269300
C	-6.86969600	3.36693300	-1.27300600
C	-7.45103200	3.62552400	-0.02382600
H	-8.12359100	4.47924800	0.10383800
H	-7.08917400	4.01291500	-2.12813300
H	-6.05482000	1.04694600	1.74555600
H	-7.59410700	2.99263200	2.04397300
H	-5.54765700	2.09265800	-2.41132500
C	-1.72373300	-2.11663300	1.18455700
H	-0.79628600	-2.67528500	1.04232100
H	-1.96648500	-2.04985000	2.25541700
C	0.41093900	-1.23798800	-2.69310300
N	0.75712700	-1.32070800	-1.35009000
H	0.72629400	-2.57316600	-4.47441300
C	1.46240500	-2.51303100	-1.23184600
C	1.53958200	-3.18295400	-2.50921500
H	2.03577200	-4.13561200	-2.68104600
C	0.87620300	-2.40076700	-3.41041300
C	1.96879100	-3.05531000	-0.04175100
N	1.09520100	-1.24984500	1.42731200
C	1.04662200	-1.11217200	2.80892400
C	1.66062600	-2.24792200	3.45530200
H	1.76132200	-2.37025800	4.53160100
C	2.12830700	-3.06222500	2.46464200
H	2.68690100	-3.98994400	2.56585800
C	1.75034000	-2.45804700	1.20776800
C	-0.17249200	-0.12686700	-3.32719500
H	-0.94358600	4.35278500	-2.51180100
C	-0.75109500	3.28981700	-2.38289400
C	-0.37441800	2.67109000	-1.13176000
H	-1.03721200	2.37643500	-4.37762400
N	-0.19088300	1.30484200	-1.29670000
C	-0.42894700	1.07232400	-2.64488400
C	-0.80500300	2.29789500	-3.31694500

C	0.62302400	0.03033000	3.50649100
H	-0.12683200	4.51099100	2.66899600
C	0.00162200	3.43706400	2.55202800
C	0.14553300	2.48784300	3.52264200
H	0.17014300	2.61846400	4.60342500
C	0.29665700	1.21995300	2.84640500
N	0.20931900	1.38538400	1.46907200
C	0.01697600	2.74784300	1.28310000
C	-0.22447700	3.38230700	0.06144800
Co	0.28814000	-0.03171700	0.08470200
C	-0.37555400	4.87532900	0.04520800
C	-1.64316100	5.46344300	0.13917400
C	0.76864400	5.69074000	-0.05385000
C	-1.79464900	6.86666600	0.13824500
H	-2.51469500	4.80748900	0.22194200
C	0.65948800	7.08917600	-0.06246000
H	1.74526800	5.20641500	-0.12510900
C	-0.63353900	7.64848100	0.03610400
H	-0.72933300	8.73676100	0.03352300
C	2.74146300	-4.33876100	-0.11138400
C	4.00924100	-4.36157600	-0.70906400
C	2.20684600	-5.53399400	0.41367600
C	4.76121600	-5.55187100	-0.79270200
H	4.41306000	-3.42509500	-1.10518200
C	2.91996600	-6.73999500	0.34914000
H	1.21779000	-5.50121200	0.87690500
C	4.19432500	-6.71936000	-0.25928500
H	4.75957500	-7.65257000	-0.31269900
C	-0.19195400	-0.11380400	-4.83448100
C	-1.33693200	-0.44091000	-5.60536100
C	1.01200900	0.24505300	-5.50963900
C	-1.26514600	-0.44509600	-7.01411400
C	1.07792800	0.23530100	-6.91467900
C	-0.06213900	-0.11460000	-7.63960700

H	-2.14939300	-0.70469900	-7.59074100
H	2.01252700	0.50325000	-7.40442000
H	-0.01508600	-0.12400400	-8.73287000
C	0.80617400	0.02372600	4.99852900
C	2.10050200	0.32260300	5.50473900
C	-0.21821500	-0.37015400	5.89986800
C	2.39859300	0.15647100	6.86622000
C	0.09048500	-0.53368000	7.26764400
C	1.38767700	-0.28505400	7.72254100
H	3.40790200	0.35434600	7.22558400
H	-0.68744700	-0.87037700	7.94878300
H	1.60999100	-0.42565000	8.78482100
C	2.36696000	-8.06460500	0.91572800
C	2.26717300	-9.11151000	-0.22217200
H	3.24642000	-9.31524600	-0.68332900
H	1.87754700	-10.06731100	0.16748900
H	1.58748900	-8.76770400	-1.01924200
C	0.96654700	-7.89865800	1.54013800
H	0.96953600	-7.18845600	2.38325500
H	0.22137800	-7.55547500	0.80346500
H	0.61665100	-8.86789000	1.93106000
C	3.32394300	-8.59226500	2.01453500
H	2.94586100	-9.54183000	2.42994600
H	4.33690900	-8.77976300	1.62492900
H	3.41262000	-7.87090500	2.84317200
C	6.15734900	-5.52669200	-1.44904800
C	6.83124200	-6.91381900	-1.45605200
H	7.82117500	-6.84261300	-1.93536100
H	6.98897300	-7.30364800	-0.43687000
H	6.24619000	-7.65637100	-2.02355700
C	6.02761800	-5.04600400	-2.91629000
H	5.38780800	-5.72703000	-3.50135700
H	5.59284400	-4.03650400	-2.98467500
H	7.01884200	-5.01390700	-3.39962300

C	7.07219400	-4.55010600	-0.66776200
H	7.18603400	-4.86705600	0.38177900
H	8.07620600	-4.51708700	-1.12416200
H	6.67302000	-3.52377100	-0.66578100
C	-3.20545500	7.48092500	0.25076100
C	1.88719100	8.01710200	-0.17315200
C	1.96550200	8.91937800	1.08415100
H	2.83646500	9.59382900	1.02011600
H	1.06691400	9.54609400	1.19920800
H	2.07136000	8.31437700	1.99944100
C	1.74877000	8.90625700	-1.43462000
H	0.84528400	9.53542500	-1.40004000
H	2.61897800	9.57814400	-1.52875900
H	1.69367600	8.29153300	-2.34800100
C	3.20937100	7.23086700	-0.28349300
H	3.39288000	6.59781500	0.59988400
H	3.23367800	6.58677400	-1.17784900
H	4.05453500	7.93405600	-0.36271900
C	-3.86366000	7.01499700	1.57388600
H	-3.96095100	5.91948700	1.62284700
H	-3.27211500	7.33981800	2.44570300
H	-4.87571400	7.44403300	1.67087400
C	-3.18071500	9.02290000	0.24307800
H	-2.75359300	9.42642800	-0.68995000
H	-4.20936100	9.41037600	0.32602700
H	-2.60729800	9.43298900	1.09090800
C	-4.06768200	7.00604400	-0.94566000
H	-5.08249000	7.43471700	-0.88142900
H	-3.62458400	7.32498500	-1.90361700
H	-4.17112000	5.91026700	-0.96967600
N	-2.54053800	-0.74516600	-4.91800900
H	-2.47092800	-0.71909500	-3.89971300
N	-1.52888600	-0.57329500	5.39570000
H	-1.71026000	-0.22549100	4.44862800

N	3.06685300	0.80581500	4.59074500
H	2.68819400	1.21129600	3.73512100
N	2.11454100	0.62607900	-4.71340100
H	1.92862600	0.64583500	-3.71117600
C	-3.77187700	-1.06188700	-5.46600700
C	-2.62846700	-1.04999000	6.09904800
C	4.43698400	0.58540100	4.59650300
C	3.36971400	1.06522900	-5.10208600
O	5.03855400	-0.03801900	5.46786100
O	3.77479900	1.10667200	-6.26429000
O	-2.57640900	-1.51874000	7.23800500
O	-3.99345100	-1.16516500	-6.67403800
C	4.21018700	1.54340800	-3.94610900
H	3.83539200	1.41270400	-2.92659600
C	5.10561100	1.17282600	3.37739700
H	4.64398900	2.05250200	2.91826900
C	5.79231700	0.22656700	2.41032500
H	5.73053800	0.47504500	1.34816500
H	5.79900800	-0.83676300	2.66002400
C	6.61801300	1.13773800	3.30793400
H	7.13237500	0.65539500	4.14127600
C	5.05127200	2.77515400	-4.18812400
H	4.99696400	3.21653200	-5.18521800
H	5.18159300	3.45781900	-3.34622000
C	5.72987100	1.42139800	-4.09294000
H	6.09374800	0.98664700	-5.02524800
C	7.30375100	2.29153200	2.65462800
C	6.51817300	1.16058100	-2.85420500
O	6.16635500	1.46770900	-1.72528600
O	6.75555200	3.16651200	2.00469600
O	7.70613400	0.56434400	-3.16010500
O	8.65167300	2.21565300	2.85453600
C	8.65919800	0.41377100	-2.06296400
H	8.10190300	0.38612800	-1.11607400

H	9.13949100	-0.56136400	-2.23740600
C	9.67473400	1.55503400	-2.10800900
H	10.13564200	1.56546300	-3.11119500
H	9.13591100	2.51282700	-2.00564600
C	9.44758100	3.25319600	2.20634700
H	10.39277800	3.24445000	2.77026500
H	8.94374300	4.22158600	2.34811600
C	9.67591600	2.97545000	0.72003400
H	8.70981200	3.06517200	0.19749200
H	10.31691400	3.79303700	0.33533400
C	10.78289600	1.44648500	-1.04126600
H	11.29622100	0.47223700	-1.14864600
H	11.54870900	2.21107500	-1.26841800
C	10.33668000	1.61828200	0.42564100
H	9.65134500	0.80527400	0.72174300
H	11.22802800	1.50004400	1.07025700
C	-4.88564300	-1.29506800	-4.47097600
H	-4.68205500	-1.15760500	-3.40622800
C	-3.95121500	-0.89252100	5.38704600
H	-3.95280200	-0.59439800	4.33734800
C	-5.06815100	-0.34188900	6.24960300
H	-5.79378800	0.31167200	5.76254500
H	-4.82783600	-0.11801700	7.29090800
C	-5.90648700	-2.34185600	-4.86476400
H	-6.38131700	-2.91067000	-4.06384600
H	-5.71806900	-2.86818900	-5.80290200
C	-6.28600800	-0.88762700	-4.97867100
H	-6.27197500	-0.45416200	-5.98042800
C	-5.07761900	-1.81416600	5.87070000
H	-4.79955600	-2.50530700	6.66838000
C	-7.31614400	-0.26326400	-4.09558300
C	-6.17262200	-2.31968300	4.99562900
O	-7.54360500	-0.97200100	-2.94095900
O	-6.36204700	-1.53418500	3.88436600

O	-6.87063500	-3.28201400	5.26111200
O	-7.92408500	0.74885900	-4.39199200
C	-8.65186800	-0.46309000	-2.12594100
H	-8.30635900	0.44822600	-1.61029300
H	-9.46604700	-0.17433800	-2.80701300
C	-9.09374400	-1.54032700	-1.14315100
H	-10.01438400	-1.16291500	-0.65892000
H	-9.39068000	-2.44780800	-1.69964300
C	-7.60010800	-1.75956100	3.14690100
C	-8.05715300	-1.88101500	-0.06278600
H	-7.17804800	-2.34844900	-0.54431100
H	-7.69678200	-0.93585900	0.38428700
C	-8.57120300	-2.82040700	1.04330300
H	-8.78957100	-3.81313000	0.61142900
H	-9.53960200	-2.44604900	1.42887100
C	-7.57671500	-2.97792700	2.21534500
H	-2.56605100	-6.03272300	-3.72169200
H	-7.72347400	-0.82522600	2.58002500
H	-8.42437600	-1.84735700	3.87282400
H	-6.55546700	-3.10604800	1.81687100
H	-7.79505500	-3.88197700	2.80304300

Intermediate (*R*)-E:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.140612 Hartree

G_corr: 1.796827 Hartree

SCF: -7569.09884556 Hartree

S: 688.899 Cal/Mol-Kelvin

H: -7566.95823356 Hartree

G: -7567.30201856 Hartree

Cartesian Coordinates:

C	3.50587600	-2.75891700	-3.58846200
C	3.50424800	-1.94532000	-2.45128200

C	2.94056200	-2.38902100	-1.23982600
C	2.38537100	-3.67989800	-1.19633700
C	2.38946200	-4.49973800	-2.33140700
C	2.95019500	-4.04396000	-3.52935200
H	3.95135600	-2.39431400	-4.51806000
H	3.97358700	-0.95870400	-2.49979400
H	1.96053900	-4.06040200	-0.26408000
H	1.95223200	-5.50054200	-2.27414500
C	3.06877100	-1.56994500	0.01081600
C	4.47912100	-0.96932500	0.30836500
H	5.18695900	-1.22993900	-0.48656500
H	4.86384500	-1.38495900	1.25291800
N	4.42434100	0.49744600	0.42428200
S	2.90177100	0.84830900	1.14650000
N	1.98687500	-0.56160400	0.43561600
O	2.38875600	2.10223600	0.60140600
O	3.02240700	0.63738500	2.60410100
C	4.71226800	1.31053700	-0.78651900
C	5.32087800	2.66176100	-0.45830400
H	3.81464600	1.45018000	-1.41648100
H	5.43356100	0.72290200	-1.37831100
C	5.04920900	3.76656800	-1.28191500
C	5.67541000	4.99816300	-1.05107200
C	6.21446200	2.81501200	0.61506100
C	6.83316600	4.04862600	0.85298800
C	6.57165800	5.14200500	0.01631500
H	7.05523700	6.10569300	0.20255200
H	7.51939800	4.15779900	1.69861000
H	4.32969400	3.66777200	-2.10182200
H	5.45206900	5.85088200	-1.69956400
H	6.39745200	1.96698700	1.28142300
C	2.22837600	-1.81770500	1.20801200
H	1.37662500	-2.49693900	1.16035400
H	2.68671300	-1.72489200	2.19531800

C	-0.73617000	-1.46556400	2.76072000
N	-0.81037600	-1.54050700	1.37370100
H	-1.14696700	-2.91267600	4.43198200
C	-1.21995500	-2.84431300	1.10734100
C	-1.44319600	-3.56573400	2.33933900
H	-1.80956800	-4.58775100	2.40389300
C	-1.11146500	-2.72291900	3.36109500
C	-1.32261300	-3.42245300	-0.16596600
N	-0.58910300	-1.39667800	-1.41331800
C	-0.35553800	-1.17166800	-2.76568900
C	-0.55371200	-2.38327600	-3.52566100
H	-0.41966600	-2.46806100	-4.60206300
C	-0.95063900	-3.34369300	-2.64285700
H	-1.19575800	-4.38392400	-2.84474600
C	-0.97931700	-2.73028600	-1.33509300
C	-0.44295300	-0.31470200	3.50817700
H	-0.51197200	4.26582500	2.95891600
C	-0.45111000	3.19716500	2.76646700
C	-0.45982700	2.59595600	1.45284300
H	-0.28795300	2.24094100	4.75570000
N	-0.40347200	1.21107400	1.54790000
C	-0.34475600	0.94949300	2.91330200
C	-0.33743900	2.18089400	3.66972700
C	-0.11451400	0.07743800	-3.36352700
H	-0.17376000	4.57069500	-2.27788000
C	-0.16565400	3.48471300	-2.21532000
C	-0.02060200	2.57833700	-3.22475900
H	0.09648200	2.76318400	-4.29138600
C	-0.08678900	1.26695900	-2.61918900
N	-0.24318400	1.36749200	-1.24113400
C	-0.30970400	2.73280400	-0.98911900
C	-0.45764200	3.33473300	0.26488300
Co	-0.38681200	-0.10847600	0.06972500
C	-0.57318900	4.82748100	0.33685300

C	0.50174100	5.60403200	0.80470600
C	-1.76426300	5.45647600	-0.06619100
C	0.40170800	7.00461800	0.88176800
H	1.42001600	5.09012700	1.09708000
C	-1.90296500	6.85429700	-0.00482800
H	-2.58683700	4.83006500	-0.41879600
C	-0.80729700	7.59825000	0.47187000
H	-0.89989000	8.68756600	0.52701300
C	-1.79246900	-4.84184000	-0.28344800
C	-3.03511400	-5.12142100	-0.88038400
C	-1.00580400	-5.90511000	0.19672200
C	-3.50555900	-6.44063000	-1.00252100
H	-3.63419800	-4.28201600	-1.23988500
C	-1.43710400	-7.23914800	0.09165300
H	-0.04355200	-5.67127300	0.65813400
C	-2.68699500	-7.47460700	-0.51089500
H	-3.03927700	-8.50711800	-0.59829100
C	-0.43701000	-0.43882400	5.00740500
C	0.72181400	-0.84375900	5.71483600
C	-1.64539800	-0.22608300	5.73273600
C	0.66361200	-1.07112400	7.10276000
C	-1.69835700	-0.46736300	7.11773700
C	-0.54360900	-0.89275400	7.77870100
H	1.55588100	-1.40382200	7.63005000
H	-2.64090200	-0.32967400	7.64468400
H	-0.58543700	-1.07899800	8.85616400
C	-0.21320400	0.15765100	-4.86674300
C	-1.51483200	0.14309200	-5.44638900
C	0.91206500	0.22580500	-5.72756500
C	-1.68346800	0.11908200	-6.84230300
C	0.74026500	0.20687400	-7.12674200
C	-0.55016400	0.14068200	-7.65709100
H	-2.69008200	0.07825700	-7.25617000
H	1.61571100	0.24915100	-7.77070100

H	-0.67467500	0.11886300	-8.74406300
C	-0.59962600	-8.42769600	0.61018700
C	-1.40532300	-9.19192100	1.69093100
H	-2.35518400	-9.58559500	1.29614200
H	-0.82272800	-10.04801600	2.07171800
H	-1.64429600	-8.53725700	2.54481600
C	0.73489900	-7.97737700	1.23876500
H	1.37961100	-7.45509100	0.51240000
H	0.58235100	-7.31265600	2.10484200
H	1.29326400	-8.85770100	1.59652700
C	-0.28056200	-9.38655100	-0.56414800
H	0.31527900	-10.24491100	-0.20987900
H	-1.19466700	-9.78657800	-1.03046800
H	0.29729000	-8.87317000	-1.35024600
C	-4.86859100	-6.78062500	-1.64158000
C	-5.75583800	-7.51302100	-0.60379200
H	-6.73587300	-7.76336800	-1.04451300
H	-5.29746500	-8.45307300	-0.25809700
H	-5.93239500	-6.88179200	0.28236200
C	-5.62419300	-5.52235800	-2.11512400
H	-5.84617700	-4.83632600	-1.28119400
H	-5.06040600	-4.96396100	-2.88024600
H	-6.58698000	-5.81477800	-2.56510300
C	-4.64752600	-7.70040400	-2.86866300
H	-4.15041800	-8.64411000	-2.59350000
H	-5.61350700	-7.95730200	-3.33573600
H	-4.02430100	-7.20338500	-3.63000400
C	1.55884700	7.89170400	1.38798300
C	-3.19842000	7.57839800	-0.42846700
C	-2.88128800	8.58252600	-1.56498900
H	-3.79805600	9.11076900	-1.87815200
H	-2.14965700	9.34450500	-1.25252200
H	-2.46958200	8.06535200	-2.44717000
C	-3.77867400	8.34548700	0.78624200

H	-3.07326300	9.09732200	1.17452500
H	-4.70527600	8.87291800	0.50171300
H	-4.01982300	7.65552000	1.61123600
C	-4.27644000	6.60091200	-0.93974000
H	-3.93796800	6.03671300	-1.82422100
H	-4.58127200	5.87551000	-0.16809100
H	-5.17723000	7.16401200	-1.23449500
C	2.78497100	7.06371600	1.82310700
H	2.54517400	6.37058800	2.64595400
H	3.20692100	6.47351800	0.99378700
H	3.57905500	7.73838600	2.18337300
C	2.00025700	8.85409100	0.25683500
H	1.17791000	9.50977300	-0.07095100
H	2.82586900	9.50062600	0.60077400
H	2.35147100	8.29293300	-0.62462000
C	1.08112900	8.71990300	2.60724600
H	1.89872800	9.35959900	2.98130300
H	0.23380300	9.37741100	2.35625900
H	0.76083000	8.06217300	3.43177400
N	1.95035100	-0.99743200	5.01258700
H	2.10845900	-0.38423700	4.20783500
N	2.19526900	0.32364500	-5.13177600
H	2.18818900	0.29511000	-4.11112600
N	-2.61224700	0.18861000	-4.56243600
H	-2.36399900	0.36851900	-3.59002800
N	-2.76775000	0.23980400	5.01147400
H	-2.57369100	0.50930900	4.04709200
C	2.94554700	-1.90579300	5.33545200
C	3.40973400	0.55761700	-5.75383300
C	-3.95726700	-0.04027100	-4.80462800
C	-4.06744700	0.43475600	5.45080800
O	-4.43653500	-0.35286400	-5.89444100
O	-4.48808700	0.11631400	6.56382200
O	3.57497100	0.61306300	-6.97364000

O	2.85337800	-2.74106100	6.23582700
C	-4.94234500	1.12349800	4.43654600
H	-4.50800700	1.42715900	3.47952500
C	-4.78975100	0.12564500	-3.56189500
H	-4.32334500	0.58502100	-2.68519100
C	-5.86061100	-0.89937900	-3.26005500
H	-6.02043100	-1.15295800	-2.20988200
H	-5.99535800	-1.70698500	-3.98287400
C	-6.26038300	0.48714000	-3.73043700
H	-6.63605600	0.55365300	-4.75321400
C	-6.03879900	2.00495800	4.98119100
H	-6.11152700	2.06659200	6.06868600
H	-6.28189700	2.90128000	4.40749200
C	-6.41318100	0.67597000	4.36100800
H	-6.70831300	-0.13143300	5.03306400
C	-6.82406000	1.44252600	-2.72702000
C	-7.04470700	0.72268000	3.01085200
O	-6.79091300	1.55849100	2.15680600
O	-6.27099800	1.78075300	-1.69278500
O	-7.95345700	-0.28136800	2.85713600
O	-8.05087800	1.87729200	-3.11969800
C	-8.66055900	-0.29641100	1.57731600
H	-7.94433200	-0.03859700	0.78294000
H	-8.98023000	-1.34309200	1.46068500
C	-9.85102600	0.66082100	1.60027600
H	-10.49119800	0.40152200	2.46189500
H	-9.47378200	1.68033500	1.78395400
C	-8.69963200	2.86712100	-2.25843500
H	-9.54252300	3.20766000	-2.87839200
H	-7.99958300	3.70468000	-2.10930500
C	-9.18283000	2.32783200	-0.90952900
H	-8.32138300	2.22335500	-0.23253000
H	-9.82904600	3.11767100	-0.47771600
C	-10.70136800	0.63626700	0.31358500

H	-11.15980700	-0.36321200	0.19279400
H	-11.54554100	1.33541300	0.45864800
C	-9.96684800	1.00796300	-0.99280200
H	-9.27944900	0.19504400	-1.28642100
H	-10.71459500	1.06490900	-1.80579600
C	4.18222500	-1.83151900	4.46751100
H	4.29484900	-0.97866700	3.79387900
C	4.57029500	0.77967500	-4.81216000
H	4.40230200	0.68495400	-3.73752400
C	5.59009500	1.81102500	-5.23883600
H	6.06698200	2.39484600	-4.44960700
H	5.40211600	2.32153100	-6.18548700
C	4.78156300	-3.15991800	4.04664900
H	5.26953200	-3.21348000	3.07205700
H	4.25370900	-4.05660300	4.37885800
C	5.47075000	-2.36163700	5.12566600
H	5.32881300	-2.70448100	6.15213800
C	5.94675400	0.33914400	-5.33817000
H	5.93441700	-0.07846300	-6.34666900
C	6.78148200	-1.68505100	4.90815100
C	7.02276500	-0.23232200	-4.47727400
O	7.03637300	-1.43607800	3.57634700
O	6.91731900	0.16143600	-3.16472500
O	7.92736500	-0.92925700	-4.89668100
O	7.54693700	-1.39902600	5.80947500
C	8.30206500	-0.76772500	3.28296900
H	8.06934600	0.29743400	3.10927200
H	8.94017100	-0.84084700	4.17492000
C	8.96034200	-1.39681200	2.05838200
H	9.94666600	-0.90923500	1.93788400
H	9.16749100	-2.46245000	2.26540000
C	8.05342700	-0.16886300	-2.30282100
C	8.14850200	-1.25372200	0.76289900
H	7.19029600	-1.78613600	0.88837900

H	7.88853900	-0.18664800	0.62632700
C	8.85521600	-1.79164400	-0.49399900
H	9.07022900	-2.86618900	-0.35600200
H	9.84270300	-1.30438900	-0.60975500
C	8.03055300	-1.61215100	-1.78829400
H	2.95755300	-4.68614100	-4.41483200
H	6.98344500	-1.91354900	-1.60128500
H	8.40154400	-2.27620200	-2.58387200
H	7.96841000	0.56251100	-1.48561500
H	8.97956100	0.03080000	-2.86322000

Intermediate (*S*)-E:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.140927 Hartree

G_corr: 1.796705 Hartree

SCF: -7569.094270 Hartree

S: 689.774 Cal/Mol-Kelvin

H: -7566.953343 Hartree

G: -7567.297565 Hartree

Cartesian Coordinates:

C	-2.27527600	-3.36234100	-2.65514200
C	-2.30383400	-2.34751200	-1.68765500
C	-3.32885900	-2.30916900	-0.73096500
C	-4.32297000	-3.30735800	-0.75308500
C	-4.29198100	-4.32069600	-1.71780100
C	-3.26747600	-4.35001700	-2.67400500
H	-1.46182100	-3.38183100	-3.38480500
H	-1.51013000	-1.59818400	-1.64479200
H	-5.10980000	-3.31584700	0.00803700
H	-5.06613700	-5.09407800	-1.71510800
C	-3.34282900	-1.29929900	0.37962800
C	-4.68306900	-0.55838500	0.68364500
H	-5.05532700	-0.81445700	1.68685900

H	-5.44816900	-0.83383400	-0.05223700
N	-4.47142900	0.89627600	0.59170500
S	-2.86839000	1.19577000	1.08733600
N	-2.16695400	-0.36512000	0.53319600
O	-2.82600300	1.21761900	2.56449700
O	-2.31595100	2.30854500	0.31429300
C	-4.96256200	1.61454700	-0.60217700
C	-6.37007000	2.16353700	-0.41313400
H	-4.26704300	2.44774500	-0.79247800
H	-4.91959000	0.96075300	-1.49376200
C	-6.89682800	2.41950400	0.86318700
C	-8.17037600	2.98914900	1.00352200
C	-7.13729600	2.48521900	-1.54720900
C	-8.40661000	3.06105100	-1.40535800
C	-8.92843900	3.31339900	-0.12909300
H	-9.92072200	3.76142700	-0.01854600
H	-8.98826200	3.30567700	-2.29930200
H	-6.29954100	2.17092100	1.74500700
H	-8.56794900	3.18566900	2.00431600
H	-6.74956400	2.28703800	-2.55235300
C	-2.39010100	-1.46189500	1.52003500
H	-1.62274000	-2.23779100	1.47274800
H	-2.71438900	-1.17855000	2.52439500
C	0.79832300	-1.09281200	-2.75586800
N	0.89822700	-1.26441600	-1.37882600
H	1.21711900	-2.40332600	-4.53363500
C	1.32158900	-2.58110400	-1.21351600
C	1.52849800	-3.21193000	-2.49529400
H	1.86661500	-4.23684800	-2.63215100
C	1.19529800	-2.29417900	-3.45066300
C	1.42275800	-3.25891800	0.00585600
N	0.80560300	-1.30646700	1.41440100
C	0.64736200	-1.16323300	2.78912500
C	0.81050900	-2.43289900	3.45660500

H	0.73787200	-2.58124800	4.53206500
C	1.11885500	-3.34978300	2.49334300
H	1.34752300	-4.40619900	2.61640600
C	1.11567200	-2.65112000	1.22922600
C	0.38183500	0.07874200	-3.40761200
H	-0.08380000	4.58738500	-2.53363600
C	0.02648800	3.51116300	-2.41945900
C	0.30887600	2.84464200	-1.16882500
H	-0.26297300	2.65651300	-4.44045000
N	0.36750200	1.46874800	-1.34929500
C	0.17705400	1.28093700	-2.71451700
C	-0.07225100	2.54256100	-3.37480300
C	0.50278300	0.05194300	3.47588300
H	0.74037900	4.59642500	2.66804000
C	0.66045700	3.51939300	2.53922500
C	0.58743700	2.55436000	3.50126700
H	0.59427900	2.67235700	4.58368100
C	0.51158500	1.28551000	2.81464900
N	0.52432500	1.47021500	1.43585800
C	0.58720100	2.84847000	1.26222700
C	0.48723400	3.52210200	0.04098600
Co	0.56747800	0.07976000	0.03300100
C	0.50264300	5.02059300	0.03098100
C	-0.60625000	5.74086900	0.49490500
C	1.63016000	5.71401500	-0.45201800
C	-0.61571600	7.15115600	0.48771300
H	-1.47413700	5.17907300	0.85189200
C	1.66391200	7.11619700	-0.46764800
H	2.48439700	5.13108400	-0.80375400
C	0.52730700	7.80807600	0.00623100
H	0.54270200	8.90043900	-0.00449000
C	1.85437600	-4.69595500	-0.00271700
C	3.20284700	-5.02177100	-0.19758700
C	0.91209500	-5.72769300	0.18103700

C	3.63874900	-6.36332500	-0.21007400
H	3.92019000	-4.20695300	-0.33478300
C	1.30361700	-7.07463100	0.17467600
H	-0.13569300	-5.45215600	0.32003400
C	2.67222400	-7.36288200	-0.02224000
H	2.98719100	-8.40892300	-0.02804500
C	0.40434100	0.10588100	-4.91250200
C	-0.74147500	-0.16354600	-5.70720000
C	1.63828400	0.40667400	-5.55861800
C	-0.64391600	-0.13417500	-7.11434700
C	1.72941300	0.42376300	-6.96216900
C	0.58406300	0.15369600	-7.71226300
H	-1.52798200	-0.34052300	-7.71218700
H	2.68684500	0.64467500	-7.43073400
H	0.64802300	0.16956500	-8.80462200
C	0.62286200	0.01051900	4.97545600
C	1.93476700	0.04663600	5.52615400
C	-0.48619400	-0.15842800	5.84541500
C	2.14646400	-0.15495500	6.89966200
C	-0.26485500	-0.34881200	7.22595700
C	1.03971500	-0.36072500	7.72486500
H	3.16298100	-0.16447500	7.29115500
H	-1.11651000	-0.50591300	7.88312400
H	1.19383800	-0.52075100	8.79638400
C	0.30156600	-8.23216100	0.36700600
C	0.31602800	-9.13853900	-0.88969200
H	1.31202600	-9.57088800	-1.07489100
H	-0.39316100	-9.97526000	-0.76916500
H	0.02472300	-8.57235000	-1.78956700
C	-1.14089800	-7.73036000	0.58113900
H	-1.23002300	-7.09985100	1.48110900
H	-1.51117000	-7.15215500	-0.28111000
H	-1.81710000	-8.59052300	0.71551400
C	0.70917000	-9.06802300	1.60646700

H	0.00299700	-9.90241100	1.75649200
H	1.71649400	-9.50071100	1.50079000
H	0.70443000	-8.45109100	2.51991700
C	5.13462600	-6.67651800	-0.42231700
C	5.42995200	-8.18999800	-0.39909600
H	6.50790400	-8.36003600	-0.55403300
H	5.16174500	-8.64970500	0.56645100
H	4.89576200	-8.72916200	-1.19886600
C	5.58597000	-6.11788700	-1.79529900
H	5.01912000	-6.58341400	-2.61828400
H	5.44272900	-5.02807800	-1.86522000
H	6.65697000	-6.32453100	-1.96175600
C	5.96404700	-6.00652400	0.70200700
H	5.66678300	-6.38491400	1.69364100
H	7.03837600	-6.21761900	0.56522700
H	5.83845500	-4.91246100	0.71084900
C	-1.86122600	7.90549400	0.99813700
C	2.88538500	7.91147700	-0.97393300
C	3.43056500	8.80096600	0.17178600
H	4.30446800	9.37969600	-0.17306500
H	2.67669700	9.51927500	0.53116200
H	3.74650400	8.18847500	1.03198100
C	2.46007800	8.80943500	-2.16291000
H	1.67550700	9.52836200	-1.87846800
H	3.32251800	9.38824900	-2.53530700
H	2.07194500	8.20357900	-2.99806000
C	4.02716900	6.99141200	-1.45194400
H	4.40412900	6.34390000	-0.64344500
H	3.71557400	6.34800800	-2.29119600
H	4.87407000	7.60281600	-1.80415000
C	-2.12084300	7.52474800	2.47747800
H	-2.28897800	6.44347100	2.60144300
H	-1.26632800	7.80666900	3.11454700
H	-3.01509500	8.04714600	2.85826600

C	-1.69881400	9.43690900	0.91754500
H	-1.54288900	9.78319100	-0.11758200
H	-2.61217100	9.92714800	1.29240900
H	-0.85786100	9.79771300	1.53264900
C	-3.08951500	7.50466200	0.14278700
H	-3.99299400	8.03007500	0.49669700
H	-2.93673700	7.76740200	-0.91688100
H	-3.29174100	6.42344700	0.19352600
N	-1.96505600	-0.46039000	-5.04960600
H	-1.92268600	-0.45321000	-4.02962700
N	-1.79746700	-0.13189800	5.29583500
H	-1.88544000	0.27809800	4.36145900
N	3.00781300	0.31304900	4.64562500
H	2.74296500	0.74480100	3.76065600
N	2.74815200	0.69271100	-4.73328500
H	2.54140600	0.71199900	-3.73499800
C	-3.17802900	-0.80172900	-5.62998900
C	-2.97721500	-0.47601500	5.94214300
C	4.33306900	-0.08452200	4.74709000
C	4.05715000	0.97537900	-5.08709500
O	4.79599800	-0.74650200	5.67327200
O	4.49267800	0.97481800	-6.23907600
O	-3.03735900	-0.92757000	7.08732100
O	-3.36797500	-0.86837700	-6.84591400
C	4.92573100	1.32291700	-3.90609600
H	4.49589700	1.28431000	-2.90072200
C	5.14503000	0.36854300	3.55815300
H	4.82853300	1.28303100	3.04689300
C	5.77069600	-0.68512300	2.66343500
H	5.80515100	-0.46530100	1.59378200
H	5.63232400	-1.73309100	2.93883600
C	6.64306700	0.14872300	3.59028500
H	7.04145700	-0.36603000	4.46669300
C	5.99542000	2.36381500	-4.13021900

H	6.06281400	2.78319100	-5.13599000
H	6.22172600	3.02814300	-3.29402800
C	6.40155400	0.90995600	-3.98577300
H	6.71149200	0.38956300	-4.89336900
C	7.50174200	1.19711100	2.96166400
C	7.06444400	0.52500400	-2.70678700
O	6.74469400	0.94110900	-1.60348000
O	7.10031300	2.12152000	2.27450800
O	8.09790000	-0.33408600	-2.93829600
O	8.81654400	0.96039000	3.23693900
C	8.92128300	-0.67259300	-1.77972400
H	8.29248800	-0.63059100	-0.87903100
H	9.24078600	-1.71045400	-1.95962900
C	10.11568700	0.27688400	-1.69448700
H	10.66292600	0.22915900	-2.65223100
H	9.73938400	1.31018000	-1.60306900
C	9.76743000	1.89278500	2.63814500
H	10.67213300	1.76675400	3.25224200
H	9.37922200	2.91550500	2.76154000
C	10.04286600	1.59484200	1.16385600
H	9.13050200	1.81351900	0.58598700
H	10.80757500	2.32375200	0.82989700
C	11.08559300	-0.04187300	-0.53898300
H	11.44283000	-1.08422600	-0.63939600
H	11.98264200	0.59202900	-0.66614200
C	10.53724600	0.16452000	0.88859400
H	9.72394900	-0.55120400	1.10023900
H	11.34297100	-0.08816700	1.60340000
C	-4.29864200	-1.13749500	-4.67044500
H	-4.14365000	-1.00741000	-3.59608300
C	-4.24178900	-0.22974900	5.15025400
H	-4.16071800	0.04942300	4.09831400
C	-5.37963800	0.40808000	5.91975000
H	-6.03178900	1.08466000	5.36448600

H	-5.19743200	0.65588500	6.96747800
C	-5.19318100	-2.28645600	-5.10180400
H	-5.61727400	-2.89960200	-4.30620900
H	-4.91193000	-2.79967800	-6.02385600
C	-5.71004700	-0.88263700	-5.24495500
H	-5.66580400	-0.44805200	-6.24646200
C	-5.44756800	-1.07293400	5.58810000
H	-5.24660300	-1.74017700	6.42829000
C	-6.85297100	-0.33282100	-4.45221100
C	-6.51357500	-1.58431300	4.68065800
O	-7.29646900	-1.16776700	-3.46118500
O	-6.59274800	-0.89082700	3.49622500
O	-7.27512500	-2.48714300	4.97618000
O	-7.38302700	0.73656500	-4.70790500
C	-8.56534900	-0.75156300	-2.85675200
H	-8.44914200	0.26487200	-2.45041800
H	-9.31651500	-0.70622200	-3.66191600
C	-8.96584200	-1.74249000	-1.77194400
H	-10.00137600	-1.48556300	-1.47854400
H	-9.00970500	-2.76249500	-2.19469400
C	-7.75646800	-1.18720800	2.65934000
C	-8.05796800	-1.70730300	-0.53395100
H	-7.05247000	-2.05538200	-0.83114100
H	-7.94365400	-0.65344700	-0.21847400
C	-8.56059200	-2.55956100	0.64529400
H	-8.65587600	-3.61106200	0.31927900
H	-9.58456100	-2.24333100	0.92336500
C	-7.64669500	-2.51006200	1.89031500
H	-3.23969300	-5.14336000	-3.42672200
H	-7.80254100	-0.32035100	1.98449800
H	-8.65105000	-1.18774100	3.30187500
H	-6.59646100	-2.65746600	1.57987600
H	-7.88131700	-3.33650800	2.57752800

Product (*R*)-2.2a

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 0.305499 Hartree

G_corr: 0.231383 Hartree

SCF: -1277.697382 Hartree

S: 148.519 Cal/Mol-Kelvin

H: -1277.391883 Hartree

G: -1277.465999 Hartree

Cartesian Coordinates:

C	4.87590000	-0.75950700	1.01699600
C	3.72890100	-0.03370600	0.67139600
C	2.75850000	-0.60540500	-0.16770400
C	2.95039900	-1.91130600	-0.65580400
C	4.09789800	-2.63410600	-0.30860400
C	5.06319900	-2.05960700	0.52969600
H	5.62680000	-0.30520800	1.67069600
H	3.57610100	0.98369400	1.04109600
H	2.20439900	-2.36300500	-1.31890400
H	4.23979800	-3.64750700	-0.69650400
H	5.96059900	-2.62430800	0.80009600
C	1.50820100	0.14179600	-0.52550400
C	0.17790000	-0.42010300	0.04449600
H	-0.19150000	-1.27160300	-0.54840400
H	0.35460000	-0.77080300	1.07479600
N	-0.82129900	0.65109800	0.02749600
S	0.01210200	2.14939700	0.21529600
N	1.55900200	1.63429600	-0.45270400
O	-0.62189700	3.17459700	-0.62580400
O	0.27060300	2.37689700	1.63809600
C	-1.98409900	0.56719800	-0.87030400
C	-3.07130000	-0.33380100	-0.30460400
H	-2.36419800	1.59379900	-0.99960400
H	-1.69419900	0.20799800	-1.87850400

C	-3.79050000	-1.18850000	-1.15580400
C	-4.82900100	-1.98589900	-0.65570400
C	-3.39810000	-0.29850000	1.06209600
C	-4.43220000	-1.09720000	1.56319600
C	-5.15240100	-1.94179900	0.70589600
H	-5.95940100	-2.56719800	1.09999600
H	-4.67740000	-1.06049900	2.62919600
H	-3.53940000	-1.23000000	-2.22220400
H	-5.38070200	-2.64759900	-1.33090400
H	-2.82599900	0.35269900	1.72979600
C	1.39980100	0.96439600	-1.77070400
H	2.27360200	1.08279500	-2.41620400
H	0.43110100	1.04299600	-2.27530400

Product *(S)*-2.2a:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 0.305499 Hartree

G_corr: 0.231389 Hartree

SCF: -1277.697382 Hartree

S: 148.506 Cal/Mol-Kelvin

H: -1277.391883 Hartree

G: -1277.465993 Hartree

Cartesian Coordinates:

C	4.87589600	-0.75948900	-1.01696000
C	3.72894000	-0.03367900	-0.67135800
C	2.75853600	-0.60544100	0.16771600
C	2.95042400	-1.91131300	0.65576700
C	4.09791300	-2.63408100	0.30864700
C	5.06315000	-2.05962900	-0.52973300
H	5.62676400	-0.30519900	-1.67068100
H	3.57614700	0.98368500	-1.04108500
H	2.20435200	-2.36303300	1.31893100
H	4.23982900	-3.64750700	0.69654200

H	5.96064100	-2.62430800	-0.80007400
C	1.50822500	0.14181500	0.52546300
C	0.17787800	-0.42006300	-0.04445800
H	-0.19154600	-1.27163300	0.54842900
H	0.35462800	-0.77076500	-1.07483800
N	-0.82127100	0.65107000	-0.02747700
S	0.01208900	2.14940900	-0.21528700
N	1.55901000	1.63425600	0.45266100
O	-0.62194000	3.17464400	0.62576300
O	0.27055400	2.37688100	-1.63806400
C	-1.98405400	0.56715800	0.87029900
C	-3.07131400	-0.33377000	0.30463400
H	-2.36415200	1.59378600	0.99957700
H	-1.69421900	0.20803700	1.87850600
C	-3.79048900	-1.18846900	1.15579900
C	-4.82902600	-1.98593600	0.65569200
C	-3.39812800	-0.29854000	-1.06206000
C	-4.43218400	-1.09716800	-1.56318100
C	-5.15238000	-1.94184800	-0.70593800
H	-5.95938400	-2.56717100	-1.10003400
H	-4.67743800	-1.06053800	-2.62922800
H	-3.53939700	-1.23003000	2.22219300
H	-5.38067300	-2.64759400	1.33087200
H	-2.82596100	0.35269700	-1.72977100
C	1.39980400	0.96441000	1.77065000
H	2.27364900	1.08284300	2.41619600
H	0.43111300	1.04296400	2.27530300

Transition State TS4:

Temperature: 313.15 Kelvin

Pressure: 1.0 Atm

H_corr: 2.136530 Hartree

G_corr: 1.801536 Hartree

SCF: -7569.074609 Hartree

S: 671.281 Cal/Mol-Kelvin

H: -7566.938079 Hartree

G: -7567.273073 Hartree

Cartesian Coordinates:

C	4.63749700	0.64401100	0.10449400
C	2.17603600	1.53064300	0.42147600
C	3.64200900	1.77798200	0.15822600
C	3.74897100	5.55651400	-0.06322100
C	3.25399800	4.26060400	0.05753600
C	4.12159200	3.12385500	0.02072500
C	5.51802800	3.39795100	-0.13725100
C	6.00303500	4.69839800	-0.25396500
C	5.12477800	5.79231200	-0.22068600
H	3.05386500	6.40028200	-0.03878700
H	2.17699100	4.12212100	0.17909100
H	6.23501000	2.57498100	-0.16613400
H	7.07849600	4.86238700	-0.37359200
H	5.50509200	6.81325300	-0.31630400
H	5.31605800	0.67453600	0.97806500
H	5.28104000	0.76526200	-0.78644300
N	4.04036400	-0.69822900	0.07839600
S	2.56836900	-0.78504300	-0.75847500
N	1.62495700	0.15077500	0.27168300
O	2.14099700	-2.18655000	-0.69677500
O	2.83306700	-0.15383900	-2.08081200
C	4.23672300	-1.63408800	1.19427400
C	5.09517300	-2.84452000	0.84399700
H	3.25485500	-1.97802300	1.56307200
H	4.71638300	-1.08053700	2.02056400
C	5.37751600	-3.79561700	1.84058300
C	6.16959800	-4.91499800	1.55753700
C	5.61157400	-3.04038600	-0.44515800
C	6.40259100	-4.16218100	-0.73167500
C	6.68794800	-5.10079600	0.26795500

H	7.30428700	-5.97659800	0.04296800
H	6.78896900	-4.30655000	-1.74560500
H	4.96563600	-3.66411600	2.84785200
H	6.37817400	-5.64698300	2.34432000
H	5.37530000	-2.31516400	-1.22871100
H	1.92162000	1.82982400	1.45854100
H	1.61389700	2.21904900	-0.22926600
C	-0.33665000	1.55884500	-2.61770700
N	-0.53231900	1.59902400	-1.24244300
H	-0.44318000	3.08453600	-4.26338500
C	-0.87714000	2.92180400	-0.97189600
C	-0.90375500	3.69805900	-2.18852100
H	-1.17703600	4.74925200	-2.24592400
C	-0.53385900	2.86331100	-3.20213000
C	-1.13982700	3.45590400	0.29484000
N	-0.63739300	1.36047700	1.53833200
C	-0.51326000	1.09511600	2.89778500
C	-0.72096900	2.29452900	3.67292100
H	-0.67431200	2.34749000	4.75859600
C	-1.01684100	3.29098100	2.78781400
H	-1.24567200	4.33408600	2.99569600
C	-0.95487400	2.71377700	1.46714000
C	-0.16664400	0.39861200	-3.38493400
H	-0.78628100	-4.15465900	-2.96619800
C	-0.62904800	-3.10235100	-2.74195000
C	-0.64720900	-2.53661300	-1.41477000
H	-0.25409300	-2.12100200	-4.69020600
N	-0.46296500	-1.15810700	-1.46815200
C	-0.27739100	-0.87715400	-2.82046500
C	-0.36114000	-2.08335800	-3.60773400
C	-0.36496900	-0.17704100	3.47075800
H	-0.63822300	-4.62939000	2.26192100
C	-0.56609600	-3.54454000	2.23055300
C	-0.39776200	-2.67315600	3.26811500

H	-0.32119000	-2.88967100	4.33264400
C	-0.37109900	-1.34601400	2.69752300
N	-0.50290700	-1.40486100	1.31400300
C	-0.62452000	-2.75477500	1.02218900
C	-0.75738200	-3.30832800	-0.25562000
Co	-0.32320500	0.10104700	0.04326300
C	-0.95079700	-4.78848600	-0.37964400
C	0.11173500	-5.60418500	-0.80750300
C	-2.19353500	-5.36312900	-0.06130500
C	-0.05196000	-6.99578100	-0.92565900
H	1.06869300	-5.12843000	-1.03305300
C	-2.39739100	-6.74996900	-0.17336000
H	-3.00404900	-4.70571300	0.26181400
C	-1.31223200	-7.53574700	-0.60519900
H	-1.45498100	-8.61710700	-0.69634000
C	-1.68065000	4.85140700	0.40822000
C	-3.05165400	5.01465000	0.67984700
C	-0.86608000	5.98595300	0.24982600
C	-3.62695400	6.29256500	0.78317600
H	-3.66504300	4.11835900	0.79498800
C	-1.40143100	7.28289000	0.35743600
H	0.19829700	5.84067900	0.05167800
C	-2.77868400	7.40279000	0.61828300
H	-3.20942000	8.40570000	0.69742000
C	-0.10101500	0.54987200	-4.87866700
C	1.11109200	0.86394600	-5.54950500
C	-1.30942900	0.45130700	-5.62928700
C	1.09498600	1.09387700	-6.94212000
C	-1.31281000	0.69300100	-7.01394700
C	-0.10767200	1.01234700	-7.64363700
H	2.02187100	1.35524300	-7.44696300
H	-2.25156700	0.63580900	-7.56212000
H	-0.10524300	1.19896600	-8.72198600
C	-0.52842200	-0.26875200	4.96527700

C	-1.85379300	-0.33523200	5.47900600
C	0.55880100	-0.19211200	5.87158300
C	-2.09208700	-0.25762500	6.86169500
C	0.31553800	-0.11454800	7.25841100
C	-1.00129000	-0.13588700	7.72549000
H	-3.11706300	-0.27478600	7.22987300
H	1.15785100	-0.03371000	7.94179700
H	-1.17996000	-0.06699700	8.80282200
C	-0.54581000	8.55731000	0.19914900
C	-1.07380900	9.38504300	-0.99957900
H	-2.12319200	9.68939400	-0.86057100
H	-0.47481100	10.30276200	-1.12651200
H	-1.01455800	8.80843700	-1.93712700
C	0.93997900	8.23679600	-0.05466200
H	1.38419100	7.67031900	0.78064700
H	1.08509600	7.66249500	-0.98502700
H	1.51120700	9.17379200	-0.15681300
C	-0.63773600	9.40705100	1.49150800
H	-0.02780600	10.32113100	1.39375400
H	-1.67098700	9.72016000	1.70900800
H	-0.26845600	8.84388800	2.36414400
C	-5.12911800	6.50937600	1.06068400
C	-5.75959000	7.29755900	-0.11493700
H	-6.83545300	7.46187300	0.06606700
H	-5.29114000	8.28557700	-0.24879500
H	-5.65445700	6.74641400	-1.06364000
C	-5.89507100	5.17969500	1.21230700
H	-5.84174600	4.56588700	0.29814800
H	-5.51668500	4.57807800	2.05497300
H	-6.95991800	5.38521600	1.40868500
C	-5.29968300	7.31756000	2.37163700
H	-4.81426000	8.30472200	2.31475500
H	-6.36945200	7.48487800	2.58332500
H	-4.86415800	6.77953700	3.22941300

C	1.08894800	-7.92763200	-1.38557000
C	-3.75092400	-7.41762400	0.14892800
C	-3.55382300	-8.46954300	1.26946100
H	-4.51292600	-8.95939500	1.50937100
H	-2.84232400	-9.25820800	0.97740000
H	-3.17308200	-8.00011500	2.19135600
C	-4.29173800	-8.11841500	-1.12281800
H	-3.60272400	-8.89504500	-1.49118400
H	-5.25984900	-8.60406200	-0.91207500
H	-4.44566500	-7.39348200	-1.93872900
C	-4.80873700	-6.40142400	0.62501600
H	-4.50146100	-5.88136500	1.54701400
H	-5.02895200	-5.63799800	-0.13858800
H	-5.75323100	-6.92555600	0.84482900
C	2.38207800	-7.15346600	-1.71192300
H	2.23431000	-6.42352900	-2.52444900
H	2.77744000	-6.61352400	-0.83667300
H	3.16252600	-7.85839400	-2.04231800
C	1.40496300	-8.94577900	-0.26104600
H	0.53157700	-9.56842700	-0.00948200
H	2.21828100	-9.62285000	-0.57338300
H	1.72597200	-8.43126800	0.65939700
C	0.64920300	-8.69167000	-2.65980300
H	1.45448400	-9.36444000	-3.00070600
H	-0.24691400	-9.30828800	-2.48563400
H	0.42051400	-7.99362500	-3.48170200
N	2.31558000	0.91453900	-4.80767700
H	2.31093300	0.48797100	-3.87386800
N	1.86837400	-0.21300900	5.33212800
H	1.91038500	-0.34817300	4.32122500
N	-2.90127600	-0.49769700	4.54692300
H	-2.60414300	-0.78444500	3.61502300
N	-2.48771600	0.09640100	-4.93120900
H	-2.34545600	-0.15960000	-3.95501600

C	3.50278100	1.51143900	-5.21133500
C	3.07292000	-0.24750400	6.02024700
C	-4.24960700	-0.19579100	4.67488100
C	-3.78111900	-0.05072100	-5.40560000
O	-4.77437400	0.26391300	5.68706700
O	-4.15312900	0.23267500	-6.54463800
O	3.18484500	-0.09232800	7.23616900
O	3.63933000	2.14428100	-6.26084800
C	-4.71478300	-0.65492400	-4.38792400
H	-4.33176400	-0.89085100	-3.39061800
C	-5.00359100	-0.46741700	3.39903500
H	-4.55277500	-1.15224900	2.67434200
C	-5.82837000	0.65467600	2.79781500
H	-5.84735500	0.72445400	1.70789700
H	-5.86850400	1.59856800	3.34596000
C	-6.51822200	-0.53075000	3.45122000
H	-6.98723100	-0.33683800	4.41786500
C	-5.78457300	-1.57743100	-4.91894100
H	-5.80984300	-1.71749400	-6.00135400
H	-6.05591600	-2.43168100	-4.29576400
C	-6.18162600	-0.20321000	-4.41541100
H	-6.44886800	0.54443300	-5.16395100
C	-7.18218200	-1.52291600	2.54966300
C	-6.88849800	-0.15745300	-3.10335100
O	-6.61963300	-0.86501000	-2.14389200
O	-6.61904800	-2.17996900	1.68955900
O	-7.89136600	0.76608500	-3.11881600
O	-8.51880600	-1.57316400	2.80250200
C	-8.71865000	0.81915200	-1.91515100
H	-8.07674800	0.63087100	-1.04223100
H	-9.08901600	1.85505200	-1.88477900
C	-9.86440300	-0.18763700	-2.00945400
H	-10.42732800	0.01529800	-2.93739400
H	-9.43577500	-1.19811800	-2.11822400

C	-9.29339400	-2.48827000	1.96589000
H	-10.22140300	-2.63031200	2.54020500
H	-8.75198500	-3.44472800	1.90201800
C	-9.57813200	-1.93521300	0.56868500
H	-8.63945800	-1.92309500	-0.00810100
H	-10.24121300	-2.67037000	0.07105600
C	-10.83360000	-0.14811700	-0.81075200
H	-11.27469300	0.86320100	-0.72889300
H	-11.67915900	-0.82254900	-1.04052000
C	-10.24451100	-0.54855900	0.55859800
H	-9.51909600	0.20852700	0.90415900
H	-11.06392100	-0.52774800	1.30152700
C	4.66115300	1.33692900	-4.25939800
H	4.51811500	0.70793400	-3.37866700
C	4.26876800	-0.58090100	5.16289300
H	4.15711300	-0.57094800	4.07608700
C	5.19055600	-1.63440000	5.74668600
H	5.67247800	-2.32052300	5.04829700
H	4.91590400	-2.03976200	6.72252700
C	5.62553100	2.49782200	-4.15093900
H	6.10304000	2.65687500	-3.18316700
H	5.37539200	3.39295800	-4.72464300
C	6.04151200	1.29303100	-4.95555900
H	5.97089100	1.38883100	-6.04084000
C	5.63654500	-0.18264900	5.72261400
H	5.61092900	0.34112300	6.67972700
C	7.11252900	0.34273000	-4.54170800
C	6.80457300	0.17891200	4.86589700
O	7.44552900	0.43526300	-3.20872700
O	6.70604900	-0.34957800	3.60285400
O	7.77107700	0.80189900	5.26255200
O	7.66330500	-0.42075800	-5.31487900
C	8.54092000	-0.43496300	-2.78673700
H	8.11207300	-1.41945100	-2.53001300

H	9.21657200	-0.57596900	-3.64257700
C	9.25673400	0.18846700	-1.59382100
H	10.14193600	-0.44099000	-1.38160600
H	9.64650500	1.18082500	-1.88548200
C	7.92820900	-0.32689900	2.79739800
C	8.38757500	0.30545500	-0.33492200
H	7.51904200	0.94289900	-0.57393400
H	7.97337900	-0.69224200	-0.09789600
C	9.11349500	0.88976400	0.88948000
H	9.51249600	1.88748400	0.63226700
H	9.99920400	0.27144100	1.13312200
C	8.21044300	1.02446300	2.13554800
H	7.25139200	1.48989100	1.84440700
H	8.66436400	1.69742200	2.87873700
H	7.74709200	-1.11780100	2.05595000
H	8.76887300	-0.62800300	3.44224400

2.5 REFERENCES

1. (a) Xiong, T.; Zhang, Q. New Amination Strategies Based on Nitrogen-Centered Radical Chemistry. *Chem. Soc. Rev.* **2016,** *45*, 3069-3087. (b) Romero, K. J.; Galliher, M. S.; Pratt, D. A.; Stephenson, C. R. J. Radicals in Natural Product Synthesis. *Chem. Soc. Rev.* **2018,** *47*, 7851-7866. (c) Jiang, H.; Studer, A. Chemistry with N-Centered Radicals Generated by Single-Electron Transfer-Oxidation Using Photoredox Catalysis. *CCS Chem.* **2019,** *1*, 38-49. (d) Xiong, P.; Xu, H.-C. Chemistry with Electrochemically Generated N-Centered Radicals. *Acc. Chem. Res.* **2019,** *52*, 3339-3350. (e) Yu, X.-Y.; Zhao, Q.-Q.; Chen, J.; Xiao, W.-J.; Chen, J.-R. When Light Meets Nitrogen-Centered Radicals: From Reagents to Catalysts. *Acc. Chem. Res.* **2020,** *53*, 1066-1083. (f) Pratley, C.; Fenner, S.; Murphy, J. A. Nitrogen-Centered Radicals in Functionalization of sp^2 Systems: Generation, Reactivity, and Applications in Synthesis. *Chem. Rev.* **2022,** *122*, 8181-8260.

2. (a) Zard, S. Z. Recent Progress in the Generation and Use of Nitrogen-Centred Radicals. *Chem. Soc. Rev.* **2008,** *37*, 1603-1618. (b) Wang, P.; Zhao, Q.; Xiao, W.; Chen, J. Recent Advances in Visible-Light Photoredox-Catalyzed Nitrogen Radical Cyclization. *Green Synthesis and Catalysis* **2020,** *1*, 42-51.

3. Zhang, X. Theoretical Study on SH2 Reaction of Methyl Radical with Three-Membered Ring. *Int. J. Quantum Chem.* **2014,** *114*, 1594-1601.

4. Lang, K.; Torker, S.; Wojtas, L.; Zhang, X. P. Asymmetric Induction and Enantiodivergence in Catalytic Radical C–H Amination via Enantiodifferentiative H-Atom Abstraction and Stereoretentive Radical Substitution. *J. Am. Chem. Soc.* **2019,** *141*, 12388-12396.

5. (a) Zard, S. Z. *Radical Reactions in Organic Synthesis*. Oxford University: 2003. (b) Curran, D. P.; Porter, N. A.; Giese, B. *Stereochemistry of Radical Reactions: Concepts, Guidelines, and Synthetic Applications*. John Wiley & Sons: 2008. (c) Narayanam, J. M. R.; Stephenson, C. R. J. Visible Light Photoredox Catalysis: Applications in Organic Synthesis. *Chem. Soc. Rev.* **2011,** *40*, 102-113. (d) Quiclet-Sire, B.; Zard, S. Z. Fun with Radicals: Some New Perspectives for Organic Synthesis. *Pure Appl. Chem.* **2011,** *83*, 519-551. (e) Chatgilialoglu, C.; Studer, A. *Stereochemistry of Radical Reactions: Concepts, Guidelines, and Synthetic Applications*. John Wiley & Sons: 2012. (f) Prier, C. K.; Rankic, D. A.; MacMillan, D. W. C. Visible Light Photoredox Catalysis with Transition Metal Complexes: Applications in Organic Synthesis. *Chem. Rev.* **2013,** *113*, 5322-5363. (g) Studer, A.; Curran, D. P. Catalysis of Radical Reactions: A Radical Chemistry Perspective. *Angew. Chem., Int. Ed.* **2016,** *55*, 58-102.

6. (a) Bar, G.; Parsons, A. F. Stereoselective Radical Reactions. *Chem. Soc. Rev.* **2003,** *32*, 251-263. (b) Brimioulle, R.; Lenhart, D.; Maturi, M. M.; Bach, T. Enantioselective Catalysis of Photochemical Reactions. *Angew. Chem., Int. Ed.* **2015,** *54*, 3872-3890. (c) Mondal, S.; Dumur, F.; Gigmes, D.; Sibi, M. P.; Bertrand, M. P.; Nechab, M. Enantioselective Radical Reactions Using Chiral Catalysts. *Chem. Rev.* **2022,** *122*, 5842-5976.

7. (a) Du, J.; Skubi, K. L.; Schultz, D. M.; Yoon, T. P. A Dual-Catalysis Approach to Enantioselective [2 + 2] Photocycloadditions Using Visible Light. *Science* **2014,** *344*, 392-6. (b) Huo, H.; Shen, X.; Wang, C.; Zhang, L.; Röse, P.; Chen, L.-A.; Harms, K.; Marsch, M.; Hilt, G.; Meggers, E. Asymmetric Photoredox Transition-Metal Catalysis Activated by Visible Light. *Nature* **2014,** *515*, 100-103. (c) Kainz, Q. M.; Matier, C. D.; Bartoszewicz, A.; Zultanski, S. L.; Peters, J. C.; Fu, G. C. Asymmetric Copper-Catalyzed C-N Cross-Couplings Induced by Visible Light. *Science* **2016,** *351*, 681-684. (d) Zhang, W.; Wang, F.; McCann, S. D.; Wang, D.; Chen, P.; Stahl, S. S.; Liu, G. Enantioselective Cyanation of Benzylic C–H bonds via Copper-Catalyzed

Radical Relay. *Science* **2016,** *353*, 1014-1018. (e) Kern, N.; Plesniak, M. P.; McDouall, J. J. W.; Procter, D. J. Enantioselective Cyclizations and Cyclization Cascades of Samarium Ketyl Radicals. *Nat. Chem.* **2017,** *9*, 1198-1204. (f) Morrill, C.; Jensen, C.; Just-Baringo, X.; Grogan, G.; Turner, N. J.; Procter, D. J. Biocatalytic Conversion of Cyclic Ketones Bearing α-Quaternary Stereocenters into Lactones in an Enantioselective Radical Approach to Medium-Sized Carbocycles. *Angew. Chem., Int. Ed.* **2018,** *57*, 3692-3696. (g) Proctor, R. S. J.; Davis, H. J.; Phipps, R. J. Catalytic Enantioselective Minisci-Type Addition to Heteroarenes. *Science* **2018,** *360*, 419-422. (h) Huang, H.-M.; McDouall, J. J. W.; Procter, D. J. SmI2-Catalysed Cyclization Cascades by Radical Relay. *Nat. Catal.* **2019,** *2*, 211-218. (i) Gu, Q.-S.; Li, Z.-L.; Liu, X.-Y. Copper(I)-Catalyzed Asymmetric Reactions Involving Radicals. *Acc. Chem. Res.* **2020,** *53*, 170-181. (j) Huo, H.; Gorsline, B. J.; Fu, G. C. Catalyst-Controlled Doubly Enantioconvergent Coupling of Racemic Alkyl Nucleophiles and Electrophiles. *Science* **2020,** *367*, 559-564. (k) Li, Z.-L.; Fang, G.-C.; Gu, Q.-S.; Liu, X.-Y. Recent Advances in Copper-Catalysed Radical-Involved Asymmetric 1,2-Difunctionalization of Alkenes. *Chem. Soc. Rev.* **2020,** *49*, 32-48. (l) Nakafuku, K. M.; Zhang, Z.; Wappes, E. A.; Stateman, L. M.; Chen, A. D.; Nagib, D. A. Enantioselective Radical C–H Amination for The Synthesis of β-Amino Alcohols. *Nature Chem.* **2020,** *12*, 697-704.

8. (a) Lu, H.; Zhang, X. P. Catalytic C–H Functionalization by Metalloporphyrins: Recent Developments and Future Directions. *Chem. Soc. Rev.* **2011,** *40*, 1899-1909. (b) Jiang, H.; Zhang, X. P. In *Oxidation: C-N Bond Formation by Oxidation (Aziridines)*, Elsevier B.V.: 2012; pp 168-182. (c) Pellissier, H.; Clavier, H. Enantioselective Cobalt-Catalyzed Transformations. *Chem. Rev.* **2014,** *114*, 2775-2823. (d) Zhang, X. P.; Cui, X. In *Asymmetric C-H Functionalization by Transition Metal-Catalyzed Carbene Transfer Reactions*, Elsevier B.V.: 2014; pp 86-120. (e) Demarteau, J.; Debuigne, A.; Detrembleur, C. Organocobalt Complexes as Sources of Carbon-Centered Radicals for Organic and Polymer Chemistries. *Chem. Rev.* **2019,** *119*, 6906-6955. (f) Lee, W.-C. C.; Zhang, X. P. Asymmetric Radical Cyclopropanation of Alkenes. *Trends Chem.* **2022,** *4*, 850-851. (g) Wang, X.; Zhang, X. P., Catalytic Radical Approach for Selective Carbene Transfers via Cobalt(II)-Based Metalloradical Catalysis. In *Transition Metal-Catalyzed Carbene Transformations*, 2022; pp 25-66.

9. (a) Ruppel, J. V.; Jones, J. E.; Huff, C. A.; Kamble, R. M.; Chen, Y.; Zhang, X. P. A Highly Effective Cobalt Catalyst for Olefin Aziridination with Azides: Hydrogen Bonding Guided Catalyst Design. *Org. Lett.* **2008,** *10*, 1995-1998. (b) Lu, H.; Jiang, H.; Wojtas, L.; Zhang, X. P. Selective Intramolecular C–H Amination through the Metalloradical Activation of Azides: Synthesis of 1,3-Diamines under Neutral and Nonoxidative Conditions. *Angew. Chem., Int. Ed.* **2010,** *49*, 10192-10196. (c) Hopmann, K. H.; Ghosh, A. Mechanism of Cobalt-Porphyrin–Catalyzed Aziridination. *ACS Catal.* **2011,** *1*, 597-600. (d) Lyaskovskyy, V.; Suarez, A. I. O.; Lu, H.; Jiang, H.; Zhang, X. P.; de Bruin, B. Mechanism of Cobalt(II) Porphyrin-Catalyzed C–H Amination with Organic Azides: Radical Nature and H-Atom Abstraction Ability of the Key Cobalt(III)–Nitrene Intermediates. *J. Am. Chem. Soc.* **2011,** *133*, 12264-12273. (e) Goswami, M.; Lyaskovskyy, V.; Domingos, S. R.; Buma, W. J.; Woutersen, S.; Troeppner, O.; Ivanović-Burmazović, I.; Lu, H.; Cui, X.; Zhang, X. P.; Reijerse, E. J.; DeBeer, S.; van Schooneveld, M. M.; Pfaff, F. F.; Ray, K.; de Bruin, B. Characterization of Porphyrin-Co(III)-'Nitrene Radical' Species Relevant in Catalytic Nitrene Transfer Reactions. *J. Am. Chem. Soc.* **2015,** *137*, 5468-5479. (f) Villanueva, O.; Weldy, N. M.; Blakey, S. B.; MacBeth, C. E. Cobalt Catalyzed sp^3 C–H Amination Utilizing Aryl Azides. *Chem. Sci.* **2015,** *6*, 6672-6675. (g) Kuijpers, P. F.; Tiekink, M. J.; Breukelaar, W. B.; Broere, D. L. J.; van Leest, N. P.; van der Vlugt, J. I.; Reek, J. N. H.; de Bruin, B. Cobalt-Porphyrin-Catalysed Intramolecular Ring-Closing C−H Amination of Aliphatic Azides: A Nitrene-Radical Approach to Saturated Heterocycles. *Chem. Eur. J.* **2017,** *23*, 7945-7952.

10. (a) Li, C.; Lang, K.; Lu, H.; Hu, Y.; Cui, X.; Wojtas, L.; Zhang, X. P. Catalytic Radical Process for Enantioselective Amination of C(sp^3)−H Bonds. *Angew. Chem., Int. Ed.* **2018,** *57*, 16837-16841.

(b) Chuentragool, P.; Yadagiri, D.; Morita, T.; Sarkar, S.; Parasram, M.; Wang, Y.; Gevorgyan, V. Aliphatic Radical Relay Heck Reaction at Unactivated C(sp3)−H Sites of Alcohols. *Angew. Chem., Int. Ed.* **2019,** *58*, 1794-1798. (c) Jin, L.-M.; Xu, P.; Xie, J.; Zhang, X. P. Enantioselective Intermolecular Radical C–H Amination. *J. Am. Chem. Soc.* **2020,** *142*, 20828-20836. (d) Lang, K.; Li, C.; Kim, I.; Zhang, X. P. Enantioconvergent Amination of Racemic Tertiary C–H Bonds. *J. Am. Chem. Soc.* **2020,** *142*, 20902-20911. (e) Lang, K.; Hu, Y.; Lee, W.-C. C.; Zhang, X. P. Combined Radical and Ionic Approach for The Enantioselective Synthesis of β-Functionalized Amines from Alcohols. *Nature Synthesis* **2022,** *1*, 548-557.

11. Jiang, H.; Lang, K.; Lu, H.; Wojtas, L.; Zhang, X. P. Intramolecular Radical Aziridination of Allylic Sulfamoyl Azides by Cobalt(II)-Based Metalloradical Catalysis: Effective Construction of Strained Heterobicyclic Structures. *Angew. Chem., Int. Ed.* **2016,** *55*, 11604-11608.

12. Hu, Y.; Lang, K.; Tao, J.; Marshall, M. K.; Cheng, Q.; Cui, X.; Wojtas, L.; Zhang, X. P. Next-Generation D2-Symmetric Chiral Porphyrins for Cobalt(II)-Based Metalloradical Catalysis: Catalyst Engineering by Distal Bridging. *Angew. Chem., Int. Ed.* **2019,** *58*, 2670-2674.

13. Stortz, C. A. Conformational Pathways of Simple Six-Membered Rings. *J. Phys. Org. Chem.* **2010,** *23*, 1173-1186.

14. (a) Tung, R. D.; Salituro, F. G.; Deininger, D. D.; Bhisetti, G. R.; Baker, C. T.; Spaltenstein, A. Preparation of Heterocyclylhydroxyalkanamides and Related Compounds as Aspartyl Protease Inhibitors. US5945413A, 1999. (b) Zhong, J.; Gan, X.; Alliston, K. R.; Groutas, W. C. Design, Synthesis, and in vitro Evaluation of Inhibitors of Human Leukocyte Elastase Based on a Functionalized Cyclic Sulfamide Scaffold. *Bioorg. Med. Chem.* **2004,** *12*, 589-93. (c) Masliah, E.; Roberts, E.; Langford, D.; Everall, I.; Crews, L.; Adame, A.; Rockenstein, E.; Fox, H. S. Patterns of Gene Dysregulation in the Frontal Cortex of Patients with HIV Encephalitis. [Erratum to Document Cited in CA142:132829]. *J. Neuroimmunol.* **2005,** *162*, 197. (d) Sparey, T.; Beher, D.; Best, J.; Biba, M.; Castro, J. L.; Clarke, E.; Hannam, J.; Harrison, T.; Lewis, H.; Madin, A.; Shearman, M.; Sohal, B.; Tsou, N.; Welch, C.; Wrigley, J. Cyclic Sulfamide Gamma-Secretase Inhibitors. *Bioorg. Med. Chem. Lett.* **2005,** *15*, 4212-6. (e) Winum, J.-Y.; Scozzafava, A.; Montero, J.-L.; Supuran, C. T. Therapeutic Potential of Sulfamides as Enzyme Inhibitors. *Med. Res. Rev.* **2006,** *26*, 767-792. (f) Benltifa, M.; García Moreno, M. I.; Ortiz Mellet, C.; García Fernández, J. M.; Wadouachi, A. Synthesis and Evaluation of Sulfamide-Type Indolizidines as Glycosidase Inhibitors. *Bioorg. Med. Chem. Lett.* **2008,** *18*, 2805-8. (g) Yang, Q.; Li, Y.; Dou, D.; Gan, X.; Mohan, S.; Groutas, C. S.; Stevenson, L. E.; Lai, Z.; Alliston, K. R.; Zhong, J.; Williams, T. D.; Groutas, W. C. Inhibition of Serine Proteases by a New Class of Cyclosulfamide-Based Carbamylating Agents. *Arch. Biochem. Biophys.* **2008,** *475*, 115-20. (h) Reitz, A. B.; Smith, G. R.; Parker, M. H. The Role of Sulfamide Derivatives in Medicinal Chemistry: A Patent Review (2006-2008). *Expert Opin. Ther. Pat.* **2009,** *19*, 1449-53. (i) Brodney, M. A.; Barreiro, G.; Ogilvie, K.; Hajos-Korcsok, E.; Murray, J.; Vajdos, F.; Ambroise, C.; Christoffersen, C.; Fisher, K.; Lanyon, L.; Liu, J.; Nolan, C. E.; Withka, J. M.; Borzilleri, K. A.; Efremov, I.; Oborski, C. E.; Varghese, A.; O'Neill, B. T. Spirocyclic Sulfamides as B-Secretase 1 (Bace-1) Inhibitors for the Treatment of Alzheimer's Disease: Utilization of Structure Based Drug Design, Watermap, and Cns Penetration Studies to Identify Centrally Efficacious Inhibitors. *J. Med. Chem.* **2012,** *55*, 9224-39.

15. Chen, Y.; Fields, K. B.; Zhang, X. P. Bromoporphyrins as Versatile Synthons for Modular Construction of Chiral Porphyrins: Cobalt-Catalyzed Highly Enantioselective and Diastereoselective Cyclopropanation. *J. Am. Chem. Soc.* **2004,** *126*, 14718-14719.

16. Jin, L.-M.; Xu, X.; Lu, H.; Cui, X.; Wojtas, L.; Zhang, X. P. Effective Synthesis of Chiral N-Fluoroaryl Aziridines through Enantioselective Aziridination of Alkenes with Fluoroaryl Azides. *Angew. Chem., Int. Ed.* **2013,** *52*, 5309-5313.

17. Lu, H.; Jiang, H.; Hu, Y.; Wojtas, L.; Zhang, X. P. Chemoselective Intramolecular Allylic C–H Aminationversus C=C Aziridination through Co(II)-based Metalloradical Catalysis. *Chem. Sci.* **2011,** *2*, 2361-2366.

18. Lu, H.; Lang, K.; Jiang, H.; Wojtas, L.; Zhang, X. P. Intramolecular 1,5-C(sp^3)–H Radical Amination via Co(II)-Based Metalloradical Catalysis for Five-Membered Cyclic Sulfamides. *Chem. Sci.* **2016,** *7*, 6934-6939.

19. Takeda, Y.; Sameera, W. M. C.; Minakata, S. Palladium-Catalyzed Regioselective and Stereospecific Ring-Opening Cross-Coupling of Aziridines: Experimental and Computational Studies. *Acc. Chem. Res.* **2020,** *53*, 1686-1702.

20. Kirai, N.; Takaya, J.; Iwasawa, N. Two Reversible σ-Bond Metathesis Pathways for Boron–Palladium Bond Formation: Selective Synthesis of Isomeric Five-Coordinate Borylpalladium Complexes. *J. Am. Chem. Soc.* **2013,** *135*, 2493-2496.

21. Horibe, T.; Tsuji, Y.; Ishihara, K. Thiourea–I2 as Lewis Base–Lewis Acid Cooperative Catalysts for Iodochlorination of Alkene with In Situ-Generated I–Cl. *ACS Catal.* **2018,** *8*, 6362-6366.

22. Van Overtveldt, M.; Heugebaert, T. S. A.; Verstraeten, I.; Geelen, D.; Stevens, C. V. Phosphonamide Pyrabactin Analogues as Abscisic Acid Agonists. *Org. Biomol. Chem.* **2015,** *13*, 5260-5264.

23. Nie, X.; Yan, Z.; Ivlev, S.; Meggers, E. Ruthenium Pybox-Catalyzed Enantioselective Intramolecular C–H Amination of Sulfamoyl Azides en Route to Chiral Vicinal Diamines. *J. Org. Chem.* **2021,** *86*, 750-761.

24. Bruker. *APEX2.* Bruker AXS Inc., Madison, Wisconsin, USA, 2012.

25. Bruker. SAINT. Data Reduction Software, 2013.

26. Sheldrick, G. M. *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany, 1996.

27. Farrugia, L. J. WinGX suite for small-molecule single-crystal crystallography. *J. Appl. Cryst.* **1999**, 837-838.

28. Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16, Revision A.03*. Gaussian, Inc., Wallingford CT, 2016.

29. (a) Schultz, N. E.; Zhao Y Fau - Truhlar, D. G.; Truhlar, D. G. Density Functionals for Inorganometallic and Organometallic Chemistry. (b) Dzik, W. I.; Xu, X.; Zhang, X. P.; Reek, J. N. H.; de Bruin, B. 'Carbene Radicals' in CoII(por)-Catalyzed Olefin Cyclopropanation. *J. Am. Chem. Soc.* **2010,** *132*, 10891-10902.

30. Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. Auxiliary Basis Sets for Main Row Atoms and Transition Metals and Their Use to Approximate Coulomb Potentials. *Theor. Chem. Acc.* **1997,** *97*, 119-124.

31. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010,** *132*, 154104.

32. Legault, C. Y. *CYLview, 1.0b*, Université de Sherbrooke: 2020.

33. Humphrey, W., Dalke, A. and Schulten, K. VMD - Visual Molecular Dynamics. *J. Mol. Graph.* **1996,** *14*, 33-38.

34. Chan, L.; Hutchison, G. R.; Morris, G. M. Understanding Ring Puckering in Small Molecules and Cyclic Peptides. *J. Chem. Inf. Model.* **2021,** *61*, 743-755.

35. Cremer, D.; Pople, J. A. General Definition of Ring Puckering Coordinates. *J. Am. Chem. Soc.* **1975,** *97*, 1354-1358.

36. (a) Hill, A. D.; Reilly, P. J. Puckering Coordinates of Monocyclic Rings by Triangular Decomposition. *J. Chem. Inf. Model.* **2007,** *47*, 1031-5. (b) Barnett, C. B.; Naidoo, K. J. Ring Puckering: A Metric for Evaluating the Accuracy of AM1, PM3, PM3CARB-1, and SCC-DFTB Carbohydrate QM/MM Simulations. *J. Phys. Chem. B* **2010,** *114*, 17142-17154.

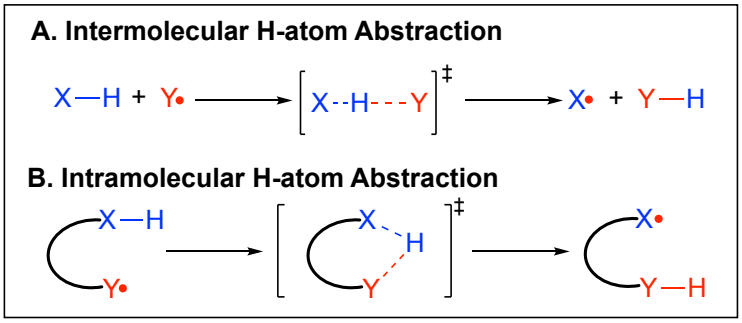
37. Cheng, H.; Gupta, K. C. An Historical Note on Finite Rotations. *Journal of Applied Mechanics* **1989,** *56*, 139-145.

CHAPTER 3 - CATALYTIC RADICAL *N*-HETEROCYCLIZATION BY METALLORADICAL C–H AMINATION INVOLVING 1,7-HYDROGEN ATOM ABSTRACTION

3.1 INTRODUCTION

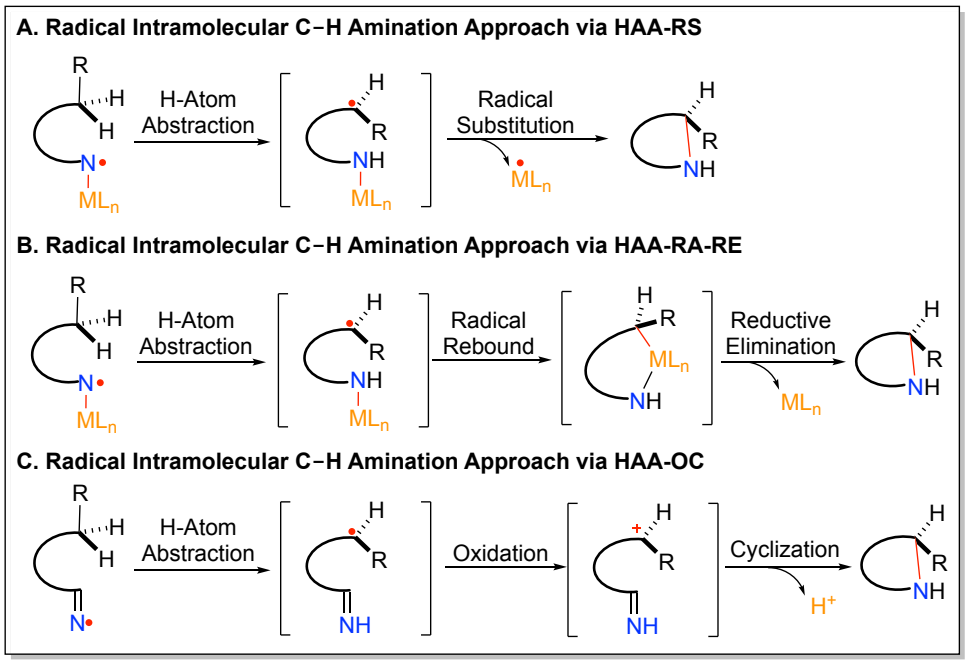
Hydrogen atom abstraction (HAA) is a well-recognized process and one of the most broadly examined pathways to access carbon-centered radicals.[1] HAA is governed by various parameters, amongst which the enthalpy change of the reaction is crucial.[2] Practical HAA reactions are generally irreversible and exothermic and associated with early transition states.[2] In addition, computational investigations have been engaged to simulate the process of HAA and to model its transition state.[3] The ideal geometry of the three atoms entangled in HAA transition state is linear (180°) in its transition state.[3] While observing linear geometry is not an issue for intermolecular HAA (Scheme 3.1.A), it is very challenging for intramolecular HAA (Scheme 3.1.B). The distortion from the ideal linear geometry induces a cost regarding its activation energy, which is also influenced by the ring size of the transition state structure.[2] While the ideal linear geometry can be more easily accommodated with 1,n-HAA at n>6, the entropic penalty from ring formation makes these reactions fairly scarce.[2]

Scheme 3.1 Intermolecular and Intramolecular Hydrogen Atom Abstraction



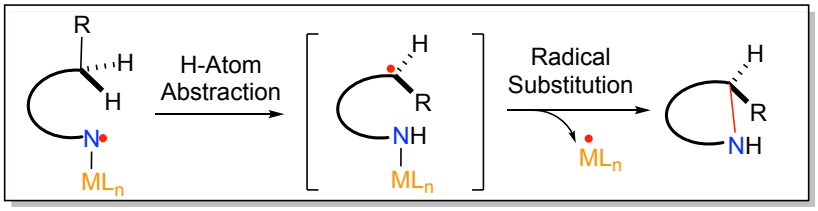
Aminyl radicals have been extensively demonstrated as versatile intermediates for forming C−N bonds.[4] Aminyl radicals have been utilized in an intramolecular manner for constructing *N*-heterocyclic structures, predominantly via radical addition (RA) to unsaturated π-bonds. HAA excuted by aminyl radicals has been gradually established as a practical approach to constructing diverse *N*-heterocyclic structures via C–N bond formation in modern organic synthesis.[5] Radical C–H amination has recently emerged for the construction of *N*-monocyclic structures utilizing intramolecular hydrogen atom abstraction (HAA) and subsequent cyclization processes, such as radical substitution (RS)[6], radical rebound-reductive elimination (RA-RE)[7] and oxidative cyclization (OC)[8] (Scheme 3.2). Consequently, numerous studies of 1,*n*-HAA have been conducted. Among these effects, intramolecular 1,5- and 1,6-C–H amination have been widely achieved through 1,5- and 1,6-HAA with aminyl radicals.[1a,9] According to the present literature, the aminyl radical triggered 1,7-HAA has not been documented. Therefore, it was open to question whether 1,7-C–H amination could be achieved through this 1,7-HAA.

Scheme 3.2 Radical Intramolecular C–H Amination Approach via HAA



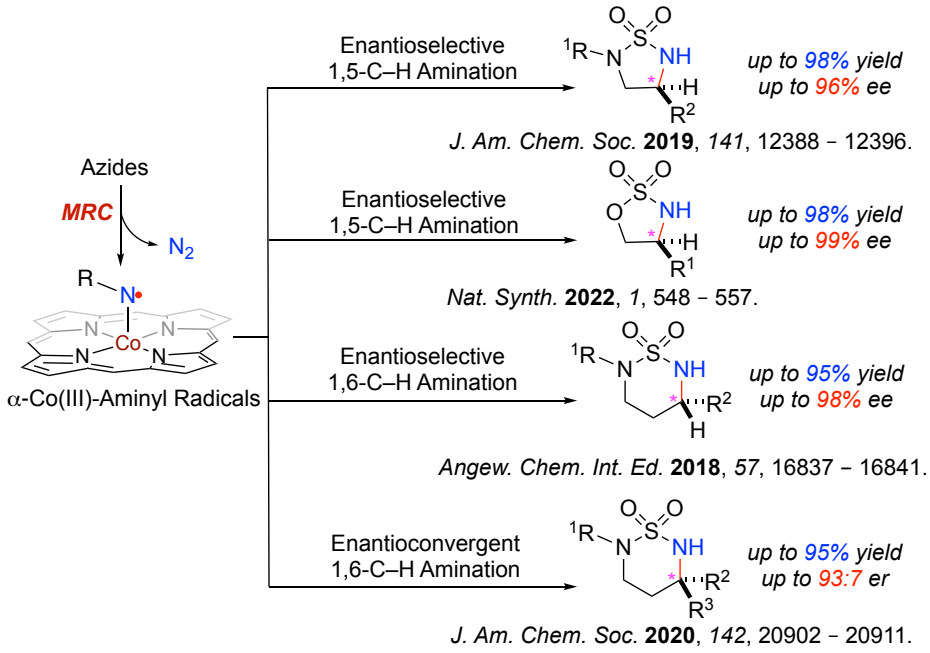
To perform 1,7-C–H amination through 1,7-HAA, it is essential to minimize the entropic penalty from the formation of 8-membered cyclic transition state of 1,7-HAA. A potential exploration could be to utilize metal-supported aminyl radicals (α-metalloalkyl aminyl radicals R(LnM)N•), where aminyl radicals are substituted on a metal complex unit (MLn) (Scheme 3.3). It could reduce the activation energy of 1,7-HAA through attractive interactions among the catalyst and substrates. Meanwhile, as M–N bonds are inherently more polarized and weaker than C–N bonds, the radical substitution step could be thermodynamically and kinetically feasible.[10] It is noted that releasing the metalloradical catalyst balances the inherent unfavored entropic change from ring closure in a certain degree. Also, this metalloradical-based 1,7-C–H amination could be readily developed as an asymmetric catalytic process to produce 7-membered *N*-cyclic compounds from various C–H substrates.

Scheme 3.3 Metalloradical Catalyzed Intramolecular C–H Amination Approach via HAA-RS



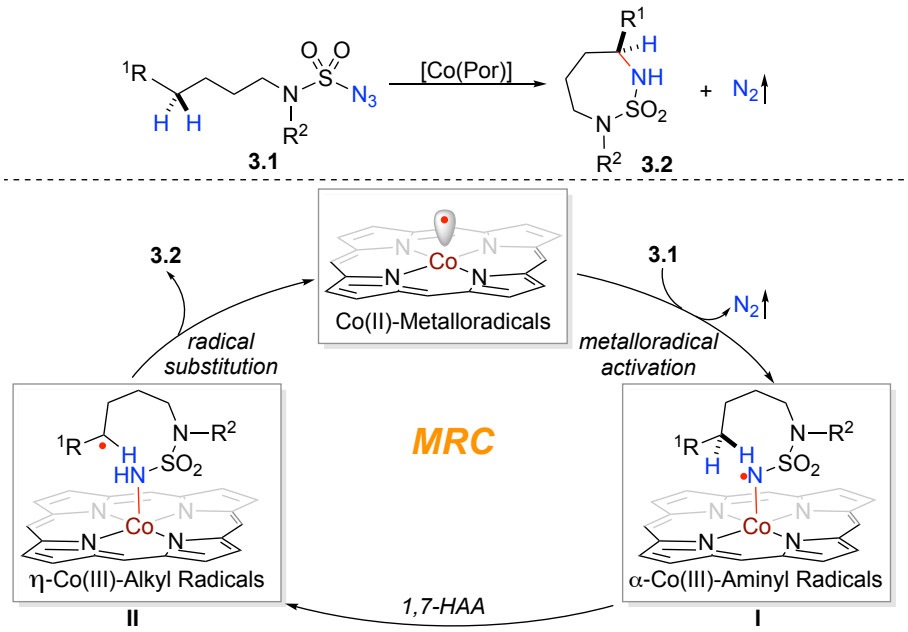
To exploit the vast prospect of HAA reactions for C–H amination, cobalt(II)-based metalloradical catalysis (MRC) has recently been established as an effective and practical strategy to address long-standing challenges regarding the control of reactivity and selectivity in the field.[6,11,10] As stable 15*e*-metalloradicals, cobalt(II) complexes of porphyrins [Co(**Por**)] have been demonstrated with unusual capability of homolytic activation of organic azides for the formation of metal-supported aminyl radicals, termed α-Co(III)-aminyl radicals.[12] These well-defined cobalt-supported *N*-centered radicals have been illustrated as pivotal intermediates to conduct C−H amination reactions. [13a,6,11,10,13b-d] With the support of a versatile ligand platform of chiral amidoporphyrins, Co(II)-based MRC has been successfully applied for the stereoselective construction of five- and six-membered *N*-heteromonocyclic sulfamides via 1,5- and 1,6-C–H amination of sulfamoyl azides, respectively (Scheme 3.4).[6,11,10] The metalloradical intramolecular C–H amination approach involves intramolecular HAA reaction of C(sp^3)–H bonds formulated by the initially generated α-Co(III)-aminyl radical intermediates, followed by intramolecular radical substitution of the ensued remote Co(III)-alkyl radicals (generated from HAA) at the nitrogen center to complete the ring closure through C–N bond formation.

Scheme 3.4 Recent Developments of Intramolecular C–H Amination via Co(II)-based Metalloradical Catalysis (MRC)



Despite 1,5- and 1,6-C–H amination being established via Co(II)-based MRC, 1,7-C–H amination via Co(II)-based MRC has yet to be developed. To broaden the synthetic applications of the metalloradical C–H amination approach, we were interested in exploring 1,7-HAA for 1,7-C–H amination and utilize it for the construction of 7-membered *N*-cyclic structures. Herein, we describe our efforts in developing a catalytic radical *N*-heterocyclization process of sulfamoyl azides to construct 7-membered cyclic sulfamides via Co(II)-based metalloradical C–H amination involving 1,7-HAA (Scheme 3.5).

Scheme 3.5 Proposed Mechanism of Co(II)-based Metalloradical 1,7-C–H Amination



Mechanistically, a potential catalytic radical pathway for 1,7-C–H amination starts with metalloradical activation of sulfamoyl azides **3.1** to produce α-Co(III)-aminyl radical intermediate **I**. Subsequently, it undergoes 1,7-HAA and delivers η-Co(III)-alkyl radical intermediate **II**. The following radical substitution of alkyl radical of intermediate **II** at its nitrogen center leads to the production of 7-membered sulfamides **3.2**. However, it is not guaranteed that α-Co(III)-aminyl radical intermediate **I** is not eligible for 1,5-HAA or 1,6-HAA. In terms of the ring strain of the TS of intramolecular 1,*n*-HAA, 1,5-HAA and 1,6-HAA are generally more favored than 1,7-HAA.[14] Thus, it was open to question whether 1,7-HAA could be favored over 1,5-HAA and 1,6-HAA through catalyst engineering and substrate design. We envisioned to address this challenging regioselectivity by fine-tuning the D_2-symmetric chiral amidoporphyrin ligand platform to adopt proper steric, electronic and chiral environment to govern the stereo-chemical course of Co(II)-based

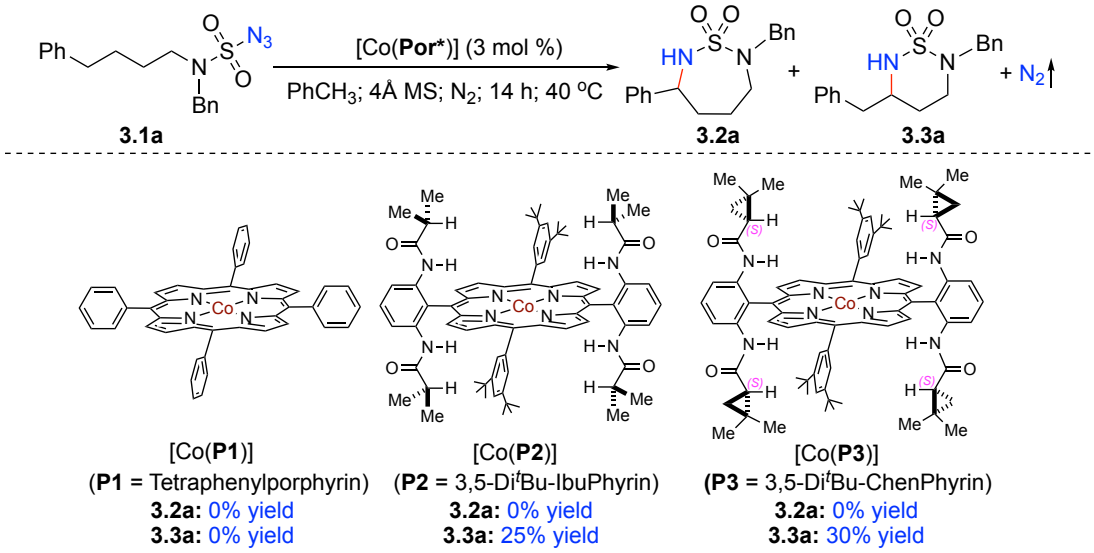
metalloradical system. Alternatively, potential modification on the substrates could inhibit 1,5-HAA and 1,6-HAA and only allow 1,7-HAA to occur. Furthermore, we were also interested in deploying 1,7-HAA beyond direct 1,7-C–H amination.

3.2 RESULTS AND DISCUSSION

3.2.1 Metalloradical 1,7-C–H Amination of Aliphatic Sulfamoyl Azide

At the outset of our effort, aliphatic *N*-benzyl-*N*-alkylsulfamoyl azide **3.1a** was selected as a model substrate to explore the proposed metalloradical 1,7-C–H amination (Table 3.1). Based on the results obtained for Chapter 2, toluene was then selected as the solvent for metalloradical amination reaction of sulfamoyl azide **3.1a**. Furthermore, the reactions were set up in the presence of 4 Å molecular sieves at 40 °C under the protection of N_2 for 14 h.

Table 3.1 Metalloradical 1,7-C–H Amination of Aliphatic Sulfamonyl Azide[a]

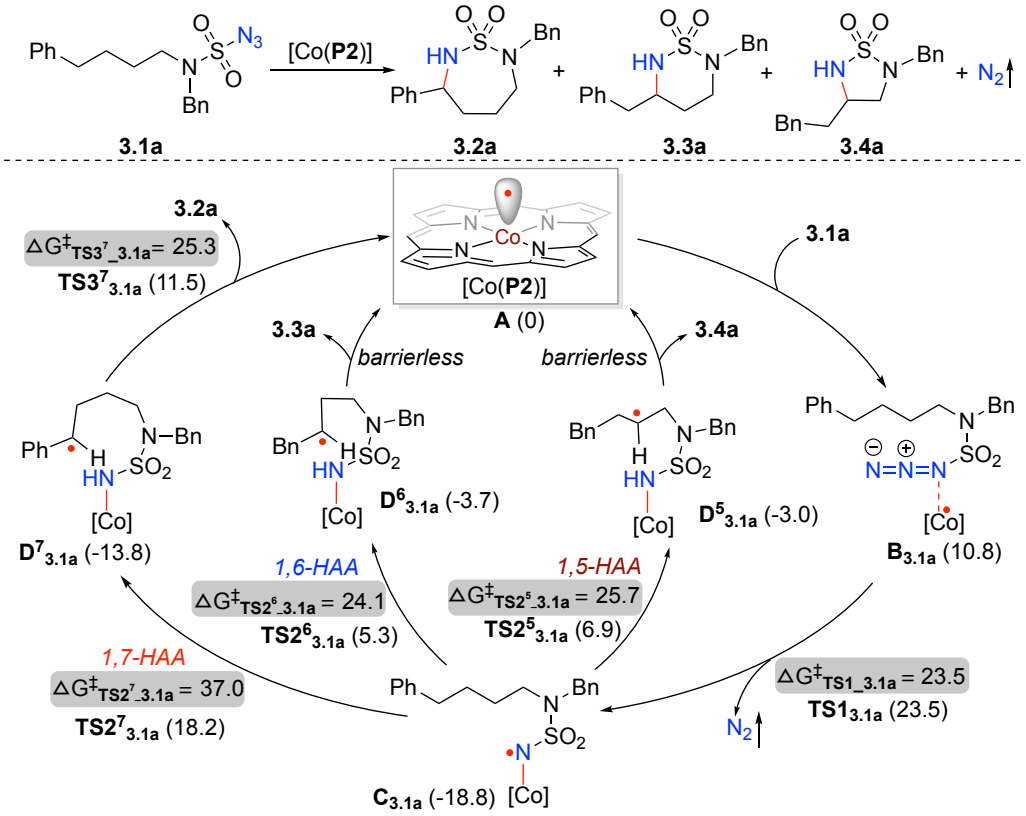


[a]Carried out with **3.1a** (0.10 mmol) in the presence of 4 Å molecular sieves by [Co(**Por***)] (3 mol %) in toluene (0.5 mL) under the protection of N_2 at 40 °C for 14 h; NMR yields.

When commercially available metalloradical catalyst [Co(**P1**)] (**P1** = Tetraphenylporphyrin) was employed in the reaction, it failed to yield 1,7-C–H amination product **3.2a** and had full recovery of sulfamoyl azide **3.1a** after 14 h. This result indicates [Co(**P1**)] might not be effective for the activation of **3.1a** under this reaction condition. When the achiral Co(II)-based amidoporphyrin [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-IbuPhyrin)[15] was assessed, it failed to afford 1,7-C–H amination product **3.2a** as well. In contrast to the result from [Co(**P1**)], 1,6-C–H amination product **3.3a** was afforded in 25% yield, suggesting that 1,6-C–H amination is more favored than 1,7-C–H amination. To further explore the ligand effects on 1,7-C–H amination, the first-generation chiral Co(II)-based amidoporphyrin [Co(**P3**)] (**P3** = 3,5-Di^{t}Bu-ChenPhyrin)[16] was deployed, it afforded **3.3a** in 30% yield, but failed to achieve 1,7-C–H amination due to the regioselectivity issue resulted from 1,6-C–H amination. In addition, the aliphatic *N*-benzyl-*N*-alkylsulfamoyl azide substrates were previously reported to prefer 1,6-C–H amination over 1,7-C–H amination under the catalyzation of various later generation of metalloradical catalysts, affording 6-membered cyclic sulfamides.[6,17] Therefore, we turned our attention to the understanding of this inherent regioselectivity issue on intramolecular C–H amination.

Computational investigation of proposed 1,7-C–H amination of substrate **3.1a** was conducted with density functional theory (DFT). In the calculation, the metalloradical catalyst [Co(**P2**)] was taken to model the reaction (Scheme 3.6). The detailed energy profiles of 1,6-C–H amination and 1,5-C–H amination were presented for comparison as well (Scheme 3.6).

Scheme 3.6 Energy Profiles of Metalloradical Intramolecular C–H Amination of Aliphatic Sulfamoyl Azide[a]



[a]Carried out with BP86/def2svp$_{Co}$//6-311G(d)$_{H, C, N, O, S}$ level of theory; Energy unit: kcal/mol.

The energy profile of proposed 1,7-C–H amination reveals weak binding of azide **3.1a** by catalyst [Co(**P2**)] through the interplay of non-covalent interactions to form the initial substrate complex intermediate $\mathbf{B}_{3.1a}$. This binding process is associated with a positive change of Gibbs free energy by 10.8 kcal/mol, resulted from unfavored entropy change. The following metalloradical activation is highly exergonic and is associated with an accessible activation barrier ($\Delta G^{\ddagger}_{TS1\_3.1a}$ = 23.5 kcal/mol), producing α-Co(III)-aminyl radical intermediate $\mathbf{C}_{3.1a}$ along with the extrusion of dinitrogen as byproduct. To perform

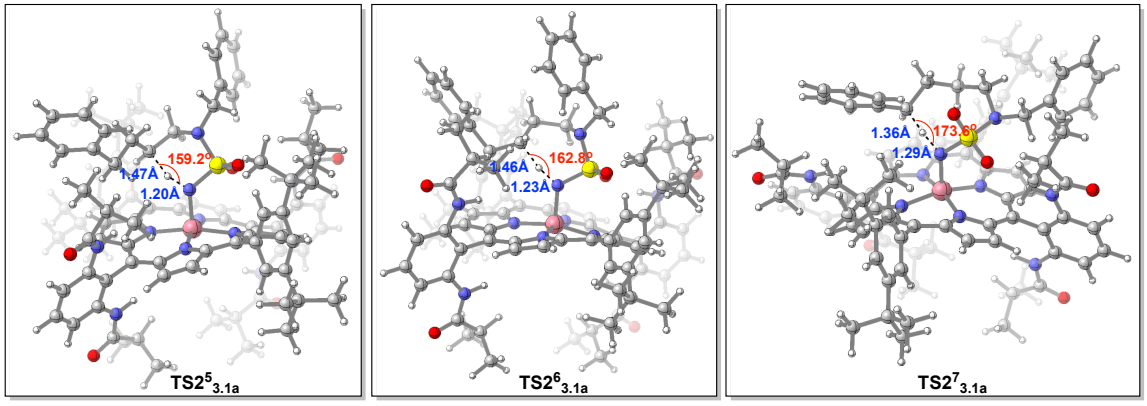
1,7-C–H amination, the intermediate $\mathbf{C_{3.1a}}$ is required to execute 1,7-HAA in the subsequent step. The 1,7-HAA process is established with a high energy barrier ($\Delta G^{\ddagger}_{\mathbf{TS2^7\_3.1a}}$ = 37.0 kcal/mol), which is inaccessible with the employed reaction condition. If successful, it would deliver η-Co(III)-alkyl radical intermediate $\mathbf{D^7_{3.1a}}$, which is endergonic by +5.0 kcal/mol. The intermediate $\mathbf{D^7_{3.1a}}$ undergoes radical substitution through high-energy 7-membered cyclic transition state ($\Delta G^{\ddagger}_{\mathbf{TS3^7\_3.1a}}$ = 25.3 kcal/mol). Thus, the computational investigation reveals the inherent difficulties in 1,7-C–H amination of aliphatic *N*-benzyl-*N*-alkylsulfamoyl azides due to the high-energy barriers of 1,7-HAA and radical substitution step.

Regarding the regioselectivity of intramolecular HAA, intermediate $\mathbf{C_{3.1a}}$ was experimentally demonstrated to undergo 1,6-HAA rather than 1,7-HAA and 1,5-HAA (Table 3.1). 1,6-HAA is computed to be more accessible ($\Delta G^{\ddagger}_{\mathbf{TS2^6\_3.1a}}$ = 24.1 kcal/mol), which is favored by 12.9 kcal/mol in comparison to 1,7-HAA (Scheme 3.6). In contrast to 1,6-HAA, 1,5-HAA is disfavored by 1.6 kcal/mol (See Experimental Section for more details). Comparing to the high-energy ring closure of in 1,7-C–H amination, ξ-Co(III)-alkyl radical intermediate $\mathbf{D^6_{3.1a}}$ could undergo rapid cyclization to produce **3.3a** through barrierless radical substitution. Thus, 1,6-C–H amination predominates the reaction among all the computed possibilities.

In addition to the energy profile, the geometries of the HAA transition states were examined to shed light on the regioselectivity among these intramolecular HAA (Scheme 3.7). In the 6-membered cyclic transition state of 1,5-HAA $\mathbf{TS2^5_{3.1a}}$, the geometry of C--(1.47Å)--H--(1.20Å)--N is bent 20.8° from linear placement. In the 7-membered cyclic

transition state of 1,6-HAA **TS$^{6}_{3.1a}$**, the geometry of C--(1.46Å)--H--(1.23Å)--N is bent 17.2° from linear placement. In the 8-membered cyclic transition state of 1,7-HAA **TS2$^{7}_{3.1a}$**, the geometry of C--(1.36Å)--H--(1.29Å)--N is bent 6.4° from linear placement. From the comparison between **TS2$^{5}_{3.1a}$** and **TS2$^{6}_{3.1a}$**, we can tell that the distortion from linear placement of C--H--N plays important role to determine the energy difference between their transition states. From the comparison between **TS2$^{6}_{3.1a}$** and **TS2$^{7}_{3.1a}$**, we can tell that the ring strain primarily contributes to the energy difference between their transition states. These findings directed us to decreasing ring strain to favor 1,7-HAA by using specific substrates, such as **3.1b** and **3.1c** (Section 4.2.2 and Section 4.2.3).

Scheme 3.7 Conformational Analysis on Transition State of Intramolecular HAA[a]

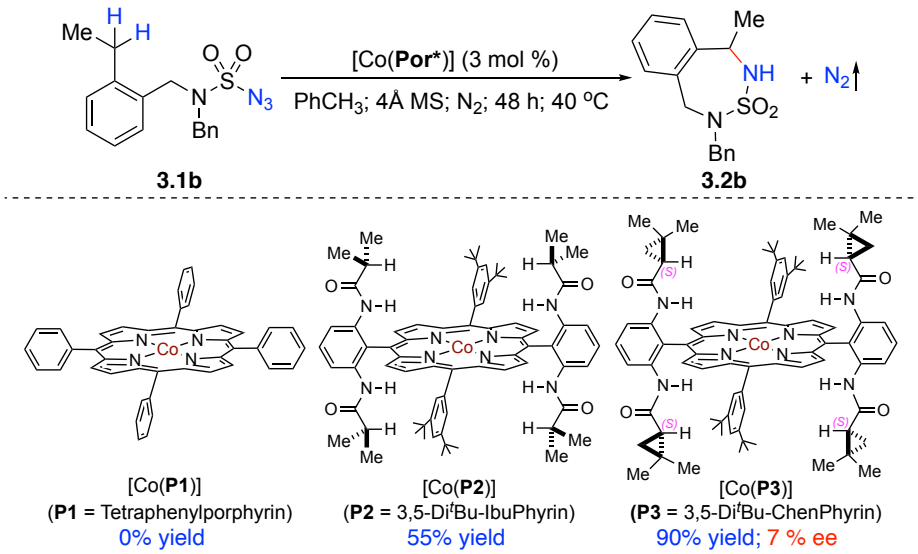


[a]Applied BP86/6-311G(d)_C, O, S, H, N/def2-svp_Co level of theory for the geometry optimization and the energy calculations.

3.2.2 Metalloradical 1,7-C–H Amination of Benzyl Sulfamoyl Azide

At the outset of our effort, benzyl *N*-benzyl-*N*-alkylsulfamoyl azide **3.1b** was selected as a model substrate to explore the proposed 1,7-C–H amination by Co(II)-based metalloradical catalysis (Table 3.2). Toluene was selected as the solvent for metalloradical amination reaction. And the reaction was set up in the presence of 4 Å molecular sieves at 40 °C under the protection of N_2 for 48 h.

Table 3.2 Metalloradical 1,7-C–H Amination of Benzyl Sulfamoyl Azide[a]

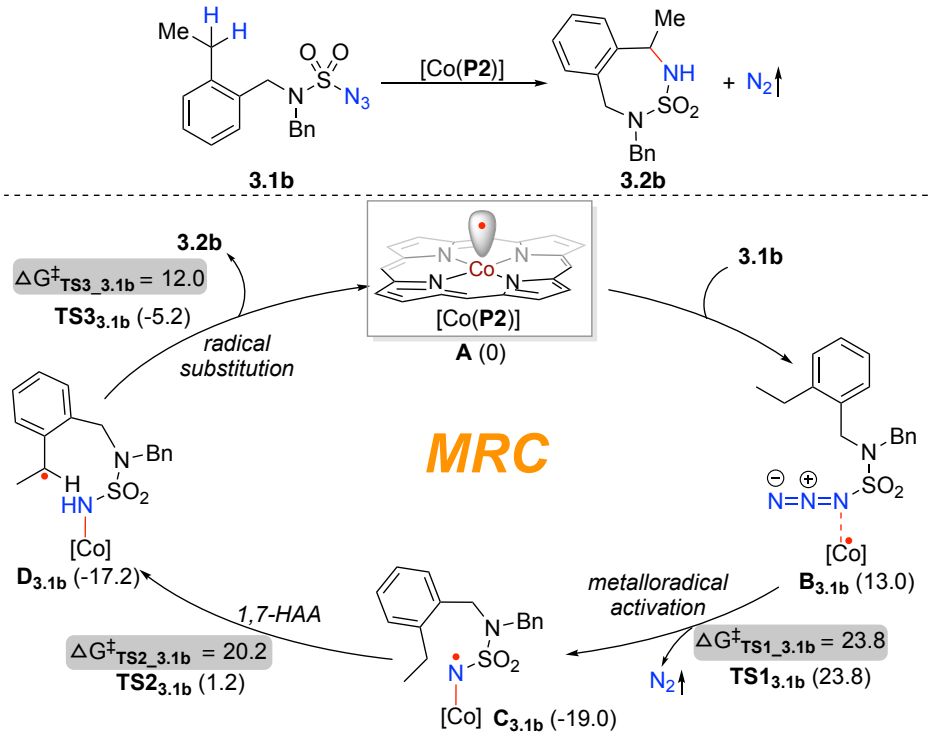


[a]Carried out with **3.1b** (0.10 mmol) in the presence of 4 Å molecular sieves by [Co(**Por***)] (3 mol %) in toluene (0.5 mL) under the protection of N_2 at 40 °C for 48 h; NMR yields.

When commercially available metalloradical catalyst [Co(**P1**)] (**P1** = Tetraphenylporphyrin) was employed into the reaction, it failed to yield 1,7-C–H amination product **3.2b** and resulted in the full recovery of starting material **3.1b** after 48 h. When achiral amidoporphyrin [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-IbuPhyrin) was employed,

3.2b was afforded in 55% yield. To further explore the ligand effects on 1,7-C–H amination, the first-generation chiral amidoporphyrin [Co(**P3**)] (**P3** = 3,5-Di^{t}Bu-ChenPhyrin) was deployed, affording **3.2b** in 90% yield along with 7% ee under the same reaction condition.

Scheme 3.8 Energy Profiles of Metalloradical 1,7-C–H Amination of Benzyl Sulfamoyl Azide[a]

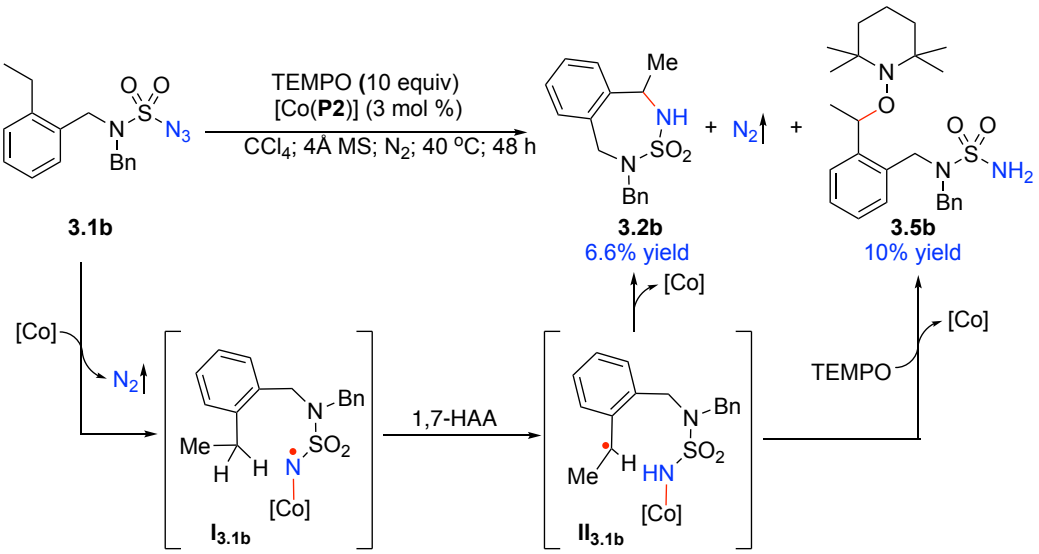


[a]Carried out with BP86/def2svp$_{Co}$//6-311G(d)$_{H, C, N, O, S}$ level of theory; Energy unit: kcal/mol.

The energy profiles of proposed mechanism suggest weak binding of azide **3.1b** by catalyst [Co(**P2**)] through the interplay of non-covalent interactions to form the substrate-catalyst adduct intermediate $\mathbf{B}_{3.1b}$. This binding process is associated with a positive change of Gibbs free energy by 13.0 kcal/mol, resulting from an unfavored entropy change. The following metalloradical activation is highly exergonic and is associated with a readily

accessible activation barrier ($\Delta G^{\ddagger}_{TS1\_3.1b}$ = 23.8 kcal/mol), producing α-Co(III)-aminyl radical intermediate $\mathbf{C_{3.1b}}$ along with the extrusion of dinitrogen as byproduct. The intermediate $\mathbf{C_{3.1b}}$ undergoes 1,7-HAA through an accessible energy barrier ($\Delta G^{\ddagger}_{TS2\_3.1b}$ = 20.2 kcal/mol) and delivers η-Co(III)-alkyl radical intermediate $\mathbf{D_{3.1b}}$, which is slightly endergonic by +1.8 kcal/mol. The intermediate $\mathbf{D_{3.1b}}$ undergoes radical substitution through a 7-membered cyclic transition state ($\Delta G^{\ddagger}_{TS3\_3.1b}$ = 12.0 kcal/mol). The overall computational investigation suggests that 1,7-C–H amination is accompanied by accessible activation energy barriers in each elemental radical reaction, consistent with experimental results.

Scheme 3.9 TEMPO Trapping Experiment of Metalloradical 1,7-C–H Amination of Benzyl Sulfamoyl Azide[a]



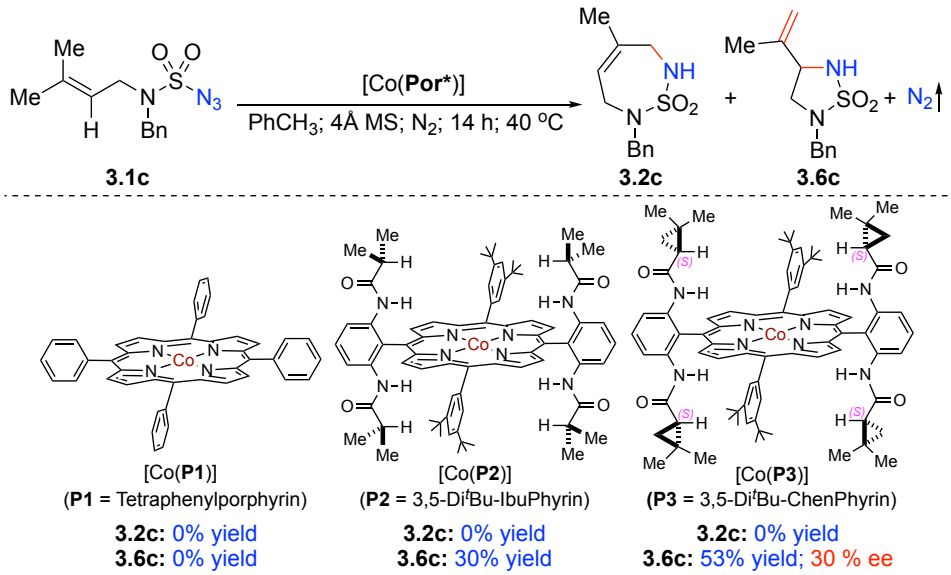
[a]Carried out with **3.1b** (0.10 mmol) in the presence of 4 Å molecular sieves and TEMPO (10 equiv) by [Co(**P2**)] (3 mol %) in carbon tetrachloride (0.5 mL) at 40 °C under the protection of N_2 for 48 h; NMR yields.

To gain more evidence and support of 1,7-HAA involved stepwise radical mechanism of 1,7-C–H amination, a radical trapping experiment was conducted with radical scavenger (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (TEMPO) (Scheme 3.8). The radical 1,7-C–H amination of azide **3.1b** was conducted with the use of catalyst [Co(**P2**)] in the presence of TEMPO (10.0 equiv). Despite adding highly excessive amount of TEMPO, 7-membered cyclic sulfamide **3.2b** was still formed in 6.6% yield via 1,7-C–H amination (Scheme 3.8). In addition to the production of **3.2b**, compound **3.5b** was also obtained from the reaction in 10% yield, generated from the radical recombination of γ-Co(III)-alkyl radical intermediate $\mathbf{II_{3.1b}}$ and TEMPO, indicating the occurrence of 1,7-HAA and its involvement in 1,7-C–H amination. It can serve as indirect evidence of 1,7-HAA triggered by aminyl radicals.

3.2.3 Metalloradical 1,7-HAA Triggered Indirect 1,5-C–H Amination of Allyl Sulfamoyl Azide

At the outset of our effort, allyl *N*-benzyl-*N*-alkylsulfamoyl azide **3.1c** was selected as a model substrate to explore 1,7-HAA triggered 1,7-C–H amination and beyond. Once again, toluene served as the solvent for metalloradical amination reaction at 40 °C, in the presence of 4 Å molecular sieves, under the protection of N_2 and 14 h as the initial reaction condition.

Table 3.3 Metalloradical 1,7-C–H Amination of Allyl Sulfamoyl Azide[a]

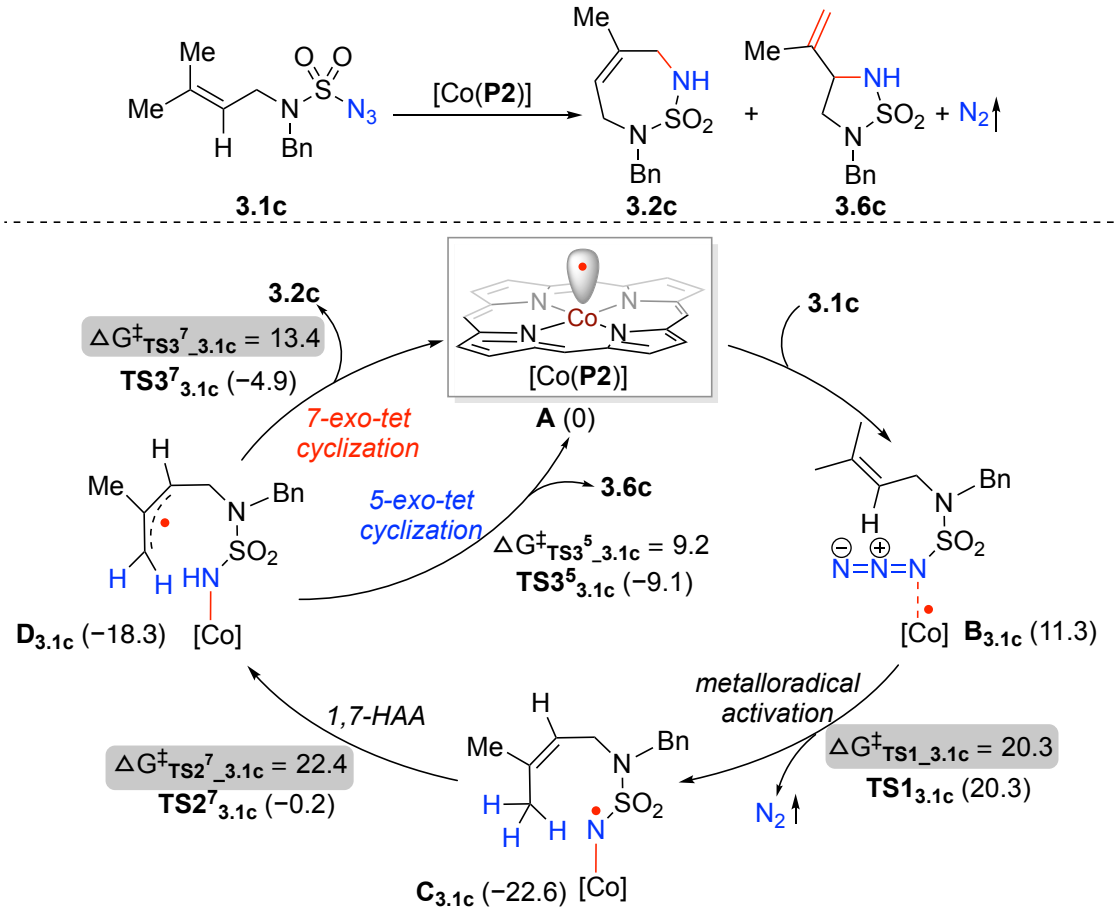


[a]Carried out with **3.1c** (0.10 mmol) in the presence of 4 Å molecular sieves by [Co(**Por***)] (3 mol %) in toluene (0.5 mL) under the protection of N_2 at 40 °C for 14 h; NMR yields.

When commercially available metalloradical catalyst [Co(**P1**)] (**P1** = Tetraphenylporphyrin) was employed into the reaction, it was not effective for the activation of azide **3.1c** under this condition and resulted in the full recovery of **3.1c** after 14 h. When the achiral Co(II)-based amidoporphyrin [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-IbuPhyrin) was tested, there was no formation of 7-membered cyclic product **3.2c** from 1,7-C–H amination. Surprisingly, 5-membered cyclic product **3.6c** was afforded in 30% yield, which was proposed to be produced from intermediate $\mathbf{D}_{\mathbf{3.1c}}$ through 5-*exo-tet* cyclization (Scheme 3.10). To further explore the ligand effects on competitions between two reaction pathways, the first-generation chiral amidoporphyrin [Co(**P3**)] (**P3** = 3,5-Di^{t}Bu-ChenPhyrin) was deployed. Similarly, it failed to achieve 1,7-C–H amination and afforded

3.6c in 53% yield along with notable asymmetric induction (30% ee). Thus, it turned our attention to the understanding of this essential selectivity.

Scheme 3.10 Energy Profiles of Metalloradical Indirect 1,5-C–H Amination Triggered by 1,7-HAA with Allyl Sulfamoyl Azide[a]



[a]Carried out with BP86/def2svp$_{Co}$//6-311G(d)$_{H, C, N, O, S}$ level of theory; Energy unit: kcal/mol.

The computational studies reveal the weak binding of azide **3.1c** by catalyst [Co(**P2**)] through the interplay of non-covalent interactions to form the initial substrate complex intermediate $\mathbf{B}_{3.1c}$. This binding process is associated with a positive change of Gibbs free

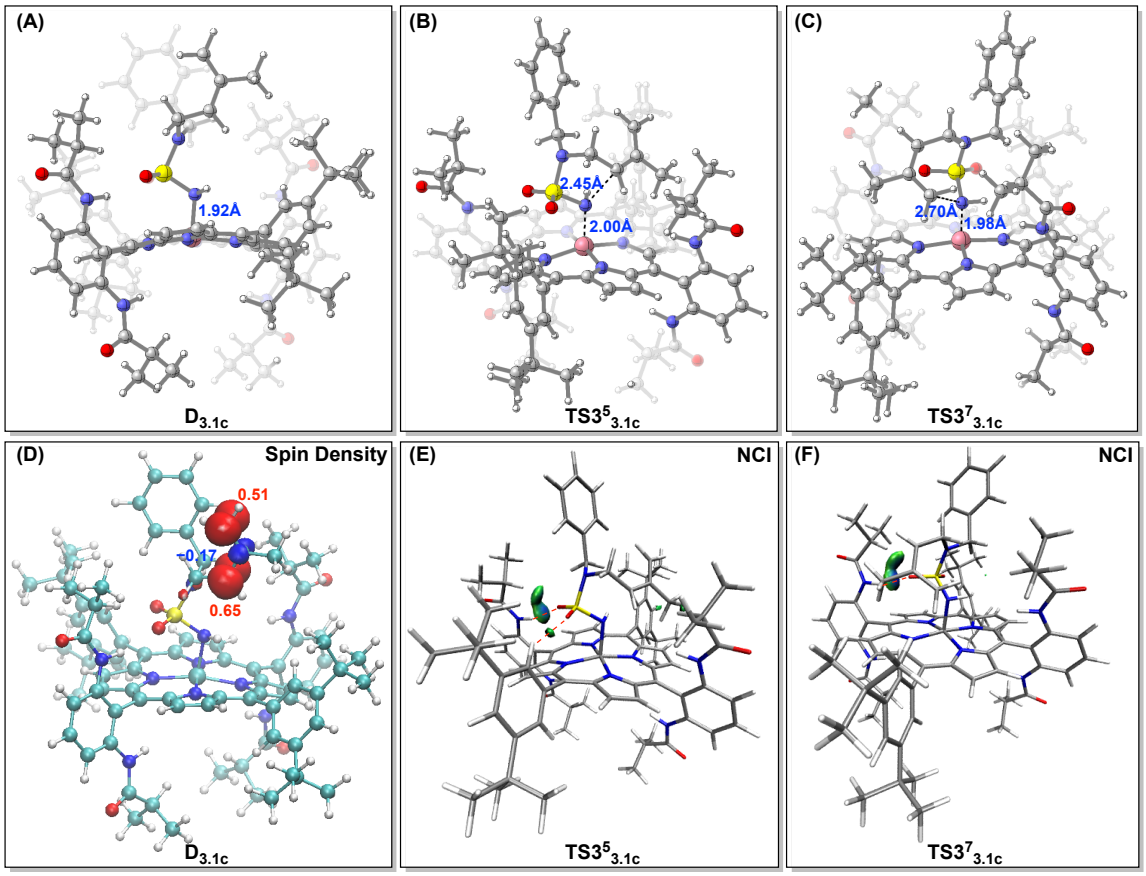
energy by 11.3 kcal/mol, resulted from unfavored entropy change. The following metalloradical activation is highly exergonic and is associated with an accessible activation barrier ($\Delta G^{\ddagger}_{\mathbf{TS1\_3.1c}}$ = 20.3 kcal/mol), producing α-Co(III)-aminyl radical intermediate $\mathbf{C_{3.1c}}$ along with the extrusion of dinitrogen as byproduct. Then, intermediate $\mathbf{C_{3.1c}}$ undergoes 1,7-HAA, associated with an accessible energy barrier ($\Delta G^{\ddagger}_{\mathbf{TS2^7\_3.1c}}$ = 22.4 kcal/mol), and delivers intermediate $\mathbf{D_{3.1c}}$. To accomplish the 1,7-C–H amination, intermediate $\mathbf{D_{3.1c}}$ is required to undergo *7-exo-tet* cyclization through 7-membered cyclic transition state ($\Delta G^{\ddagger}_{\mathbf{TS3^7\_3.1c}}$ = 13.4 kcal/mol) to produce 7-membered cyclic product **3.2c**.

While the computational investigation suggests 1,7-C–H amination goes through reasonable activation energy barriers in all elemental radical reactions (Scheme 3.9), the resonance of allyl alkyl radical on intermediate $\mathbf{D_{3.1c}}$ potentially creates an opportunity for *5-exo-tet* cyclization to occur. Comparing to *7-exo-tet* cyclization process, *5-exo-tet* cyclization is favored by a 4.2 kcal/mol ($\Delta G^{\ddagger}_{\mathbf{TS3^5\_3.1c}}$ = 9.2 kcal/mol) to produce 5-membered cyclic product **3.6c**. Accordingly, indirect 1,5-C–H amination predominates the reaction.

In addition to the energy profile, the spin density of intermediate $\mathbf{D_{3.1c}}$ was analyzed to study the regioselectivity between *5-exo-tet* cyclization and *7-exo-tet* cyclization. (Scheme 3.7). Furthermore, the geometries of their transition states $\mathbf{TS3^5_{3.1c}}$ and $\mathbf{TS3^7_{3.1c}}$ were examined along with the non-covalent interactions (NCI) among substrate and catalyst. The spin density plot of intermediate $\mathbf{D_{3.1c}}$ presents more radical character located on the secondary carbon (0.65 e^-) rather than the primary carbon (0.51 e^-), indicating that the resonance of this allyl radical favors 5-*exo-tet* cyclization (Scheme 3.11 D). The NCI

plot of **TS3^5$_{3.1c}$** presents the existence of two attractive interactions, C(sp^2)–H---O and N–H---O (indicated by green solid surface in Scheme 3.11 E). However, the NCI plot of **TS3^7$_{3.1c}$** presents the existence of only one attractive interaction, N–H---O (indicated by green solid surface in Scheme 3.11 F). The H-bonding of C(sp^2)–H---O type is typically evaluated to be 3–5 kcal/mol.[18] Consistently, the additional H-bonding C(sp^2)–H---O in **TS3^5$_{3.1c}$** could lead to 4.2 kcal/mol lower than **TS3^7$_{3.1c}$**, driving *5-exo-tet* cyclization more favored than *7-exo-tet* cyclization kinetically.

Scheme 3.11 Conformational Analysis on the Regioselectivity of Radical Substitution[a]



[a]Applied BP86/6-311G(d)$_{\_C,\ O,\ S,\ H,\ N}$/def2-svp$_{_Co}$ level of theory; Green solid surface indicates attractive interactions in NCI plots; Spin density unit: e^-.

3.2.4 Computational Study of 1,7-HAA

In the computation of metalloradical 1,7-C–H amination of **3.1a**, 1,7-HAA process encounters an inaccessibly high activation energy barrier of 37.0 kcal/mol. However, it only takes 20.2 kcal/mol and 22.4 kcal/mol for **3.1b** and **3.1c**, respectively (Table 3.4). Such dramatic free energy differences ($\Delta\Delta G^{\ddagger}$ = 16.8, 14.6 kcal/mol) among these three transition states was largely influenced by the enthalpy ($\Delta\Delta H^{\ddagger}$ = 10.6, 10.5 kcal/mol) (Table 3.4).

Table 3.4 Energy Profiles of 1,7-HAA Transition States[a]

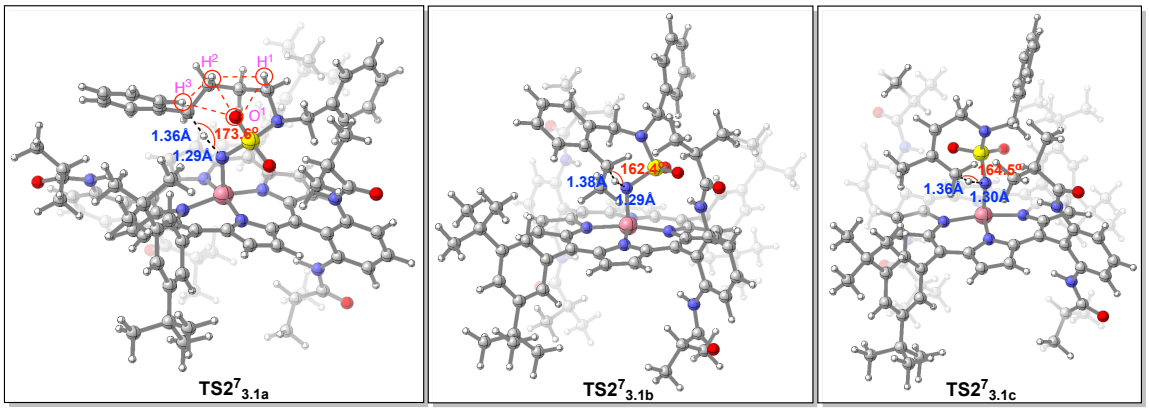
Parameter	$TS2^{7}_{3.1a}$	$TS2^{7}_{3.1b}$	$TS2^{7}_{3.1c}$
$\Delta G^{\ddagger}$	37.0	20.2	22.4
$\Delta H^{\ddagger}$	29.5	18.9	19.0
$-T\Delta S^{\ddagger}$	7.5	1.3	3.4

[a]Energy unit: kcal/mol.

To ascertain the origins of the enthalpy differences among $\mathbf{TS2^{7}_{3.1a}}$, $\mathbf{TS2^{7}_{3.1b}}$, and $\mathbf{TS2^{7}_{3.1c}}$, their structures were analyzed for comparison (Scheme 3.12). In $\mathbf{TS2^{7}_{3.1a}}$, the geometry of C--(1.36Å)--H--(1.28Å)--N is bent 6.4° from linear placement. In $\mathbf{TS2^{7}_{3.1b}}$, the geometry of C--(1.36Å)--H--(1.28Å)--N is bent 17.8° from linear placement. In $\mathbf{TS2^{7}_{3.1c}}$, the geometry of C--(1.36Å)--H--(1.28Å)--N is bent 15.5° from linear placement. From this information, we can tell there is a negative correlation between the distortion degree from the linear placement and activation barriers. Now, we can rule out the possibility that the linear placement is primarily attributed to the big difference among the activation barriers. Therefore, enthalpy reflects the ring strain of the cyclic transition states.

Torsional strain (also known as Pitzer strain) are typically the dominant source of ring strain for common rings (5-, 6-, 7-membered). However, for medium-sized rings, angle strain (also known as Baeyer strain) and transannular strain (also known as Prelog strain) are the primary sources of ring strain. In **TS2$^{7}_{3.1a}$**, the angle ∠C–C–N is around 116.9°, the angles ∠C–C–C are around 116°; In **TS2$^{7}_{3.1b}$**, the angle ∠C–C–N are around 115.7°; In **TS2$^{7}_{3.1c}$**, the angle ∠C–C–N are around 117.3°. Theses information basically rules out the possibility that angle strain are one of the primary sources of ring strain in the cyclic HAA transition states. In **TS2$^{7}_{3.1a}$**, transannular strain can be represented by the steric repulsion from H^1, H^2, H^3, O^1. The distances among them are H^1--H^2: 2.27 Å, H^2--H^3: 2.35 Å, H^1--O^1: 2.61 Å, H^2--O^1: 2.51 Å, H^3--O^1: 2.39 Å. This transannular strain doesn't exist in **TS2$^{7}_{3.1a}$** and **TS2$^{7}_{3.1c}$** due to the presence of C=C double bond. Thus, it concludes the existence of transannular strain leads to the high strain of **TS2$^{7}_{3.1a}$**.

Scheme 3.12 Conformational Analysis on 1,7-HAA Transition States



[a]Applied BP86/6-311G(d)$_{\_C, O, S, H, N}$/def2-svp$_{_Co}$ level of theory.

3.3 CONCLUSIONS

In summary, we have explored 1,7-HAA enabled by metal-supported aminyl radical and demonstrated the application of 1,7-HAA to intramolecular C–H amination reactions. The intramolecular C–H amination reactions can be referred to *N*-heterocyclization, which starts with the generation of metal-supported aminyl radical and follows by subsequent radical H-atom abstraction and radical substitution via metalloradical catalysis (MRC), as a catalytic approach for the construction of *N*-heterocyclic compounds from C–H substrates through C–N bond formation.

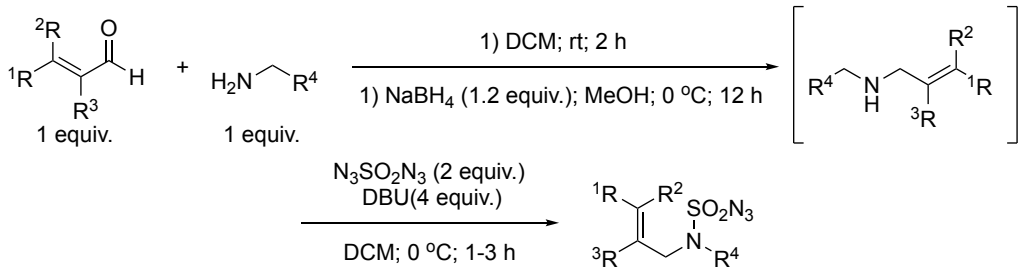
In addition, the activation energy of 1,7-HAA is high in general, but it can be altered by the variation of substrate structures. Based on the experimental and computational studies, we have discovered that benzyl substrate **3.1b** and allyl substrate **3.1c** have significantly lower energy barrier than aliphatic substrate **3.1a** by decreasing the transannular strain. The following radical substitution can also be influenced to afford different products. Thus, we believe further substrate design and catalyst modification can lead to the development of the stereoselective version of this work and the new discovery of *N*-heterocyclization reactions.

3.4 EXPERIMENTAL SECTION

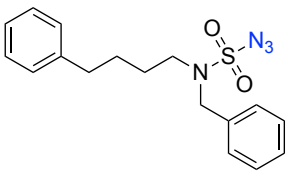
3.4.1 General Considerations

All C–H amination reactions were performed under a nitrogen atmosphere in oven-dried glassware following standard Schlenk techniques. 4 Å molecular sieves were dried in a vacuum oven prior to use. Gas tight syringes were used to transfer liquid reagents and solvents in catalytic reactions. Anhydrous solvents were purchased from Sigma-Aldrich and used without further purification. Thin layer chromatography was performed on Merck TLC plates (silica gel 60 F254). Flash column chromatography was performed with silica gel (60 Å, 230-4mesh, 32-63 μm). ^{1}H NMR and ^{13}C NMR were recorded on Inova400, Inova500, Inova6instruments with chemical shifts reported relative to residual solvent. Infrared spectra were measured with a Nicolet Avatar 320 spectrometer with a Smart Miracle accessory. HRMS data was obtained on an Agilent 11LC/MS/TOF mass spectrometer. HPLC measurements were carried out on a Shimadzu HPLC system. Optical rotations were recorded on the Rudolph Research Analytical, Autopol® IV, Automatic Polarimeter.

3.4.2 General Procedure for Preparation of Sulfamoyl Azides



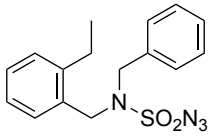
To a solution of amine (1.0 equiv) in dry DCM was added the solution and aldehyde (1.0 equiv) in dry DCM dropwise and the reaction was stirred for 2 h at room temperature. The solvent of the reaction mixture was removed directly under reduced pressure. The residue was dissolved in MeOH, and $NaBH_4$ (1.2 equiv) was added by portion. The reaction mixture was extracted 3 times with EtOAc, and the solvent was removed directly under reduced pressure. The crude product (secondary amine) was used directly for next step without any further treatment after dried over Na_2SO_4. A mixture of crude secondary amine from the previous step and DBU (4 equiv) in DCM was added dropwise to a solution of $N_3SO_2N_3$ (2 equiv., 0.3 M in DCM) at 0 °C. After the reaction was completed based on TLC (1~3 h), the majority of the solvent was removed under reduced pressure at room temperature. Purification of this mixture by silica gel column chromatography afforded the allyl sulfamoyl azide. Note: Some azides could be explosive and should be handled carefully.



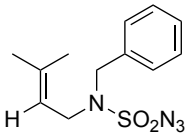
(((Azidosulfonyl)(4-phenylbutyl)amino)methyl)benzene

3.1a. Colorless oil. Yield: 61%. R_f = 0.6 (16:1 Hexanes/EtOAc). ^1H NMR (6MHz, $CDCl_3$)

δ 7.33-7.41 (m, 3H), 7.33 – 7.29 (m, 2H), 7.24-7.29 (m, 2H), 7.16-7.21 (m, 1H), 7.11 (d, *J* = 7.5 Hz, 2H), 4.42 (s, 2H), 3.23 (t, *J* = 6.9 Hz, 2H), 2.55 (t, *J* = 6.8 Hz, 2H), 1.50-1.64 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.96, 134.98, 129.20, 128.84, 128.77, 128.72, 128.68, 126.26, 52.77, 48.81, 35.52, 28.44, 27.04. IR (neat, cm^{-1}): 2125.12, 1382.20, 1218.12, 1165.18. HRMS (DART$^+$) ($[M+NH_4]^+$): Calcd. For $C_{17}H_{24}N_5O_2S$: 362.16452, found 362.16416.



1-(((Azidosulfonyl)(benzyl)amino)methyl)-2-ethylbenzene 3.1b. Colorless oil. Yield: 64% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 5H), 7.26 – 7.15 (m, 4H), 4.50 (s, 2H), 4.41 (s, 2H), 2.52 (q, *J* = 7.6 Hz, 2H), 1.11 (t, *J* = 7.6, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.36, 131.75, 128.60, 126.42, 126.21, 126.12, 126.00, 125.73, 123.66, 49.08, 46.56, 22.61, 12.25. IR (neat, cm^{-1}): 2128.02, 1382.10, 1167.24. HRMS (DART$^+$) ($[M+NH_4]^+$): Calcd. for $C_{16}H_{22}N_5O_2S$: 348.14887, found 348.14898.

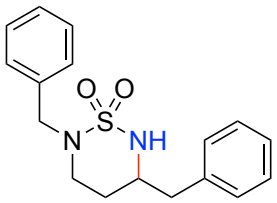


(((Azidosulfonyl)(3-methylbut-2-en-1-yl)amino)methyl)benzene 3.1c. Colorless oil. Yield: 60% (Method II). R_f = 0.6 (16:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.42 – 7.29 (m, 5H), 5.27 (t, *J* = 7.3 Hz, 1H), 4.42 (s, 2H), 3.83 (d, *J* = 7.3 Hz, 2H), 1.77 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.52, 137.05, 131.05, 131.05, 130.70, 130.55, 119.03, 79.58, 79.37, 79.16, 53.51, 47.91, 28.34, 20.10.

IR (neat, cm^{-1}): 2122.06, 1376.36, 1205.89, 1163.07. HRMS ($DART^+$) ($[M+NH_4]^+$): Calcd. for $C_{12}H_{20}N_5O_2S$: 298.13322, found 298.13388.

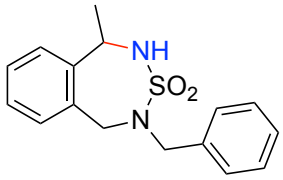
3.4.3 General Procedure for [Co(Por)]-Catalyzed C–H Amination

An oven dried Schlenk tube was charged with catalyst [Co(**Por**)](3 mol %) and 4Å molecular sieves (50 mg). This reaction vessel was evacuated and backfilled with nitrogen several times. Under nitrogen atmosphere, the allyl sulfamoyl azide **3.1** (0.1 mmol) was added followed by the addition of 0.5 mL of toluene. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at 40 ºC for 14 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum, and purified by flash column chromatography. The fractions containing product were collected and concentrated by rotary evaporation to obtain the target compound.

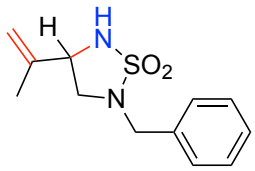


2,5-Dibenzyl-1,2,6-thiadiazinane 1,1-dioxide 3.3a was obtained with catalyst **[Co(P3)]** in toluene. White solid. Yield: 28%. R_f = 0.4 (2:1 Hexanes/EtOAc). ^1H NMR (5MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 8H), 7.17 (dt, *J* = 8.1, 1.9 Hz, 2H), 4.46 (d, *J* = 13.9 Hz, 1H), 4.02 – 3.81 (m, 3H), 3.33 – 3.22 (m, 1H), 3.13 – 3.03 (m, 1H), 2.92 – 2.72 (m, 2H), 1.71 – 1.45 (m, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 135.89, 135.56, 129.53, 129.00, 128.93, 128.79, 128.10, 127.35, 57.18, 51.94, 47.54, 41.66, 28.56.

IR (neat, cm^{-1}): 1332.14, 1216.76, 1163.88. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{17}H_{21}N_2O_2S$: 317.13183, found 317.13179.



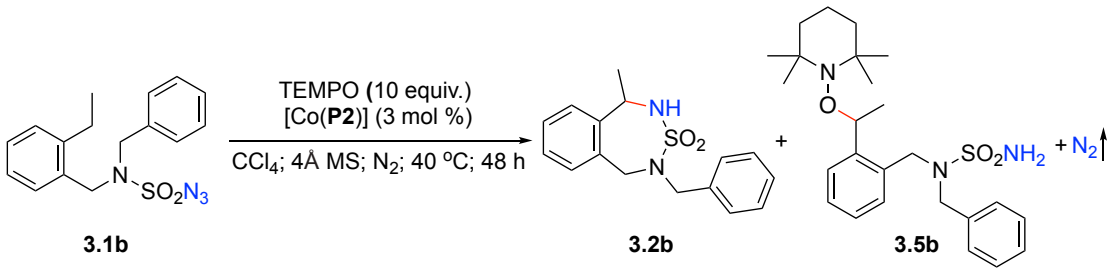
4-benzyl-1-methyl-1,2,4,5-tetrahydrobenzo[*d*][1,2,7] thiadiazepine 3,3-dioxide 3.2b was obtained with catalyst **[Co(P3)]** in toluene through the general procedure for 48 h. Light yellow solid. Yield: 90 %. R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -1.6(*c* = 1.0, $CHCl_3$).^{1}H NMR (6MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 4H), 7.35 – 7.23 (m, 4H), 6.98 (d, *J* = 7.4 Hz, 1H), 4.91 – 4.77 (m, 2H), 4.49 (d, *J* = 14.0 Hz, 1H), 4.29 (d, *J* = 10.5 Hz, 1H), 3.86 (d, *J* = 16.0 Hz, 1H), 3.31 (d, *J* = 14.0 Hz, 1H), 1.71 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$ δ 142.54, 135.56, 134.85, 132.15, 129.17, 128.99, 128.89, 128.22, 128.12, 125.61, 50.92, 50.32, 50.03, 19.83. HPLC analysis: *ee* = 8 %. IC (90% hexanes: 10% isopropanol, 0.8 mL/min): t_{major} = 62.088 min, t_{minor} = 43.138 min. IR (neat, cm^{-1}): 3283.19, 1348.38, 1338.12, 1158.23. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{16}H_{19}N_2O_2S$: 303.11617, found 303.11648.



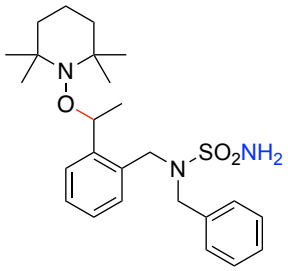
2-benzyl-4-(prop-1-en-2-yl)-1,2,5-thiadiazolidine 1,1-dioxide 3.6c was obtained with catalyst **[Co(P3)]** in toluene through the general procedure. Light yellow solid. Yield: 45%. (53% NMR yield) R_f = 0.4 (2:1 Hexanes/EtOAc). $[\alpha]_D^{20}$ = -8.398(*c* = 0.5, $CHCl_3$).^{1}H NMR (6MHz, $CDCl_3$) δ 7.37 – 7.24 (m, 5H), 5.01 (s, 1H), 4.88 (s, 1H), 4.45 (bs, 1H), 4.28 (d, *J* = 13.8 Hz, 1H), 4.17 (dd, *J* = 9.0, 8.3 Hz, 1H), 3.93 (d, *J*

= 13.8 Hz, 1H), 3.31 (t, J = 8.3 Hz, 1H), 2.93 (t, J = 9.0 Hz, 1H), 1.70 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.64, 137.32, 131.15, 130.99, 130.57, 116.42, 59.44, 54.12, 52.84, 20.14. HPLC analysis: *ee* = 27 %. IC (70% hexanes: 30% isopropanol, 1.0 mL/min): t_{major} = 10.754 min, t_{minor} = 12.011 min. IR (neat, cm^{-1}): 3269.22, 1455.04, 1297.31, 1162.96, 1073.46. HRMS (DART$^+$) ([M+H]$^+$) Calcd. for $C_{16}H_{17}N_2O_2S$: 301.10052, found 301.09971.

3.4.4 General Procedure for TEMPO Trapping Experiment



An oven dried Schlenk tube was charged with catalyst [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-IbuPhyrin) (3 mol %) and 4Å molecular sieves (50 mg). This reaction vessel was evacuated and backfilled with nitrogen several times. Under nitrogen atmosphere, the allyl sulfamoyl azide substrate **3.1b** (0.2 mmol) and TEMPO (10 equiv) were added followed by the addition of 1 mL of CCl_4. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at 40 ºC for 48 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum, and purified by flash column chromatography. The fractions containing product were collected and afford **3.2b** and **3.5b**. Meanwhile, **3.1b** has 60% remained after the reaction.

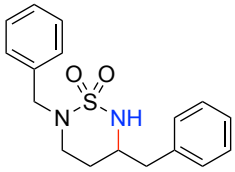


***N*-benzyl-*N*-(2-(1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethyl)benzyl)-λ^2-azanesulfonamide 3.5b**. White solid. Yield: 5%. (10% NMR yield) R_f = 0.4 (2:1 Hexanes/EtOAc). ^{1}H NMR (6MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.8 Hz, 1H), 7.28 – 7.44 (m, 7H), 7.15 – 7.22 (m, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 5.27 (s, 2H), 5.18 (q, *J* = 6.5 Hz, 1H), 4.78 (d, *J* = 15.3 Hz, 1H), 4.56 (d, *J* = 15.9 Hz, 1H), 4.09 (d, *J* = 15.3 Hz, 1H), 4.02 (d, *J* = 15.9 Hz, 1H), 1.44 (d, *J* = 6.5 Hz, 3H), 1.38 (s, 5H), 1.20 (s, 4H), 1.06 (s, 3H), 0.56 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.14, 137.95, 132.96, 132.25, 131.09, 130.86, 130.72, 130.16, 130.12, 128.88, 81.46, 62.93, 62.08, 51.87, 50.06, 42.62, 42.40, 35.73, 35.42, 26.58, 22.96, 22.84, 19.22.IR (neat, cm^{-1}): 2929.27, 1455.26, 1351.55, 1158.86, 1132.54, 1063.82, 1045.33. HRMS (DART$^+$) ([M+H]$^+$): Calcd. for $C_{25}H_{38}N_3O_3S$: 460.26284, found 460.26430.

3.4.5 X-Ray Crystallographic Information

The X-ray diffraction data were collected using Bruker-AXS SMART-APEXII CCD diffractometer (Cu K_α, λ = 1.54178 Å). Indexing was performed using *APEX2*[19] (Difference Vectors method). Data integration and reduction were performed using SaintPlus.[20] Absorption correction was performed by multi-scan method implemented in SADABS.[21] Space group were determined using XPREP implemented in APEX2.[19] The structure was solved using SHELXS-97 (direct methods) and refined using SHELXL97

contained in WinGX v1.70.01program.[22]



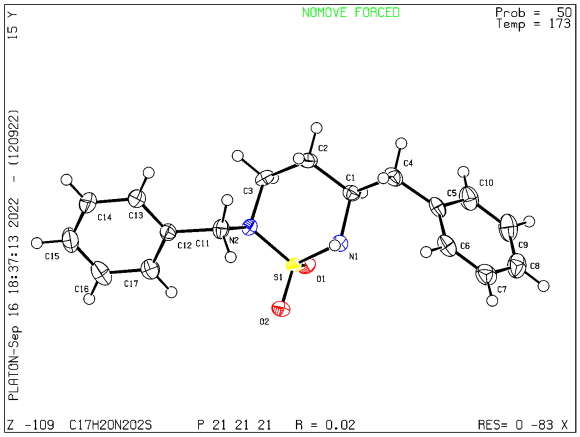


Table 3.5 Crystal Data and Structure Refinement for (±)-**3.3a**		
Identification code	(±)-3.3a	
Empirical formula	C17 H20 N2 O2 S	
Formula weight	316.41	
Temperature	173(2) K	
Wavelength	1.54178 ≈	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.2232(4) ≈	α= 90∞.
	b = 9.4098(6) ≈	β= 90∞.
	c = 27.4374(16) ≈	γ = 90∞.
Volume	1606.71(17) $\approx^3$	
Z	4	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	1.859 mm^{-1}	

F(000)	672
Crystal size	0.420 x 0.3x 0.180 mm^3
Theta range for data collection	4.969 to 66.632∞.
Index ranges	-7<=h<=7, -11<=k<=11, -32<=l<=32
Reflections collected	27354
Independent reflections	2849 [R(int) = 0.0368]
Completeness to theta = 66.632∞	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6020
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2849 / 0 / 203
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0229, wR2 = 0.0604
R indices (all data)	R1 = 0.0230, wR2 = 0.0605
Absolute structure parameter	0.004(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.183 and -0.306 e.≈$^{-3}$

3.4.6 Details on DFT Calculations

In the investigation of C–H amination reaction via 1,7-HAA, catalyst [Co(**P2**)] was modeled for the DFT calculations. The geometry optimizations were performed with the Gaussian 16[23] at the BP86[24]/def2-svp[25]// 6-311G*$_{H, C, N, O, S}$ level of theory in the gas phase at room temperature. Gas-phase Hessian matrix calculations were applied to the

characterization of all minima (without imaginary frequency) and transition states (with only one imaginary frequency). Thermochemical parameters such as internal energy, enthalpy, entropy, Gibbs free energy and thermal corrections were obtained from these calculations. The structures were displayed by CYLview[26] and VMD[27].

Intermediate $A_{3.1a}$

$A_{[Co(II)(\mathbf{P2})]}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -0.6444 cm-1

G_corr: 1.303862 Hartree

H_corr: 1.538533 Hartree

SCF: -5071.844772 Hartree

S: 493.906 Cal/Mol-Kelvin

H: -5070.306239 Hartree

G: -5070.540910 Hartree

Cartesian Coordinates:

H	9.34557400	-0.14040400	-3.78545600
H	9.47145500	0.54656400	-2.14976100
C	8.75950000	0.19265700	-2.91205200
H	8.14622900	1.05428500	-3.22278500
H	9.71603800	1.52630400	1.38664100
H	9.35824500	-2.51245300	-2.82716300
C	9.35441100	0.90304800	2.22112500
H	9.83675900	1.27520200	3.13960600
H	9.48208400	-1.87248100	-1.17248600
C	8.77080200	-2.15200900	-1.96566200
H	8.83790400	-0.00596300	-0.02882900
C	7.87092900	-0.96256900	-2.38579200
H	7.71186800	3.09209200	1.79248100
H	9.70860400	-0.12865900	2.06072200
H	7.58078900	-1.77234300	-4.38581500

C	7.74555200	-0.00345800	-0.02029700
C	6.96179800	-1.43261100	-3.53954400
C	7.42990200	2.44785900	2.64143500
H	7.94496100	2.82671100	3.54050400
H	6.31366800	-0.62227700	-3.91209900
C	7.06418100	-0.47294200	-1.16513400
C	7.82154600	0.97252100	2.37529500
H	8.16611400	-2.99423300	-1.59134000
C	7.07840200	0.46452300	1.12208300
H	0.81818200	5.26259400	-6.18211000
H	1.72879900	4.14059400	-5.13937400
H	6.34700900	2.56485000	2.80506700
C	0.78327600	4.27924800	-5.68848900
H	6.31991800	-2.27843400	-3.24294700
C	5.66200300	-0.46917300	-1.13933400
C	7.42014900	0.10667500	3.59609100
H	7.93893700	0.45844200	4.50403100
H	4.53043500	2.61025100	-0.32965100
H	0.72392500	3.50111900	-6.46679500
C	5.66809200	0.46031300	1.10286900
O	-0.37802100	6.52365900	-4.06136400
H	7.69005500	-0.95036000	3.43833700
H	5.08757500	-0.81911300	-2.00003500
H	2.60443000	4.53152000	-0.30965700
H	-0.21123300	7.60998600	-2.16269900
C	4.95644600	-0.00278200	-0.01173100
C	3.45322700	2.48798400	-0.24176800
H	0.00000000	8.84732300	0.00037300
C	-0.11942100	7.07818100	-1.21736900
C	-0.34905400	5.34352200	-3.71821200
C	-0.00000100	7.75293400	0.00032000
C	2.48839300	3.45192900	-0.23521700
C	-0.43637600	4.20313800	-4.75023000
H	5.10347700	0.81318300	1.97116800

H	6.33756700	0.14909300	3.79443200
H	-1.81277000	5.31660100	-6.01802200
C	-0.11975200	5.66991700	-1.21896300
N	-0.23309500	4.91174900	-2.40530200
C	0.11941700	7.07806200	1.21794400
C	-1.75558100	4.32955500	-5.53426700
C	3.45714200	-0.00221300	-0.00797900
C	2.78078800	1.21745300	-0.10422100
H	0.21123200	7.60977500	2.16332600
H	-0.42381200	3.22481200	-4.23235900
H	-1.81989500	3.55424000	-6.31496400
C	-0.00000400	4.95247700	0.00018400
H	-0.22114400	3.90204400	-2.26496800
C	0.11974600	5.66979800	1.21940000
C	1.22215600	2.77229200	-0.10253700
H	4.53211300	-2.61405100	0.30641100
H	-0.78962400	-3.50321000	-6.45534400
N	1.40027900	1.39276800	-0.04645300
O	0.37795900	6.52325900	4.06189300
C	-0.00000300	3.44824300	0.00011200
C	2.78100200	-1.22187600	0.09056100
H	-0.88332400	-5.26459700	-6.17016500
C	3.45436900	-2.49225200	0.22390600
H	-2.63244400	4.22368800	-4.87497300
N	0.23308800	4.91151400	2.40566500
C	-0.84025000	-4.28153100	-5.67661300
C	0.34905600	5.34315600	3.71861800
H	-1.77831900	-4.14139700	-5.11522800
H	-1.72891400	4.14020100	5.13959700
H	0.22112600	3.90182200	2.26523300
H	1.75563700	-3.56190000	-6.33726500
H	0.42367800	3.22439300	4.23256600
H	1.74964200	-5.32414000	-6.03940900
N	1.40036800	-1.39732100	0.03948700

C	0.43627800	4.20266900	4.75053100
C	2.48973400	-3.45642900	0.22160100
C	-1.22216100	2.77227900	0.10268400
C	1.70033300	-4.33676900	-5.55545200
C	-0.78340200	4.27875600	5.68875600
Co	0.00000300	-0.00229100	0.00000200
C	0.39174000	-4.20791700	-4.75431400
C	1.22269700	-2.77690500	0.09600500
H	2.60622200	-4.53605700	0.29481700
H	-2.60444700	4.53148500	0.30990200
C	-2.48840400	3.45190100	0.23537100
N	-1.40028000	1.39275900	0.04646600
H	-0.81827500	5.26205800	6.18246600
H	0.38782200	-3.22963400	-4.23623400
H	-0.72411800	3.50055300	6.46699400
C	0.31528500	-5.34820500	-3.72137000
H	2.58588900	-4.23172800	-4.90778800
C	1.75546300	4.32894100	5.53462400
H	2.63234300	4.22309400	4.87534900
H	0.20200700	-3.90661900	-2.26702700
N	0.21233300	-4.91634100	-2.40735800
O	0.34057400	-6.52839500	-4.06463800
C	0.00001100	-3.45286800	0.00006300
C	-3.45323700	2.48795400	0.24178800
C	-2.78079100	1.21743600	0.10416400
H	1.81268700	5.31593500	6.01847900
N	-1.40035300	-1.39732600	-0.03948700
H	1.81971000	3.55354500	6.31524600
C	0.10921600	-5.67447500	-1.22007400
H	-2.58585700	-4.23154600	4.90809700
C	-1.22267500	-2.77691100	-0.09594200
C	0.00001100	-4.95709500	0.00010600
H	-4.53044900	2.61021400	0.32964000
C	0.10891800	-7.08275200	-1.21847500

C	-2.78098500	-1.22188600	-0.09067800
C	-3.45713800	-0.00222700	0.00782600
C	-1.70025400	-4.33650700	5.55571000
H	0.19254000	-7.61452900	-2.16457800
H	-0.20198000	-3.90648300	2.26717400
C	-0.10919600	-5.67440200	1.22032800
H	-1.75554600	-3.56159900	6.33748400
N	-0.21231000	-4.91619700	2.40756600
H	-6.34698000	2.56523500	-2.80507400
H	-1.74948200	-5.32385500	6.03972200
H	-5.10335000	0.81335800	-1.97135200
C	0.00000600	-7.75751600	0.00018900
C	-2.48969900	-3.45644400	-0.22160900
C	-0.10890400	-7.08267900	1.21881300
C	-3.45433600	-2.49226900	-0.22404400
C	-0.39172100	-4.20763300	4.75448000
C	-0.31525800	-5.34798300	3.72160500
H	-0.38788900	-3.22938300	4.23633800
C	-7.42987600	2.44810800	-2.64155400
C	-5.66801700	0.46040100	-1.10312300
C	-4.95643900	-0.00279900	0.01147800
H	-6.33717400	0.14959200	-3.79472700
H	-7.94489400	2.82702800	-3.54061600
H	0.00000300	-8.85190800	0.00022200
H	-2.60618000	-4.53607400	-0.29479000
H	-7.71198500	3.09219400	-1.79253700
H	-0.19252900	-7.61440000	2.16494700
O	-0.34059200	-6.52815300	4.06493800
C	-7.41977700	0.10704800	-3.59651600
H	-7.93849100	0.45889000	-4.50447000
H	-4.53207100	-2.61407700	-0.30664900
C	-7.82139200	0.97269300	-2.37565000
C	-7.07832600	0.46460100	-1.12242900
C	-5.66207000	-0.46929600	1.13899200

C	0.84033400	-4.28112000	5.67670500
H	-5.08769600	-0.81930600	1.99970100
H	0.78972000	-3.50274500	6.45538200
H	-7.68960300	-0.95003300	-3.43893600
H	0.88348800	-5.26414700	6.17032700
C	-7.74554900	-0.00349800	0.01986000
H	1.77836100	-4.14098000	5.11524900
C	-7.06424900	-0.47308000	1.16469900
C	-9.35426600	0.90304000	-2.22164900
H	-9.83655600	1.27532500	-3.14010700
H	-9.71603800	1.52609800	-1.38708000
H	-6.31390900	-0.62258200	3.91168700
H	-8.83790200	-0.00601700	0.02831700
H	-9.70837400	-0.12873200	-2.06148500
H	-8.14649000	1.05397600	3.22237500
C	-6.96200800	-1.43290400	3.53905200
H	-6.32010200	-2.27870700	3.24245700
C	-7.87107000	-0.96281400	2.38526600
C	-8.75971300	0.19235000	2.91154200
H	-9.47162700	0.54628800	2.14922600
H	-7.58105100	-1.77268200	4.38526700
C	-8.77087600	-2.15225200	1.96498800
H	-8.16613500	-2.99443200	1.59065200
H	-9.48210700	-1.87269000	1.17177900
H	-9.34583800	-0.14078800	3.78488200
H	-9.35837200	-2.51277500	2.82642100

$A_{\underline{3.1a}}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.284192 Hartree

H_corr: 0.367138 Hartree

SCF: -1427.65981 Hartree

S: 174.575 Cal/Mol-Kelvin

H: -1427.292671 Hartree

G: -1427.375618 Hartree

Cartesian Coordinates:

H	-4.77631900	2.54561100	-2.24890200
H	-6.14677300	2.36816000	-0.16649800
C	-4.52840900	1.79779100	-1.48935500
C	-5.29534200	1.69874600	-0.32281300
C	-3.43714400	0.93915700	-1.68595000
H	-2.83989900	1.01807200	-2.60130900
C	-4.96889600	0.73728700	0.64582600
H	-5.56789800	0.65339600	1.55790200
C	-3.10631600	-0.02768000	-0.72333300
C	-3.88210400	-0.12026700	0.44700800
H	-2.32059900	-2.02134100	-0.97176800
C	-1.95270400	-0.98488500	-0.95522400
H	-1.46899700	-0.78249300	-1.92869600
H	-3.62611100	-0.87055100	1.20177100
H	3.43248400	3.18054600	-2.51546200
C	3.43347800	2.50832000	-1.65120600
H	4.70814100	1.03040900	-2.60009200
C	4.15110600	1.30475800	-1.69889500
C	2.72434400	2.85887800	-0.49611500
H	2.17742900	3.80857100	-0.46620900
C	4.15688400	0.46044200	-0.58128500
N	-0.95040900	-0.88925200	0.13933400
C	2.71252700	2.01649200	0.63295900
C	3.44445400	0.81624000	0.57290600
H	-0.59562600	1.05233400	-0.53338900
H	0.09554700	3.04462600	0.88424400
O	-1.04356600	-3.41504700	0.46725800
H	4.71529700	-0.48031800	-0.60473800
N	3.17073000	-3.18363400	-0.63471300
N	0.92382900	-2.46188600	-0.99962100

C	1.93456700	2.40486200	1.87701700
S	-0.11473600	-2.28367000	0.49710400
N	2.08118200	-2.84121400	-0.75727200
H	3.45251800	0.14831600	1.44111700
C	0.39173300	2.40558900	1.73764900
C	-0.16850200	0.38032000	0.22826700
H	2.24588100	3.42031400	2.18462500
C	-0.28050800	1.02314900	1.61699000
H	-1.35488100	1.12504000	1.84832200
H	2.21664400	1.73592100	2.70928900
H	-0.02033700	2.90124600	2.63458600
H	0.87850900	0.20167600	-0.06353900
O	0.78610500	-2.02960200	1.62720500
H	0.13811700	0.33307900	2.36860000

Intermediate $B_{3.1a}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.608977 Hartree

H_corr: 1.90818 Hartree

SCF: -6499.508175 Hartree

S: 629.727 Cal/Mol-Kelvin

H: -6497.599994 Hartree

G: -6497.899198 Hartree

Cartesian Coordinates:

H	-8.09539800	-4.94967200	-1.66140300
H	-8.49057800	-4.07301900	-0.16418500
C	-7.70083900	-4.24050800	-0.91363300
H	-6.85103300	-4.72193400	-0.40282300
H	-9.52839100	-1.80251700	2.58250200
H	-8.87755100	-2.97151900	-3.08042200
C	-9.53226000	-0.70295300	2.50053300
H	-10.16367900	-0.31651000	3.31707900

H	-9.30367900	-2.06132900	-1.61412000
C	-8.48214900	-2.28482400	-2.31265000
H	-8.61667200	-1.86176200	0.50705200
C	-7.26335000	-2.92067600	-1.59743000
H	-7.44937900	-1.59862900	4.09180000
H	-10.02154900	-0.42883500	1.55127500
H	-6.64075400	-3.94499400	-3.41329900
C	-7.58570800	-1.50074700	0.49904500
C	-6.20626100	-3.25901700	-2.66757300
C	-7.53555000	-0.50359200	3.99697700
H	-8.19267800	-0.14379100	4.80679800
H	-5.32353200	-3.75948900	-2.23776100
C	-6.72576800	-1.94634300	-0.52863600
C	-8.11404700	-0.10804100	2.61517500
H	-8.20217900	-1.34277100	-2.81193300
C	-7.17125100	-0.61164500	1.50220700
H	1.77616100	-6.20944500	4.72698000
H	0.44697400	-5.56078100	3.73645800
H	-6.53608100	-0.07262500	4.16549500
C	1.54130000	-5.68728800	3.78677800
H	-5.86526800	-2.35998800	-3.20737100
C	-5.40389000	-1.47697900	-0.52743600
C	-8.22974600	1.43484100	2.52991800
H	-8.89807000	1.81449700	3.32138700
H	-4.02226900	-1.60301400	2.82047800
H	1.85308500	-6.32824000	2.94557800
C	-5.83511600	-0.16442700	1.46674500
O	2.07413700	-3.93527300	6.10804800
H	-8.64227700	1.74827600	1.55695400
H	-4.69964000	-1.79744700	-1.29857300
H	-2.01837700	-1.31315300	4.63089200
H	1.41368300	-2.36400500	7.38066500
C	-4.94559300	-0.58901700	0.46819400
C	-3.07855400	-1.07558200	2.70121500

H	0.62902700	-0.56453400	8.92080500
C	0.99009200	-1.44094400	6.99105100
C	1.88038700	-3.50333700	4.97190800
C	0.54481100	-0.42497200	7.83850500
C	-2.07199300	-0.93114800	3.61300500
C	2.27160400	-4.33239100	3.73694000
H	-5.47309600	0.54431500	2.21722400
H	-7.25363900	1.92958900	2.65388600
H	4.12430700	-5.01629000	4.66285500
C	0.88710900	-1.27111400	5.59470700
N	1.31938600	-2.26550300	4.68611900
C	-0.00383400	0.76220500	7.35009000
C	3.80071300	-4.52445200	3.73234800
C	-3.53892600	-0.07411300	0.43929200
C	-2.68075600	-0.34979600	1.51422700
H	-0.35011700	1.55280100	8.01315900
H	1.97725600	-3.79798500	2.81828900
H	4.10783000	-5.15160800	2.87950000
C	0.33253700	-0.07600300	5.06382800
H	1.20897300	-2.03698000	3.69607700
C	-0.11149800	0.93768500	5.95791900
C	-1.02796500	-0.17231200	2.96639700
H	-5.16628900	1.10569200	-1.58798600
H	-0.02567000	-1.68502400	-7.23512500
N	-1.39705000	0.16261500	1.67202900
O	-1.24294800	3.38080400	7.23772000
C	0.19158200	0.14921900	3.58308200
C	-3.16698000	0.78656300	-0.60632000
H	-0.29297800	-0.25440500	-8.27111800
C	-4.10456900	1.34041300	-1.55700200
H	4.32966900	-3.56071800	3.65413500
N	-0.65268700	2.11333700	5.39017100
C	-0.16954900	-0.59202200	-7.23035800
C	-1.17425400	3.23328200	6.01864100

H	0.74701300	-0.13060700	-6.82830500
H	0.18075200	5.49081600	5.08564200
H	-0.66407300	2.12589400	4.37095100
H	-2.53246500	-2.00548400	-6.94923700
H	-1.52127100	3.99906900	4.00501700
H	-2.89452000	-0.57053400	-7.95112800
N	-1.89773500	1.31182200	-0.81582500
C	-1.68172800	4.32007600	5.05205700
C	-3.41103700	2.21911100	-2.33963900
C	1.26886200	0.68496300	2.86437200
C	-2.67411200	-0.91231300	-6.92847500
C	-0.89304200	5.61976600	5.29813400
Co	-0.28133800	1.01539400	0.28993100
C	-1.41033000	-0.21128200	-6.39831100
C	-2.03737500	2.17681700	-1.89858000
H	-3.78066500	2.84082700	-3.15313300
H	2.84361000	0.72083000	4.46978900
C	2.58899200	0.86984400	3.42197600
N	1.26393400	0.99241200	1.50959800
H	-0.99585800	5.92832000	6.34975100
H	-1.24098200	-0.51942300	-5.35225600
H	-1.27290200	6.43279200	4.65829900
C	-1.61052700	1.31288200	-6.47227700
H	-3.55388100	-0.69294600	-6.30167000
C	-3.19095500	4.52965000	5.27793100
H	-3.76555000	3.61507600	5.05857300
H	-1.16695300	1.40334000	-4.46738000
N	-1.41488200	1.98128900	-5.27086500
O	-1.91062100	1.86119600	-7.53171500
C	-0.99130000	2.84790400	-2.55097000
C	3.40678400	1.22677500	2.38873200
C	2.58015200	1.31327100	1.20553600
H	-3.37962900	4.80541700	6.32681800
N	0.79489300	2.02070900	-1.03099800

H	-3.57336200	5.33590600	4.63117200
C	-1.51923900	3.36645300	-5.00339800
H	1.23119700	7.22622400	-0.20402300
C	0.35051600	2.68509300	-2.16795700
C	-1.31126800	3.80449200	-3.66808300
H	4.47240200	1.44449400	2.41485000
C	-1.81498700	4.29914300	-6.01808600
C	2.18205700	2.11300800	-1.07676900
C	3.05186300	1.75400000	-0.03852400
C	0.36047300	7.70296100	0.27458800
H	-1.97107600	3.94298100	-7.03413500
H	-1.00361000	4.83081300	-1.39104500
C	-1.40672500	5.19429700	-3.37631900
H	0.56659700	7.78338400	1.35420900
N	-1.20257800	5.59393000	-2.03683400
H	6.44040400	-1.48485400	0.79692300
H	0.26030100	8.71895000	-0.13725400
H	4.90300400	-0.17166700	-0.30251400
C	-1.90100200	5.65445200	-5.69474700
C	1.46785400	3.17319200	-2.94080000
C	-1.70296500	6.12062900	-4.39391200
C	2.60203600	2.78478900	-2.28547500
C	-0.93300000	6.90382500	0.02595800
C	-1.21737300	6.86705400	-1.48732300
H	-0.79247600	5.87487000	0.40877900
C	7.48364300	-1.16941200	0.63948000
C	5.36237500	0.82076300	-0.33125600
C	4.52791100	1.94061100	-0.21724800
H	6.13166000	-1.41930400	-1.79090700
H	8.10127100	-2.08027800	0.55738000
H	-2.13105500	6.37381100	-6.48683700
H	1.37872800	3.72468600	-3.87512300
H	7.80692900	-0.62126500	1.53961400
H	-1.77212400	7.17779100	-4.14438400

O	-1.43180700	7.89800800	-2.12241100
C	7.18439700	-1.10565400	-1.86998900
H	7.80014700	-2.01473900	-1.98179700
H	3.63758100	2.95536000	-2.57174400
C	7.63877300	-0.29494500	-0.63007600
C	6.75645100	0.96331300	-0.49428200
C	5.09024400	3.23304200	-0.25540700
C	-2.13344100	7.54232200	0.74875900
H	4.42223800	4.09074800	-0.14901900
H	-1.93350000	7.63401600	1.82867500
H	7.28755000	-0.51012300	-2.79193200
H	-2.32429900	8.54794600	0.34394200
C	7.28026900	2.26450300	-0.52735000
H	-3.05084900	6.94506300	0.62043300
C	6.47214500	3.41681100	-0.40668400
C	9.13323500	0.04529100	-0.79978700
H	9.71769200	-0.88476900	-0.89192100
H	9.53325800	0.59829300	0.06608500
H	5.55378200	5.89231900	0.67120000
H	8.35785500	2.39682600	-0.64902600
H	9.32223200	0.64182800	-1.70756700
H	7.65330400	4.80405400	1.69626700
C	6.09284500	5.94911500	-0.28877100
H	5.34867400	5.94369300	-1.10209900
C	7.12590500	4.81409200	-0.44039900
C	8.14681900	4.93348300	0.71916400
H	8.94574700	4.17879100	0.64543800
H	6.60481000	6.92470200	-0.31999500
C	7.85984000	5.00705500	-1.79139300
H	7.15771900	4.93467900	-2.63813800
H	8.64768100	4.25268800	-1.94487800
H	8.62581700	5.92738200	0.70905600
H	8.33805300	6.00059700	-1.83086500
H	-2.73409000	-8.07442300	-1.57899100

H	-3.58872800	-7.05705900	-3.69693700
C	-2.50353300	-7.03265300	-1.82140400
C	-2.98184800	-6.46310000	-3.00704400
C	-1.72118800	-6.26999800	-0.94283300
H	-1.34497500	-6.72149700	-0.01839500
C	-2.68069400	-5.12613400	-3.30735400
H	-3.05490700	-4.67444100	-4.23079000
C	-1.41678400	-4.92985700	-1.23380600
C	-1.90676300	-4.36397200	-2.42531900
H	-1.18801500	-3.26364800	0.12230100
C	-0.59429300	-4.11055700	-0.25867400
H	-0.31005800	-4.72411600	0.61463800
H	-1.67668300	-3.32115500	-2.66426600
H	3.67186400	-9.32877500	-0.74525700
C	4.05763600	-8.30858500	-0.83973200
H	4.97817300	-8.30320300	1.12589200
C	4.79109600	-7.73587100	0.20915900
C	3.82787600	-7.58412600	-2.01543600
H	3.26933200	-8.05176000	-2.83440000
C	5.29200700	-6.43537600	0.06884100
N	0.62262100	-3.54385500	-0.91122600
C	4.31844500	-6.27217500	-2.16895500
C	5.05522200	-5.71272900	-1.10927900
H	1.07691500	-5.48025300	-1.51438800
H	2.02305700	-6.15786500	-3.77148700
O	2.63489300	-1.99662700	-0.64669300
H	5.87616100	-5.98218200	0.87576800
N	-0.08919700	-0.71714400	-3.05616900
N	0.19366000	-0.88942100	-0.68894500
C	4.08361400	-5.50328100	-3.45751500
S	1.28885800	-2.22993000	-0.11192400
N	0.09983600	-0.86178200	-1.93373400
H	5.45388500	-4.69729500	-1.21033900
C	2.60646200	-5.21968100	-3.82121900

C	1.58537900	-4.50418600	-1.54938100
H	4.53063800	-6.07698900	-4.29063300
C	1.89408600	-4.12513000	-3.00246600
H	0.93446900	-3.89366500	-3.49613700
H	4.63673700	-4.54796100	-3.42117200
H	2.57632800	-4.90855500	-4.88045800
H	2.49773600	-4.59872900	-0.94279100
O	1.00729300	-2.22671600	1.32731200
H	2.49163800	-3.19737100	-3.02062800

Transition State $TS1_{3.1a}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -542.8332 cm-1

G_corr: 1.610546 Hartree

H_corr: 1.905221 Hartree

SCF: -6499.489688 Hartree

S: 620.197 Cal/Mol-Kelvin

H: -6497.584466 Hartree

G: -6497.879142 Hartree

Cartesian Coordinates:

H	-7.74104700	-5.20919900	-2.11088600
H	-8.21342500	-4.44833600	-0.57309700
C	-7.40310000	-4.52287600	-1.31576000
H	-6.53279600	-4.98112200	-0.81862200
H	-9.46186700	-2.38025300	2.25955300
H	-8.61662400	-3.20315200	-3.43293300
C	-9.52534100	-1.27981400	2.23357500
H	-10.19784700	-0.97183000	3.05060200
H	-9.12988100	-2.41323100	-1.92603400
C	-8.28169600	-2.54062300	-2.61691100
H	-8.49837300	-2.27259000	0.20504100
C	-7.03773000	-3.14108500	-1.91449700

H	-7.43587800	-2.14028200	3.83749900
H	-10.00529800	-0.98343900	1.28630100
H	-6.32109100	-4.01382400	-3.77384000
C	-7.48831300	-1.85888200	0.24656100
C	-5.94283100	-3.34975300	-2.97941300
C	-7.58277500	-1.04847900	3.79509100
H	-8.28116500	-0.76895900	4.60195200
H	-5.03871500	-3.82209200	-2.56322300
C	-6.58062500	-2.20095300	-0.77993500
C	-8.14628100	-0.61477000	2.41854000
H	-8.05402000	-1.55425200	-3.05331200
C	-7.14852200	-1.00779700	1.30904600
H	1.50456200	-6.42964900	4.31743900
H	0.20618200	-5.65839500	3.37343100
H	-6.61518700	-0.57041900	4.01542300
C	1.29313300	-5.84020200	3.41193400
H	-5.64807900	-2.40083100	-3.45764000
C	-5.28581100	-1.66508600	-0.71616500
C	-8.34584800	0.92191400	2.40709700
H	-9.05397200	1.22330300	3.19755800
H	-3.98812900	-1.83831800	2.70738000
H	1.57229500	-6.44273400	2.53196400
C	-5.83715400	-0.49253800	1.33781000
O	1.92506700	-4.25336500	5.83055900
H	-8.75099200	1.26205500	1.44003200
H	-4.54527300	-1.90600800	-1.48208700
H	-2.03291200	-1.51148800	4.56550200
H	1.37821000	-2.73208200	7.19428400
C	-4.90224100	-0.81498100	0.34216800
C	-3.06800400	-1.26486200	2.62220700
H	0.66776200	-1.01156700	8.85390400
C	0.97085600	-1.77750900	6.86872200
C	1.74320500	-3.75059300	4.72204800
C	0.56561000	-0.80473400	7.78399300

C	-2.08587800	-1.10164500	3.55868600
C	2.08810300	-4.52129300	3.43799700
H	-5.53388300	0.19246200	2.13494600
H	-7.40233200	1.46223700	2.58304800
H	3.90847800	-5.35052000	4.30938200
C	0.84627400	-1.52473400	5.48597800
N	1.23464100	-2.47273600	4.51245300
C	0.03407400	0.42178100	7.38056000
C	3.60588500	-4.78692700	3.41293900
C	-3.52684500	-0.22643000	0.37793300
C	-2.68332800	-0.49121700	1.46522700
H	-0.28222300	1.17706500	8.09744200
H	1.81626400	-3.91784100	2.55608000
H	3.87859100	-5.37283200	2.52046200
C	0.31018500	-0.28458700	5.04443600
H	1.12365200	-2.19236900	3.53385000
C	-0.09601100	0.68297400	6.00419800
C	-1.06145800	-0.28887400	2.95370600
H	-5.17756000	1.01989400	-1.58423100
H	0.33612500	-1.10486700	-7.35343600
N	-1.43145700	0.08363600	1.66996300
O	-1.16054200	3.06265100	7.44907400
C	0.15094500	0.02635000	3.58306700
C	-3.17417300	0.70324100	-0.61408300
H	-0.04524300	0.36922500	-8.28886600
C	-4.12733700	1.29644600	-1.52331400
H	4.18036500	-3.84647100	3.39042400
N	-0.62445800	1.90095500	5.51757300
C	0.10932700	-0.02907100	-7.27418900
C	-1.11786500	2.98835400	6.22256900
H	0.99053200	0.47185600	-6.84131900
H	0.21934100	5.31670800	5.44195600
H	-0.65469300	1.97752600	4.50178000
H	-2.13696700	-1.63778900	-7.08197200

H	-1.47262300	3.88801400	4.26630200
H	-2.61137000	-0.17440500	-7.99102000
N	-1.93000800	1.29995000	-0.76142000
C	-1.63342300	4.13562800	5.33322800
C	-3.46992900	2.27682800	-2.21078000
C	1.22472500	0.58270200	2.87934100
C	-2.36118000	-0.56222300	-6.99173400
C	-0.85464400	5.42136300	5.66644200
Co	-0.29865000	0.91136600	0.29491900
C	-1.15113200	0.19660900	-6.41593500
C	-2.09899800	2.25309600	-1.76502500
H	-3.86071900	2.95527500	-2.96686100
H	2.79547900	0.57858000	4.48450500
C	2.54331000	0.75508100	3.44057700
N	1.22038200	0.93239900	1.53361200
H	-0.95551000	5.65448100	6.73738400
H	-0.95170800	-0.16762700	-5.39357400
H	-1.24362600	6.27399600	5.08648900
C	-1.46842500	1.70177200	-6.38460600
H	-3.25208700	-0.45179000	-6.35203000
C	-3.14428800	4.31697200	5.57495300
H	-3.71220100	3.41429700	5.29655700
H	-1.12032900	1.66457700	-4.36015400
N	-1.37565300	2.28909100	-5.12735900
O	-1.76879500	2.30602900	-7.41291800
C	-1.07847600	3.00993700	-2.35254300
C	3.36148000	1.13988400	2.41786800
C	2.53680000	1.25919600	1.23839800
H	-3.33304300	4.52138900	6.64004200
N	0.73238400	2.09201000	-0.91505700
H	-3.53491400	5.16115100	4.98393800
C	-1.57469200	3.64497000	-4.77788900
H	0.88930400	7.32066000	0.28862700
C	0.26780200	2.83192400	-1.99562300

C	-1.42298000	4.01696200	-3.41422700
H	4.42624300	1.36009200	2.44954200
C	-1.90319600	4.62244700	-5.73988900
C	2.12011400	2.17740300	-0.98584000
C	3.00366600	1.75395000	0.01425200
C	-0.00618400	7.73634200	0.77850200
H	-2.01705200	4.32192400	-6.77918300
H	-1.21702300	4.91717100	-1.07055500
C	-1.59791500	5.37876700	-3.04156000
H	0.18103700	7.76335000	1.86416300
N	-1.43899900	5.70633600	-1.67604000
H	6.32311500	-1.56350800	0.73266200
H	-0.13900400	8.76961100	0.42279400
H	4.80791100	-0.19011000	-0.30757600
C	-2.07158900	5.94879200	-5.33855100
C	1.37057900	3.37435200	-2.74843200
C	-1.92448400	6.34749800	-4.00871300
C	2.51727400	2.93078100	-2.14980200
C	-1.26477300	6.90495400	0.46402400
C	-1.52450900	6.94323800	-1.05356800
H	-1.09080200	5.86180900	0.79113600
C	7.37176900	-1.26199700	0.58489200
C	5.28948500	0.79192600	-0.31559500
C	4.47815400	1.92556200	-0.17213200
H	6.01388200	-1.41100600	-1.85048900
H	7.97319200	-2.18061100	0.47526500
H	-2.32629400	6.70048000	-6.09211000
H	1.26412200	3.99557600	-3.63590200
H	7.70504600	-0.74716200	1.50101500
H	-2.05545200	7.38284300	-3.69988900
O	-1.77838900	7.99769000	-1.63228000
C	7.07285000	-1.11711500	-1.92148800
H	7.67000300	-2.03459400	-2.06084400
H	3.54748100	3.11598500	-2.44556700

C	7.54374200	-0.35340300	-0.65823600
C	6.68451300	0.91579700	-0.48533400
C	5.06052000	3.20981400	-0.18394200
C	-2.49907000	7.45645700	1.20102800
H	4.40943400	4.07671600	-0.04987900
H	-2.31842000	7.49561200	2.28746300
H	7.18803200	-0.49665100	-2.82542300
H	-2.72274400	8.47500900	0.84894700
C	7.23047200	2.20841100	-0.49178400
H	-3.39095500	6.83325800	1.02500000
C	6.44456900	3.37222000	-0.33873000
C	9.04414800	-0.03572800	-0.81859900
H	9.61117200	-0.97355400	-0.93628400
H	9.45404700	0.48569400	0.06222600
H	5.58258400	5.83378100	0.81370700
H	8.30947000	2.32428400	-0.61744700
H	9.24498700	0.58146900	-1.70992700
H	7.67464400	4.68273400	1.78624500
C	6.11298700	5.90696000	-0.15004300
H	5.36081700	5.93810100	-0.95550100
C	7.12329300	4.75789400	-0.34330200
C	8.15914500	4.82878200	0.80696600
H	8.94385600	4.06266800	0.70456500
H	6.64259000	6.87346500	-0.15996300
C	7.84542200	4.97225500	-1.69744500
H	7.13275400	4.93490900	-2.53764500
H	8.61695700	4.20751900	-1.87946600
H	8.65560700	5.81401400	0.81688900
H	8.34187300	5.95735800	-1.71688700
H	-2.43149400	-7.94915300	-1.98767700
H	-3.17359100	-6.88625900	-4.12603900
C	-2.21995800	-6.89264700	-2.17955300
C	-2.63516000	-6.29800100	-3.37668400
C	-1.52183700	-6.13764700	-1.22615000

H	-1.19111800	-6.61019900	-0.29472900
C	-2.35485500	-4.94344400	-3.61230800
H	-2.67747100	-4.47225000	-4.54581400
C	-1.23853200	-4.78050400	-1.45173900
C	-1.66485100	-4.19009400	-2.65580000
H	-1.17696700	-3.19327100	0.00863600
C	-0.50707600	-3.96741500	-0.39906800
H	-0.21570300	-4.61792700	0.44697600
H	-1.44424400	-3.13483900	-2.84104700
H	3.85802100	-9.09891300	-1.23448400
C	4.23774000	-8.07367000	-1.17608500
H	5.08341700	-8.32866300	0.80680600
C	4.92547800	-7.64416100	-0.03223100
C	4.04527300	-7.19872300	-2.25177100
H	3.52268500	-7.55522200	-3.14668200
C	5.41598100	-6.33344200	0.02333500
N	0.67656100	-3.27389700	-0.96088500
C	4.52674500	-5.87511400	-2.20892800
C	5.21423100	-5.45961100	-1.05447500
H	1.31699100	-5.13832500	-1.61522200
H	2.33506000	-5.61953500	-3.90357300
O	2.57356000	-1.63696500	-0.48983400
H	5.96293000	-5.98915400	0.90655600
N	-0.38282000	-0.08645400	-2.96407700
N	0.01590400	-0.72781900	-0.60743700
C	4.35032400	-4.94629300	-3.39809100
S	1.18467900	-1.91945200	-0.07756000
N	0.15793700	-0.74328100	-2.19429500
H	5.60259200	-4.43655700	-1.00129200
C	2.89389400	-4.66714700	-3.84126500
C	1.73902500	-4.12110200	-1.57854500
H	4.88662000	-5.38826500	-4.25885600
C	2.09532500	-3.65575800	-2.99758600
H	1.14817200	-3.44389900	-3.52247400

H	4.85686200	-3.98659300	-3.19204600
H	2.92736800	-4.27705700	-4.87430100
H	2.62696500	-4.16889700	-0.92966800
O	0.86919700	-2.09030200	1.36182900
H	2.64059100	-2.69852400	-2.93861500

Intermediate $C_{3.1a}$

C_{N2}:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: -0.013118 Hartree

H_corr: 0.00864 Hartree

SCF: -109.557996 Hartree

S: 45.794 Cal/Mol-Kelvin

H: -109.549356 Hartree

G: -109.571114 Hartree

Cartesian Coordinates:

N	0.00000000	0.00000000	0.55384100
N	0.00000000	0.00000000	-0.55384100

$C_{[Co(Por)]3.1a}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.606063 Hartree

H_corr: 1.896263 Hartree

SCF: -6389.981446 Hartree

S: 610.777 Cal/Mol-Kelvin

H: -6388.085183 Hartree

G: -6388.375383 Hartree

Cartesian Coordinates:

H	-9.15721000	0.42643000	0.95168500
H	-8.98150900	-1.09963400	0.05651600

C	-8.42604400	-0.24016200	0.46384300
H	-7.98300400	0.30750800	-0.38359500
H	-8.52193400	-4.43169100	-1.42546700
H	-8.72841800	-0.75471700	3.16838200
C	-7.97473000	-5.23595400	-0.90646100
H	-8.28344000	-6.18963100	-1.36442900
H	-8.55320000	-2.31389100	2.33012000
C	-8.00645600	-1.41646100	2.66049100
H	-7.86615800	-3.04871300	0.25721000
C	-7.33661900	-0.67483700	1.47578800
H	-6.54843600	-4.27800000	-3.08194000
H	-8.30562000	-5.25676800	0.14502000
H	-7.41116800	1.24377400	2.50053500
C	-6.79774200	-2.82693500	0.20785000
C	-6.65706900	0.59628000	2.02415700
C	-6.07842900	-5.11230600	-2.53573500
H	-6.42656900	-6.05456300	-2.99149600
H	-6.17519600	1.18384400	1.22574300
C	-6.33436800	-1.62434500	0.78618100
C	-6.44642900	-5.07170600	-1.03121200
H	-7.25773900	-1.73528200	3.40407200
C	-5.94334900	-3.74871700	-0.41650400
H	-0.48478600	3.39394400	-7.20705600
H	-1.42397200	2.66551100	-5.87914200
H	-4.99069800	-5.04968300	-2.69765600
C	-0.55062400	3.29639900	-6.11211200
H	-5.89783200	0.36231600	2.78850400
C	-4.95969700	-1.35403400	0.72113400
C	-5.77169200	-6.26302600	-0.30535800
H	-6.11558000	-7.21911500	-0.73500000
H	-3.54786100	-2.23696000	-2.61071500
H	-0.73087200	4.29779300	-5.68728700
C	-4.56867100	-3.43959800	-0.46071500
O	1.23173000	1.25794100	-7.42900400

H	-6.01906200	-6.26466600	0.76882300
H	-4.55130500	-0.43561400	1.14816300
H	-1.50222300	-2.27214900	-4.39723900
H	1.27267900	-0.81881700	-7.81640000
C	-4.06830400	-2.25374500	0.09783800
C	-2.48741000	-2.08835700	-2.42129700
H	1.59410800	-3.23933700	-8.31697200
C	1.29276800	-1.55532400	-7.01630000
C	1.00238100	1.33639100	-6.22255600
C	1.47456600	-2.91390000	-7.27884600
C	-1.46018800	-2.10589400	-3.32261800
C	0.75440000	2.69668300	-5.55128900
H	-3.86272900	-4.14269800	-0.91211000
H	-4.67437200	-6.23418800	-0.39591200
H	2.11266200	3.72528300	-6.91240200
C	1.13654000	-1.11805000	-5.68351700
N	0.93903700	0.24365100	-5.36204500
C	1.50821600	-3.87082600	-6.26249900
C	1.95387700	3.62135800	-5.82804600
C	-2.60254200	-1.95878100	0.08966200
C	-1.90738400	-1.85052700	-1.12168000
H	1.65216000	-4.92919000	-6.47122900
H	0.64920200	2.55883700	-4.46240600
H	1.77612200	4.62261800	-5.40266700
C	1.16769500	-2.06977600	-4.62653900
H	0.73040900	0.46070100	-4.38206100
C	1.35344900	-3.44770800	-4.93011000
C	-0.25610100	-1.80815800	-2.59063800
H	-3.52035800	-2.75436400	2.67451600
H	-0.91748200	4.72784100	5.23084600
N	-0.53174700	-1.65816600	-1.24064300
O	1.64448700	-6.41571300	-4.87699500
C	1.00145700	-1.65728800	-3.19327800
C	-1.93045600	-1.91530900	1.32226800

H	-0.57726300	4.07256900	6.85702700
C	-2.50443000	-2.38198600	2.56378700
H	2.88142600	3.22505400	-5.38428600
N	1.39287300	-4.35564100	-3.84633700
C	-0.52099200	3.85777700	5.77881400
C	1.52827900	-5.73578100	-3.85935100
H	0.54117100	3.74191500	5.50874600
H	3.71270700	-6.43029700	-2.26167300
H	1.29926300	-3.92782600	-2.92634200
H	-3.23192900	3.65387800	5.22098600
H	1.41626400	-5.60131600	-1.68382400
H	-2.96509600	2.95844800	6.84526700
N	-0.60618000	-1.55570400	1.50879300
C	1.52180800	-6.38262900	-2.46101800
C	-1.52200400	-2.31201300	3.51030300
C	2.07730500	-1.08300000	-2.51018600
C	-2.82850000	2.78578200	5.76688700
C	2.85487800	-7.12212300	-2.24209400
Co	0.63192600	-0.85528500	0.12977500
C	-1.33450400	2.59042000	5.45082200
C	-0.35907000	-1.75509300	2.86216200
H	-1.56831500	-2.59441400	4.56043400
H	3.60770800	-1.02300300	-4.15008700
C	3.33175400	-0.74412300	-3.13509100
N	2.05677700	-0.63167200	-1.19134500
H	3.00461100	-7.86951000	-3.03616700
H	-1.22333000	2.36483000	4.37296900
H	2.85687400	-7.64195900	-1.27029000
C	-0.78942800	1.42191200	6.29094900
H	-3.42260500	1.90079400	5.48689900
C	0.32404100	-7.34562300	-2.35757300
H	-0.63537700	-6.81452100	-2.46804900
H	-0.23670300	0.51716500	4.53366200
N	-0.22216600	0.39682800	5.54617100

O	-0.85756200	1.43167500	7.51824900
C	0.79950800	-1.36595700	3.54776500
C	4.04066200	-0.00783700	-2.22929700
C	3.25293500	0.05202000	-1.02302200
H	0.38362900	-8.10645300	-3.15083300
N	1.96260600	-0.46869100	1.54265600
H	0.31984500	-7.85870100	-1.38218600
C	0.39884600	-0.78928600	5.99737700
H	5.16456100	-4.54847400	3.16264900
C	1.83519000	-0.66639500	2.91089000
C	0.92110400	-1.67140800	5.01505600
H	5.02901600	0.43284700	-2.34043100
C	0.51791600	-1.10226500	7.36577500
C	3.09619300	0.32365100	1.39299600
C	3.71113800	0.61889800	0.17234000
C	4.73588200	-5.56324000	3.12772400
H	0.11038900	-0.41436200	8.10391400
H	1.93208000	-3.38067200	3.46758000
C	1.57255100	-2.86503800	5.42874100
H	5.07095800	-6.04240900	2.19362200
N	2.08258000	-3.71161300	4.41964200
H	4.41208300	4.34841000	-2.68624200
H	5.14353300	-6.13370200	3.97640000
H	3.86911500	3.07254000	-0.83940100
C	1.15860400	-2.28622000	7.73769800
C	2.90291700	-0.00393200	3.61869300
C	1.68910400	-3.17251400	6.79780200
C	3.65533400	0.64840300	2.68211500
C	3.19682900	-5.53461400	3.20172200
C	2.77145000	-4.91041900	4.54367400
H	2.81403900	-4.92222900	2.36269800
C	5.37450700	4.87473300	-2.59302300
C	4.83877600	2.75686200	-0.44441900
C	4.92924400	1.48467100	0.13683000

H	3.75852000	5.31318000	-0.36093700
H	5.25712000	5.86976500	-3.05507100
H	1.24914800	-2.52650400	8.80148400
H	3.03380700	-0.02754900	4.69907200
H	6.12295000	4.31568700	-3.17856900
H	2.18918700	-4.09279900	7.09371100
O	3.04026800	-5.44861300	5.61532600
C	4.73956800	5.81198700	-0.33351000
H	4.61668800	6.81820500	-0.76945400
H	4.53242600	1.27298000	2.83613300
C	5.81531600	5.01541200	-1.11449500
C	5.95935900	3.61222000	-0.49057600
C	6.15727800	1.03990600	0.66811800
C	2.60405800	-6.95124900	3.09175000
H	6.20595000	0.03654200	1.09763600
H	2.94230000	-7.44328500	2.16556200
H	5.02637500	5.93260800	0.72422100
H	2.92805600	-7.56176700	3.94827700
C	7.16665500	3.13799300	0.04529800
H	1.50204900	-6.93254800	3.08630000
C	7.29677700	1.85603300	0.62473500
C	7.13198500	5.81701100	-1.07715100
H	6.97502900	6.80871600	-1.53183000
H	7.93638400	5.32106600	-1.64542400
H	8.33578300	-0.77240400	1.00987700
H	8.04708300	3.78405900	0.01344300
H	7.48812700	5.98249600	-0.04673000
H	9.42419200	0.73358900	-0.77539200
C	8.61686600	-0.02145000	1.76658800
H	7.90940700	-0.09979200	2.60860500
C	8.66408300	1.40351800	1.17850000
C	9.71289400	1.41922700	0.03800300
H	9.83365700	2.42328100	-0.39827700
H	9.61245000	-0.29915000	2.14928900

C	9.11216400	2.37393500	2.30037000
H	8.38860900	2.38040600	3.13204900
H	9.21156400	3.40859100	1.93608400
H	10.69859400	1.10042300	0.41757200
H	10.09193900	2.06792300	2.70494700
H	-6.25835200	4.41485300	-3.46933700
H	-7.12798800	2.16926700	-2.79273200
C	-5.58644500	3.67740800	-3.01884400
C	-6.07415700	2.42094300	-2.63708600
C	-4.23565700	3.99478200	-2.82303200
H	-3.86196300	4.98094000	-3.12139600
C	-5.20315700	1.48804200	-2.05574500
H	-5.57259700	0.50258500	-1.75476600
C	-3.35604700	3.06188500	-2.24844600
C	-3.85285400	1.80627400	-1.86311300
H	-1.36178500	2.96686000	-3.01897500
C	-1.87390900	3.38365000	-2.13778800
H	-1.71672300	4.47905600	-2.16591900
H	-3.17170200	1.08104000	-1.40842400
H	-3.69179300	10.09110800	0.55881700
C	-4.13019700	9.08799300	0.57059000
H	-5.58259300	9.52978600	-0.97980900
C	-5.19091800	8.77479300	-0.29102300
C	-3.63560500	8.12233200	1.45500300
H	-2.81325400	8.38051600	2.13257500
C	-5.74971300	7.49120800	-0.25810000
N	-1.22379100	2.83631700	-0.93177900
C	-4.18566700	6.82631200	1.49870900
C	-5.25024900	6.52760700	0.62930300
H	-0.46371600	4.61689000	-0.05103300
H	-1.57365700	5.95408900	1.74329400
O	1.39584400	2.60653400	-0.92048900
H	-6.58180900	7.23706900	-0.92235000
N	-0.13889500	0.78144200	0.08700000

C	-3.62238900	5.78738600	2.44993900
S	0.14839800	1.83413800	-1.18379800
H	-5.69704600	5.52768700	0.64917200
C	-2.29814600	5.14837100	1.96607100
C	-1.10125500	3.75188500	0.22379300
H	-4.37061100	4.99221600	2.61803900
C	-2.46026800	4.24187300	0.73656900
H	-2.99111200	4.79351800	-0.05781300
H	-3.44505900	6.25800500	3.43367700
H	-1.86024000	4.56454400	2.79694600
H	-0.57778500	3.20178800	1.02068600
O	-0.02390100	1.26947000	-2.55315100
H	-3.09131100	3.37019700	0.98424700

Transition State $TS2^{7}_{3.1a}$ (1,7-HAA):

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -1275.2684 cm-1

G_corr: 1.611522 Hartree

H_corr: 1.889821 Hartree

SCF: -6389.928006 Hartree

S: 585.729 Cal/Mol-Kelvin

H: -6388.038185 Hartree

G: -6388.316484 Hartree

Cartesian Coordinates:

H	-9.10681200	-0.60987200	-3.23723600
H	-9.17876300	0.52625400	-1.86907600
C	-8.51384700	-0.15206800	-2.42726500
H	-8.20056700	-0.95540900	-1.74087700
H	-9.19039600	3.36591900	0.50710700
H	-8.33905400	1.24835200	-4.81589800
C	-8.54415000	4.25536600	0.42470600
H	-8.97466200	5.03321900	1.07602400

H	-8.42905600	2.42789900	-3.48967700
C	-7.77050700	1.69598500	-3.98323000
H	-8.12087700	2.52041500	-1.29360200
C	-7.28561800	0.59104000	-3.01066800
H	-7.69367900	2.55382300	2.44071900
H	-8.60010600	4.62867300	-0.61124400
H	-7.05531300	-0.83606200	-4.63728000
C	-7.09052600	2.23558900	-1.06956800
C	-6.44667200	-0.41825400	-3.81898800
C	-7.11805400	3.48776000	2.33327000
H	-7.58712400	4.25265300	2.97502300
H	-6.10144700	-1.26720300	-3.20772000
C	-6.48507700	1.23315500	-1.85837600
C	-7.09361500	3.96104300	0.85811500
H	-6.91851400	2.24823500	-4.41259500
C	-6.42600200	2.87679100	-0.01345900
H	-0.05536900	-7.94368100	-2.80784000
H	-1.03003800	-6.51058500	-3.20604600
H	-6.10511200	3.30269700	2.72394700
C	-0.00820900	-6.85781700	-2.98170700
H	-5.56543500	0.06005400	-4.27824500
C	-5.16668500	0.86287300	-1.55168900
C	-6.28317200	5.27733800	0.75377400
H	-6.74105000	6.06201500	1.37940000
H	-4.90777900	-0.86824000	0.66318000
H	0.61793300	-6.67141200	-3.86948500
C	-5.09395700	2.49562600	0.24470600
O	-0.55625800	-7.63845900	-0.22991400
H	-6.25688500	5.64497600	-0.28528800
H	-4.66129000	0.08148400	-2.12260100
H	-3.69208900	-3.03937300	1.76111500
H	-1.71156000	-7.47863900	1.52262900
C	-4.45789800	1.49749200	-0.50984400
C	-3.84322700	-1.06536900	0.76871100

H	-2.70843100	-7.45799100	3.80611100
C	-1.76193900	-6.55797700	2.09925500
C	-0.26895300	-6.47672600	-0.51196200
C	-2.31067800	-6.53089500	3.38173300
C	-3.23404500	-2.15334100	1.32581100
C	0.57891400	-6.14596300	-1.75083500
H	-4.53661800	2.96542900	1.06035600
H	-5.24241700	5.15152700	1.09156400
H	2.05642100	-7.68429700	-1.26567000
C	-1.24421700	-5.37298200	1.53472100
N	-0.63894100	-5.36898800	0.25512100
C	-2.35702900	-5.36263200	4.14403000
C	2.02865300	-6.60514800	-1.48529300
C	-3.04609200	1.10788200	-0.19186800
C	-2.79915500	-0.15952500	0.35461100
H	-2.76914400	-5.34695300	5.15109800
H	0.58873700	-5.05690500	-1.92233600
H	2.65769100	-6.41370800	-2.36984000
C	-1.31593400	-4.15470000	2.27080700
H	-0.30798200	-4.46386500	-0.09365600
C	-1.85340200	-4.17212000	3.58945300
C	-1.81106600	-1.92560800	1.24642100
H	-3.17086900	3.82122300	-1.13982600
H	6.97871500	3.39919500	-1.76659000
N	-1.55239400	-0.68548100	0.67447100
O	-2.89323200	-3.51530500	6.30578800
C	-0.84967200	-2.85291800	1.68309300
C	-2.02849500	2.06562500	-0.32326900
H	6.93792800	4.91568500	-0.82615100
C	-2.23972400	3.42993600	-0.73616100
H	2.47487900	-6.06666700	-0.63366900
N	-1.84121100	-2.95899100	4.31731100
C	6.31868100	4.09733800	-1.22694800
C	-2.32426000	-2.69329900	5.59001200

H	5.87412000	3.55144600	-0.38107300
H	-0.10681700	-1.69466900	6.94957000
H	-1.39725100	-2.17691100	3.83825500
H	6.55194900	4.64734400	-3.92431500
H	-1.63524000	-0.65099600	5.25164200
H	6.50782300	6.20220900	-3.04214600
N	-0.71179900	1.88821800	0.09762200
C	-2.07660000	-1.25089400	6.07063900
C	-1.07734700	4.10905800	-0.48015400
C	0.52145800	-2.61286300	1.54567200
C	5.89953500	5.35151600	-3.38339300
C	-1.08394900	-1.28230800	7.24962100
Co	0.18642000	0.14525100	0.35176600
C	5.24052700	4.65828100	-2.18090700
C	-0.13672500	3.15317800	0.04191500
H	-0.86755000	5.16775500	-0.62186200
H	1.33976900	-4.59078400	2.23373900
C	1.53350500	-3.60937100	1.80586100
N	1.09740300	-1.44668200	1.06318200
H	-1.48282600	-1.91023500	8.06119100
H	4.61238900	3.82297100	-2.53839400
H	-0.91743700	-0.26757200	7.64626400
C	4.37926500	5.66872300	-1.40442200
H	5.15454700	5.74305500	-4.09347600
C	-3.41699000	-0.61732400	6.48334300
H	-4.10958900	-0.53930600	5.62969100
H	2.98409900	4.18275300	-1.12245500
N	3.17545200	5.16116600	-0.90611300
O	4.77049100	6.81756600	-1.21312200
C	1.15215600	3.49320400	0.50958900
C	2.72097500	-3.08412700	1.38830100
C	2.45384900	-1.73040300	0.96272000
H	-3.90073900	-1.23309000	7.25665400
N	1.91153400	1.13229000	0.55439300

H	-3.26111300	0.39462300	6.89135800
C	2.34983700	5.74974400	0.08451500
H	0.35282000	3.29828800	5.55714600
C	2.10552700	2.49880300	0.75546600
C	1.42610300	4.94054100	0.81129100
H	3.70645100	-3.54404000	1.40549500
C	2.44714400	7.12910800	0.36122900
C	3.17052400	0.57329200	0.66228700
C	3.45941000	-0.79748000	0.70004500
C	-0.70252800	3.52593300	5.77890200
H	3.14316200	7.73252700	-0.21584800
H	-0.08681300	3.71993200	2.44450600
C	0.69551200	5.54411400	1.88379500
H	-1.12849500	2.66705900	6.32240500
N	-0.11666700	4.70930400	2.68491500
H	5.68408800	-2.49332300	-3.13467700
H	-0.72840800	4.40205500	6.44565200
H	4.95522600	-1.02065100	-1.51027000
C	1.67817000	7.68931900	1.38047300
C	3.48486800	2.76709000	1.09207100
C	0.81720700	6.91757000	2.15971500
C	4.15692300	1.58450800	0.96693500
C	-1.51095900	3.81074500	4.49515200
C	-0.89284100	5.03284900	3.78988200
H	-1.44659400	2.92517700	3.83415200
C	6.73460900	-2.79758800	-3.00688600
C	5.52750800	-1.29516300	-0.61937700
C	4.88893400	-1.23870900	0.62579400
H	6.47753400	-0.01726900	-2.90962900
H	7.18742100	-2.86576900	-4.01076500
H	1.76521300	8.76115900	1.58315000
H	3.87516100	3.74377100	1.37128400
H	6.73799800	-3.80674200	-2.56363300
H	0.24042900	7.34562000	2.97725000

O	-1.06251300	6.17346500	4.21526500
C	7.50313100	-0.39905500	-2.78736400
H	7.96504000	-0.44082300	-3.78852600
H	5.21373300	1.38365400	1.13112700
C	7.52682800	-1.79938700	-2.12505700
C	6.86852700	-1.71919900	-0.73216300
C	5.59925600	-1.59230300	1.79126000
C	-2.98770500	4.08830500	4.81571400
H	5.08333600	-1.52884000	2.75215900
H	-3.42761400	3.25329100	5.38411100
H	8.06506400	0.33313800	-2.18442000
H	-3.07647500	5.00668800	5.41508300
C	7.54490100	-2.06125400	0.44853500
H	-3.58238000	4.22831100	3.89858300
C	6.93846800	-2.00277400	1.72312900
C	8.99264400	-2.27388600	-2.05876300
H	9.41589300	-2.31264100	-3.07570600
H	9.08201700	-3.28538100	-1.62933400
H	6.05046900	-2.93040900	4.27008200
H	8.58549200	-2.38732400	0.38405500
H	9.62404200	-1.59010500	-1.46744700
H	7.38523400	-4.54626900	2.76494200
C	6.92920900	-2.26462800	4.27302000
H	6.57921300	-1.23365100	4.44664500
C	7.75411700	-2.38606300	2.97547200
C	8.23791200	-3.85253000	2.84695000
H	8.87612800	-4.00141300	1.96173400
H	7.55171200	-2.54867900	5.13703300
C	8.98266600	-1.44939500	3.09572200
H	8.67056100	-0.39674800	3.19420500
H	9.64437900	-1.52140000	2.21814800
H	8.82681100	-4.14176900	3.73391600
H	9.58002000	-1.71133800	3.98551800
H	-5.52597700	-5.18142000	-5.30956700

H	-7.15763600	-4.90833900	-3.43396100
C	-5.20584400	-4.73674600	-4.36203800
C	-6.11994600	-4.58234700	-3.31276800
C	-3.87446900	-4.32955000	-4.19789300
H	-3.16031100	-4.46067400	-5.01836500
C	-5.69541800	-4.01458600	-2.10227800
H	-6.40194800	-3.90209900	-1.27356800
C	-3.43713000	-3.76546300	-2.98649700
C	-4.36532700	-3.60889900	-1.94134500
H	-1.60813400	-3.90925300	-1.88379400
C	-1.97596200	-3.40931000	-2.78734700
H	-1.39060800	-3.79454000	-3.64661100
H	-4.03290000	-3.16929700	-0.99700400
H	4.00489700	1.00183900	-5.75264000
C	3.33496500	1.69457700	-5.23357900
H	4.46098700	3.46167900	-5.80596500
C	3.59667100	3.07394200	-5.25854400
C	2.21167200	1.20065700	-4.56622800
H	2.00224400	0.12707000	-4.54562600
C	2.74678300	3.95406100	-4.57234600
N	-1.73664900	-1.93671700	-2.60562200
C	1.33098100	2.08138500	-3.89122700
C	1.64143600	3.46152200	-3.87210800
H	-3.24314100	-1.54387500	-3.93935300
H	-0.30980300	0.21537300	-4.95329600
O	0.69742900	-1.63451700	-3.58261400
H	2.93897200	5.03087500	-4.59043600
N	0.36446700	-0.25779800	-1.49424600
C	0.04398900	1.61016300	-3.34467200
S	0.00321600	-1.69402700	-2.26547900
H	0.96922500	4.15452800	-3.35519500
C	-0.87516600	0.95355500	-4.36161100
C	-2.19494200	-1.22565300	-3.82734500
H	-0.47295300	2.36904800	-2.73479000

C	-2.15677400	0.30932800	-3.79356700
H	-3.01497900	0.65822800	-4.39257700
H	0.27240700	0.68106400	-2.37398100
H	-1.15104400	1.75119400	-5.08164100
H	-1.65372600	-1.59915700	-4.72156300
O	0.33930400	-2.81184900	-1.34570800
H	-2.35107500	0.65953600	-2.76690800

Intermediate $D^{7}_{3.1a}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.605188 Hartree

H_corr: 1.895006 Hartree

SCF: -6389.972537 Hartree

S: 609.974 Cal/Mol-Kelvin

H: -6388.07753 Hartree

G: -6388.367349 Hartree

Cartesian Coordinates:

H	-8.97454500	-1.41423100	-2.43875700
H	-8.79483300	-2.35789700	-0.94362400
C	-8.24073300	-1.78327000	-1.70251300
H	-7.56152900	-2.47837500	-2.22221600
H	-8.33951800	-4.06357100	2.24226900
H	-9.19714600	0.73834600	-1.09151700
C	-8.03068100	-3.52474700	3.15322800
H	-8.32840600	-4.14315200	4.01554000
H	-8.99656000	-0.15091000	0.43787500
C	-8.45112200	0.35564800	-0.37456900
H	-7.95114400	-2.14439100	1.09321700
C	-7.45733300	-0.59661100	-1.08734900
H	-6.02475700	-5.19628700	2.22912500
H	-8.60530000	-2.58559000	3.21082000
H	-7.54761100	0.51963600	-2.95298400

C	-6.88503300	-1.91730700	1.02328300
C	-6.78241600	0.17670900	-2.23780000
C	-5.79592100	-4.65267100	3.16050400
H	-6.12634000	-5.27764000	4.00734100
H	-6.07058800	-0.45486300	-2.79445000
C	-6.43779500	-1.12315800	-0.05551900
C	-6.50896200	-3.27757300	3.19294500
H	-7.92688900	1.22183300	0.06083500
C	-6.01997200	-2.41891600	2.00767600
H	2.21177900	-6.02463500	-5.57722400
H	0.75800000	-5.20296700	-4.96104200
H	-4.70122500	-4.55281800	3.23014400
C	1.80921000	-5.05137300	-5.25686300
H	-6.24804500	1.07360700	-1.88494000
C	-5.06764900	-0.82798900	-0.12861000
C	-6.17194000	-2.55587200	4.52221300
H	-6.51179300	-3.15683200	5.38269100
H	-3.11238200	-3.75443000	0.36981900
H	1.82416400	-4.36665700	-6.12063400
C	-4.65069800	-2.10431800	1.89419600
O	3.06759800	-6.64553000	-3.11572100
H	-6.66818000	-1.57310800	4.57677800
H	-4.67584300	-0.21487900	-0.94267800
H	-0.77377600	-5.13942100	0.39765000
H	2.80907100	-7.57477100	-1.23479900
C	-4.16655900	-1.31458100	0.84033700
C	-2.09921400	-3.36609200	0.44382100
H	2.75662700	-8.67482700	1.00171100
C	2.53727800	-7.01338200	-0.34369100
C	2.67460200	-5.49228100	-2.94392300
C	2.50597200	-7.61285800	0.91631700
C	-0.92627700	-4.06390700	0.46207800
C	2.65240800	-4.48132500	-4.10137300
H	-3.94117600	-2.45976800	2.64736400

H	-5.08928000	-2.39078400	4.63952400
H	4.58621400	-5.15540100	-4.86048100
C	2.21627300	-5.64495100	-0.47229100
N	2.23825700	-4.98549400	-1.72179500
C	2.16833100	-6.90313000	2.07059700
C	4.10243700	-4.21506500	-4.55300200
C	-2.71054700	-0.96040800	0.78760000
C	-1.76230600	-1.96902800	0.58536600
H	2.15089900	-7.37257100	3.05235200
H	2.21056000	-3.53089300	-3.75929000
H	4.11721900	-3.51875100	-5.40720900
C	1.85883300	-4.89851800	0.68448300
H	1.93183900	-4.00796300	-1.73080400
C	1.84463600	-5.53924700	1.95474200
C	0.13502400	-3.09461800	0.56884900
H	-4.33932200	1.22886100	1.59280800
H	1.51952900	5.42282300	-3.85192400
N	-0.37975500	-1.80410100	0.63274600
O	1.60869000	-6.24848300	4.84335300
C	1.49047800	-3.44485200	0.59970100
C	-2.33187300	0.35600400	1.08203700
H	1.45605400	6.94207300	-2.91632100
C	-3.26460100	1.37277700	1.50856500
H	4.70287800	-3.76892800	-3.74376400
N	1.50927800	-4.74940200	3.07931000
C	1.28504600	5.85524000	-2.86580800
C	1.41682400	-5.11244600	4.41433700
H	1.99130300	5.43138100	-2.13357600
H	3.14521500	-3.38483800	5.75641000
H	1.31974700	-3.76998100	2.87185400
H	-0.91211500	5.73492100	-4.53471800
H	0.86298000	-3.03174700	4.77056200
H	-1.08769600	7.22271000	-3.56071100
N	-1.02915300	0.83914700	1.11977200

C	1.05485200	-3.94983700	5.35881800
C	-2.53336200	2.48626100	1.80624000
C	2.50346400	-2.48400100	0.52646800
C	-1.15589000	6.12478900	-3.53299900
C	2.24051500	-3.68843600	6.30793700
Co	0.62738100	-0.11457200	0.58927600
C	-0.18228800	5.56558000	-2.48367400
C	-1.15200800	2.15927500	1.54672700
H	-2.87979500	3.44966100	2.17565600
H	4.29966700	-3.82669900	0.40763000
C	3.89862900	-2.81608500	0.36378500
N	2.31713000	-1.10808900	0.48008900
H	2.47865200	-4.60244600	6.87345100
H	-0.31678600	4.46867300	-2.41632600
H	1.99536300	-2.88958800	7.02664500
C	-0.46928700	6.20611100	-1.11369600
H	-2.19946200	5.85747400	-3.30355100
C	-0.22008100	-4.31081500	6.14215100
H	-1.08453300	-4.44584300	5.47195000
H	-0.34807000	4.32220000	-0.30853000
N	-0.50613800	5.29819900	-0.06037000
O	-0.61563700	7.41861800	-0.98384200
C	-0.10847300	3.08360400	1.69004400
C	4.55806100	-1.64614700	0.12509700
C	3.57889700	-0.58873000	0.20848500
H	-0.06883600	-5.25199800	6.69226200
N	1.67674900	1.53816700	0.91187100
H	-0.46991900	-3.51909600	6.86705000
C	-0.61860700	5.55049100	1.32482800
H	2.08344100	2.47855700	6.76367900
C	1.21327700	2.77870900	1.33802000
C	-0.42287900	4.45866700	2.21232400
H	5.61948100	-1.49038100	-0.05493700
C	-0.91369000	6.83097200	1.83257400

C	3.00501800	1.75930500	0.55338100
C	3.91064500	0.76836000	0.15608800
C	1.18570600	2.16998200	7.32370200
H	-1.05618500	7.65615900	1.13752500
H	-0.08295700	2.69612200	3.97712100
C	-0.52035200	4.67562000	3.61356800
H	1.39153700	1.19012900	7.78414600
N	-0.30312000	3.56585900	4.46043400
H	6.09737600	-0.45414100	-3.91046700
H	1.01851100	2.90346900	8.12720700
H	4.89053400	0.75162300	-2.33815100
C	-1.00607800	7.00869400	3.21482600
C	2.26832100	3.76117500	1.29001700
C	-0.81494100	5.95785000	4.11496400
C	3.36481800	3.14024100	0.76259900
C	-0.05478600	2.09321200	6.41399900
C	-0.35143100	3.49363400	5.84574600
H	0.15466800	1.38753100	5.58713600
C	7.12277600	-0.07828400	-4.05019600
C	5.64470000	1.08744900	-1.62003700
C	5.29401900	1.15748400	-0.26538800
H	5.25571100	1.98581000	-4.22837900
H	7.35876200	-0.14853800	-5.12557900
H	-1.23514000	8.00490500	3.60556900
H	2.16064100	4.79794200	1.60284900
H	7.80602500	-0.75294600	-3.50853300
H	-0.88517400	6.10285800	5.19139000
O	-0.60667000	4.44399100	6.58201600
C	6.30543000	2.29446400	-4.35169400
H	6.53804900	2.25560900	-5.42940800
H	4.34575700	3.56177900	0.55472600
C	7.27713900	1.38331000	-3.55963400
C	6.93452700	1.45543400	-2.05736900
C	6.24463300	1.58572900	0.68308800

C	-1.28868600	1.59288200	7.18864600
H	5.95184800	1.61656900	1.73514800
H	-1.08734000	0.61193400	7.64880700
H	6.38928600	3.34368700	-4.02380400
H	-1.54584500	2.30505900	7.98759600
C	7.85579600	1.87612200	-1.08602900
H	-2.16704900	1.48748900	6.53132800
C	7.54164800	1.94581300	0.28958200
C	8.71874600	1.84267100	-3.85777000
H	8.91133000	1.77768000	-4.94095900
H	9.46891200	1.21008700	-3.35486700
H	7.77700700	1.41834000	3.08364700
H	8.86160600	2.16109600	-1.40297800
H	8.89132700	2.88944800	-3.55712500
H	9.52754900	0.40815100	1.48385500
C	8.09542000	2.41884500	2.74733800
H	7.24731600	3.11154300	2.87589600
C	8.61760200	2.40359700	1.29623500
C	9.82759200	1.43781200	1.22929100
H	10.28299800	1.41516800	0.22668700
H	8.89617600	2.75290300	3.42694000
C	9.08446000	3.83654800	0.93622200
H	8.24602300	4.55078400	0.98209600
H	9.51338100	3.88932700	-0.07682400
H	10.60881500	1.75054200	1.94279200
H	9.85948500	4.17709400	1.64368100
H	-4.51540000	-3.02743500	-6.97842500
H	-5.95708300	-3.72994000	-5.06038600
C	-4.13551900	-2.96769600	-5.95368900
C	-4.94331200	-3.35930700	-4.87969000
C	-2.83569400	-2.49742800	-5.71787200
H	-2.20432700	-2.19662200	-6.56158100
C	-4.44593800	-3.27463400	-3.57002700
H	-5.07024400	-3.58290900	-2.72562900

C	-2.32712800	-2.41739300	-4.41074300
C	-3.14854400	-2.80563700	-3.33683500
H	-0.32051500	-2.81831600	-3.75675800
C	-0.89675200	-1.97706100	-4.16778100
H	-0.42375500	-1.68504800	-5.12634900
H	-2.75786600	-2.73860500	-2.31694200
H	-6.66407700	5.31128300	-5.26142600
C	-6.34092800	5.14186800	-4.22912000
H	-7.82916700	6.48179400	-3.38263400
C	-6.99773800	5.80195100	-3.17512900
C	-5.27988200	4.27681700	-3.97595300
H	-4.78126400	3.78126900	-4.81378500
C	-6.57129700	5.58416500	-1.85122000
N	-0.82410400	-0.86955800	-3.17203200
C	-4.82729900	4.03302400	-2.63889700
C	-5.51304800	4.72305900	-1.58598700
H	-1.96425500	0.15008500	-4.59477600
H	-2.11296500	3.04261600	-3.70794200
O	1.64984900	0.01548400	-3.51911500
H	-7.07218400	6.09889600	-1.02508100
N	0.54104300	0.34804400	-1.27454500
C	-3.75064100	3.16337700	-2.32804700
S	0.78269000	-0.71075800	-2.54714700
H	-5.18275200	4.56382400	-0.55391900
C	-2.92283000	2.39097700	-3.30805000
C	-1.37789000	0.41177400	-3.69815100
H	-3.47088900	3.07516900	-1.27051200
C	-2.28751000	1.12770500	-2.69787100
H	-3.07899200	0.42766300	-2.38082800
H	1.29918400	1.03306300	-1.40596400
H	-3.52403900	2.11369600	-4.19458200
H	-0.56180700	1.07243900	-4.04535400
O	1.17121500	-2.08935900	-2.16602800
H	-1.70558100	1.37863800	-1.79681700

Transition State $TS3^{7}_{3.1a}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -96.3375 cm-1

G_corr: 1.615988 Hartree

H_corr: 1.894365 Hartree

SCF: -6389.943042 Hartree

S: 585.895 Cal/Mol-Kelvin

H: -6388.048676 Hartree

G: -6388.327054 Hartree

Cartesian Coordinates:

N	0.17531800	-0.17667300	-1.66244100
H	-9.10308700	-0.69650500	-3.19855100
H	-9.18100800	0.48160900	-1.86686600
C	-8.51331200	-0.21269500	-2.40138300
H	-8.20148400	-0.99341500	-1.68870700
H	-9.20924100	3.37275300	0.43458500
H	-8.33496300	1.11601900	-4.83005200
C	-8.56274700	4.26032500	0.33538400
H	-8.99725200	5.05281700	0.96613400
H	-8.42611200	2.33480600	-3.53946700
C	-7.76742000	1.58821200	-4.01023800
H	-8.13090400	2.48307600	-1.33712600
C	-7.28408200	0.51390700	-3.00329500
H	-7.72154200	2.59823200	2.38870800
H	-8.61274800	4.60944200	-0.70929800
H	-7.05032200	-0.96501300	-4.58299400
C	-7.09933000	2.20901500	-1.10516100
C	-6.44309300	-0.51974300	-3.77816000
C	-7.14768000	3.53155300	2.26735600
H	-7.62282900	4.30727800	2.89148500
H	-6.09623900	-1.34732000	-3.13888600

C	-6.48703800	1.19128300	-1.86871000
C	-7.11461100	3.97660700	0.78362500
H	-6.91461200	2.12746700	-4.45435300
C	-6.43965100	2.87686900	-0.06262500
H	0.06663000	-7.99596500	-2.74585100
H	-0.86356100	-6.55340200	-3.20732000
H	-6.13680800	3.35647100	2.66776400
C	0.13977300	-6.91255100	-2.92555000
H	-5.56203100	-0.05549000	-4.25206000
C	-5.16635800	0.83807700	-1.55290900
C	-6.30573800	5.29215300	0.65950900
H	-6.76994300	6.08824300	1.26582800
H	-4.92024400	-0.85795500	0.67772400
H	0.81605600	-6.74281500	-3.77924100
C	-5.10704500	2.50655200	0.20872500
O	-0.59074400	-7.66052400	-0.21663000
H	-6.27198000	5.63902000	-0.38649800
H	-4.65494100	0.04785900	-2.10613200
H	-3.70764400	-3.03014000	1.77009800
H	-1.71830700	-7.48181100	1.55254900
C	-4.46206500	1.49711300	-0.52285800
C	-3.85530100	-1.05562500	0.77952400
H	-2.74063900	-7.43548600	3.82556300
C	-1.77026300	-6.55606700	2.12098100
C	-0.24839900	-6.50836700	-0.47512500
C	-2.33415300	-6.51433700	3.39648200
C	-3.24693100	-2.14548300	1.33465800
C	0.66862900	-6.19921900	-1.66995200
H	-4.55589400	2.99412100	1.01803800
H	-5.26750800	5.17504200	1.00789000
H	2.09660200	-7.75492800	-1.09780300
C	-1.24100100	-5.37856900	1.55247700
N	-0.60951800	-5.39339500	0.28481300
C	-2.38257600	-5.33840300	4.14641500

C	2.09540200	-6.67639200	-1.32242600
C	-3.05070300	1.11453100	-0.19414600
C	-2.80843600	-0.15157500	0.36205100
H	-2.80312100	-5.31111600	5.14975900
H	0.70503100	-5.11162500	-1.84916000
H	2.77503600	-6.49710400	-2.17139200
C	-1.32034200	-4.14992000	2.27075200
H	-0.22948100	-4.50044900	-0.04083600
C	-1.86953600	-4.15484100	3.58509500
C	-1.82219000	-1.92055400	1.24882900
H	-3.17744500	3.84306200	-1.12197800
H	7.05787500	3.49899100	-1.56639000
N	-1.56369300	-0.68135900	0.67752400
O	-2.90167700	-3.48010600	6.30056700
C	-0.85577800	-2.85270000	1.66999500
C	-2.03428900	2.07634400	-0.31946700
H	6.96249200	5.03563200	-0.66385900
C	-2.24753500	3.44733400	-0.71953100
H	2.50093300	-6.14008700	-0.44946100
N	-1.86006900	-2.93598000	4.30291100
C	6.37103400	4.19250200	-1.05493400
C	-2.33678500	-2.66270000	5.57582400
H	5.92602700	3.65604800	-0.20338100
H	-0.10058800	-1.65838900	6.89288900
H	-1.42007900	-2.15682900	3.81519500
H	6.62861100	4.68005100	-3.76735600
H	-1.66096000	-0.61923700	5.21864900
H	6.54638200	6.25115500	-2.91683700
N	-0.72060700	1.89836300	0.10178800
C	-2.08572700	-1.21788500	6.04714400
C	-1.08899900	4.12665200	-0.44770900
C	0.51647500	-2.61830500	1.51457400
C	5.95759600	5.38315200	-3.24820100
C	-1.07174000	-1.24333200	7.20826500

Co	0.17379900	0.15492000	0.35790300
C	5.29558200	4.70402000	-2.03948000
C	-0.14807800	3.16293800	0.06578900
H	-0.88360000	5.18863300	-0.57224900
H	1.33884500	-4.58732600	2.23299400
C	1.52987700	-3.61423400	1.78501400
N	1.09068900	-1.46189400	1.01024200
H	-1.45636800	-1.86594300	8.03081400
H	4.69332000	3.84361600	-2.38370200
H	-0.89693000	-0.22644600	7.59578400
C	4.39593200	5.71223600	-1.30136500
H	5.21581400	5.75030500	-3.97474200
C	-3.42019000	-0.58747800	6.48248100
H	-4.12621900	-0.50897900	5.63997600
H	3.06071600	4.18682900	-0.97196500
N	3.20723700	5.18089600	-0.79537200
O	4.74841600	6.87980600	-1.15078600
C	1.14501600	3.48898900	0.53538200
C	2.71592500	-3.09665800	1.35626700
C	2.44610500	-1.74700500	0.91450700
H	-3.89035400	-1.20594100	7.26198900
N	1.90467300	1.12217800	0.50782000
H	-3.25976400	0.42390100	6.89025400
C	2.36021300	5.75369500	0.18843000
H	0.26638700	3.18760300	5.57396600
C	2.09802500	2.48473100	0.75146600
C	1.42094400	4.92800700	0.87697300
H	3.70173300	-3.55565300	1.38061000
C	2.45456700	7.12667200	0.49432300
C	3.16616500	0.55850700	0.61817600
C	3.45259500	-0.81391600	0.65118800
C	-0.79166100	3.41594700	5.78170200
H	3.16105800	7.74071200	-0.05862400
H	-0.12317900	3.67849200	2.45592600

C	0.67498900	5.51072900	1.95097900
H	-1.23087500	2.54854300	6.30061400
N	-0.14961500	4.66143300	2.72250500
H	5.68642500	-2.59914400	-3.14628000
H	-0.82569100	4.27912600	6.46481200
H	4.95123600	-1.08664900	-1.55708300
C	1.66651100	7.66648100	1.51018500
C	3.47540000	2.74105300	1.10300400
C	0.79240600	6.87850700	2.25734300
C	4.14975800	1.56218300	0.94959000
C	-1.57596900	3.72897000	4.48968800
C	-0.94210600	4.96354300	3.82162000
H	-1.50179500	2.85716700	3.81190200
C	6.74001900	-2.89043000	-3.01320400
C	5.52319600	-1.33828000	-0.65903100
C	4.88350100	-1.25538800	0.58396000
H	6.45763300	-0.11236300	-2.98228900
H	7.19201100	-2.97761200	-4.01603400
H	1.75030700	8.73372300	1.73712200
H	3.86404200	3.70696600	1.41991300
H	6.75338900	-3.88884900	-2.54651600
H	0.20166800	7.28909200	3.07390100
O	-1.11426100	6.09517700	4.27013900
C	7.48707200	-0.48093200	-2.85089400
H	7.94909200	-0.54173000	-3.85103900
H	5.20529300	1.35786400	1.11791600
C	7.52376200	-1.86490800	-2.15550100
C	6.86595600	-1.75853900	-0.76394300
C	5.59607900	-1.58263500	1.75569900
C	-3.05763100	4.00405300	4.78897700
H	5.07936100	-1.50149000	2.71480300
H	-3.51067600	3.15702700	5.32852300
H	8.04151900	0.27087600	-2.26540900
H	-3.15522700	4.90822700	5.40829000

C	7.54385700	-2.07347400	0.42331900
H	-3.63404700	4.16767000	3.86412600
C	6.93628900	-1.99151600	1.69611700
C	8.99393900	-2.32427400	-2.07979900
H	9.41721100	-2.38205900	-3.09588000
H	9.09262500	-3.32497300	-1.62783600
H	6.04853800	-2.87352600	4.25863700
H	8.58572400	-2.39684500	0.36578000
H	9.61907400	-1.62181500	-1.50392300
H	7.38973100	-4.51334800	2.78534000
C	6.92559700	-2.20565500	4.25046400
H	6.57257000	-1.17266700	4.40477300
C	7.75208400	-2.34869700	2.95612100
C	8.24038200	-3.81586700	2.85556400
H	8.88017000	-3.97932600	1.97402600
H	7.54798800	-2.47217400	5.12016400
C	8.97779700	-1.40638700	3.05996600
H	8.66240900	-0.35303600	3.13864700
H	9.64041200	-1.49272100	2.18432400
H	8.82892900	-4.08691000	3.74852800
H	9.57526700	-1.64988000	3.95494700
H	-5.32892600	-5.50196800	-5.14074200
H	-6.95563700	-5.12554200	-3.27883400
C	-5.01221400	-4.98565400	-4.22911300
C	-5.92341400	-4.77352200	-3.18756200
C	-3.68816000	-4.54272900	-4.10324400
H	-2.97681800	-4.71650600	-4.91823600
C	-5.50295200	-4.11437700	-2.02283500
H	-6.20667100	-3.95640600	-1.19927700
C	-3.25581800	-3.88644700	-2.93749900
C	-4.17983700	-3.67477600	-1.89855600
H	-1.40324800	-3.95283000	-1.86770300
C	-1.80066000	-3.49051500	-2.77771500
H	-1.22346600	-3.88735600	-3.63656700

H	-3.85280900	-3.16389900	-0.98873600
H	3.58788200	1.89529000	-6.41183300
C	2.98672200	2.37173100	-5.63143200
H	4.12278800	4.22105000	-5.66924500
C	3.29552800	3.67566900	-5.20651200
C	1.90935300	1.68768700	-5.07551800
H	1.68108300	0.67131800	-5.40515200
C	2.54549300	4.27378500	-4.17864600
N	-1.59414200	-2.00611800	-2.64599600
C	1.11416700	2.28974000	-4.05435500
C	1.49048800	3.58357300	-3.58698500
H	-3.20501400	-1.68692000	-3.87270500
H	-0.27605300	0.04012200	-4.91253000
O	0.82457100	-1.61208600	-3.69362900
H	2.77959000	5.28894900	-3.84693600
C	-0.11608400	1.71678400	-3.60558700
S	0.11607600	-1.70973400	-2.38303400
H	0.89163400	4.05653300	-2.80215500
C	-0.91927900	0.82659200	-4.47913900
C	-2.16311800	-1.33469300	-3.84298400
H	-0.61961800	2.19679800	-2.76086600
C	-2.16152400	0.19569200	-3.82410400
H	-3.06329400	0.53142100	-4.36266400
H	1.10811600	0.16037700	-1.95309100
H	-1.22331500	1.44040100	-5.35594100
H	-1.67788200	-1.71142400	-4.76819600
O	0.53417000	-2.80270200	-1.47071400
H	-2.27168100	0.54305800	-2.78586200

Intermediate $E_{\underline{3.1a}}$:

E = $A_{[Co(II)(\mathbf{P2})]}$ + **3.2a**

Product 3.2a:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.285471 Hartree

H_corr: 0.357352 Hartree

SCF: -1318.169175 Hartree

S: 151.286 Cal/Mol-Kelvin

H: -1317.811823 Hartree

G: -1317.883704 Hartree

Cartesian Coordinates:

H	2.00054100	2.04350400	0.96015900
C	-1.10258100	0.37097700	1.70138400
N	-1.11883500	0.73920600	0.27032800
S	0.21009200	1.66405000	-0.31051400
N	1.37233500	1.24819900	0.83537400
O	0.04141900	3.12054700	-0.12156200
O	0.45196900	1.16425900	-1.67969400
C	-2.40354500	1.22592500	-0.28496500
C	-3.43496000	0.11451100	-0.34173000
H	-2.20251500	1.59033000	-1.30644300
H	-2.79028700	2.08734300	0.29331300
C	-3.15282500	-1.08197100	-1.02665500
C	-4.11357700	-2.09515000	-1.10960900
C	-4.69359000	0.27283300	0.25992200
C	-5.65865400	-0.74162700	0.17717800
C	-5.37009200	-1.92784100	-0.50734500
H	-6.12090500	-2.72140000	-0.57302400
H	-6.63564300	-0.60360600	0.65088600
H	-2.17227100	-1.20715300	-1.49642300
H	-3.88461900	-3.01893100	-1.65037300
H	-4.92341100	1.20098100	0.79540500
C	4.32667800	-0.93957100	1.02847900
C	3.21582300	-0.42619000	0.33541600
C	5.49609000	-1.29975600	0.34647100
C	3.29851400	-0.26934300	-1.06046900

C	5.56987700	-1.14290700	-1.04324800
H	6.35219500	-1.69439600	0.90286200
C	4.46969900	-0.62555500	-1.74105400
H	2.44844500	0.14146200	-1.61330500
H	6.48334700	-1.41727400	-1.58007200
H	4.52209900	-0.49488800	-2.82655200
C	1.94850000	-0.08915700	1.11731400
H	2.22957400	-0.03075700	2.18718700
C	0.86506500	-1.17898700	1.00024900
C	-0.36076100	-0.96977400	1.91019600
H	-2.15417200	0.26155900	2.01105700
H	-0.66565500	1.17658300	2.31480800
H	-1.06342400	-1.79750400	1.71322900
H	-0.06606700	-1.05194700	2.97264900
H	1.34122400	-2.14206600	1.24718400
H	0.54322000	-1.25817100	-0.05118600
H	4.27727200	-1.05726100	2.11779800

Transition State $TS2^{5}_{3.1a}$ (1,5-HAA)

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -1201.3038 cm-1

G_corr: 1.604493 Hartree

H_corr: 1.889007 Hartree

SCF: -6389.938859 Hartree

S: 598.81 Cal/Mol-Kelvin

H: -6388.049852 Hartree

G: -6388.334366 Hartree

Cartesian Coordinates:

H	-8.31470900	-2.77443200	-3.94782500
H	-8.87233600	-1.84803600	-2.53639200
C	-7.98032100	-2.27028300	-3.02533200
H	-7.56103600	-3.03661900	-2.35306500

H	-9.92342600	0.40563400	0.14249700
H	-7.88731700	-0.61413000	-5.24544600
C	-9.57421000	1.44666900	0.24151100
H	-10.28211100	1.96619100	0.90749800
H	-8.43398300	0.35795900	-3.85978600
C	-7.55662500	-0.13369800	-4.30898000
H	-8.47914700	0.16592400	-1.57718300
C	-6.92770700	-1.18265900	-3.35728800
H	-8.43663700	-0.21027100	2.15195500
H	-9.64119800	1.92955300	-0.74744200
H	-6.12474000	-2.34862500	-5.01142200
C	-7.43626300	0.17219900	-1.25247800
C	-5.75545600	-1.85957300	-4.09549200
C	-8.16954300	0.85639800	2.22832500
H	-8.91126800	1.34692800	2.88117700
H	-5.27112000	-2.63733900	-3.48274400
C	-6.47936300	-0.48639000	-2.05543500
C	-8.15181200	1.52805900	0.83194600
H	-6.82914000	0.65263600	-4.56901700
C	-7.10323400	0.82716700	-0.05700100
H	2.11986900	-7.76456800	-2.71380900
H	0.59748400	-6.98734700	-3.20895500
H	-7.19124500	0.92096100	2.73013900
C	1.65612800	-6.79982300	-2.96910800
H	-4.98511800	-1.13292100	-4.40207300
C	-5.14431800	-0.47379200	-1.62539200
C	-7.77933300	3.02403900	0.98648900
H	-8.51484500	3.53921300	1.62710800
H	-4.60849300	-2.35002200	0.41490000
H	2.14033800	-6.40387300	-3.87619200
C	-5.74893000	0.82286800	0.33505500
O	1.37927800	-7.58767800	-0.21863300
H	-7.76713500	3.53282100	0.00847300
H	-4.36891600	-0.97541900	-2.20888000

H	-2.93927600	-4.17987300	1.53331400
H	0.05704800	-7.88037500	1.43858400
C	-4.76688900	0.18376100	-0.43592200
C	-3.55210600	-2.24399500	0.65166600
H	-0.88626900	-8.21705100	3.72017200
C	-0.23591700	-7.03005000	2.04993200
C	1.19320200	-6.41153500	-0.52769700
C	-0.75732600	-7.20154600	3.33281100
C	-2.71747900	-3.16076700	1.22285800
C	1.80880200	-5.81298400	-1.80176800
H	-5.44563700	1.30668500	1.26814600
H	-6.78823300	3.15870700	1.44780500
H	3.82760100	-6.41433500	-1.21422100
C	-0.06372200	-5.72764100	1.53539400
N	0.46696100	-5.50615500	0.24397400
C	-1.11882900	-6.11962700	4.13785900
C	3.29548600	-5.50065200	-1.52510400
C	-3.33660200	0.17120500	0.00996400
C	-2.78181700	-1.03921900	0.44892600
H	-1.51726000	-6.25582900	5.14134500
H	1.29782500	-4.86647500	-2.04693000
H	3.77960000	-5.11209700	-2.43555700
C	-0.43140500	-4.60490200	2.32865000
H	0.38624600	-4.55561400	-0.13449500
C	-0.95435200	-4.81597800	3.63553300
C	-1.42393300	-2.53414200	1.34276000
H	-4.21038200	2.85863200	-0.49778200
H	4.96317100	4.55764300	-2.57409600
N	-1.47474600	-1.22349800	0.88672800
O	-2.06026000	-4.57092000	6.39286400
C	-0.28301700	-3.20453400	1.80867400
C	-2.62348800	1.37658300	0.08679700
H	4.96729800	5.97819500	-1.49441600
C	-3.20225700	2.67963500	-0.13068400

H	3.41025400	-4.74140000	-0.73594400
N	-1.27976200	-3.67365700	4.40394000
C	4.38913000	5.09133700	-1.79932600
C	-1.78765500	-3.59809400	5.69187600
H	4.29556500	4.42252600	-0.92880300
H	-0.07401300	-2.05889500	7.26741200
H	-1.10296600	-2.78266400	3.94223600
H	3.74055500	5.85312100	-4.37705300
H	-1.67388000	-1.43316700	5.43799300
H	3.67702300	7.32303700	-3.35833200
N	-1.30457400	1.50028600	0.51982000
C	-1.99859100	-2.16141200	6.20592100
C	-2.26499800	3.60187800	0.24750800
C	0.99058700	-2.63015900	1.73079900
C	3.15864400	6.38502300	-3.60807600
C	-1.15128500	-1.95369300	7.47512200
Co	0.01338100	0.03912100	0.70909600
C	3.01043400	5.51630300	-2.35050000
C	-1.08760100	2.86960700	0.64000200
H	-2.34750600	4.68719900	0.25788800
H	2.26121800	-4.35355900	2.40871500
C	2.21436100	-3.34221000	2.01009100
N	1.27110700	-1.34226700	1.28772000
H	-1.42449300	-2.70124600	8.23538400
H	2.43638700	4.60699900	-2.60893900
H	-1.32050400	-0.94986500	7.89755200
C	2.26799200	6.30765000	-1.26137900
H	2.17962300	6.63802300	-4.04239200
C	-3.49706500	-1.94571100	6.49092800
H	-4.10271000	-2.03294900	5.57429600
H	1.24618600	4.58415500	-0.79759400
N	1.32479600	5.56916900	-0.54674800
O	2.52959100	7.48582600	-1.03260800
C	0.09681300	3.48525000	1.08638000

C	3.24382600	-2.51593900	1.66107100
C	2.65725000	-1.26605000	1.24145300
H	-3.85501000	-2.70010700	7.20821500
N	1.42853200	1.38954000	1.03399100
H	-3.67228300	-0.94656500	6.92214800
C	0.63761200	5.95496600	0.62772600
H	-0.16775000	2.88227800	6.32686900
C	1.28779200	2.75965700	1.22748700
C	0.05083400	4.94633800	1.44160400
H	4.31359700	-2.70288900	1.72528500
C	0.52672500	7.31225600	0.99133500
C	2.79474200	1.15869800	1.04821500
C	3.40293700	-0.10265100	1.03043800
C	-1.23921100	2.88805700	6.58507800
H	0.98482800	8.06751800	0.35696900
H	-0.96434600	3.36552900	3.13766100
C	-0.61198500	5.33535100	2.64375100
H	-1.47031400	1.94034000	7.09776800
N	-1.13323500	4.31372700	3.46987600
H	5.76354600	-2.66523600	-2.21321000
H	-1.41403300	3.71450500	7.29128800
H	4.72998500	-0.88482400	-1.13620300
C	-0.14647100	7.65614000	2.16371000
C	2.57835200	3.37184900	1.44367100
C	-0.71298700	6.69287900	2.99954000
C	3.51415100	2.39229100	1.26554000
C	-2.12828300	3.06158400	5.33662100
C	-1.79926900	4.41707000	4.68331400
H	-1.90719700	2.24013600	4.62822400
C	6.86313500	-2.61665100	-2.18922000
C	5.42411300	-0.63497500	-0.32837300
C	4.88999900	-0.21042300	0.89506800
H	5.77398400	-0.19951700	-3.04661800
H	7.23582500	-2.95349300	-3.17177600

H	-0.22825100	8.71233500	2.43821000
H	2.73481400	4.42477600	1.66944800
H	7.21398000	-3.33430700	-1.42957400
H	-1.22653600	6.96100400	3.92079200
O	-2.09427400	5.47844200	5.22880300
C	6.87298900	-0.21659700	-2.98164400
H	7.26121600	-0.52407400	-3.96770500
H	4.59740200	2.47589300	1.32048200
C	7.37250100	-1.18635900	-1.88088200
C	6.81927900	-0.73414500	-0.51390900
C	5.74980400	0.10143600	1.96734800
C	-3.62129400	3.01461800	5.70207900
H	5.30652800	0.41056600	2.91691500
H	-3.86463800	2.07736300	6.22795700
H	7.21512500	0.81339400	-2.78755200
H	-3.87356700	3.86024600	6.35950500
C	7.64706700	-0.41372600	0.57294000
H	-4.26127100	3.08029200	4.80749600
C	7.14146300	-0.00106000	1.82589200
C	8.91395400	-1.20295500	-1.91833400
H	9.25699100	-1.51963400	-2.91681300
H	9.33930600	-1.91106600	-1.18800800
H	6.72254600	-0.05753000	4.64529200
H	8.73007800	-0.48876000	0.45049900
H	9.34443700	-0.20638000	-1.72465900
H	8.32737800	-1.78475200	3.60355000
C	7.38872300	0.73612500	4.26874500
H	6.78904600	1.65051200	4.12754200
C	8.11902000	0.31495800	2.97719900
C	8.96730000	-0.94285100	3.29252000
H	9.55504500	-1.27374900	2.42183600
H	8.12578200	0.94802000	5.06036700
C	9.05722000	1.47307500	2.55350400
H	8.48360000	2.38834900	2.33329100

H	9.64330500	1.22210500	1.65538500
H	9.67561500	-0.73329100	4.11210100
H	9.77050900	1.70570900	3.36246500
H	-0.97597600	-4.51066700	-8.15606100
H	-2.23357800	-6.09180700	-6.68102300
C	-0.92427300	-4.40744700	-7.06759100
C	-1.62949300	-5.29182000	-6.24206100
C	-0.15847100	-3.38011200	-6.50056700
H	0.38305400	-2.68499500	-7.15281200
C	-1.55972700	-5.14345300	-4.84957900
H	-2.11012300	-5.82921200	-4.19783800
C	-0.07222500	-3.23085500	-5.10501300
C	-0.78511400	-4.12358300	-4.28318600
H	1.74176400	-2.51661600	-4.12996900
C	0.79114700	-2.12042700	-4.52392300
H	1.06752200	-1.41873800	-5.33237300
H	-0.73762100	-4.01142900	-3.19539800
H	2.22548700	4.39084500	-6.95791600
C	1.36408500	4.56782500	-6.30557800
H	0.74101600	6.36698600	-7.34671100
C	0.53377800	5.67639800	-6.52356600
C	1.09737000	3.68647600	-5.25142200
H	1.75671900	2.82602800	-5.08862100
C	-0.55712300	5.89807000	-5.67400800
N	0.17750000	-1.33429700	-3.43615400
C	-0.00717500	3.88653300	-4.39888700
C	-0.82424300	5.00841500	-4.62360700
H	-1.89603800	-1.61943600	-2.95396600
H	-1.51912500	1.74569800	-4.76477000
O	2.18134000	-1.82544300	-1.91200600
H	-1.20600400	6.76586300	-5.82913100
N	0.34310400	-0.11842100	-1.14863500
C	-0.34906100	2.86716100	-3.32777100
S	0.71364000	-1.64244400	-1.83318900

H	-1.68522300	5.18501500	-3.96928200
C	-0.77374600	1.52728800	-3.96865600
C	-1.24316400	-0.93375100	-3.52377100
H	-1.15615600	3.25082500	-2.68027300
C	-1.36767900	0.49490900	-3.04686800
H	-2.31552200	0.76213400	-2.55973000
H	0.51999500	2.67437800	-2.67270300
H	0.09667500	1.08587900	-4.48403300
H	-1.53051400	-1.03056900	-4.58759100
O	-0.05269100	-2.78876900	-1.25055900
H	-0.48885500	0.35064500	-1.87757700

Intermediate $D^5_{3.1a}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.604751 Hartree

H_corr: 1.894143 Hartree

SCF: -6389.954958 Hartree

S: 609.076 Cal/Mol-Kelvin

H: -6388.060815 Hartree

G: -6388.350207 Hartree

Cartesian Coordinates:

H	-9.10424200	-0.06520600	-2.58997600
H	-9.10387800	-1.02884600	-1.09624400
C	-8.45215100	-0.54120700	-1.83820100
H	-7.86891400	-1.32683400	-2.34476900
H	-9.03264800	-2.72146600	2.13262600
H	-9.02809400	2.10255300	-1.24618500
C	-8.65531000	-2.23803800	3.04886100
H	-9.06923900	-2.79400500	3.90570900
H	-9.02157900	1.18883800	0.28078100
C	-8.37555100	1.60624400	-0.50788000
H	-8.30476800	-0.90762400	0.98486400

C	-7.51753000	0.51313300	-1.19412600
H	-6.93979700	-4.22491300	2.16309500
H	-9.06510500	-1.21550500	3.09416200
H	-7.38132400	1.63429700	-3.05485300
C	-7.21453100	-0.86006600	0.93747500
C	-6.69936200	1.17518600	-2.32074500
C	-6.64179000	-3.72483900	3.09926900
H	-7.08890300	-4.28331400	3.93898500
H	-6.07647600	0.44401800	-2.86119200
C	-6.61962300	-0.16230000	-0.13651100
C	-7.11476600	-2.24949600	3.11857400
H	-7.73911000	2.37832000	-0.04505900
C	-6.46534300	-1.48943900	1.94324500
H	1.25523700	-5.18505400	-6.49092000
H	-0.09695300	-4.26782200	-5.78672700
H	-5.54737100	-3.80909000	3.19046200
C	0.98354600	-4.23614300	-6.00360500
H	-6.04471400	1.97642400	-1.93988100
C	-5.21814700	-0.10130500	-0.18297300
C	-6.68758600	-1.59135200	4.45479900
H	-7.14064900	-2.12451500	5.30774900
H	-3.81455200	-3.24424500	0.17455000
H	1.16380700	-3.41360100	-6.71494200
C	-5.06044700	-1.40385900	1.85998100
O	1.77924400	-6.38814500	-4.18137400
H	-7.01265600	-0.53907900	4.50047500
H	-4.71036700	0.41756100	-0.99881200
H	-1.74204100	-4.97848000	-0.14184000
H	1.34357000	-7.59062700	-2.50075800
C	-4.43220700	-0.71573500	0.81228800
C	-2.74737000	-3.03882300	0.22048300
H	1.10978100	-9.06361600	-0.50377700
C	1.18215500	-7.16713600	-1.51200900
C	1.61071200	-5.23506500	-3.78686600

C	1.05284600	-7.97731000	-0.38285500
C	-1.70892700	-3.91098800	0.06674900
C	1.81768700	-4.03604400	-4.72585200
H	-4.43411400	-1.86616800	2.62890500
H	-5.59518300	-1.61037800	4.59399700
H	3.67850900	-4.85694300	-5.52669700
C	1.11132200	-5.76401500	-1.37531300
N	1.25290900	-4.89687300	-2.48261300
C	0.85816900	-7.44863000	0.89495200
C	3.32057500	-3.92700300	-5.05728800
C	-2.93586100	-0.60951100	0.78564800
C	-2.17319400	-1.74309300	0.49287200
H	0.76603500	-8.08305700	1.77451300
H	1.50436800	-3.10681700	-4.22209700
H	3.49958700	-3.09274300	-5.75495200
C	0.89599900	-5.19734100	-0.08842600
H	1.13976200	-3.89523700	-2.29955400
C	0.78165500	-6.05209000	1.04320700
C	-0.49542600	-3.14713600	0.22065200
H	-4.19209100	1.79269300	1.64408300
H	3.43584600	5.39023600	-2.55994300
N	-0.78219600	-1.81346800	0.48922100
O	0.42688200	-7.23424700	3.76068900
C	0.78107700	-3.71255600	0.10517800
C	-2.34810600	0.60481300	1.15969700
H	3.41535200	6.77550700	-1.43404900
C	-3.10586100	1.74666800	1.61055600
H	3.92236800	-3.74442200	-4.15238500
N	0.60475200	-5.43951800	2.30595500
C	3.04438600	5.75079500	-1.59519300
C	0.44997800	-6.02242100	3.55435500
H	3.45655000	5.10634100	-0.80199200
H	2.46791000	-4.94233500	5.14826400
H	0.60142800	-4.42072800	2.28892300

H	1.34916000	6.26879200	-3.71358700
H	0.30839000	-3.97842500	4.30589600
H	1.21373200	7.65300200	-2.59042300
N	-0.98096700	0.84938800	1.26789000
C	0.31225600	-5.00991700	4.70798100
C	-2.20494900	2.69400500	2.00534700
C	1.94203800	-2.93653000	0.15250800
C	0.93930500	6.59876100	-2.74540500
C	1.51593100	-5.16398700	5.65758800
Co	0.49505400	-0.31857900	0.64823800
C	1.49960700	5.73726800	-1.60435800
C	-0.89201000	2.13783900	1.79221100
H	-2.39560700	3.68160000	2.42084900
H	3.47859600	-4.52369900	-0.25826400
C	3.25957200	-3.46927200	-0.10237800
N	1.99619900	-1.56584100	0.36532400
H	1.56649800	-6.19611500	6.03713700
H	1.16453300	4.69141300	-1.74329400
H	1.42292100	-4.48140600	6.51800300
C	0.99941200	6.26455700	-0.24761100
H	-0.15912400	6.54378400	-2.80161300
C	-1.01687300	-5.25824000	5.44400800
H	-1.88388400	-5.09639400	4.78306300
H	0.75596100	4.30628700	0.31322100
N	0.64433500	5.26126400	0.65209400
O	0.96279400	7.46432000	0.01175900
C	0.29090000	2.82301000	2.10985800
C	4.11518700	-2.40810800	-0.12006900
C	3.33131500	-1.23226600	0.18076500
H	-1.05720000	-6.29667000	5.80659900
N	1.80940200	1.06709700	1.22369900
H	-1.11547500	-4.58258700	6.30923800
C	0.33965200	5.37071600	2.02776100
H	1.61837400	1.28011600	7.25835600

C	1.55605600	2.29876500	1.81759400
C	0.18548400	4.16923200	2.77194600
H	5.19083900	-2.40708300	-0.28196700
C	0.19469200	6.61950400	2.66389800
C	3.17082000	1.07857500	0.95400000
C	3.90057900	0.02553500	0.39353500
C	0.61624000	1.08059200	7.67154600
H	0.31037300	7.52809700	2.07625200
H	-0.04548900	2.19302800	4.31527100
C	-0.08342800	4.24681800	4.16635600
H	0.59282300	0.03468100	8.01813700
N	-0.19252800	3.03057600	4.87682700
H	6.01709500	-0.68623100	-3.82048000
H	0.47105500	1.73841600	8.54212000
H	4.99136400	0.36357000	-2.03289900
C	-0.08413600	6.65860800	4.03177900
C	2.77970200	3.04741400	1.98648900
C	-0.22066500	5.49808400	4.79662700
C	3.77322700	2.30799300	1.41303000
C	-0.49045600	1.33265100	6.62989500
C	-0.46767700	2.81730000	6.22042400
H	-0.29728900	0.69491300	5.74590500
C	7.10302200	-0.50964600	-3.86354500
C	5.75665300	0.37903400	-1.25123400
C	5.35296600	0.22114600	0.08065700
H	5.70066400	1.88843600	-3.59450700
H	7.37922300	-0.39549300	-4.92552500
H	-0.19400200	7.63119100	4.52133900
H	2.84658900	4.02367100	2.46289900
H	7.60604400	-1.41146100	-3.47746700
H	-0.42899500	5.53392400	5.86432800
O	-0.67641600	3.71151700	7.03738000
C	6.79615200	1.98958000	-3.64067800
H	7.07227600	2.13351900	-4.69907800

H	4.82966500	2.55044000	1.32167100
C	7.51957600	0.74814000	-3.06028000
C	7.11527200	0.56633700	-1.58271800
C	6.31530800	0.23851300	1.11019700
C	-1.88093400	0.98573600	7.19379500
H	5.97703700	0.09944500	2.13968500
H	-1.90926600	-0.05950900	7.54208900
H	7.07319900	2.90339600	-3.08974800
H	-2.11640700	1.64247700	8.04515400
C	8.04606400	0.57812400	-0.53265900
H	-2.67087400	1.11473000	6.43623000
C	7.67647300	0.41338600	0.82081900
C	9.03823900	0.95066600	-3.23552600
H	9.27376900	1.07730900	-4.30472100
H	9.61720800	0.08461100	-2.87422600
H	7.65674200	-0.73527800	3.43172100
H	9.10356600	0.71825000	-0.76798700
H	9.39992500	1.85126600	-2.71209300
H	9.27457200	-1.69969600	1.67275900
C	8.17492400	0.23236700	3.32871300
H	7.46590400	1.03293800	3.59704700
C	8.76286300	0.42720100	1.91626500
C	9.77394000	-0.71720800	1.65306600
H	10.26966900	-0.61357900	0.67498700
H	8.98608900	0.25028900	4.07466500
C	9.50725700	1.78594200	1.88668200
H	8.81472300	2.62228500	2.07681000
H	9.99418500	1.96947700	0.91595400
H	10.56081100	-0.72024400	2.42641400
H	10.29144600	1.81140800	2.66232700
H	-5.27591400	-1.71679000	-6.94440800
H	-6.67777800	-2.73686600	-5.14283000
C	-4.85493200	-1.88425400	-5.94807400
C	-5.64061900	-2.45343400	-4.93861100

C	-3.52355500	-1.53233900	-5.68507000
H	-2.90869500	-1.09493600	-6.47963000
C	-5.08938400	-2.66362800	-3.66517600
H	-5.69598400	-3.11541000	-2.87404400
C	-2.96061300	-1.74656500	-4.41485800
C	-3.76042000	-2.31187400	-3.40462000
H	-0.97237800	-2.34475800	-3.85518400
C	-1.50200600	-1.42871800	-4.15377700
H	-1.02701900	-1.05674500	-5.08436200
H	-3.32745800	-2.47841100	-2.41366400
H	-2.54786100	7.61726000	-5.95010700
C	-2.74746600	7.26628900	-4.93265700
H	-2.81854500	9.26166900	-4.08567000
C	-2.90121400	8.18845700	-3.88906900
C	-2.85159600	5.89282400	-4.67788300
H	-2.73333100	5.17791300	-5.50031100
C	-3.16184000	7.72809400	-2.59124400
N	-1.33171700	-0.45303900	-3.03651600
C	-3.11513100	5.41644100	-3.38034500
C	-3.26774700	6.35431600	-2.34162200
H	-2.83623000	0.71630300	-3.82868000
H	-1.05509700	3.56811100	-3.39745500
O	1.08112100	0.45689800	-3.57730500
H	-3.28173500	8.44093300	-1.76969100
N	0.49716300	0.39370300	-1.12209600
C	-3.18679900	3.93195600	-3.09816200
S	0.38364800	-0.37833200	-2.56614100
H	-3.47629600	6.00347000	-1.32442600
C	-1.80740700	3.35062800	-2.61804900
C	-1.80751400	0.89229800	-3.44363200
H	-3.50699000	3.38950600	-4.00392400
C	-1.85864500	1.88746300	-2.33449600
H	-2.28166700	1.54631400	-1.38215600
H	-3.94187600	3.72696200	-2.31997000

H	-1.51166700	3.91178200	-1.71389800
H	-1.21660400	1.28619300	-4.29747700
O	0.79453200	-1.78872500	-2.39898500
H	0.02272200	1.30898400	-1.20007700

Transition State $TS2^{6}_{3.1a}$ (1,6-HAA)

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -1442.26 cm-1

G_corr: 1.602514 Hartree

H_corr: 1.889422 Hartree

SCF: -6389.939544 Hartree

S: 603.848 Cal/Mol-Kelvin

H: -6388.050122 Hartree

G: -6388.337030 Hartree

Cartesian Coordinates:

H	8.14382500	1.59103500	-4.76225400
H	8.61153300	1.99072500	-3.09339000
C	7.75829600	1.72550700	-3.73736800
H	7.06563500	2.58289800	-3.74523000
H	9.63922200	2.32612400	0.40693200
H	8.44007700	-0.90212900	-4.29014700
C	9.48660900	1.55340800	1.17836800
H	10.15518300	1.79625400	2.02014600
H	8.91556400	-0.55624500	-2.61198600
C	8.05200300	-0.74138800	-3.27004700
H	8.49668200	1.00959500	-1.02910900
C	7.04547600	0.43647800	-3.25547200
H	7.73621200	3.68207500	1.49574500
H	9.81657300	0.58479000	0.76775100
H	6.33628600	-0.03025900	-5.25984000
C	7.43444700	0.94491400	-0.78301200

C	5.91406000	0.11304300	-4.25196800
C	7.67257600	2.89473500	2.26448500
H	8.37190100	3.15525400	3.07693500
H	5.17574100	0.92890800	-4.31985100
C	6.52197400	0.64994900	-1.81967800
C	8.02647200	1.50703300	1.67251000
H	7.57234600	-1.67675900	-2.93850300
C	7.03207700	1.16569000	0.54307100
H	-0.60946000	4.20991000	-7.15041300
H	0.60787900	3.39855100	-6.13307100
H	6.65407500	2.91797800	2.68304400
C	-0.42883900	3.33789300	-6.50321900
H	5.38187400	-0.81523800	-3.98599200
C	5.16018600	0.57402400	-1.49074300
C	7.92801400	0.43403500	2.78591500
H	8.62781800	0.66590900	3.60648600
H	3.99029300	3.12934700	-1.19442700
H	-0.51812200	2.42605700	-7.11721100
C	5.65458300	1.07853200	0.83111100
O	-1.51725800	5.71735300	-5.14694100
H	8.18158000	-0.56594500	2.39709900
H	4.41403500	0.35524700	-2.25806200
H	1.90439100	4.86040300	-1.41210200
H	-1.30448800	7.16297800	-3.62913200
C	4.71662600	0.78302400	-0.16843100
C	2.94853700	2.96928400	-0.92569200
H	-1.07642300	8.92600200	-1.88175700
C	-1.09892900	6.89859000	-2.59429100
C	-1.35221800	4.64104300	-4.57230200
C	-0.96834500	7.87295000	-1.60348700
C	1.90504500	3.84236700	-1.02752200
C	-1.44338800	3.31418600	-5.34484800
H	5.29271900	1.26310200	1.84692900
H	6.91687500	0.37955200	3.21940600

H	-3.16450600	4.00279300	-6.49816400
C	-0.96250600	5.53537300	-2.25349500
N	-1.08490600	4.50584400	-3.21401000
C	-0.70583400	7.54968000	-0.27064900
C	-2.88333800	3.14413500	-5.86854400
C	3.25325100	0.72966300	0.15046300
C	2.43352700	1.76773400	-0.30947300
H	-0.60591800	8.31209100	0.49956600
H	-1.20402100	2.47612000	-4.66993400
H	-2.97059300	2.22706000	-6.47464300
C	-0.69258100	5.17657500	-0.90440600
H	-0.96516300	3.54330100	-2.87795400
C	-0.56821700	6.19446200	0.08060100
C	0.74107100	3.16491600	-0.51194600
H	4.67562100	-1.30595300	1.57022200
H	-3.08568000	-5.96178600	-0.49087700
N	1.07025000	1.89243500	-0.06598400
O	-0.19070500	7.78284600	2.57647100
C	-0.53498200	3.74049000	-0.49219700
C	2.76125500	-0.27787000	0.99122700
H	-3.03779300	-6.83018700	1.06653500
C	3.59641000	-1.22993800	1.68222200
H	-3.60865600	3.07228800	-5.04210200
N	-0.30771500	5.78491200	1.40915400
C	-2.62968600	-5.96983700	0.51248500
C	-0.14145200	6.55448000	2.54997700
H	-2.93937000	-5.04813300	1.03050300
H	-2.00567500	5.64599200	4.41610000
H	-0.24007200	4.77631000	1.53864700
H	-1.13957800	-7.35841700	-1.36369900
H	0.14634600	4.65666800	3.58836900
H	-0.99549400	-8.24218000	0.18341200
N	1.42529300	-0.45983000	1.34020800
C	0.11364000	5.73640900	3.83048200

C	2.77750700	-1.97408400	2.48406800
C	-1.67006800	3.00922700	-0.13169700
C	-0.67566900	-7.34315000	-0.36392000
C	-1.03876600	5.98491900	4.82227700
Co	-0.14823900	0.49312000	0.59294100
C	-1.09272200	-6.08309200	0.40813100
C	1.43206600	-1.51178600	2.25408600
H	3.04543300	-2.78327100	3.16067800
H	-3.26242800	4.53430500	-0.54983400
C	-3.01401700	3.51556900	-0.25874800
N	-1.68467700	1.68621100	0.30039600
H	-1.12104400	7.06059600	5.04125800
H	-0.71287700	-5.18798200	-0.12161400
H	-0.86059200	5.44975500	5.76917000
C	-0.50299900	-6.12494200	1.83038500
H	0.41722500	-7.40061200	-0.48783300
C	1.46966700	6.14998200	4.43147700
H	2.30386800	5.92354300	3.74760000
H	-0.19988400	-4.10182100	1.66541700
N	-0.06845800	-4.88978300	2.29959600
O	-0.46730000	-7.16439000	2.48379000
C	0.30614200	-2.09692100	2.85622400
C	-3.85525400	2.47966000	0.02747400
C	-3.02992500	1.35158700	0.38358900
H	1.47815600	7.23273500	4.62925000
N	-1.35139900	-0.69683700	1.64617000
H	1.65299800	5.62123800	5.38099900
C	0.34797900	-4.53881800	3.60482800
H	-0.61196200	1.01378700	7.37856900
C	-1.00045800	-1.72434400	2.51037700
C	0.51943600	-3.15903800	3.90021500
H	-4.94284700	2.47308100	0.03339400
C	0.58807100	-5.51194600	4.59465700
C	-2.73075200	-0.78458100	1.52162200

C	-3.54669700	0.14598000	0.86895100
C	0.41864100	1.33855400	7.59566400
H	0.45422200	-6.56295200	4.34716100
H	0.79973200	-0.78638900	4.70511200
C	0.90655000	-2.77880200	5.21580700
H	0.43661400	2.44040400	7.59161900
N	1.02987300	-1.39775300	5.48722600
H	-6.10118300	0.53065100	-3.09932300
H	0.67801800	0.99060500	8.60724600
H	-4.87506100	-0.36529200	-1.37396300
C	0.98160800	-5.10315900	5.87036900
C	-2.17576800	-2.43557400	2.95834500
C	1.14066800	-3.75624700	6.20145600
C	-3.24098500	-1.88677300	2.30339000
C	1.42150000	0.77446700	6.57146600
C	1.41820800	-0.76311400	6.65870400
H	1.11305300	1.09568900	5.55809200
C	-7.18258200	0.33843700	-3.02381900
C	-5.55832300	-0.34688300	-0.52017100
C	-5.01779300	-0.09693000	0.74865800
H	-5.72043000	-2.01893500	-2.73432700
H	-7.56067200	0.14679900	-4.04257600
H	1.16697600	-5.86283200	6.63592500
H	-2.16849900	-3.25797300	3.67115000
H	-7.66248600	1.25879500	-2.65211300
H	1.43926300	-3.44081400	7.19941000
O	1.73703400	-1.34605900	7.69291600
C	-6.81299000	-2.13589500	-2.66470800
H	-7.19179400	-2.35527700	-3.67759200
H	-4.28948400	-2.16938400	2.36524100
C	-7.49390000	-0.86446700	-2.09802000
C	-6.93956200	-0.57797500	-0.68732800
C	-5.86387200	-0.05799600	1.87580200
C	2.84750200	1.29070200	6.84019400

H	-5.42274200	0.16383000	2.85035000
H	2.87061600	2.39243500	6.83171800
H	-7.01781400	-3.01222100	-2.02775300
H	3.19426700	0.94297100	7.82530500
C	-7.75268900	-0.53415400	0.45569200
H	3.56047800	0.92855200	6.08178400
C	-7.24406000	-0.27081900	1.74724200
C	-9.01874500	-1.09307100	-2.09900900
H	-9.36310000	-1.29277600	-3.12684300
H	-9.57076400	-0.21053200	-1.73539800
H	-6.97152700	1.06075900	4.25639900
H	-8.82616100	-0.70536300	0.34620200
H	-9.30873900	-1.96014800	-1.48251700
H	-8.78224800	1.87844500	2.61675700
C	-7.47754900	0.08146600	4.27584800
H	-6.72733300	-0.68856000	4.52052800
C	-8.20789600	-0.21963900	2.95123600
C	-9.26262600	0.89169100	2.71970200
H	-9.85761700	0.71315600	1.81019200
H	-8.20425300	0.10498000	5.10421400
C	-8.92554900	-1.58530400	3.09575000
H	-8.20123800	-2.39793400	3.26979500
H	-9.50737000	-1.84338200	2.19686600
H	-9.96250700	0.94124000	3.57122000
H	-9.62399700	-1.56428000	3.94961800
H	-1.73788700	-5.84802800	-4.44249400
H	-0.73114800	-6.18458500	-6.70484400
C	-1.41198500	-4.98412200	-5.03028200
C	-0.85140900	-5.17395900	-6.30278500
C	-1.56759000	-3.69254500	-4.51608000
H	-2.01287100	-3.54331900	-3.52672200
C	-0.45363500	-4.06468900	-7.05772600
H	-0.01983800	-4.20389400	-8.05282500
C	-1.16980200	-2.57010900	-5.26658700

C	-0.61445600	-2.77085700	-6.54054700
H	-1.20892600	-0.42369200	-5.51779200
C	-1.36310200	-1.17021300	-4.71373000
H	-2.38983000	-1.04621700	-4.33980800
H	-0.31225900	-1.90450100	-7.13997500
H	2.49100000	-7.35410100	-2.97892200
C	3.03645800	-6.46817300	-2.63883000
H	4.98050200	-7.25183700	-3.19980000
C	4.43182000	-6.41160400	-2.76344000
C	2.33557900	-5.39410300	-2.07828100
H	1.24536300	-5.44881300	-1.99124800
C	5.11740700	-5.27277300	-2.32359200
N	-0.45769500	-0.89302500	-3.58011200
C	3.01307800	-4.24495100	-1.62841200
C	4.41166100	-4.19807200	-1.76483900
H	1.34379700	0.17982700	-3.40725500
H	0.31437500	-2.99839300	-2.07978600
O	-2.50797500	-0.04942500	-2.31498600
H	6.20727700	-5.21975000	-2.41197400
N	-0.33911400	-0.56870200	-0.97763000
C	2.25106900	-3.07124200	-1.01253400
S	-1.03793500	0.14299800	-2.35097800
H	4.95565400	-3.31338200	-1.41608500
C	1.26287400	-2.45002100	-1.97603400
C	0.98228600	-0.75943700	-3.85603900
H	2.98777400	-2.31691000	-0.68936700
C	1.78919200	-1.95403300	-3.30125300
H	1.74874700	-2.78698700	-4.02942600
H	1.73110300	-3.40631600	-0.09800900
H	0.54571300	-1.34566900	-1.33529300
H	1.12817900	-0.66181300	-4.94478100
O	-0.55906800	1.53250700	-2.62241700
H	2.85161200	-1.66291400	-3.22007000

Intermediate $D^6_{3.1a}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.603274 Hartree

H_corr: 1.894338 Hartree

SCF: -6389.954643 Hartree

S: 612.595 Cal/Mol-Kelvin

H: -6388.060306 Hartree

G: -6388.351369 Hartree

Cartesian Coordinates:

H	8.11626300	2.25541600	-4.28863200
H	8.41062200	2.84658200	-2.63741000
C	7.64141200	2.43390000	-3.30902900
H	6.86568700	3.20531000	-3.44372200
H	9.10169800	3.63123100	0.86074000
H	8.64507300	-0.13027600	-3.55992100
C	8.97041400	2.92545900	1.69747800
H	9.53745000	3.32547300	2.55363100
H	8.93378600	0.39811200	-1.88663000
C	8.15515600	0.06525100	-2.59104100
H	8.22841700	2.05989000	-0.50552500
C	7.03225100	1.11942100	-2.75811800
H	6.98073800	4.85798100	1.66006000
H	9.43552800	1.96593200	1.41698300
H	6.53854400	0.40658600	-4.75468100
C	7.16331400	1.89495900	-0.32821000
C	6.02448700	0.58748700	-3.79682600
C	6.93912800	4.14825400	2.50235700
H	7.53689500	4.56676100	3.32970100
H	5.21133400	1.30573500	-3.99205000
C	6.37537900	1.39781600	-1.38978500
C	7.48821200	2.75924900	2.08937100
H	7.75037500	-0.88994900	-2.21876500

C	6.63277600	2.19484600	0.93574800
H	-0.04247100	2.38577600	-7.92654400
H	1.12353000	2.10058500	-6.60976500
H	5.89306800	4.09463000	2.84289800
C	0.18420100	1.74254100	-7.06241400
H	5.57446900	-0.36879600	-3.48262200
C	5.00866000	1.19283000	-1.14964000
C	7.41477500	1.79748100	3.30194000
H	8.01707900	2.18800000	4.13951100
H	3.54722600	3.53961700	-1.32706100
H	0.35306600	0.71599400	-7.42831500
C	5.25411600	1.97696700	1.13428400
O	-1.48853900	4.09286400	-6.48274900
H	7.80429300	0.79958900	3.04130900
H	4.35656200	0.81327300	-1.93959100
H	1.29649300	4.81179100	-2.16713200
H	-1.73463900	5.86525500	-5.37433500
C	4.43766700	1.47670500	0.10925200
C	2.51016500	3.26010600	-1.15664000
H	-2.12066200	7.98521000	-4.12240400
C	-1.69278700	5.88576000	-4.28771100
C	-1.24295600	3.23131800	-5.63848700
C	-1.90809200	7.06393000	-3.57099400
C	1.38185300	3.90529600	-1.57113900
C	-0.97858800	1.77444500	-6.05337900
H	4.79270000	2.22140100	2.09549000
H	6.38344300	1.67098400	3.66764800
H	-2.59318400	1.80900800	-7.52367600
C	-1.41672300	4.68785700	-3.59347000
N	-1.19104100	3.46576500	-4.26754400
C	-1.86218500	7.10647900	-2.17606000
C	-2.26765800	1.19469400	-6.66955900
C	2.96773400	1.29260900	0.32688300
C	2.08289100	2.12512300	-0.37223200

H	-2.03144100	8.02684400	-1.62037200
H	-0.70554500	1.17959300	-5.16669500
H	-2.09743100	0.16592500	-7.02827400
C	-1.36178100	4.70172400	-2.17282800
H	-0.96803000	2.65121900	-3.68528500
C	-1.58888800	5.91887100	-1.47350400
C	0.26033700	3.14857200	-1.07362600
H	4.45904900	-0.35134100	2.14332700
H	-1.61254100	-6.62790700	0.49919500
N	0.69323400	2.07224300	-0.30856300
O	-1.94713200	8.07038200	0.56086600
C	-1.06912100	3.45533100	-1.38690700
C	2.51138400	0.38477600	1.29320700
H	-1.57554600	-7.19830600	2.18996100
C	3.37273500	-0.34488200	2.19168000
H	-3.08897500	1.16410700	-5.93549300
N	-1.53055300	5.87769000	-0.06087400
C	-1.40276200	-6.32716800	1.53864400
C	-1.70706500	6.90145000	0.85712600
H	-2.12595000	-5.54318100	1.81513700
H	-3.73530400	6.08858000	2.59150700
H	-1.33682500	4.95734700	0.33135400
H	0.84595900	-7.25377300	0.21680000
H	-1.33801900	5.37900200	2.37657300
H	0.98254800	-7.79015600	1.91671500
N	1.17268900	0.15383900	1.60811700
C	-1.58195200	6.45776200	2.32737300
C	2.56519900	-0.97695800	3.09488100
C	-2.12944700	2.62400000	-1.01518100
C	1.05511900	-6.92085900	1.24619400
C	-2.92837500	6.69160400	3.03870800
Co	-0.41094800	0.69782600	0.55380700
C	0.05433600	-5.83820700	1.68075600
C	1.20513900	-0.68980800	2.71344900

H	2.85064900	-1.60552400	3.93635500
H	-3.82475400	3.66664700	-2.05282000
C	-3.48811200	2.82089200	-1.45646900
N	-2.02805300	1.47585400	-0.23476300
H	-3.21495100	7.75173600	2.96256400
H	0.18948800	-4.94434100	1.04223300
H	-2.85642100	6.42652000	4.10609100
C	0.30558500	-5.46910800	3.15400900
H	2.09348000	-6.55451800	1.27991200
C	-0.44722800	7.25250400	2.99952700
H	0.52821700	7.04557400	2.52991800
H	0.17393400	-3.49735900	2.59680100
N	0.32566900	-4.10273600	3.40348900
O	0.44470600	-6.33272700	4.01723300
C	0.09221800	-1.25134700	3.35836000
C	-4.21023500	1.75810300	-0.99729600
C	-3.30713600	0.93315600	-0.23214500
H	-0.64265200	8.33223700	2.91287200
N	-1.57099300	-0.41158300	1.71364500
H	-0.37260500	6.99695700	4.06905300
C	0.43205700	-3.43004900	4.64178400
H	-2.01338600	2.52329700	6.87030000
C	-1.20261000	-1.14628000	2.83450300
C	0.31126700	-2.01499800	4.63568000
H	-5.27041600	1.55379700	-1.12819500
C	0.65429100	-4.11721000	5.85152000
C	-2.89576100	-0.75426900	1.48084000
C	-3.72278900	-0.17562400	0.51146200
C	-1.08959800	3.06450900	7.13192800
H	0.74520900	-5.20141400	5.83568400
H	0.08549000	0.47946800	4.88996400
C	0.40814400	-1.30580200	5.86419900
H	-1.23086400	4.12590800	6.87134100
N	0.26672300	0.09906500	5.81788000

H	-5.66022200	-1.25975300	-3.67475800
H	-0.94968900	2.98975700	8.22115800
H	-4.60060800	-1.46271800	-1.64242100
C	0.74869000	-3.38884200	7.03929200
C	-2.32197700	-1.91076500	3.33377300
C	0.62861900	-1.99792100	7.07016100
C	-3.35454800	-1.70813200	2.46405300
C	0.13656500	2.48407200	6.40262500
C	0.34440800	1.02472900	6.84877000
H	-0.04763400	2.52255300	5.31174900
C	-6.70152800	-1.61735900	-3.66926500
C	-5.40307600	-1.35183200	-0.90749600
C	-5.10753100	-0.69854200	0.29693300
H	-4.97817100	-3.52756300	-2.58738700
H	-6.88691000	-2.12216200	-4.63272900
H	0.92121000	-3.92637400	7.97678500
H	-2.29458600	-2.54118900	4.22060600
H	-7.35980800	-0.73446000	-3.61746200
H	0.70036200	-1.43506200	7.99894700
O	0.56002300	0.73891300	8.02465700
C	-6.04052600	-3.81577900	-2.61101700
H	-6.22241800	-4.34554400	-3.56164600
H	-4.35263300	-2.13959900	2.48993100
C	-6.97588900	-2.58617000	-2.49143600
C	-6.69388100	-1.86094100	-1.15956700
C	-6.11535200	-0.53075200	1.26833000
C	1.41002300	3.29192100	6.71656200
H	-5.86750000	0.00336400	2.18852600
H	1.27347200	4.35257700	6.45050500
H	-6.21396000	-4.52712500	-1.78676900
H	1.63986200	3.22962100	7.79124500
C	-7.67241800	-1.67838200	-0.17023600
H	2.28148900	2.91024600	6.16008400
C	-7.41370800	-1.01343900	1.04916100

C	-8.43353300	-3.07728900	-2.59996000
H	-8.58194400	-3.58698300	-3.56590900
H	-9.15612600	-2.24560900	-2.55527900
H	-7.72485900	0.92487300	3.12120500
H	-8.67999200	-2.06126400	-0.34838700
H	-8.68827600	-3.79949200	-1.80657800
H	-9.35553500	0.97706300	1.12728700
C	-8.08367200	-0.09300700	3.34626300
H	-7.27899700	-0.63305700	3.87209400
C	-8.54989800	-0.83694500	2.07814300
C	-9.70201900	-0.02216400	1.43798000
H	-10.11744800	-0.52311600	0.54941200
H	-8.92589900	0.00529500	4.05039400
C	-9.08115000	-2.22889400	2.50381800
H	-8.28488700	-2.83221900	2.96988200
H	-9.47563100	-2.79999100	1.64863900
H	-10.52541400	0.11256200	2.15994000
H	-9.89847500	-2.12064500	3.23700500
H	-0.20270800	-6.85890700	-2.11089600
H	0.73989700	-7.87395000	-4.19022500
C	-0.02003100	-6.23319700	-2.99009900
C	0.50505600	-6.80560300	-4.15899500
C	-0.32467000	-4.86827100	-2.94808100
H	-0.73876600	-4.42195600	-2.03816700
C	0.72028600	-6.00396000	-5.28596900
H	1.12816000	-6.44138400	-6.20250100
C	-0.11149000	-4.05472000	-4.07591300
C	0.41206200	-4.63660300	-5.24194900
H	-0.34481100	-2.14647600	-5.05754500
C	-0.49533900	-2.58644300	-4.05120400
H	-1.56321300	-2.48704400	-3.80738200
H	0.57756400	-4.01352400	-6.12822200
H	4.75155400	-7.30041500	-2.19176600
C	5.15322300	-6.34622500	-1.83606200

H	7.22481800	-6.95929900	-2.03797800
C	6.53910700	-6.15641800	-1.75011000
C	4.27572500	-5.31812100	-1.46926400
H	3.19407000	-5.47298500	-1.54467400
C	7.03970200	-4.92948000	-1.29597100
N	0.25210300	-1.79957800	-3.04581200
C	4.76619600	-4.08232400	-1.00931600
C	6.15877500	-3.90216800	-0.93266200
H	1.90571700	-0.49854100	-2.94483800
H	1.60068000	-3.00990400	-0.98310800
O	-2.06555600	-0.89977600	-2.36343800
H	8.12046500	-4.76880400	-1.22716800
N	-0.09902100	-0.71300800	-0.71513800
C	3.81340900	-2.96751300	-0.56566000
S	-0.64080700	-0.52110500	-2.30418400
H	6.55809400	-2.94567800	-0.57610200
C	2.58620100	-2.79994400	-1.40883500
C	1.65495900	-1.47906700	-3.37858100
H	4.39181500	-2.01977500	-0.55870500
C	2.65823900	-2.54438200	-2.87731800
H	2.48047100	-3.48249100	-3.44180100
H	3.52154800	-3.13778600	0.48613500
H	0.93034700	-0.81853700	-0.78067300
H	1.74927000	-1.36078800	-4.47547600
O	-0.24949800	0.77491800	-2.93429600
H	3.67429800	-2.21642300	-3.16584500

Product 2a[a](6-member ring)

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.285357 Hartree

H_corr: 0.3571 Hartree

SCF: -1318.181474 Hartree

S: 150.996 Cal/Mol-Kelvin

H: -1317.824374 Hartree

G: -1317.896117 Hartree

Cartesian Coordinates:

C	-1.15271000	-0.57035500	1.26260000
N	-1.38065100	0.38096600	0.14565200
S	-0.01105500	1.41018000	-0.07050000
N	1.10608900	0.16847800	-0.44546700
O	0.33412800	2.08582400	1.20405200
O	-0.20875900	2.20971300	-1.28562700
C	-2.62904700	1.17153400	0.28980100
C	-3.84297600	0.31507100	-0.01977400
H	-2.56842500	2.00421100	-0.43034200
H	-2.71682500	1.61393000	1.30223200
C	-4.93243400	0.27039100	0.86492100
C	-6.07127600	-0.48822900	0.55851100
C	-3.90558700	-0.42202100	-1.21670300
C	-5.03949600	-1.18249900	-1.52161800
C	-6.12692000	-1.21659300	-0.63566400
H	-7.01377800	-1.81105500	-0.87637700
H	-5.07820700	-1.74907000	-2.45744800
H	-4.89136500	0.83722700	1.80189900
H	-6.91337000	-0.51238900	1.25731300
H	-3.05271500	-0.39595400	-1.90157400
C	4.61828700	-0.64132100	1.06561900
C	3.78779200	-1.05175100	0.00485000
C	5.82005500	0.03164000	0.81804900
C	4.19614100	-0.76926100	-1.31261300
C	6.21361300	0.30892700	-0.49881900
H	6.45382100	0.33890200	1.65577200
C	5.39879300	-0.09342200	-1.56384300
H	3.56718200	-1.08997800	-2.15047800
H	7.15362400	0.83432200	-0.69275100

H	5.69980800	0.11446100	-2.59530100
C	2.46786200	-1.74585200	0.27836900
H	2.58803100	-2.47746500	1.09678300
H	2.14137100	-2.30763200	-0.61348700
C	1.33683400	-0.77482300	0.68422800
C	0.01669100	-1.51328700	0.95292600
H	-2.08405600	-1.15023700	1.36239000
H	-0.98942200	-0.02828100	2.21649000
H	0.15311300	-2.20163300	1.80490200
H	-0.23686500	-2.11830000	0.06565100
H	1.98141600	0.63615100	-0.72354600
H	1.64750100	-0.22179900	1.59396800
H	4.32128700	-0.85760600	2.09814900

Product 2a[b](5 member)

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.281936 Hartree

H_corr: 0.356885 Hartree

SCF: -1318.172045 Hartree

S: 157.743 Cal/Mol-Kelvin

H: -1317.81516 Hartree

G: -1317.890109 Hartree

Cartesian Coordinates:

C	0.59305400	0.03010700	-0.09677800
N	1.77390500	-0.84356000	-0.07910000
S	1.21925200	-2.49159400	0.12652700
N	-0.39933500	-2.16618200	-0.40485700
O	1.15670000	-2.90157700	1.54610500
O	1.94185500	-3.32548600	-0.83704000
C	2.86274800	-0.47696400	0.84653400
C	3.58296300	0.77162700	0.37052700
H	3.56830800	-1.32559000	0.87381700

H	2.48512500	-0.33849200	1.87944600
C	3.79113200	1.85324200	1.24095100
C	4.48591100	2.99265600	0.81053000
C	4.07385100	0.85016500	-0.94582700
C	4.76342900	1.98816900	-1.37770400
C	4.97297900	3.06259400	-0.50002300
H	5.51403100	3.95152100	-0.83881000
H	5.14380100	2.03658300	-2.40291800
H	3.40983000	1.80303400	2.26706700
H	4.64282600	3.82740700	1.50081900
H	3.90455900	0.01127800	-1.62803900
C	-4.19792100	1.85515400	0.39831800
C	-3.99526800	0.47037900	0.25851700
C	-5.46803000	2.41782500	0.21872200
C	-5.09944500	-0.33872600	-0.06545000
C	-6.55907100	1.60084100	-0.10515300
H	-5.60672700	3.49700400	0.33806400
C	-6.37109100	0.21951600	-0.24614100
H	-4.96299200	-1.42124600	-0.17050300
H	-7.55279200	2.03804700	-0.24215600
H	-7.21892800	-0.42750300	-0.49216400
C	-2.61089800	-0.13104900	0.41342600
H	-2.71197100	-1.13860700	0.85692700
H	-2.02906200	0.47022500	1.13290700
C	-1.86931800	-0.21092400	-0.94208300
C	-0.43888500	-0.76805500	-0.91910800
H	0.85905300	0.98092600	-0.58546300
H	0.22321900	0.24845300	0.92855900
H	-0.97139000	-2.25071400	0.44492600
H	-0.07169700	-0.80966500	-1.95908300
H	-1.82494500	0.79983300	-1.38551800
H	-2.46435400	-0.82232400	-1.64180000
H	-3.35120400	2.50070400	0.65911900

Intermediate $A_{3.1b}$

$A_{[Co(II)(\mathbf{P2})]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -0.6444 cm-1

G_corr: 1.303862 Hartree

H_corr: 1.538533 Hartree

SCF: -5071.844772 Hartree

S: 493.906 Cal/Mol-Kelvin

H: -5070.306239 Hartree

G: -5070.54091 Hartree

Cartesian Coordinates:

H	9.34557400	-0.14040400	-3.78545600
H	9.47145500	0.54656400	-2.14976100
C	8.75950000	0.19265700	-2.91205200
H	8.14622900	1.05428500	-3.22278500
H	9.71603800	1.52630400	1.38664100
H	9.35824500	-2.51245300	-2.82716300
C	9.35441100	0.90304800	2.22112500
H	9.83675900	1.27520200	3.13960600
H	9.48208400	-1.87248100	-1.17248600
C	8.77080200	-2.15200900	-1.96566200
H	8.83790400	-0.00596300	-0.02882900
C	7.87092900	-0.96256900	-2.38579200
H	7.71186800	3.09209200	1.79248100
H	9.70860400	-0.12865900	2.06072200
H	7.58078900	-1.77234300	-4.38581500
C	7.74555200	-0.00345800	-0.02029700
C	6.96179800	-1.43261100	-3.53954400
C	7.42990200	2.44785900	2.64143500
H	7.94496100	2.82671100	3.54050400
H	6.31366800	-0.62227700	-3.91209900
C	7.06418100	-0.47294200	-1.16513400

C	7.82154600	0.97252100	2.37529500
H	8.16611400	-2.99423300	-1.59134000
C	7.07840200	0.46452300	1.12208300
H	0.81818200	5.26259400	-6.18211000
H	1.72879900	4.14059400	-5.13937400
H	6.34700900	2.56485000	2.80506700
C	0.78327600	4.27924800	-5.68848900
H	6.31991800	-2.27843400	-3.24294700
C	5.66200300	-0.46917300	-1.13933400
C	7.42014900	0.10667500	3.59609100
H	7.93893700	0.45844200	4.50403100
H	4.53043500	2.61025100	-0.32965100
H	0.72392500	3.50111900	-6.46679500
C	5.66809200	0.46031300	1.10286900
O	-0.37802100	6.52365900	-4.06136400
H	7.69005500	-0.95036000	3.43833700
H	5.08757500	-0.81911300	-2.00003500
H	2.60443000	4.53152000	-0.30965700
H	-0.21123300	7.60998600	-2.16269900
C	4.95644600	-0.00278200	-0.01173100
C	3.45322700	2.48798400	-0.24176800
H	0.00000000	8.84732300	0.00037300
C	-0.11942100	7.07818100	-1.21736900
C	-0.34905400	5.34352200	-3.71821200
C	-0.00000100	7.75293400	0.00032000
C	2.48839300	3.45192900	-0.23521700
C	-0.43637600	4.20313800	-4.75023000
H	5.10347700	0.81318300	1.97116800
H	6.33756700	0.14909300	3.79443200
H	-1.81277000	5.31660100	-6.01802200
C	-0.11975200	5.66991700	-1.21896300
N	-0.23309500	4.91174900	-2.40530200
C	0.11941700	7.07806200	1.21794400
C	-1.75558100	4.32955500	-5.53426700

C	3.45714200	-0.00221300	-0.00797900
C	2.78078800	1.21745300	-0.10422100
H	0.21123200	7.60977500	2.16332600
H	-0.42381200	3.22481200	-4.23235900
H	-1.81989500	3.55424000	-6.31496400
C	-0.00000400	4.95247700	0.00018400
H	-0.22114400	3.90204400	-2.26496800
C	0.11974600	5.66979800	1.21940000
C	1.22215600	2.77229200	-0.10253700
H	4.53211300	-2.61405100	0.30641100
H	-0.78962400	-3.50321000	-6.45534400
N	1.40027900	1.39276800	-0.04645300
O	0.37795900	6.52325900	4.06189300
C	-0.00000300	3.44824300	0.00011200
C	2.78100200	-1.22187600	0.09056100
H	-0.88332400	-5.26459700	-6.17016500
C	3.45436900	-2.49225200	0.22390600
H	-2.63244400	4.22368800	-4.87497300
N	0.23308800	4.91151400	2.40566500
C	-0.84025000	-4.28153100	-5.67661300
C	0.34905600	5.34315600	3.71861800
H	-1.77831900	-4.14139700	-5.11522800
H	-1.72891400	4.14020100	5.13959700
H	0.22112600	3.90182200	2.26523300
H	1.75563700	-3.56190000	-6.33726500
H	0.42367800	3.22439300	4.23256600
H	1.74964200	-5.32414000	-6.03940900
N	1.40036800	-1.39732100	0.03948700
C	0.43627800	4.20266900	4.75053100
C	2.48973400	-3.45642900	0.22160100
C	-1.22216100	2.77227900	0.10268400
C	1.70033300	-4.33676900	-5.55545200
C	-0.78340200	4.27875600	5.68875600
Co	0.00000300	-0.00229100	0.00000200

C	0.39174000	-4.20791700	-4.75431400
C	1.22269700	-2.77690500	0.09600500
H	2.60622200	-4.53605700	0.29481700
H	-2.60444700	4.53148500	0.30990200
C	-2.48840400	3.45190100	0.23537100
N	-1.40028000	1.39275900	0.04646600
H	-0.81827500	5.26205800	6.18246600
H	0.38782200	-3.22963400	-4.23623400
H	-0.72411800	3.50055300	6.46699400
C	0.31528500	-5.34820500	-3.72137000
H	2.58588900	-4.23172800	-4.90778800
C	1.75546300	4.32894100	5.53462400
H	2.63234300	4.22309400	4.87534900
H	0.20200700	-3.90661900	-2.26702700
N	0.21233300	-4.91634100	-2.40735800
O	0.34057400	-6.52839500	-4.06463800
C	0.00001100	-3.45286800	0.00006300
C	-3.45323700	2.48795400	0.24178800
C	-2.78079100	1.21743600	0.10416400
H	1.81268700	5.31593500	6.01847900
N	-1.40035300	-1.39732600	-0.03948700
H	1.81971000	3.55354500	6.31524600
C	0.10921600	-5.67447500	-1.22007400
H	-2.58585700	-4.23154600	4.90809700
C	-1.22267500	-2.77691100	-0.09594200
C	0.00001100	-4.95709500	0.00010600
H	-4.53044900	2.61021400	0.32964000
C	0.10891800	-7.08275200	-1.21847500
C	-2.78098500	-1.22188600	-0.09067800
C	-3.45713800	-0.00222700	0.00782600
C	-1.70025400	-4.33650700	5.55571000
H	0.19254000	-7.61452900	-2.16457800
H	-0.20198000	-3.90648300	2.26717400
C	-0.10919600	-5.67440200	1.22032800

H	-1.75554600	-3.56159900	6.33748400
N	-0.21231000	-4.91619700	2.40756600
H	-6.34698000	2.56523500	-2.80507400
H	-1.74948200	-5.32385500	6.03972200
H	-5.10335000	0.81335800	-1.97135200
C	0.00000600	-7.75751600	0.00018900
C	-2.48969900	-3.45644400	-0.22160900
C	-0.10890400	-7.08267900	1.21881300
C	-3.45433600	-2.49226900	-0.22404400
C	-0.39172100	-4.20763300	4.75448000
C	-0.31525800	-5.34798300	3.72160500
H	-0.38788900	-3.22938300	4.23633800
C	-7.42987600	2.44810800	-2.64155400
C	-5.66801700	0.46040100	-1.10312300
C	-4.95643900	-0.00279900	0.01147800
H	-6.33717400	0.14959200	-3.79472700
H	-7.94489400	2.82702800	-3.54061600
H	0.00000300	-8.85190800	0.00022200
H	-2.60618000	-4.53607400	-0.29479000
H	-7.71198500	3.09219400	-1.79253700
H	-0.19252900	-7.61440000	2.16494700
O	-0.34059200	-6.52815300	4.06493800
C	-7.41977700	0.10704800	-3.59651600
H	-7.93849100	0.45889000	-4.50447000
H	-4.53207100	-2.61407700	-0.30664900
C	-7.82139200	0.97269300	-2.37565000
C	-7.07832600	0.46460100	-1.12242900
C	-5.66207000	-0.46929600	1.13899200
C	0.84033400	-4.28112000	5.67670500
H	-5.08769600	-0.81930600	1.99970100
H	0.78972000	-3.50274500	6.45538200
H	-7.68960300	-0.95003300	-3.43893600
H	0.88348800	-5.26414700	6.17032700
C	-7.74554900	-0.00349800	0.01986000

H	1.77836100	-4.14098000	5.11524900
C	-7.06424900	-0.47308000	1.16469900
C	-9.35426600	0.90304000	-2.22164900
H	-9.83655600	1.27532500	-3.14010700
H	-9.71603800	1.52609800	-1.38708000
H	-6.31390900	-0.62258200	3.91168700
H	-8.83790200	-0.00601700	0.02831700
H	-9.70837400	-0.12873200	-2.06148500
H	-8.14649000	1.05397600	3.22237500
C	-6.96200800	-1.43290400	3.53905200
H	-6.32010200	-2.27870700	3.24245700
C	-7.87107000	-0.96281400	2.38526600
C	-8.75971300	0.19235000	2.91154200
H	-9.47162700	0.54628800	2.14922600
H	-7.58105100	-1.77268200	4.38526700
C	-8.77087600	-2.15225200	1.96498800
H	-8.16613500	-2.99443200	1.59065200
H	-9.48210700	-1.87269000	1.17177900
H	-9.34583800	-0.14078800	3.78488200
H	-9.35837200	-2.51277500	2.82642100

A_{1b}:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.259858 Hartree

H_corr: 0.337951 Hartree

SCF: -1388.340915 Hartree

S: 164.359 Cal/Mol-Kelvin

H: -1388.002965 Hartree

G: -1388.081057 Hartree

Cartesian Coordinates:

C	0.13583500	0.54882400	1.20334600
H	-0.82905100	0.79097600	1.68069100

H	0.79681500	0.15538600	1.98720300
N	-0.12060100	-0.57058600	0.25276100
S	0.46790900	-2.08224300	0.52259100
N	1.69269900	-2.17116000	-0.81684300
O	-0.52968500	-3.11374000	0.19851600
O	1.20362900	-2.09023300	1.79195400
C	-1.01755400	-0.34615600	-0.90141100
C	-2.46113100	-0.06921900	-0.50960100
H	-0.95981500	-1.23514200	-1.54793000
H	-0.60973200	0.49850200	-1.48099700
C	-3.11850100	1.06638000	-1.01110400
C	-4.46112900	1.31432700	-0.69261700
C	-3.16892000	-0.95569300	0.32256700
C	-4.50715200	-0.70486600	0.64642300
C	-5.15734200	0.43004900	0.14016100
H	-6.20433800	0.62261200	0.39382600
H	-5.04794100	-1.40357000	1.29229600
H	-2.57518700	1.76291700	-1.65916800
H	-4.96072500	2.20214400	-1.09275400
H	-2.67063600	-1.85178400	0.70430100
N	1.98172100	-3.33749500	-1.14696800
N	2.31577900	-4.36306000	-1.53802400
C	0.70156500	1.79845700	0.55204300
C	-0.16985700	2.88177900	0.34359000
C	2.07064900	1.91743600	0.18927800
C	0.27483700	4.07886100	-0.23015800
H	-1.21853300	2.78214100	0.64461400
C	2.49767700	3.12735300	-0.38570800
C	1.61716800	4.19641700	-0.60000700
H	-0.42085900	4.91007000	-0.37994200
H	3.54741700	3.24615400	-0.66693800
H	1.98803500	5.12350800	-1.04867500
C	3.03994200	0.77142600	0.42942800
H	2.92383100	0.41759100	1.47053300

H	2.73817900	-0.09050200	-0.19250500
C	4.52297000	1.06504700	0.17421000
H	4.72250200	1.31076400	-0.88171200
H	4.89188400	1.90044100	0.79203300
H	5.12854100	0.17903100	0.42078500

Intermediate $B_{3.1b}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.585724 Hartree

H_corr: 1.878666 Hartree

SCF: -6460.187033 Hartree

S: 616.549 Cal/Mol-Kelvin

H: -6458.308367 Hartree

G: -6458.601309 Hartree

Cartesian Coordinates:

H	9.04000600	3.09049600	1.69306900
H	9.36324400	1.38606500	1.30025500
C	8.56152400	2.11730700	1.48942300
H	8.03025200	1.80264700	2.40252600
H	9.98026400	-2.00516400	0.03540100
H	8.84568200	3.66795900	-0.79213700
C	9.61820000	-2.37474400	-0.93819600
H	10.20888200	-3.27125200	-1.18768000
H	9.16955800	1.97567900	-1.23360500
C	8.37189700	2.68676900	-0.96644600
H	8.83096000	-0.09594900	-0.35182900
C	7.58679700	2.23498000	0.29069400
H	8.19336100	-3.47534700	1.17067400
H	9.84236900	-1.61212000	-1.70230000
H	7.05755300	4.28221700	0.80670100
C	7.74971000	-0.24398900	-0.30229200
C	6.54599500	3.32294300	0.62360900

C	7.91471400	-3.83824100	0.16780900
H	8.54074700	-4.71717900	-0.06220800
H	5.96750500	3.07957700	1.52947300
C	6.93438800	0.86266400	0.02265700
C	8.11911000	-2.73473000	-0.90068100
H	7.70316100	2.78169900	-1.83764100
C	7.22889300	-1.52150000	-0.55898200
H	2.91514600	4.47664400	6.12472600
H	3.32727500	3.43965400	4.73382400
H	6.86829400	-4.17861400	0.21462100
C	2.63531100	4.21910700	5.09140900
H	5.83455200	3.48023300	-0.20331900
C	5.54785600	0.66012600	0.08840600
C	7.72165700	-3.28869400	-2.29204400
H	8.34371100	-4.16234500	-2.55087500
H	4.75426500	-0.76955000	2.47981900
H	2.77750200	5.11314200	4.46173100
C	5.82969100	-1.68221700	-0.48937100
O	1.14302400	2.67204900	7.20177500
H	7.86304100	-2.52739000	-3.07683500
H	4.86991500	1.48036300	0.33474200
H	2.95978000	-0.98490900	4.51168800
H	0.79128600	0.72587700	7.97836500
C	4.98785300	-0.60771200	-0.17059400
C	3.66851900	-0.80316600	2.42214000
H	0.48331800	-1.55466300	8.94135400
C	0.61428000	-0.13256500	7.33425800
C	1.00934300	2.53865000	5.98562400
C	0.44061000	-1.41537400	7.85660500
C	2.76912200	-0.91696800	3.44221100
C	1.16958400	3.74321600	5.04127900
H	5.37806600	-2.66255900	-0.66894800
H	6.66885200	-3.61092600	-2.32306100
H	0.38530300	5.12201600	6.53411100

C	0.56142200	0.05875700	5.93789600
N	0.72643900	1.33617400	5.35163500
C	0.21435400	-2.52500700	7.04033700
C	0.20509900	4.85986400	5.48050000
C	3.50397300	-0.79392600	-0.07816700
C	2.91084200	-0.78117700	1.19127000
H	0.07932800	-3.52421400	7.45015500
H	0.92609800	3.44100900	4.00886400
H	0.35147200	5.76605100	4.86887000
C	0.33256500	-1.04891900	5.07833600
H	0.63917100	1.37140000	4.33359400
C	0.15979000	-2.34193800	5.64605900
C	1.45530500	-0.91729300	2.84207800
H	4.42135700	-1.19569500	-2.75941600
H	-1.64567700	3.82887900	-6.41236500
N	1.54945900	-0.85838700	1.45698500
O	-0.32561900	-5.23625300	6.16891600
C	0.26626100	-0.89488600	3.58324800
C	2.76755600	-1.06432300	-1.23937600
H	-1.62745100	2.70672800	-7.80658300
C	3.36394500	-1.31125300	-2.53229700
H	-0.84804500	4.54837500	5.38489300
N	-0.06039200	-3.41829800	4.75714600
C	-1.68023100	2.76821600	-6.70916900
C	-0.29105000	-4.75622000	5.03720200
H	-2.65383000	2.35857300	-6.39500300
H	-2.70354100	-5.34969600	3.77909500
H	-0.06539900	-3.16061100	3.77096300
H	0.88361400	3.67629500	-6.15177100
H	-0.38513600	-5.02400900	2.87405500
H	0.99339900	2.57235700	-7.55095700
N	1.39088500	-1.26282200	-1.29413800
C	-0.52080200	-5.63060400	3.78992400
C	2.36241200	-1.73046400	-3.36101200

C	-0.98958400	-0.75534300	2.97474300
C	0.84588700	2.61873000	-6.46042500
C	-1.96531400	-6.16724800	3.81565800
Co	0.07533600	-0.90389200	0.14589500
C	-0.51157100	1.99230000	-6.07943000
C	1.13864100	-1.67677300	-2.59753000
H	2.42604700	-2.02839600	-4.40606000
H	-2.28211700	-0.56616600	4.80412500
C	-2.21611600	-0.58462100	3.71781200
N	-1.23869500	-0.75082400	1.60863500
H	-2.13777300	-6.74011500	4.73986200
H	-0.61432900	2.01903200	-4.98012900
H	-2.14929300	-6.83142500	2.95558500
C	-0.53772600	0.53592300	-6.57547500
H	1.68680600	2.09438500	-5.97855800
C	0.50393900	-6.77912900	3.78076300
H	1.53670200	-6.40226900	3.70247600
H	-0.31210100	-0.06024800	-4.62144300
N	-0.40444400	-0.41680000	-5.57288500
O	-0.64736000	0.27219200	-7.77172400
C	-0.12550100	-1.95045700	-3.14382900
C	-3.21940200	-0.45920900	2.80139100
C	-2.61452200	-0.58751600	1.49381800
H	0.42525800	-7.35973500	4.71247700
N	-1.40524300	-1.22182700	-1.13541000
H	0.32211900	-7.45716600	2.93111800
C	-0.34539100	-1.82458500	-5.69374700
H	-1.81494800	-7.01828400	-1.41156500
C	-1.31362100	-1.68951800	-2.44350500
C	-0.20396400	-2.58904200	-4.50517000
H	-4.28455000	-0.32933900	2.98010700
C	-0.42127100	-2.46822600	-6.94573400
C	-2.76725100	-1.04664600	-0.91101500
C	-3.35707800	-0.69019400	0.30977600

C	-0.82356600	-7.49555400	-1.34697600
H	-0.53194700	-1.86493900	-7.84427100
H	0.05422800	-4.16056200	-2.55747900
C	-0.13317300	-4.00701800	-4.60145200
H	-0.68569500	-7.85859500	-0.31561100
N	0.01177700	-4.73425900	-3.39894100
H	-5.79534500	3.01747800	2.05160600
H	-0.82046200	-8.36288300	-2.02459400
H	-4.80803600	1.58628400	0.58432800
C	-0.35235300	-3.86140400	-7.00161800
C	-2.62504900	-1.80848900	-3.03498700
C	-0.20886200	-4.64386500	-5.85441500
C	-3.52155900	-1.37725800	-2.09876700
C	0.30281000	-6.52097900	-1.73593500
C	0.12503000	-6.10306400	-3.20772200
H	0.24563100	-5.63025600	-1.08133300
C	-6.88952400	2.90566500	2.10682200
C	-5.44951100	0.70078200	0.55180600
C	-4.84997500	-0.55495500	0.39064900
H	-6.04002500	3.21183500	-0.54547500
H	-7.31993800	3.91250200	2.24251300
H	-0.41183200	-4.35525700	-7.97649200
H	-2.81670600	-2.16260900	-4.04630400
H	-7.12127500	2.31340000	3.00728700
H	-0.15432300	-5.72989300	-5.90120300
O	0.09833900	-6.93754700	-4.11048500
C	-7.12642300	3.10464400	-0.40233700
H	-7.55145300	4.11715600	-0.29269900
H	-4.60428300	-1.31078800	-2.18267600
C	-7.47026100	2.23803500	0.83490600
C	-6.85017100	0.83570900	0.66198000
C	-5.66202100	-1.70697100	0.33772800
C	1.69012600	-7.16974600	-1.56459600
H	-5.17348200	-2.67762200	0.22634600

H	1.83215900	-7.51697200	-0.52836700
H	-7.54135500	2.66040300	-1.32208300
H	1.78681400	-8.03555000	-2.23765900
C	-7.62373000	-0.33311700	0.60432400
H	2.50180200	-6.46265000	-1.80109800
C	-7.05712900	-1.61696400	0.44319600
C	-9.00509500	2.19120300	0.97882200
H	-9.39659900	3.21355000	1.10734900
H	-9.32168700	1.60600700	1.85806100
H	-6.48399700	-4.34449300	1.05495000
H	-8.70972400	-0.25186100	0.69008600
H	-9.49278600	1.76517900	0.08651500
H	-8.10273800	-3.05085300	2.58620600
C	-7.18289600	-4.16761300	0.22096300
H	-6.60721400	-4.18085800	-0.71915700
C	-7.97519500	-2.85626300	0.39769100
C	-8.77724700	-2.95212500	1.72003500
H	-9.40761000	-2.06426700	1.88633300
H	-7.87925500	-5.02141600	0.19064000
C	-8.96027200	-2.72380000	-0.79106700
H	-8.41943500	-2.66128100	-1.74961400
H	-9.59331500	-1.82649400	-0.70507800
H	-9.44110400	-3.83322200	1.70386000
H	-9.62922800	-3.60004500	-0.83535400
C	0.85642100	5.18937300	0.54011000
H	0.77630900	5.41237300	1.62008800
H	1.90764400	4.95726200	0.32524900
N	0.06646700	3.94286100	0.22067600
S	0.81319900	2.54507700	0.84357700
N	0.17240600	1.29425900	-0.28195000
O	0.26178200	2.10267200	2.13139900
O	2.25926800	2.68347500	0.63491200
C	-1.41595400	4.01884500	0.48636700
C	-2.25866600	3.99951800	-0.77553400

H	-1.59657800	4.94380000	1.05609600
H	-1.69932900	3.18584500	1.14748400
C	-2.69289800	2.77573100	-1.31722400
C	-3.48625700	2.74410900	-2.47122900
C	-2.65355900	5.19469500	-1.40306500
C	-3.45065100	5.16529300	-2.55426600
C	-3.86512500	3.94065000	-3.09454300
H	-4.48985300	3.91868500	-3.99253700
H	-3.75170700	6.10466800	-3.02807100
H	-2.42152900	1.83565000	-0.82632300
H	-3.81639700	1.78115000	-2.87173700
H	-2.33730900	6.15665200	-0.98901300
N	0.40902900	1.56730100	-1.48315200
N	0.54808600	1.66072600	-2.61514600
C	0.39387400	6.39644100	-0.24988000
C	-0.31194300	7.40829400	0.42806100
C	0.68379900	6.54973800	-1.62764400
C	-0.74987000	8.56087000	-0.23396600
H	-0.51498900	7.29251300	1.49879400
C	0.22883900	7.71036100	-2.27889200
C	-0.48238000	8.70701800	-1.60019800
H	-1.29420400	9.33594000	0.31342000
H	0.44053100	7.83234400	-3.34708800
H	-0.82237000	9.59797900	-2.13714400
C	1.50637000	5.53828500	-2.40228200
H	1.37849100	4.53328300	-1.97301700
H	1.11894400	5.47758300	-3.43373900
C	3.00480600	5.90393600	-2.44588500
H	3.16159600	6.88650200	-2.91935600
H	3.44066500	5.95341200	-1.43478200
H	3.57365800	5.15544500	-3.02037300

Transition State TS1:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -540.5161 cm-1

G_corr: 1.585706 Hartree

H_corr: 1.875692 Hartree

SCF: -6460.169795 Hartree

S: 610.327 Cal/Mol-Kelvin

H: -6458.294103 Hartree

G: -6458.584089 Hartree

Cartesian Coordinates:

H	8.69009500	3.85412500	1.35189900
H	9.16334100	2.14880500	1.17486300
C	8.29930000	2.82590600	1.26668300
H	7.78036300	2.58153300	2.20796200
H	10.08829600	-1.29958700	0.34427700
H	8.49030300	4.10545700	-1.18664800
C	9.77637400	-1.81916100	-0.57669600
H	10.44609600	-2.68490600	-0.70607200
H	8.96618300	2.40683900	-1.41351200
C	8.10562500	3.07287300	-1.24213000
H	8.78697700	0.43631900	-0.28474800
C	7.33928300	2.71292100	0.05563100
H	8.41363900	-2.76197800	1.64647500
H	9.94769200	-1.14249500	-1.43014000
H	6.62899000	4.75397000	0.31159100
C	7.72144200	0.20293300	-0.22588600
C	6.20394700	3.73908500	0.24416500
C	8.18516100	-3.27300100	0.69690500
H	8.88851200	-4.11579100	0.58635400
H	5.63075900	3.55960000	1.16793800
C	6.81027800	1.26727700	-0.04601700
C	8.31332900	-2.30139400	-0.50344900
H	7.44702200	3.00261600	-2.12321700
C	7.31639300	-1.13692100	-0.32633500

H	2.56460600	5.20284000	5.44864900
H	3.00772600	4.02577100	4.18254600
H	7.17123500	-3.69523500	0.78006700
C	2.28316700	4.80814600	4.45984500
H	5.49705500	3.73257600	-0.60119600
C	5.44477900	0.95685600	0.03521100
C	7.99040200	-3.06107900	-1.81466100
H	8.69125100	-3.90133700	-1.95547500
H	4.73342600	-0.27097000	2.58501600
H	2.37044300	5.62434900	3.72377400
C	5.93481800	-1.40841600	-0.25042600
O	0.88535600	3.45870900	6.77057800
H	8.07811700	-2.39634400	-2.68978600
H	4.69350000	1.73730500	0.17473400
H	2.91625800	-0.40580600	4.60612600
H	0.59915300	1.62421800	7.78273200
C	5.00135900	-0.37754100	-0.07305000
C	3.65292300	-0.37578400	2.51781300
H	0.39855200	-0.52444600	9.03166500
C	0.47804900	0.68131700	7.25420100
C	0.75446800	3.17362600	5.58065000
C	0.36564500	-0.53046100	7.93770200
C	2.74314200	-0.45021100	3.53262600
C	0.84251200	4.25953300	4.49498700
H	5.57232800	-2.43934200	-0.30705500
H	6.97092400	-3.47839400	-1.81025300
H	0.00896500	5.77326400	5.82314100
C	0.43712200	0.68979000	5.84377200
N	0.53653300	1.88726400	5.09878600
C	0.21182200	-1.74855700	7.27291000
C	-0.17114900	5.37350400	4.81359100
C	3.53742100	-0.66707700	0.03326500
C	2.92082500	-0.52422700	1.28209900
H	0.12390500	-2.69124900	7.80954300

H	0.60240600	3.82025200	3.51231200
H	-0.07883600	6.20206600	4.09162700
C	0.28456000	-0.53535200	5.13856800
H	0.44333000	1.80198000	4.08213900
C	0.17091100	-1.75168900	5.86651400
C	1.44376800	-0.58939800	2.92060200
H	4.51871300	-1.47616600	-2.53095000
H	-0.92718700	2.94036800	-6.92568700
N	1.56315700	-0.66094100	1.53813800
O	-0.16341700	-4.57544000	6.75830800
C	0.24148700	-0.57268000	3.63722200
C	2.83652100	-1.16111800	-1.07537700
H	-0.97768600	1.63578100	-8.14875800
C	3.46402900	-1.60116000	-2.29653400
H	-1.20839600	5.00207200	4.77616200
N	0.02414300	-2.94529200	5.12273900
C	-1.03373000	1.85334700	-7.07149900
C	-0.13535500	-4.24699900	5.57392700
H	-2.03619900	1.56101600	-6.71920500
H	-2.48674600	-5.17916300	4.40425300
H	0.02458400	-2.82142800	4.11120700
H	1.58377700	2.65342100	-6.60473300
H	-0.19071000	-4.79876300	3.46348900
H	1.62733300	1.35679800	-7.83212800
N	1.47192500	-1.43625200	-1.10668600
C	-0.28906500	-5.28988000	4.45076800
C	2.49711300	-2.21122100	-3.04712100
C	-1.00212100	-0.54255900	2.99334900
C	1.47454800	1.56805900	-6.76209200
C	-1.68913400	-5.92614300	4.54792300
Co	0.12791000	-0.81539200	0.20818400
C	0.07381900	1.09619300	-6.31902500
C	1.25741500	-2.07021100	-2.32790600
H	2.59375000	-2.68654800	-4.02149200

H	-2.34417400	-0.22412700	4.76305700
C	-2.24819900	-0.32264400	3.68345100
N	-1.21751800	-0.65725600	1.62559000
H	-1.82661100	-6.38326400	5.53988000
H	-0.03224100	1.28392100	-5.23654000
H	-1.81478500	-6.71015000	3.78361700
C	-0.04960100	-0.40991600	-6.60580900
H	2.27279100	1.06187800	-6.19530900
C	0.81929500	-6.34933200	4.58997300
H	1.82179000	-5.90880600	4.46478500
H	0.05654900	-0.73404300	-4.57901700
N	-0.02656800	-1.21969600	-5.47398400
O	-0.13791000	-0.83249500	-7.75724200
C	0.01195400	-2.43655500	-2.86042900
C	-3.22383800	-0.25223200	2.73008200
C	-2.58613800	-0.47406100	1.45432000
H	0.77443100	-6.81053200	5.58829800
N	-1.31183200	-1.37375200	-1.04322100
H	0.69799600	-7.14239800	3.83435300
C	-0.06336600	-2.63190700	-5.40812400
H	-2.11410100	-7.08737200	-0.59872100
C	-1.18909200	-2.03594200	-2.26156300
C	-0.03478300	-3.24627500	-4.12670300
H	-4.29195400	-0.09866100	2.86703800
C	-0.12183000	-3.43158800	-6.56840700
C	-2.67166700	-1.12521400	-0.90161700
C	-3.29277000	-0.63948200	0.25650000
C	-1.17219000	-7.62816500	-0.41135900
H	-0.14817500	-2.94684600	-7.54187500
H	0.01822700	-4.56157800	-1.97902900
C	-0.05522000	-4.66565500	-4.03512600
H	-1.11999800	-7.86008500	0.66471200
N	-0.01880600	-5.23580600	-2.74240600
H	-5.66468100	3.30054300	1.50887900

H	-1.20879200	-8.57578600	-0.96998000
H	-4.69037000	1.68856800	0.22981300
C	-0.14522300	-4.82152500	-6.44176800
C	-2.48216000	-2.19822000	-2.88138600
C	-0.11139900	-5.45555800	-5.19844800
C	-3.39375300	-1.59707100	-2.06054300
C	0.05302300	-6.80594300	-0.85112000
C	-0.01483900	-6.57276300	-2.37198200
H	0.03991900	-5.83512200	-0.31928700
C	-6.76061100	3.21098900	1.56660900
C	-5.35170700	0.81929000	0.28876100
C	-4.78231300	-0.46014400	0.27895700
H	-5.87970400	3.21022200	-1.09302700
H	-7.17537900	4.23305600	1.58706800
H	-0.19021100	-5.43374100	-7.34781200
H	-2.64951800	-2.69470900	-3.83541600
H	-7.00927700	2.72473100	2.52435000
H	-0.12742800	-6.53963600	-5.10394900
O	-0.05488000	-7.51399700	-3.16167000
C	-6.96879200	3.13567100	-0.95174800
H	-7.37668900	4.16091400	-0.95966500
H	-4.46907800	-1.50575600	-2.19754400
C	-7.34300500	2.41860600	0.36918000
C	-6.75091600	0.99408400	0.35927800
C	-5.61813300	-1.59491800	0.33623100
C	1.36818400	-7.53504500	-0.51480700
H	-5.15058300	-2.58222600	0.34204500
H	1.42622300	-7.75619300	0.56322000
H	-7.38194800	2.59967900	-1.82208700
H	1.42387600	-8.48528300	-1.06775500
C	-7.54963700	-0.15782400	0.41658600
H	2.24960200	-6.93161200	-0.78643300
C	-7.01203600	-1.46391200	0.40575600
C	-8.87976600	2.41743200	0.49958900

H	-9.25056000	3.45530400	0.51015900
H	-9.21757700	1.93929600	1.43408300
H	-6.51313500	-4.12122300	1.32032200
H	-8.63443600	-0.04411600	0.47495700
H	-9.36780100	1.90615400	-0.34660200
H	-8.12188800	-2.63262900	2.67408200
C	-7.19473600	-4.02014900	0.45968500
H	-6.60547300	-4.14807500	-0.46331600
C	-7.95824100	-2.68031900	0.47960600
C	-8.78116600	-2.61355900	1.79088700
H	-9.39206300	-1.69892500	1.84911800
H	-7.91055600	-4.85669600	0.50943300
C	-8.92265800	-2.65630200	-0.73300900
H	-8.36680200	-2.71009300	-1.68343600
H	-9.53565500	-1.74147800	-0.75549600
H	-9.46589000	-3.47592200	1.85917300
H	-9.61125600	-3.51736700	-0.69331700
C	0.66628100	4.93364100	0.07010000
H	0.61930700	5.23940000	1.13371100
H	1.71458000	4.69527400	-0.15310100
N	-0.11136300	3.66844400	-0.13072600
S	0.64552900	2.32081400	0.62350000
N	0.05540900	1.00605800	-0.36432600
O	0.05544300	2.06330000	1.96191700
O	2.10030800	2.54336100	0.51210300
C	-1.58251500	3.76437300	0.12438700
C	-2.41476400	3.84862800	-1.14491000
H	-1.76908900	4.64372000	0.76488100
H	-1.88644000	2.88515400	0.71204200
C	-2.65416400	2.69239600	-1.91093900
C	-3.43126600	2.75233800	-3.07392100
C	-2.99000300	5.06194300	-1.55921800
C	-3.77070700	5.12442300	-2.72140700
C	-3.98921500	3.97116700	-3.48528200

H	-4.59802000	4.01886200	-4.39353000
H	-4.20581700	6.07972700	-3.03082800
H	-2.23112300	1.73760300	-1.58518300
H	-3.61047600	1.84152700	-3.65324800
H	-2.81391100	5.97149400	-0.97689400
N	0.52104700	1.41767800	-1.82512400
N	0.48425200	0.81423400	-2.79859200
C	0.18066200	6.08800800	-0.78627500
C	-0.43611100	7.17947300	-0.14694000
C	0.37470000	6.12276500	-2.18868200
C	-0.87525800	8.29630800	-0.86724800
H	-0.56861500	7.15355400	0.94073200
C	-0.08340300	7.24663600	-2.89899800
C	-0.70328800	8.32447100	-2.25596900
H	-1.34755900	9.13519700	-0.34706500
H	0.05218600	7.27342700	-3.98623900
H	-1.04647700	9.18544500	-2.83829500
C	1.09970400	5.01731100	-2.93112300
H	0.95732100	4.05689400	-2.41317800
H	0.64249800	4.89842100	-3.92879400
C	2.60594400	5.30857000	-3.09760500
H	2.77296400	6.24218400	-3.65919100
H	3.10743500	5.41789700	-2.12227200
H	3.10607600	4.49070600	-3.64127900

Intermediate $C_{3.1b}$

C_{N2}:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: -0.013118 Hartree

H_corr: 0.00864 Hartree

SCF: -109.557996 Hartree

S: 45.794 Cal/Mol-Kelvin

H: -109.549356 Hartree

G: -109.571114 Hartree

Cartesian Coordinates:

N	0.00000000	0.00000000	0.55384100
N	0.00000000	0.00000000	-0.55384100

$C_{[Co(III)]\ 3.1b}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.583161 Hartree

H_corr: 1.86719 Hartree

SCF: -6350.664231 Hartree

S: 597.79 Cal/Mol-Kelvin

H: -6348.797041 Hartree

G: -6349.08107 Hartree

Cartesian Coordinates:

H	-9.02405900	-2.93788600	-0.54303100
H	-9.30014300	-1.36038000	0.23035700
C	-8.51893800	-2.06825500	-0.08925000
H	-7.99156500	-2.41588200	0.81411300
H	-9.81574800	2.07106600	1.40401800
H	-8.81393900	-1.82259200	-2.83506100
C	-9.43660700	2.96533100	0.88252200
H	-10.00340400	3.83048100	1.26336600
H	-9.08904800	-0.22283300	-2.10797800
C	-8.31306700	-0.96487500	-2.35463200
H	-8.71053000	0.81153800	-0.11064200
C	-7.53241900	-1.43031100	-1.09961800
H	-8.00286100	2.44188100	3.19788700
H	-9.67255600	2.86582700	-0.18985900
H	-7.05953000	-3.35652100	-1.99392600
C	-7.62632300	0.86840100	0.01030800
C	-6.52202000	-2.51099600	-1.53396600

C	-7.70734600	3.35230100	2.65121900
H	-8.31006300	4.19177500	3.03758200
H	-5.94844700	-2.90801600	-0.68092700
C	-6.84292900	-0.21494900	-0.44590200
C	-7.92966800	3.18377700	1.12692400
H	-7.63617200	-0.50830900	-3.09513400
C	-7.07225800	2.00817900	0.61312500
H	-2.79498900	-7.18632400	2.68930500
H	-3.47594500	-5.61544300	2.19256100
H	-6.65335400	3.56068500	2.89407200
C	-2.68943500	-6.35637200	1.97358900
H	-5.80386800	-2.13129100	-2.27852600
C	-5.45199900	-0.13634800	-0.28186600
C	-7.50756400	4.48566600	0.40055800
H	-8.10830600	5.33870900	0.75906400
H	-4.62838800	-0.42491700	2.55753700
H	-2.85973700	-6.74248100	0.95606200
C	-5.66965500	2.05602900	0.75166500
O	-1.13705800	-6.05528900	4.46741700
H	-7.65809700	4.39891300	-0.68810900
H	-4.79145800	-0.93997100	-0.61462200
H	-2.82330100	-1.45155100	4.31950300
H	-0.72856700	-4.89152700	6.17246500
C	-4.86210800	0.99906500	0.31006900
C	-3.54223600	-0.40898600	2.50206700
H	-0.29236500	-3.56418500	8.23700700
C	-0.51392200	-3.82678600	6.11585300
C	-1.04928100	-5.27052200	3.52381400
C	-0.26754500	-3.06863200	7.26142800
C	-2.63850600	-0.91835600	3.38903700
C	-1.28398500	-5.73586800	2.07964000
H	-5.19163600	2.91809700	1.22707700
H	-6.44792600	4.73121900	0.57497600
H	-0.21905500	-7.61584600	2.39404700

C	-0.48600100	-3.20398800	4.84921300
N	-0.73398800	-3.91917500	3.65648400
C	0.00725500	-1.70066100	7.20532100
C	-0.19554700	-6.75993800	1.70134500
C	-3.37529500	1.03864700	0.47215300
C	-2.78843200	0.23969700	1.45767800
H	0.19561100	-1.11240700	8.10136900
H	-1.21969300	-4.87588900	1.39250100
H	-0.35947500	-7.13262800	0.67752800
C	-0.20299100	-1.81360200	4.76103000
H	-0.68550200	-3.38664200	2.78284200
C	0.03924100	-1.06947500	5.94874700
C	-1.32759200	-0.63620400	2.85975200
H	-4.23878300	3.11248000	-1.28524600
H	-1.45743000	0.30706400	-7.28498900
N	-1.42492000	0.09935300	1.68126500
O	0.64379800	1.01998400	7.98924400
C	-0.14566800	-1.10654100	3.43756200
C	-2.61037400	1.92304600	-0.29551500
H	-1.26534900	1.96465100	-7.92915300
C	-3.17452000	2.96811500	-1.11388000
H	0.81300300	-6.31584500	1.74605000
N	0.30268700	0.31319900	5.80922000
C	-0.99087900	1.28879600	-7.10527600
C	0.57861400	1.25896800	6.78509800
H	0.10226700	1.15480000	-7.12859300
H	2.99601900	2.51936300	6.17400600
H	0.28190800	0.65800300	4.85068900
H	-3.46303000	0.99546000	-5.87517700
H	0.72034300	2.67907000	5.13392800
H	-3.36247000	2.66588500	-6.49826200
N	-1.22249800	2.01004300	-0.28545000
C	0.80298800	2.68173800	6.23797800
C	-2.13253600	3.72356500	-1.57127200

C	1.09288700	-0.96569700	2.79918100
C	-3.00258700	1.98331700	-5.71245500
C	2.21642700	3.15361500	6.62654100
Co	0.03161900	0.69397100	0.50400300
C	-1.46388200	1.87582600	-5.76567000
C	-0.92117800	3.09526700	-1.10213700
H	-2.16391900	4.61535800	-2.19409400
H	2.36870300	-2.21435500	4.15736600
C	2.29627100	-1.61757500	3.25027100
N	1.33467900	-0.24724300	1.63650800
H	2.33866900	3.11279800	7.71966300
H	-1.13319500	1.21233500	-4.94391900
H	2.38567700	4.19128600	6.29593900
C	-0.86597400	3.28074600	-5.57245700
H	-3.35231700	2.36367600	-4.73918400
C	-0.27818900	3.61722100	6.81163200
H	-1.28950700	3.31253200	6.49665000
H	-0.34201100	2.70521200	-3.67369900
N	-0.30632300	3.49556500	-4.31663400
O	-0.92133800	4.13069700	-6.45788000
C	0.35747100	3.48174900	-1.52743400
C	3.26394100	-1.34697600	2.32541600
C	2.66886100	-0.49049600	1.32791900
H	-0.24591300	3.59906300	7.91178900
N	1.55058800	1.62492200	-0.38127100
H	-0.11462700	4.65412800	6.47583200
C	0.18877500	4.69776500	-3.76334900
H	4.08120400	5.97808600	1.67716300
C	1.50100400	2.72738500	-1.22240200
C	0.51181200	4.71166800	-2.37849700
H	4.30431700	-1.66400700	2.32560600
C	0.36423600	5.85880600	-4.54185900
C	2.85572500	1.15850400	-0.46789300
C	3.39615600	0.11623700	0.29653500

C	3.43922200	6.65426400	2.26474800
H	0.11095800	5.82872400	-5.59968900
H	1.09479100	5.00992300	0.05645000
C	0.99780300	5.91342800	-1.79258300
H	3.58591100	6.42195200	3.33195100
N	1.28280400	5.89683000	-0.40866700
H	5.04766200	-4.33118200	-0.10278700
H	3.77737500	7.68593800	2.08355200
H	4.30811200	-2.22760600	-0.67067400
C	0.85018600	7.01891300	-3.93550600
C	2.79355300	2.96947400	-1.81717700
C	1.16799600	7.07001000	-2.57675200
C	3.62260500	1.97639500	-1.37759000
C	1.95586400	6.51067100	1.87582500
C	1.78181900	6.90980400	0.39856100
H	1.65195000	5.45601600	2.02022100
C	6.13937800	-4.44860000	-0.18789900
C	5.13239300	-1.56014400	-0.40259800
C	4.82451400	-0.28843400	0.10043400
H	5.06342000	-3.37712600	-2.53257600
H	6.33551500	-5.46340200	-0.57351100
H	0.98449400	7.91782600	-4.54499500
H	3.01450600	3.78425700	-2.50407000
H	6.56347000	-4.38442700	0.82759500
H	1.54123700	7.97820700	-2.10731000
O	2.06884100	8.03706500	0.00174000
C	6.15539400	-3.51976100	-2.53930900
H	6.35617200	-4.52325700	-2.95131100
H	4.66766700	1.81107000	-1.62963300
C	6.76842900	-3.38508100	-1.12295700
C	6.47023100	-1.97665700	-0.56780100
C	5.86987000	0.58957200	0.45507300
C	1.05805200	7.40807300	2.74855300
H	5.60862300	1.56655500	0.86778600

H	1.20057200	7.17934600	3.81710600
H	6.58702500	-2.77647700	-3.22962900
H	1.31023900	8.46674200	2.58351900
C	7.48232300	-1.07440900	-0.20661900
H	-0.00944900	7.27221800	2.51019800
C	7.21227800	0.21221700	0.30984800
C	8.28047400	-3.67095900	-1.22564700
H	8.43913100	-4.68604600	-1.62443000
H	8.77930100	-3.62440000	-0.24352600
H	7.29082300	2.38296000	2.16045200
H	8.52505100	-1.37819800	-0.32296600
H	8.79035100	-2.96918700	-1.90621300
H	8.63875300	0.25354500	2.69832500
C	7.89797500	2.49736200	1.24736100
H	7.30347500	3.05597400	0.50569200
C	8.38221600	1.13940200	0.69967400
C	9.23804300	0.45530000	1.79547500
H	9.65969200	-0.50275500	1.45269900
H	8.76638300	3.12359400	1.50861100
C	9.26307400	1.40785400	-0.54660900
H	8.68329000	1.90064000	-1.34424600
H	9.68350700	0.47919900	-0.96375800
H	10.08124200	1.10492600	2.08535700
H	10.10798000	2.06700600	-0.28460300
C	-0.58016400	-2.43797500	-3.24726900
H	-1.59796800	-2.81475400	-3.45162800
H	-0.63398200	-1.33826000	-3.24729900
N	-0.15159200	-2.84121500	-1.88211800
S	-0.87061400	-1.98681100	-0.59007600
N	-0.05955200	-0.54422800	-0.81504700
O	-0.51560300	-2.74806700	0.64061200
O	-2.31930700	-1.78759300	-0.88226200
C	0.29872700	-4.22252500	-1.65799200
C	-0.69821500	-5.31913700	-2.02144000

H	0.57194500	-4.29675700	-0.59443900
H	1.22400400	-4.36674900	-2.24056000
C	-0.21482900	-6.54309900	-2.51821900
C	-1.09085900	-7.59411100	-2.81528900
C	-2.08321500	-5.16185300	-1.84317500
C	-2.96264200	-6.20940900	-2.15231000
C	-2.47104100	-7.42926500	-2.63504400
H	-3.15947900	-8.24574400	-2.87405700
H	-4.03902600	-6.06899900	-2.01239000
H	0.86131400	-6.67277100	-2.67908900
H	-0.69536300	-8.54023300	-3.19830600
H	-2.48298500	-4.21391800	-1.46927200
C	0.36763800	-2.94292500	-4.32326400
C	-0.07407800	-3.98001400	-5.16651700
C	1.66779900	-2.40937800	-4.50055500
C	0.74415900	-4.49917700	-6.17528400
H	-1.07699500	-4.39283300	-5.01737400
C	2.48228400	-2.95279400	-5.51257100
C	2.03520700	-3.98522300	-6.34416600
H	0.37727800	-5.30518000	-6.81794700
H	3.49152400	-2.54782600	-5.65082600
H	2.69332200	-4.38604200	-7.12180600
C	2.18829400	-1.23877000	-3.68743200
H	1.63592300	-1.13943600	-2.74047300
H	3.24152200	-1.42899900	-3.41251100
C	2.11295100	0.08579600	-4.47282400
H	2.71307200	0.04231600	-5.39649200
H	1.07572600	0.31005000	-4.77098000
H	2.48224700	0.92576400	-3.86388000

Transition State $TS2^{7}_{3.1b}$(1,7-HAA) :

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -1430.1519 cm-1

G_corr: 1.578676 Hartree

H_corr: 1.860614 Hartree

SCF: -6350.627632 Hartree

S: 593.388 Cal/Mol-Kelvin

H: -6348.767018 Hartree

G: -6349.048956 Hartree

Cartesian Coordinates:

H	9.63956900	1.92469700	-1.05280300
H	9.29119100	2.53082000	0.58254800
C	8.82975200	2.11986600	-0.32936500
H	8.17624200	2.89911500	-0.75456500
H	8.58600900	3.35975000	4.08554700
H	9.80116300	-0.47321900	-0.18482000
C	8.17698900	2.63594600	4.80963300
H	8.38527500	3.02890300	5.81811800
H	9.46560300	0.08148100	1.47177400
C	8.99369600	-0.25079600	0.53347500
H	8.30724600	1.78000700	2.48468400
C	8.03531900	0.81990500	-0.04640900
H	6.28962100	4.53766500	4.09419800
H	8.73453800	1.69052200	4.70547600
H	8.31240800	0.10397200	-2.08352100
C	7.25300000	1.60917300	2.25485200
C	7.48057400	0.29516100	-1.38600700
C	5.96376100	3.80431400	4.84988300
H	6.21216700	4.20873000	5.84589500
H	6.80681100	1.02119500	-1.86927600
C	6.91722400	1.11233100	0.97563300
C	6.65798200	2.43587100	4.63406400
H	8.45687500	-1.19043300	0.74323900
C	6.29191400	1.89023500	3.23792800
H	2.08636700	2.46518500	-7.53342400
H	2.89709400	2.17344700	-5.97048400

H	4.86692400	3.72533200	4.78763700
C	2.12802100	1.79320500	-6.66191000
H	6.92946000	-0.65122800	-1.26309400
C	5.56083500	0.89907500	0.68937500
C	6.17428400	1.43926000	5.71746500
H	6.42101700	1.81558400	6.72483400
H	4.17235600	3.25046600	0.05756600
H	2.44895900	0.79742500	-7.00987500
C	4.93885700	1.65774600	2.91366400
O	0.04566400	3.97836100	-6.42818200
H	6.65718600	0.45582900	5.59515900
H	5.24012000	0.50559500	-0.27743700
H	2.32729400	4.50653300	-1.49933700
H	0.02914200	5.80153300	-5.32322000
C	4.56927400	1.17011900	1.65361700
C	3.13964100	2.96747600	-0.13211800
H	-0.44532300	7.91632200	-4.09556200
C	-0.10931000	5.79855400	-4.24456200
C	0.31484800	3.13113800	-5.57776300
C	-0.38357900	6.97351000	-3.54317300
C	2.21680500	3.59708300	-0.91217000
C	0.74533800	1.71291200	-5.98298300
H	4.15206000	1.86743200	3.64491100
H	5.08437200	1.28442000	5.67878800
H	-0.44588700	1.77046100	-7.80614500
C	-0.02588600	4.57507900	-3.54648800
N	0.27404300	3.35850200	-4.20516800
C	-0.57388900	6.98641400	-2.15970800
C	-0.30709700	1.11470900	-6.93312700
C	3.12851700	0.93454400	1.31819700
C	2.48982200	1.81423400	0.44254200
H	-0.78128200	7.90519100	-1.61419100
H	0.83317700	1.08268800	-5.08231500
H	0.01091700	0.12161200	-7.29103700

C	-0.23729100	4.55295000	-2.14289900
H	0.54191900	2.56908700	-3.60997700
C	-0.49754900	5.77153600	-1.45488800
C	0.99195000	2.84407200	-0.79737800
H	4.16371200	-1.03500700	3.06952200
H	2.10255600	-7.29271400	-1.95732300
N	1.16229500	1.74300600	0.03766200
O	-1.11075100	7.89913400	0.54490600
C	-0.21214500	3.26839400	-1.36242100
C	2.47752900	-0.17285900	1.86398900
H	2.31929400	-8.16634500	-0.41430700
C	3.12788500	-1.10968200	2.74684200
H	-1.28564500	1.00102900	-6.43823800
N	-0.67628700	5.70351400	-0.05405000
C	1.71386800	-7.40806700	-0.93248600
C	-0.95387900	6.71858700	0.84973400
H	0.68384800	-7.79386400	-0.99271900
H	-3.21496600	6.34433600	2.47969100
H	-0.57818800	4.77084700	0.34449300
H	3.60142000	-5.37831400	-1.16611800
H	-1.03111000	5.14134000	2.35357800
H	3.88107900	-6.19654800	0.39333100
N	1.15585300	-0.54346300	1.63793300
C	-1.02606200	6.24767300	2.31546100
C	2.20557300	-2.06155300	3.06751800
C	-1.42706700	2.61769900	-1.10814500
C	3.21093900	-5.50572000	-0.14367200
C	-2.32000000	6.77139300	2.96058000
Co	-0.15653500	0.30997500	0.41011900
C	1.77406700	-6.07341900	-0.17817500
C	0.99113300	-1.71667600	2.36975400
H	2.31805100	-2.92619500	3.71863800
H	-2.82267100	4.01157500	-2.17836100
C	-2.69710000	3.12309700	-1.56273600

N	-1.59760500	1.47199700	-0.33667200
H	-2.37323400	7.86593200	2.86022900
H	1.12033100	-5.34210000	-0.69000100
H	-2.35259000	6.51552600	4.03209300
C	1.27192300	-6.26116700	1.26411100
H	3.25814500	-4.52549100	0.35675800
C	0.22212700	6.75859000	3.06401400
H	1.15224000	6.36458700	2.62328300
H	0.61954300	-4.31015300	1.19013300
N	0.67318700	-5.12595100	1.80056300
O	1.42663500	-7.31450400	1.87715900
C	-0.18560400	-2.46629100	2.48300900
C	-3.65507000	2.28507000	-1.06817600
C	-2.97287100	1.25390600	-0.32549700
H	0.26485400	7.85818400	3.02243600
N	-1.57015400	-0.92871000	1.10290800
H	0.19130100	6.45370700	4.12280800
C	0.20873500	-4.91501200	3.11740600
H	-3.93523800	-0.34561100	5.40400600
C	-1.37633700	-2.08571800	1.84888700
C	-0.22188300	-3.60822300	3.46521400
H	-4.73225400	2.33563200	-1.20925100
C	0.15868900	-5.95495300	4.06770400
C	-2.94072500	-0.88700300	0.86823100
C	-3.63177300	0.15338300	0.23709600
C	-3.45952800	0.12520000	6.27945800
H	0.49380200	-6.94962700	3.78184100
H	-0.96868100	-1.36700400	4.35734600
C	-0.68543900	-3.36189500	4.78894500
H	-3.73479500	1.19252300	6.28457000
N	-1.07336500	-2.04241800	5.11296100
H	-6.36220600	-1.91156400	-3.12048400
H	-3.87409600	-0.34277800	7.18593900
H	-5.18640500	-1.58447000	-1.15928700

C	-0.31108200	-5.68057400	5.35315800
C	-2.62234000	-2.78577600	2.04726200
C	-0.73163900	-4.40448300	5.73324200
C	-3.59374900	-2.03506100	1.45434000
C	-1.92632000	-0.03926800	6.25288100
C	-1.58686900	-1.54146300	6.30107700
H	-1.54042700	0.40291800	5.31436100
C	-7.45275000	-1.81836800	-2.99624800
C	-5.78859300	-0.86636400	-0.59435700
C	-5.12845700	0.10104800	0.17649500
H	-6.36796200	-3.55286200	-1.08998900
H	-7.92766800	-2.58473100	-3.63212700
H	-0.34796200	-6.49143300	6.08720400
H	-2.72639300	-3.71370300	2.60616300
H	-7.74886700	-0.82790600	-3.37861200
H	-1.09145700	-4.19278100	6.73841800
O	-1.78188300	-2.21165800	7.31284800
C	-7.45755000	-3.40428700	-1.02673700
H	-7.93587400	-4.18738400	-1.63928500
H	-4.66522100	-2.21826600	1.43013900
C	-7.88374200	-1.99828000	-1.51903100
C	-7.19706800	-0.92223300	-0.65193000
C	-5.88871300	1.03390100	0.91247500
C	-1.26565200	0.67426300	7.44468500
H	-5.35648300	1.77259600	1.51589500
H	-1.54728700	1.73956700	7.46523200
H	-7.75792300	-3.56485000	0.02170100
H	-1.58855000	0.20862100	8.38802000
C	-7.91720800	0.02186700	0.09518700
H	-0.16635500	0.61275400	7.39640800
C	-7.29018500	1.00889900	0.88730300
C	-9.42235900	-1.91380800	-1.45586100
H	-9.86313600	-2.70094000	-2.08898700
H	-9.80048900	-0.94670200	-1.82619400

H	-6.65701600	3.62088100	1.83786800
H	-9.00877800	-0.00489700	0.06713500
H	-9.80409100	-2.06550800	-0.43278500
H	-8.44588500	3.38098700	-0.00517100
C	-7.30044900	3.00856700	2.49090500
H	-6.65930000	2.50570700	3.23346600
C	-8.15369300	2.00518600	1.68867200
C	-9.05279000	2.80704300	0.71410500
H	-9.72468100	2.15217100	0.13713500
H	-7.95929800	3.69929100	3.04173300
C	-9.04604700	1.22409700	2.68611200
H	-8.43382800	0.64433200	3.39603500
H	-9.72016500	0.52003000	2.17318000
H	-9.68262800	3.52061300	1.27188800
H	-9.67302200	1.92092000	3.26785100
C	0.84517000	-3.15392000	-2.62120300
H	1.56010800	-3.95176100	-2.89387300
H	0.82802800	-3.10552900	-1.52103600
N	1.35604300	-1.87652000	-3.10801800
S	1.55374100	-0.58285900	-2.02125600
N	0.12564600	-0.75601200	-1.13518300
O	1.64779300	0.61815100	-2.90296400
O	2.69812300	-0.83358900	-1.10946400
C	1.91906100	-1.81705200	-4.46051600
C	3.12146900	-2.72796000	-4.67313900
H	2.19443500	-0.76806800	-4.64953300
H	1.12649600	-2.07551700	-5.18922100
C	3.21572300	-3.51110100	-5.83539700
C	4.33944000	-4.31645900	-6.06706800
C	4.16575900	-2.77675600	-3.73177300
C	5.28546800	-3.58608200	-3.95952400
C	5.37804800	-4.35535300	-5.12879400
H	6.25465500	-4.98667800	-5.30422600
H	6.09230300	-3.61496800	-3.22039100

H	2.40141300	-3.49084200	-6.56888500
H	4.39846400	-4.91992400	-6.97838200
H	4.09046800	-2.18513700	-2.81317000
C	-0.54807100	-3.54015800	-3.11245500
C	-0.79223000	-4.90991800	-3.28714300
C	-1.62284600	-2.61158800	-3.28392000
C	-2.06913400	-5.40631200	-3.58060500
H	0.04262200	-5.61182300	-3.18098200
C	-2.91036300	-3.14083500	-3.55286600
C	-3.13684900	-4.51070600	-3.70327800
H	-2.22430100	-6.48155400	-3.71001100
H	-3.74719300	-2.45136100	-3.68988200
H	-4.14300700	-4.87473300	-3.93268800
C	-1.43276400	-1.14379300	-3.23558900
H	-0.78832000	-0.88035100	-2.04160000
H	-0.58153700	-0.80757700	-3.84016800
C	-2.62468900	-0.22829600	-3.37948200
H	-3.07934400	-0.32565500	-4.38483800
H	-3.41644000	-0.42692200	-2.64117200
H	-2.32278100	0.82313400	-3.27064600

Intermediate $D_{3.1b}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.581102 Hartree

H_corr: 1.866084 Hartree

SCF: -6350.659374 Hartree

S: 599.793 Cal/Mol-Kelvin

H: -6348.793291 Hartree

G: -6349.078272 Hartree

Cartesian Coordinates:

H	-9.02148400	-3.13072200	-2.11495200
H	-9.38137300	-2.11477900	-0.70008500

C	-8.56356200	-2.54075100	-1.30280900
H	-7.99775800	-3.23314000	-0.65828500
H	-10.08318700	0.34196900	1.94118100
H	-8.92577200	-1.06738400	-3.62381500
C	-9.77876100	1.40006200	1.88405700
H	-10.39087300	1.95629000	2.61260900
H	-9.28906100	-0.01070900	-2.23990100
C	-8.47197300	-0.50048400	-2.79307600
H	-8.93823500	0.00139900	0.01537000
C	-7.63938800	-1.44346000	-1.88814700
H	-8.25375200	-0.00440200	3.72433800
H	-10.03724100	1.78018700	0.88193800
H	-7.06123900	-2.69712500	-3.57051700
C	-7.85749600	0.06770600	0.16049300
C	-6.57064000	-2.12931600	-2.76290500
C	-8.03238900	1.07269900	3.64734800
H	-8.67815900	1.60483000	4.36645900
H	-5.95666800	-2.83966900	-2.18622200
C	-7.01629700	-0.62828700	-0.73603900
C	-8.28342600	1.59154600	2.20896700
H	-7.83978200	0.29123300	-3.22734900
C	-7.36434700	0.83730200	1.22533200
H	-3.71747000	-7.11070200	-1.22264900
H	-3.93443300	-5.41370000	-0.71643400
H	-6.98825700	1.22295100	3.96430200
C	-3.41945800	-6.07196800	-1.43482000
H	-5.89287400	-1.40000200	-3.23543400
C	-5.63020900	-0.54314400	-0.53779600
C	-7.96717900	3.10720700	2.14849000
H	-8.61062800	3.66335900	2.85126400
H	-4.73075300	-2.00555600	1.91895200
H	-3.77101400	-5.80928100	-2.44610300
C	-5.96468800	0.90893300	1.38523700
O	-1.56394700	-7.51695700	0.44166000

H	-8.14342300	3.50879100	1.13704500
H	-4.92689700	-1.05339400	-1.19913700
H	-2.82540400	-3.70329100	2.87124700
H	-0.75379500	-7.53215000	2.38454600
C	-5.10169800	0.22684200	0.51768000
C	-3.64853500	-1.91439300	1.85774300
H	-0.08365100	-7.58882700	4.78341700
C	-0.49138800	-6.61718300	2.91056400
C	-1.44125200	-6.35173000	0.06612500
C	-0.11763800	-6.63093500	4.25503200
C	-2.69521700	-2.76314800	2.33898500
C	-1.88695200	-5.92496600	-1.34140200
H	-5.53148200	1.49285800	2.20324300
H	-6.92056700	3.32166700	2.41674800
H	-1.38238400	-7.86885300	-2.18952600
C	-0.54157000	-5.39127700	2.21250800
N	-0.92798100	-5.32316300	0.85397100
C	0.20984600	-5.46409200	4.94831500
C	-1.18085000	-6.80511900	-2.38876300
C	-3.61634900	0.29449900	0.69444300
C	-2.95696200	-0.80292000	1.25307100
H	0.49327900	-5.47697400	5.99906600
H	-1.62035900	-4.86890500	-1.51110200
H	-1.54273100	-6.56759100	-3.40282000
C	-0.19764300	-4.18742100	2.88772500
H	-0.86998800	-4.40446000	0.40432200
C	0.16869700	-4.23684100	4.26269100
C	-1.41689700	-2.19354400	1.99114200
H	-4.66511700	2.77868100	-0.21391300
H	-0.06897200	3.48690100	-6.73934000
N	-1.58020900	-0.95727200	1.36562900
O	1.05231900	-3.65123700	7.05260200
C	-0.20494900	-2.85841600	2.18830200
C	-2.93262200	1.45935100	0.34179300

H	-0.36429200	5.23953700	-6.51346100
C	-3.59418200	2.68127600	-0.05080900
H	-0.08864800	-6.65805800	-2.37630700
N	0.46889400	-3.01197000	4.90284600
C	0.05494100	4.33491600	-6.04799900
C	0.87728500	-2.77609700	6.20705700
H	1.13460000	4.50367000	-5.90605800
H	3.26679900	-1.33412400	6.14437900
H	0.37135000	-2.18636100	4.31398000
H	-2.28358800	2.90377900	-5.61082200
H	0.90274200	-0.66900100	5.63976800
H	-2.65345100	4.63252600	-5.36845700
N	-1.56120600	1.65442100	0.45414800
C	1.10285700	-1.28767400	6.53572400
C	-2.63254700	3.64602200	-0.12575400
C	1.01791400	-2.31368700	1.77304500
C	-2.15254400	3.75670800	-4.92566700
C	2.56913800	-1.08169200	6.95935300
Co	-0.17422400	0.26662100	0.72493500
C	-0.65092300	4.04949300	-4.71449000
C	-1.37314100	3.00116700	0.16207800
H	-2.74579600	4.70253800	-0.36102700
H	2.37730000	-4.03150200	2.25792400
C	2.27150800	-3.01783500	1.87654700
N	1.21043500	-1.03228300	1.27058700
H	2.80583000	-1.72546500	7.82027400
H	-0.18087300	3.16189800	-4.24850700
H	2.74695700	-0.03321700	7.24907700
C	-0.50752700	5.26096800	-3.77752200
H	-2.66241700	3.51398300	-3.97925200
C	0.13162300	-0.86591500	7.65442200
H	-0.92007100	-0.96262500	7.33908400
H	-0.23955800	3.92496300	-2.23958100
N	-0.28629600	4.92288400	-2.44580300

O	-0.61359200	6.41498500	-4.18602100
C	-0.14527200	3.67175300	0.12855700
C	3.24205000	-2.16910800	1.42891000
C	2.58709300	-0.93749100	1.06074500
H	0.27957200	-1.50193100	8.54059400
N	1.24363200	1.64283800	0.52577700
H	0.30524400	0.18272700	7.94601700
C	-0.20712900	5.77216500	-1.31996200
H	2.28464900	4.82127000	4.97803900
C	1.07680200	2.99940700	0.26700700
C	-0.13430300	5.16686800	-0.03757900
H	4.31516700	-2.33756500	1.37491100
C	-0.19412900	7.17644700	-1.43977700
C	2.62008600	1.43844000	0.46640700
C	3.27581900	0.21977500	0.68041400
C	1.39363300	5.02392600	5.59430700
H	-0.25496300	7.62325100	-2.43001300
H	-0.04647400	4.33198000	2.33630700
C	-0.05741100	5.99245000	1.11773300
H	1.40495500	4.32918200	6.44976100
N	-0.00673600	5.34946400	2.37502800
H	6.07031200	-2.87658300	-1.74893100
H	1.47468000	6.05172100	5.97977300
H	4.83897500	-0.95749500	-1.21564400
C	-0.11148000	7.95748400	-0.28522700
C	2.35233000	3.64800900	0.08833500
C	-0.04347500	7.39420400	0.99097400
C	3.30670400	2.67645500	0.18556600
C	0.09382400	4.86695600	4.78368400
C	0.08029100	5.90349900	3.64422800
H	0.05923300	3.84357000	4.36300600
C	7.15630500	-2.73415300	-1.63540900
C	5.43643200	-0.47401300	-0.43670400
C	4.77354400	0.18172200	0.60920800

H	6.00883200	-0.70582800	-3.16194900
H	7.65128800	-3.27528700	-2.45981200
H	-0.10130000	9.04734000	-0.38409000
H	2.48066000	4.71051300	-0.10935000
H	7.46382400	-3.20605000	-0.68765700
H	0.01716600	8.00733900	1.88822400
O	0.13956900	7.10954000	3.87399100
C	7.09499300	-0.61220400	-3.00806500
H	7.59312900	-1.11915600	-3.85185200
H	4.38514200	2.77705400	0.08660400
C	7.54696800	-1.23526700	-1.66361900
C	6.84680500	-0.50770100	-0.49700000
C	5.52559300	0.80935400	1.62429000
C	-1.14863200	5.07760000	5.67002500
H	4.98697100	1.30269800	2.43648900
H	-1.14253400	4.37728100	6.52098100
H	7.35304100	0.45856700	-3.05483200
H	-1.15955200	6.10490100	6.06536400
C	7.55971100	0.12943000	0.52970000
H	-2.08265900	4.92054400	5.10636100
C	6.92685500	0.79216100	1.60411100
C	9.08407700	-1.13738600	-1.58322000
H	9.53333000	-1.66454600	-2.44052100
H	9.48346600	-1.60474200	-0.66803000
H	6.27374900	1.40913800	4.31153100
H	8.65141700	0.11282100	0.50165100
H	9.43587100	-0.09308400	-1.62017200
H	8.05472900	-0.39660400	3.85263600
C	6.92016600	2.13292300	3.78842500
H	6.28100900	2.93084800	3.37573500
C	7.78199700	1.45951000	2.70115200
C	8.66992400	0.38861400	3.38371300
H	9.34976000	-0.10121000	2.66878100
H	7.57285600	2.59580900	4.54628000

C	8.68579200	2.54363300	2.06167900
H	8.08242800	3.32581100	1.57243900
H	9.36501800	2.12204000	1.30396700
H	9.29067600	0.84946800	4.17069900
H	9.30817200	3.02808800	2.83302900
C	-0.86215500	-0.46503500	-4.20009600
H	-1.87102500	-0.79603000	-4.50931900
H	-0.99721200	0.43742000	-3.58416200
N	-0.23794500	-1.49718100	-3.32086900
S	-0.90193000	-1.50045800	-1.73266000
N	0.00910500	-0.22262200	-1.12215400
O	-0.57171000	-2.83576500	-1.15758200
O	-2.32085400	-1.08533500	-1.74840500
C	-0.01878000	-2.83695400	-3.94544000
C	1.44340200	-3.22758100	-4.06406900
H	-0.47589400	-2.80366200	-4.94712900
H	-0.55975000	-3.59938800	-3.36615900
C	2.12162100	-3.78872600	-2.96607700
C	3.45659900	-4.19489600	-3.08667500
C	2.13038200	-3.07693400	-5.28085600
C	3.46647800	-3.48086900	-5.40253200
C	4.13244400	-4.04400000	-4.30621100
H	5.17178800	-4.37290200	-4.40306700
H	3.98536100	-3.36154000	-6.35894300
H	1.59153600	-3.91353100	-2.01718000
H	3.96507300	-4.64794700	-2.22971900
H	1.61435800	-2.63930400	-6.14187600
C	-0.03282300	-0.15956400	-5.42882000
C	-0.51366400	-0.55487600	-6.68029600
C	1.22080500	0.55201800	-5.34193700
C	0.19819300	-0.30095900	-7.86576700
H	-1.47638100	-1.07616300	-6.73563700
C	1.92770000	0.78953500	-6.56440900
C	1.43090000	0.36991300	-7.79423900

H	-0.20596300	-0.62294000	-8.82973000
H	2.88493700	1.31695300	-6.52725800
H	2.00027900	0.56990600	-8.70754000
C	1.72797400	1.01084600	-4.10052700
H	0.98490000	-0.54512400	-1.22692800
H	1.16433300	0.77319900	-3.19510500
C	3.00446000	1.77615400	-3.93816000
H	3.89035500	1.16488600	-4.20029000
H	3.04849900	2.67063300	-4.58711700
H	3.13778200	2.11291100	-2.89995600

Transition State $TS3^{7}_{3.1b}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -108.4346 cm-1

G_corr: 1.586958 Hartree

H_corr: 1.865396 Hartree

SCF: -6350.646043 Hartree

S: 586.021 Cal/Mol-Kelvin

H: -6348.780648 Hartree

G: -6349.059085 Hartree

Cartesian Coordinates:

H	-9.16681000	-2.52920900	-2.20282200
H	-9.40840900	-1.75095700	-0.62165400
C	-8.64291800	-2.07375600	-1.34502300
H	-8.03581700	-2.85701200	-0.86258800
H	-9.88541500	0.28009800	2.41572200
H	-9.16901700	-0.24980900	-3.36628700
C	-9.56476000	1.33131700	2.50342000
H	-10.11198500	1.77051300	3.35350300
H	-9.41322500	0.57169200	-1.80774300
C	-8.64643200	0.17826900	-2.49373000
H	-8.88801600	0.23836200	0.38095500

C	-7.75599100	-0.89448300	-1.81757900
H	-7.94318400	-0.35880600	3.98400900
H	-9.88645600	1.86728400	1.59519100
H	-7.32287500	-1.86137400	-3.71909500
C	-7.79848900	0.27368800	0.45384000
C	-6.76541300	-1.42944900	-2.87153900
C	-7.70405400	0.71463700	4.05998500
H	-8.28426900	1.13353600	4.89980400
H	-6.11587500	-2.22091300	-2.46422100
C	-7.03655100	-0.27346500	-0.60218800
C	-8.04641200	1.45593500	2.74308400
H	-8.04175200	1.03083300	-2.84404400
C	-7.21523600	0.85857900	1.58832200
H	-4.60798000	-6.62196800	-0.17631700
H	-4.40930400	-4.89801100	0.24534500
H	-6.63669700	0.80217100	4.31726300
C	-4.23471900	-5.65132900	-0.53941500
H	-6.11857300	-0.63195100	-3.27196100
C	-5.63799200	-0.22705900	-0.49799900
C	-7.70465900	2.95935500	2.89784000
H	-8.28532600	3.40354600	3.72423700
H	-4.58493100	-1.83223700	2.12075200
H	-4.82655600	-5.36139800	-1.42316400
C	-5.80631500	0.89210200	1.65390100
O	-2.07135500	-7.36585700	0.76330100
H	-7.94384100	3.51657500	1.97715300
H	-4.99296600	-0.63315900	-1.27981100
H	-2.63670200	-3.50046000	3.03369900
H	-0.83202800	-7.40979200	2.47315700
C	-5.02060200	0.35616400	0.62574700
C	-3.50912900	-1.76422000	1.97264700
H	0.27404800	-7.46228600	4.70617800
C	-0.42942600	-6.50182000	2.91618500
C	-1.96735600	-6.21330600	0.34533000

C	0.18777300	-6.51324600	4.16783000
C	-2.53239900	-2.59824100	2.43394000
C	-2.73832600	-5.75394600	-0.90350000
H	-5.30342600	1.33828700	2.51757400
H	-6.63744900	3.11947400	3.11825600
H	-2.81333400	-7.76881900	-1.72624800
C	-0.55078300	-5.28662900	2.20981300
N	-1.19944500	-5.22230100	0.95291300
C	0.68973400	-5.35202200	4.75748100
C	-2.51549200	-6.75891000	-2.04656500
C	-3.52314600	0.39110700	0.70006500
C	-2.84736800	-0.69950900	1.25600200
H	1.15830000	-5.35974200	5.73979100
H	-2.38702100	-4.75427900	-1.20967700
H	-3.11506800	-6.48300500	-2.92986700
C	-0.02028500	-4.08966800	2.76818800
H	-1.20686000	-4.30695200	0.49309600
C	0.58341300	-4.13628900	4.05766800
C	-1.27574700	-2.07889700	1.94546700
H	-4.59320000	2.92034300	-0.03249100
H	-0.96326000	4.09539000	-6.56970600
N	-1.47216800	-0.87913300	1.26981200
O	1.98645500	-3.55740100	6.62629600
C	-0.06779200	-2.78037100	2.03252400
C	-2.84537200	1.54493900	0.29874700
H	-0.74985400	5.83802500	-6.22865500
C	-3.51435800	2.79866800	0.03726800
H	-1.45731200	-6.80544400	-2.35303700
N	1.04585300	-2.91829400	4.60684500
C	-0.60282800	4.82440300	-5.82627900
C	1.69314700	-2.68518000	5.81035900
H	0.48104000	4.67073200	-5.69548600
H	4.08605500	-1.34237900	5.30269300
H	0.87713000	-2.09776000	4.02652600

H	-3.24711200	4.07256300	-5.44287600
H	1.69820000	-0.58698400	5.21110600
H	-3.12482600	5.81913200	-5.09047700
N	-1.46773200	1.71702500	0.31908800
C	2.02958300	-1.20404200	6.06810600
C	-2.54608300	3.75914600	-0.01632800
C	1.12052100	-2.29435900	1.46079900
C	-2.88738200	4.81335900	-4.71032300
C	3.55429300	-1.05417500	6.22397000
Co	-0.09560900	0.29263700	0.47009500
C	-1.36565200	4.67158400	-4.49986200
C	-1.27781600	3.08305400	0.14386100
H	-2.66375400	4.83429700	-0.13912500
H	2.48141300	-4.04535200	1.81921200
C	2.36087700	-3.03258500	1.43986400
N	1.29726200	-1.02997000	0.91673800
H	3.91393700	-1.69967400	7.03986600
H	-1.16423700	3.66725900	-4.08148900
H	3.82091900	-0.01135700	6.46106500
C	-0.90197200	5.75525400	-3.50851600
H	-3.44471600	4.66098200	-3.77206200
C	1.28803400	-0.73323000	7.33355200
H	0.19426300	-0.78980100	7.20974900
H	-0.63207900	4.26301100	-2.12706600
N	-0.55084900	5.27125600	-2.25506000
O	-0.88046600	6.94263900	-3.82627300
C	-0.04130300	3.74516000	0.13235800
C	3.30351600	-2.21362400	0.88684800
C	2.64881800	-0.96245200	0.58517700
H	1.56551900	-1.36703900	8.18975300
N	1.32905300	1.66805400	0.26797800
H	1.55075600	0.30989100	7.57365500
C	-0.22943700	5.99147500	-1.08071100
H	2.97761400	4.34746200	4.81605600

C	1.17845500	3.04757900	0.16982800
C	-0.00641300	5.24998200	0.11111500
H	4.36034300	-2.41318900	0.72326100
C	-0.14163500	7.39739500	-1.07173500
C	2.69349600	1.44497900	0.11791200
C	3.33002100	0.19836100	0.19571300
C	2.15054200	4.52005400	5.52371200
H	-0.30501600	7.94344600	-1.99871700
H	0.32969500	4.18535000	2.36735000
C	0.26439100	5.95466000	1.31767000
H	2.20824000	3.75110900	6.31102900
N	0.43386800	5.19134800	2.49407600
H	5.94376200	-2.62673900	-2.75144400
H	2.30225100	5.50624800	5.98826000
H	4.71966600	-0.75885400	-1.94290300
C	0.14790500	8.05350300	0.12635000
C	2.45903700	3.68801500	-0.01325800
C	0.34558900	7.36025100	1.32191200
C	3.39342100	2.69358500	-0.07491100
C	0.78243200	4.47552200	4.81959800
C	0.70660500	5.61532800	3.78647900
H	0.67538700	3.49833800	4.31098600
C	7.03171300	-2.45791100	-2.76461300
C	5.38582700	-0.37232800	-1.16542300
C	4.81864900	0.14292700	0.00703500
H	5.68019800	-0.31503300	-3.92672900
H	7.42991700	-2.88287700	-3.70227200
H	0.21521100	9.14579800	0.12916100
H	2.60477300	4.76245800	-0.10830400
H	7.46849100	-3.02194000	-1.92404400
H	0.55863400	7.87515200	2.25690200
O	0.86931600	6.78905600	4.11452100
C	6.77413600	-0.20053200	-3.87306100
H	7.19560500	-0.59097100	-4.81511400

H	4.46710400	2.78711000	-0.22276800
C	7.37893200	-0.95224100	-2.66086300
C	6.78572200	-0.38893400	-1.35243500
C	5.66069600	0.63243700	1.02739800
C	-0.37260900	4.63570400	5.82740700
H	5.19628200	1.01963700	1.93706000
H	-0.32176200	3.85547000	6.60406300
H	6.99788900	0.87771800	-3.82236300
H	-0.31102300	5.61908400	6.31853800
C	7.58904200	0.11152500	-0.31735900
H	-1.35607100	4.56220700	5.33527700
C	7.05511500	0.62253400	0.88591800
C	8.91286600	-0.80524800	-2.72732200
H	9.28232300	-1.20646200	-3.68520300
H	9.41958700	-1.36475300	-1.92398400
H	6.63857700	0.88707900	3.69583300
H	8.67406800	0.10705700	-0.44264400
H	9.23087300	0.24877700	-2.66771100
H	8.35022900	-0.84762200	2.85899600
C	7.24706900	1.67137600	3.21667000
H	6.58463500	2.51574400	2.96437200
C	8.00679500	1.14231100	1.98335600
C	8.93463400	-0.00967300	2.44518700
H	9.54575100	-0.40430400	1.61802400
H	7.96641000	2.03302100	3.96933300
C	8.86796700	2.29846800	1.41531500
H	8.23574700	3.13839300	1.08361600
H	9.47661500	1.97757600	0.55515800
H	9.62482700	0.34378200	3.22998100
H	9.55834300	2.67801800	2.18761200
C	-1.38636400	-1.32224600	-4.59839700
H	-2.02756900	-1.98141100	-5.21083900
H	-2.04694100	-0.52996200	-4.21385700
N	-0.87302100	-2.08586800	-3.44828900

S	-1.23951800	-1.53784300	-1.88453300
N	-0.04392600	-0.40032300	-1.48099400
O	-1.16902700	-2.76335700	-1.04958700
O	-2.50102600	-0.77046000	-1.96364200
C	-0.45420200	-3.49175500	-3.65489900
C	0.99793200	-3.82994300	-3.35660500
H	-0.65354700	-3.69270600	-4.72062800
H	-1.11279400	-4.15732200	-3.07602100
C	1.31734200	-4.66251100	-2.27067300
C	2.63881500	-5.06946600	-2.04331500
C	2.03424100	-3.39476500	-4.20388500
C	3.35478800	-3.80023000	-3.97933200
C	3.65986200	-4.64520500	-2.90166900
H	4.69006900	-4.97496400	-2.73628200
H	4.14683100	-3.47092200	-4.65934400
H	0.52290700	-4.99460300	-1.59630400
H	2.86654800	-5.72458700	-1.19731300
H	1.80256100	-2.74720800	-5.05534300
C	-0.24210300	-0.78418500	-5.42551800
C	0.04577600	-1.33353800	-6.67734300
C	0.63499700	0.20580900	-4.86392200
C	1.20305000	-0.97108700	-7.38618800
H	-0.63847200	-2.07591100	-7.10373500
C	1.83831600	0.50443000	-5.57121900
C	2.11115900	-0.06625200	-6.81225800
H	1.40426500	-1.40839600	-8.36845000
H	2.53688700	1.23466700	-5.15500900
H	3.02745000	0.20416500	-7.34553100
C	0.27784900	0.93444400	-3.68774600
H	0.84707500	-0.92182900	-1.55487700
H	-0.77082100	0.95567300	-3.39356700
C	1.16178000	1.97539000	-3.09193100
H	2.18983600	1.61833300	-2.91853300
H	1.24572600	2.85542700	-3.76058400

H	0.76492100	2.31424900	-2.13043400

Intermediate $E_{3.1b}$:

$E_{[3.2b]}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.262117 Hartree

H_corr: 0.328319 Hartree

SCF: -1278.861017 Hartree

S: 139.334 Cal/Mol-Kelvin

H: -1278.532698 Hartree

G: -1278.5989 Hartree

Cartesian Coordinates:

C	0.07168000	-0.00155500	1.27642600
H	-0.88200800	0.33655500	1.71149500
H	0.62873600	-0.49862700	2.08506000
N	-0.27887600	-1.05582200	0.28751100
S	0.96599300	-2.15791400	-0.02246800
N	2.14897000	-1.16988100	-0.78492000
O	0.52308900	-3.10531700	-1.05239000
O	1.44189400	-2.62157200	1.29420300
C	-1.04942900	-0.60400800	-0.89407300
C	-2.45812600	-0.19615900	-0.49984100
H	-1.08708300	-1.45486400	-1.59120500
H	-0.53502300	0.22746400	-1.41047800
C	-3.01055500	1.00450500	-0.97501800
C	-4.32898400	1.35993100	-0.65631500
C	-3.24495100	-1.03335100	0.31209400
C	-4.55846600	-0.67646200	0.63678100
C	-5.10574400	0.52053800	0.15152900
H	-6.13386700	0.79761500	0.40458400
H	-5.16063300	-1.33756800	1.26808400
H	-2.40311500	1.66661500	-1.60184100

H	-4.74697400	2.29738500	-1.03674900
H	-2.81356100	-1.96475700	0.69153300
C	0.81956400	1.20315600	0.71735200
C	2.12916400	1.11399600	0.17251500
C	0.17143300	2.45002600	0.74112500
C	2.72976100	2.28357600	-0.32186300
C	0.78731300	3.60785700	0.25195200
H	-0.84087000	2.50977000	1.15516300
C	2.07405300	3.52116300	-0.28488200
H	3.73669400	2.23970100	-0.74467000
H	0.26260500	4.56739300	0.28946400
H	2.57341900	4.41275300	-0.67651900
C	2.86777000	-0.22766200	0.13777800
H	2.86031000	-0.65788700	1.15807700
H	2.79990300	-1.79831000	-1.27070300
C	4.33056200	-0.15581100	-0.31029700
H	4.90482500	0.54136000	0.31763000
H	4.79887200	-1.14832600	-0.21332400
H	4.42109000	0.16695900	-1.36033400

Intermediate $A_{3.1c}$

$A_{[Co(II)(\mathbf{P2})]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -0.6444 cm-1

G_corr: 1.303862 Hartree

H_corr: 1.538533 Hartree

SCF: -5071.844772 Hartree

S: 493.906 Cal/Mol-Kelvin

H: -5070.306239 Hartree

G: -5070.54091 Hartree

Cartesian Coordinates:

H	9.34557400	-0.14040400	-3.78545600

H	9.47145500	0.54656400	-2.14976100
C	8.75950000	0.19265700	-2.91205200
H	8.14622900	1.05428500	-3.22278500
H	9.71603800	1.52630400	1.38664100
H	9.35824500	-2.51245300	-2.82716300
C	9.35441100	0.90304800	2.22112500
H	9.83675900	1.27520200	3.13960600
H	9.48208400	-1.87248100	-1.17248600
C	8.77080200	-2.15200900	-1.96566200
H	8.83790400	-0.00596300	-0.02882900
C	7.87092900	-0.96256900	-2.38579200
H	7.71186800	3.09209200	1.79248100
H	9.70860400	-0.12865900	2.06072200
H	7.58078900	-1.77234300	-4.38581500
C	7.74555200	-0.00345800	-0.02029700
C	6.96179800	-1.43261100	-3.53954400
C	7.42990200	2.44785900	2.64143500
H	7.94496100	2.82671100	3.54050400
H	6.31366800	-0.62227700	-3.91209900
C	7.06418100	-0.47294200	-1.16513400
C	7.82154600	0.97252100	2.37529500
H	8.16611400	-2.99423300	-1.59134000
C	7.07840200	0.46452300	1.12208300
H	0.81818200	5.26259400	-6.18211000
H	1.72879900	4.14059400	-5.13937400
H	6.34700900	2.56485000	2.80506700
C	0.78327600	4.27924800	-5.68848900
H	6.31991800	-2.27843400	-3.24294700
C	5.66200300	-0.46917300	-1.13933400
C	7.42014900	0.10667500	3.59609100
H	7.93893700	0.45844200	4.50403100
H	4.53043500	2.61025100	-0.32965100
H	0.72392500	3.50111900	-6.46679500
C	5.66809200	0.46031300	1.10286900

O	-0.37802100	6.52365900	-4.06136400
H	7.69005500	-0.95036000	3.43833700
H	5.08757500	-0.81911300	-2.00003500
H	2.60443000	4.53152000	-0.30965700
H	-0.21123300	7.60998600	-2.16269900
C	4.95644600	-0.00278200	-0.01173100
C	3.45322700	2.48798400	-0.24176800
H	0.00000000	8.84732300	0.00037300
C	-0.11942100	7.07818100	-1.21736900
C	-0.34905400	5.34352200	-3.71821200
C	-0.00000100	7.75293400	0.00032000
C	2.48839300	3.45192900	-0.23521700
C	-0.43637600	4.20313800	-4.75023000
H	5.10347700	0.81318300	1.97116800
H	6.33756700	0.14909300	3.79443200
H	-1.81277000	5.31660100	-6.01802200
C	-0.11975200	5.66991700	-1.21896300
N	-0.23309500	4.91174900	-2.40530200
C	0.11941700	7.07806200	1.21794400
C	-1.75558100	4.32955500	-5.53426700
C	3.45714200	-0.00221300	-0.00797900
C	2.78078800	1.21745300	-0.10422100
H	0.21123200	7.60977500	2.16332600
H	-0.42381200	3.22481200	-4.23235900
H	-1.81989500	3.55424000	-6.31496400
C	-0.00000400	4.95247700	0.00018400
H	-0.22114400	3.90204400	-2.26496800
C	0.11974600	5.66979800	1.21940000
C	1.22215600	2.77229200	-0.10253700
H	4.53211300	-2.61405100	0.30641100
H	-0.78962400	-3.50321000	-6.45534400
N	1.40027900	1.39276800	-0.04645300
O	0.37795900	6.52325900	4.06189300
C	-0.00000300	3.44824300	0.00011200

C	2.78100200	-1.22187600	0.09056100
H	-0.88332400	-5.26459700	-6.17016500
C	3.45436900	-2.49225200	0.22390600
H	-2.63244400	4.22368800	-4.87497300
N	0.23308800	4.91151400	2.40566500
C	-0.84025000	-4.28153100	-5.67661300
C	0.34905600	5.34315600	3.71861800
H	-1.77831900	-4.14139700	-5.11522800
H	-1.72891400	4.14020100	5.13959700
H	0.22112600	3.90182200	2.26523300
H	1.75563700	-3.56190000	-6.33726500
H	0.42367800	3.22439300	4.23256600
H	1.74964200	-5.32414000	-6.03940900
N	1.40036800	-1.39732100	0.03948700
C	0.43627800	4.20266900	4.75053100
C	2.48973400	-3.45642900	0.22160100
C	-1.22216100	2.77227900	0.10268400
C	1.70033300	-4.33676900	-5.55545200
C	-0.78340200	4.27875600	5.68875600
Co	0.00000300	-0.00229100	0.00000200
C	0.39174000	-4.20791700	-4.75431400
C	1.22269700	-2.77690500	0.09600500
H	2.60622200	-4.53605700	0.29481700
H	-2.60444700	4.53148500	0.30990200
C	-2.48840400	3.45190100	0.23537100
N	-1.40028000	1.39275900	0.04646600
H	-0.81827500	5.26205800	6.18246600
H	0.38782200	-3.22963400	-4.23623400
H	-0.72411800	3.50055300	6.46699400
C	0.31528500	-5.34820500	-3.72137000
H	2.58588900	-4.23172800	-4.90778800
C	1.75546300	4.32894100	5.53462400
H	2.63234300	4.22309400	4.87534900
H	0.20200700	-3.90661900	-2.26702700

N	0.21233300	-4.91634100	-2.40735800
O	0.34057400	-6.52839500	-4.06463800
C	0.00001100	-3.45286800	0.00006300
C	-3.45323700	2.48795400	0.24178800
C	-2.78079100	1.21743600	0.10416400
H	1.81268700	5.31593500	6.01847900
N	-1.40035300	-1.39732600	-0.03948700
H	1.81971000	3.55354500	6.31524600
C	0.10921600	-5.67447500	-1.22007400
H	-2.58585700	-4.23154600	4.90809700
C	-1.22267500	-2.77691100	-0.09594200
C	0.00001100	-4.95709500	0.00010600
H	-4.53044900	2.61021400	0.32964000
C	0.10891800	-7.08275200	-1.21847500
C	-2.78098500	-1.22188600	-0.09067800
C	-3.45713800	-0.00222700	0.00782600
C	-1.70025400	-4.33650700	5.55571000
H	0.19254000	-7.61452900	-2.16457800
H	-0.20198000	-3.90648300	2.26717400
C	-0.10919600	-5.67440200	1.22032800
H	-1.75554600	-3.56159900	6.33748400
N	-0.21231000	-4.91619700	2.40756600
H	-6.34698000	2.56523500	-2.80507400
H	-1.74948200	-5.32385500	6.03972200
H	-5.10335000	0.81335800	-1.97135200
C	0.00000600	-7.75751600	0.00018900
C	-2.48969900	-3.45644400	-0.22160900
C	-0.10890400	-7.08267900	1.21881300
C	-3.45433600	-2.49226900	-0.22404400
C	-0.39172100	-4.20763300	4.75448000
C	-0.31525800	-5.34798300	3.72160500
H	-0.38788900	-3.22938300	4.23633800
C	-7.42987600	2.44810800	-2.64155400
C	-5.66801700	0.46040100	-1.10312300

C	-4.95643900	-0.00279900	0.01147800
H	-6.33717400	0.14959200	-3.79472700
H	-7.94489400	2.82702800	-3.54061600
H	0.00000300	-8.85190800	0.00022200
H	-2.60618000	-4.53607400	-0.29479000
H	-7.71198500	3.09219400	-1.79253700
H	-0.19252900	-7.61440000	2.16494700
O	-0.34059200	-6.52815300	4.06493800
C	-7.41977700	0.10704800	-3.59651600
H	-7.93849100	0.45889000	-4.50447000
H	-4.53207100	-2.61407700	-0.30664900
C	-7.82139200	0.97269300	-2.37565000
C	-7.07832600	0.46460100	-1.12242900
C	-5.66207000	-0.46929600	1.13899200
C	0.84033400	-4.28112000	5.67670500
H	-5.08769600	-0.81930600	1.99970100
H	0.78972000	-3.50274500	6.45538200
H	-7.68960300	-0.95003300	-3.43893600
H	0.88348800	-5.26414700	6.17032700
C	-7.74554900	-0.00349800	0.01986000
H	1.77836100	-4.14098000	5.11524900
C	-7.06424900	-0.47308000	1.16469900
C	-9.35426600	0.90304000	-2.22164900
H	-9.83655600	1.27532500	-3.14010700
H	-9.71603800	1.52609800	-1.38708000
H	-6.31390900	-0.62258200	3.91168700
H	-8.83790200	-0.00601700	0.02831700
H	-9.70837400	-0.12873200	-2.06148500
H	-8.14649000	1.05397600	3.22237500
C	-6.96200800	-1.43290400	3.53905200
H	-6.32010200	-2.27870700	3.24245700
C	-7.87107000	-0.96281400	2.38526600
C	-8.75971300	0.19235000	2.91154200
H	-9.47162700	0.54628800	2.14922600

H	-7.58105100	-1.77268200	4.38526700
C	-8.77087600	-2.15225200	1.96498800
H	-8.16613500	-2.99443200	1.59065200
H	-9.48210700	-1.87269000	1.17177900
H	-9.34583800	-0.14078800	3.78488200
H	-9.35837200	-2.51277500	2.82642100

A_{1a}:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.214209 Hartree

H_corr: 0.288571 Hartree

SCF: -1234.663938 Hartree

S: 156.509 Cal/Mol-Kelvin

H: -1234.375366 Hartree

G: -1234.449729 Hartree

Cartesian Coordinates:

C	0.30342700	1.58405400	0.54565900
N	0.61545300	0.14724500	0.28083900
S	2.17353700	-0.33509900	0.60187300
N	3.03100900	0.44233200	-0.80896900
O	2.28265800	-1.78742100	0.42308200
O	2.64515900	0.33533500	1.81718600
C	-0.04077400	-0.47552900	-0.90160500
C	-1.30765900	-1.23339000	-0.54502800
H	0.67845000	-1.16302700	-1.37319300
H	-0.25671600	0.31825500	-1.63670800
C	-2.48863300	-1.02219500	-1.27378700
C	-3.64443200	-1.76233300	-0.99039800
C	-1.29878800	-2.19899300	0.47674400
C	-2.45429500	-2.93361100	0.76563200
C	-3.63038300	-2.71850100	0.03263500
H	-4.53264400	-3.29504500	0.25898500

H	-2.43490300	-3.68261200	1.56344200
H	-2.50683200	-0.26886600	-2.06919200
H	-4.55839300	-1.58673900	-1.56649400
H	-0.37940300	-2.37488600	1.04289000
N	4.20820200	0.06263200	-0.94881500
N	5.29808300	-0.22423300	-1.16755300
C	-1.57450600	3.66014600	-0.85711100
C	-1.98460400	2.67214100	0.20891000
C	-1.16674900	1.76981600	0.79034500
H	0.67565200	2.20106100	-0.29144100
H	0.87316500	1.86272000	1.44587300
H	-1.65176200	4.69540100	-0.47831100
H	-2.25554300	3.60031900	-1.72487900
H	-0.54787600	3.52134900	-1.22405800
C	-3.43337400	2.76580200	0.62642200
H	-3.67156000	3.77287300	1.01451300
H	-3.68919700	2.03069000	1.40350000
H	-4.10437500	2.59904200	-0.23572800
H	-1.58177800	1.10746600	1.55966200

Intermediate $B_{3.1c}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.539956 Hartree

H_corr: 1.829647 Hartree

SCF: -6306.512525 Hartree

S: 609.707 Cal/Mol-Kelvin

H: -6304.682878 Hartree

G: -6304.972569 Hartree

Cartesian Coordinates:

H	-9.19221000	3.00638000	-0.75848400
H	-8.95888300	1.90682400	-2.13676100
C	-8.44053500	2.41457900	-1.30809900

H	-7.71301200	3.11606200	-1.74822900
H	-8.52330300	-0.67122300	-4.69122800
H	-9.56187000	1.01968900	0.80405400
C	-8.18928900	-1.69999100	-4.47757600
H	-8.45839900	-2.31844000	-5.34927200
H	-9.32483300	-0.12389500	-0.53796500
C	-8.80120900	0.45106400	0.24229600
H	-8.17408800	-0.19096500	-2.50803800
C	-7.74249400	1.41176800	-0.35479500
H	-6.20015100	-0.20854100	-5.70649000
H	-8.76578000	-2.07883400	-3.61739600
H	-7.89297600	2.77923500	1.33111400
C	-7.11309100	-0.18212600	-2.24819100
C	-7.11046300	2.21049600	0.80269600
C	-5.95089200	-1.26409700	-5.50985000
H	-6.25756800	-1.85600100	-6.38893100
H	-6.36434200	2.93851800	0.44349600
C	-6.69778400	0.59758800	-1.14640100
C	-6.66809500	-1.77792600	-4.23602000
H	-8.33423100	-0.26761000	0.93507300
C	-6.21915300	-0.93702200	-3.02255300
H	-1.91570100	6.73608400	4.23518900
H	-2.63523000	5.36583600	3.35080300
H	-4.85536800	-1.33831000	-5.42524300
C	-1.82774900	5.65548400	4.04318300
H	-6.62613400	1.55513300	1.54456300
C	-5.33277600	0.60215200	-0.82435800
C	-6.29312600	-3.26242500	-3.99907800
H	-6.59600400	-3.87887300	-4.86238300
H	-3.90463600	2.43145700	-2.15359300
H	-1.98411300	5.11993400	4.99417300
C	-4.85605600	-0.90223100	-2.66603700
O	-0.20699100	7.38341100	2.21303100
H	-6.79937500	-3.66079300	-3.10428500

H	-4.96809200	1.18905000	0.02138700
H	-2.01423900	4.37525900	-1.99719500
H	0.06864300	7.95573500	0.17673700
C	-4.39995100	-0.14288600	-1.57712000
C	-2.87464200	2.34440100	-1.81579200
H	0.59564900	8.68087400	-2.15182100
C	0.26876500	7.22508300	-0.60393500
C	-0.22444600	6.15349000	2.18014600
C	0.56896500	7.61356900	-1.91079200
C	-1.92468200	3.32031800	-1.74513700
C	-0.43885400	5.33075200	3.46136600
H	-4.12056200	-1.45838500	-3.25445300
H	-5.20910600	-3.39792500	-3.85907800
H	0.68644400	6.74713100	4.67901600
C	0.23090000	5.85226700	-0.28205200
N	-0.04991500	5.39706400	1.02711800
C	0.83793800	6.68550100	-2.91894600
C	0.68004700	5.66727500	4.46511100
C	-2.93762000	-0.10212300	-1.25491500
C	-2.25533100	1.11791600	-1.36472500
H	1.07416900	6.99138200	-3.93652600
H	-0.39380100	4.25451800	3.22718300
H	0.52721000	5.12239800	5.41085200
C	0.49294300	4.88223900	-1.28535500
H	-0.11332600	4.38331200	1.13898800
C	0.80185600	5.31424900	-2.60518200
C	-0.71914000	2.69454700	-1.25644000
H	-4.00905300	-2.72833000	-0.85606300
H	2.45819200	-4.59062900	5.51425100
N	-0.91608800	1.33313400	-1.05525400
O	1.45660300	5.52189400	-5.50869100
C	0.45808200	3.40681600	-0.99228700
C	-2.27372900	-1.29614500	-0.93378200
H	2.32804900	-6.28641300	4.96338600

C	-2.93227300	-2.57815100	-0.81894400
H	1.67226800	5.39071200	4.07337000
N	1.06816400	4.31535900	-3.56917700
C	2.32887200	-5.23695100	4.63095600
C	1.36783400	4.44797800	-4.91601100
H	3.19889600	-5.08858200	3.97141200
H	3.77629400	3.15317500	-5.49682300
H	1.02390000	3.36083900	-3.21450100
H	-0.07502300	-4.41375200	5.74373800
H	1.49993700	2.27003700	-4.92894000
H	-0.28618300	-6.10045000	5.19358600
N	-0.89614700	-1.44494000	-0.80931000
C	1.58253600	3.10848000	-5.64683200
C	-1.95143400	-3.52173700	-0.69779600
C	1.63037300	2.77822000	-0.55128400
C	-0.19695400	-5.05638600	4.85652100
C	2.99123100	3.09002200	-6.26776400
Co	0.45591900	-0.01448700	-0.58702100
C	1.00797000	-4.91064400	3.90857600
C	-0.69213500	-2.81757500	-0.71503800
H	-2.05464900	-4.60254300	-0.61960700
H	2.93044700	4.57851900	-0.19880100
C	2.83619400	3.49422400	-0.20513800
N	1.82723200	1.40686100	-0.46143400
H	3.11388700	3.94734100	-6.94713300
H	1.05806200	-3.86725100	3.54528700
H	3.15139200	2.16329000	-6.84253300
C	0.83354600	-5.87398000	2.72053000
H	-1.14231500	-4.78131700	4.35999200
C	0.49301200	2.94399400	-6.72383200
H	-0.51532700	2.90711300	-6.28042900
H	0.88401700	-4.23795400	1.47947800
N	0.79226700	-5.25351400	1.48042900
O	0.74232400	-7.08817400	2.89340800

C	0.55411500	-3.46453300	-0.74165500
C	3.78086100	2.55520200	0.08981100
C	3.16633400	1.26172600	-0.11253100
H	0.52527100	3.79215100	-7.42498400
N	1.89572200	-1.38535200	-0.51457100
H	0.64839200	2.01444500	-7.29547300
C	0.67864200	-5.83611100	0.19722800
H	2.56322200	-3.44110800	-5.62018500
C	1.76489600	-2.76028800	-0.68904500
C	0.58130700	-4.95948300	-0.91490500
H	4.81287800	2.70906000	0.39698300
C	0.66483900	-7.23193000	0.00636400
C	3.26161200	-1.17602600	-0.35818800
C	3.87444900	0.05417100	-0.08442200
C	1.70526800	-3.51864100	-6.30765600
H	0.72619900	-7.88631300	0.87370700
H	0.44820400	-3.62147700	-3.03607400
C	0.49653700	-5.51054100	-2.22318200
H	1.72187400	-2.64011300	-6.97300300
N	0.42823000	-4.60473300	-3.30464900
H	5.95380500	-0.38806800	4.18013400
H	1.84260200	-4.42137100	-6.92296000
H	5.11960900	-0.90792200	2.10203200
C	0.56826900	-7.73846200	-1.29156500
C	3.06002700	-3.39841100	-0.71343400
C	0.48891600	-6.90594800	-2.41016900
C	3.98572100	-2.41817800	-0.49881000
C	0.36749100	-3.59661400	-5.54466200
C	0.36886000	-4.86225600	-4.66627500
H	0.27216200	-2.69684300	-4.90711300
C	7.05269800	-0.32041000	4.20547400
C	5.83531400	-0.47788000	1.39504400
C	5.34440300	0.07465800	0.20409800
H	6.21857800	-2.71074600	3.01946000

H	7.39088500	-0.74358200	5.16674000
H	0.55893000	-8.82315600	-1.43684100
H	3.22132600	-4.46428800	-0.86492800
H	7.32211900	0.74836200	4.19089100
H	0.42202500	-7.30496400	-3.42070100
O	0.33724700	-5.98751200	-5.16074500
C	7.30914800	-2.57215900	3.08470600
H	7.64599700	-3.02146900	4.03446100
H	5.06811500	-2.51192000	-0.44514900
C	7.70862400	-1.07638100	3.02250600
C	7.21391100	-0.47071200	1.69241900
C	6.24683900	0.64021300	-0.72016500
C	-0.82669800	-3.64666000	-6.51317100
H	5.84487800	1.05438900	-1.64751600
H	-0.81357100	-2.77917200	-7.19275800
H	7.76926300	-3.13966800	2.25908600
H	-0.78224400	-4.56521300	-7.11769900
C	8.08077200	0.09899400	0.74741600
H	-1.78772300	-3.64358100	-5.97378300
C	7.62597000	0.65782600	-0.46763800
C	9.23956100	-0.98123000	3.18143800
H	9.54083400	-1.42569200	4.14403900
H	9.59236900	0.06334200	3.17873500
H	7.25847600	2.62627100	-2.49729600
H	9.15312800	0.11182000	0.95545500
H	9.77388400	-1.52846500	2.38726500
H	8.72759600	3.21500700	-0.46060800
C	7.96798300	1.81499600	-2.72905600
H	7.42689200	1.03371400	-3.28788900
C	8.64429500	1.25586800	-1.46077000
C	9.41462400	2.41242100	-0.77516000
H	9.96244300	2.07214900	0.11781200
H	8.73227500	2.23158500	-3.40517200
C	9.64742800	0.15715000	-1.89383500

H	9.12870100	-0.67976000	-2.38940200
H	10.20429200	-0.25464500	-1.03733000
H	10.15107400	2.84935400	-1.47088700
H	10.38507700	0.56834000	-2.60384500
C	-1.63762000	-0.62021200	4.58310500
N	-1.87765100	0.38135600	3.48338200
S	-0.53819100	1.14642800	2.86480000
N	0.26373600	-0.05246200	1.68076400
O	0.42423600	1.34405800	3.95348700
O	-0.97074300	2.21327200	1.96221800
C	-2.99551900	0.10228600	2.54358100
C	-4.32646300	0.09308200	3.27170500
H	-2.97952300	0.89255300	1.77807500
H	-2.82907800	-0.85999800	2.02676600
C	-5.20234600	-0.99502600	3.12417300
C	-6.45238100	-0.99424100	3.76021300
C	-4.71476600	1.18183400	4.07326900
C	-5.95998000	1.18136300	4.71073800
C	-6.83280900	0.09373500	4.55510700
H	-7.80709500	0.09592000	5.05314500
H	-6.25335300	2.03532400	5.32889400
H	-4.90873500	-1.84588000	2.50001900
H	-7.12591000	-1.84755000	3.63599700
H	-4.03107300	2.02608000	4.20135800
N	1.11271100	-0.75876000	2.26173900
N	1.92989200	-1.45512800	2.67094600
C	-3.58901000	-1.29552800	6.93162500
C	-2.46929100	-0.28485800	6.97328900
C	-1.64314300	0.00877500	5.94785600
H	-2.42730800	-1.37522600	4.47134300
H	-0.68058700	-1.13938900	4.39980500
H	-4.53001200	-0.83931600	7.28448600
H	-3.78358600	-1.70989600	5.93292800
H	-3.37811900	-2.13947200	7.61320100

C	-2.30524600	0.41367800	8.30312100
H	-3.22518600	0.96146000	8.57662600
H	-1.46959600	1.12915200	8.29728200
H	-2.12622600	-0.31452200	9.11480500
H	-0.85882900	0.75798900	6.10244600

Transition State TS1:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -538.8493 cm-1

G_corr: 1.540895 Hartree

H_corr: 1.826607 Hartree

SCF: -6306.49918 Hartree

S: 601.332 Cal/Mol-Kelvin

H: -6304.672573 Hartree

G: -6304.958285 Hartree

Cartesian Coordinates:

H	-8.78652400	-1.13646800	-3.10884300
H	-9.05037100	-0.79013300	-1.38479400
C	-8.27417600	-0.93289700	-2.15310300
H	-7.69339300	-1.82891100	-1.88036700
H	-9.56367000	0.38885700	2.06829200
H	-8.72158900	1.36520800	-3.63808200
C	-9.22425900	1.37416900	2.42827500
H	-9.78330600	1.59484700	3.35206200
H	-8.98225500	1.76208000	-1.92448400
C	-8.20908300	1.54060300	-2.67697400
H	-8.51750400	0.85077200	0.10936300
C	-7.35527500	0.30744800	-2.28797900
H	-7.67410500	-0.67774800	3.46187400
H	-9.51303200	2.13322800	1.68262100
H	-6.89864100	-0.14203800	-4.36818300

C	-7.42985000	0.83821600	0.20929100
C	-6.35226400	0.03932500	-3.42824000
C	-7.41586900	0.33505100	3.81241700
H	-8.00931400	0.54163300	4.71907500
H	-5.73367800	-0.85155000	-3.23023900
C	-6.65321300	0.57377400	-0.94026400
C	-7.71027000	1.39473300	2.72104900
H	-7.58123700	2.44001800	-2.78644500
C	-6.86293300	1.08847900	1.46833800
H	0.36415100	-8.12962500	1.16121900
H	-1.06009800	-7.10950900	0.85546400
H	-6.35444500	0.32827600	4.10674400
C	0.00302700	-7.25373900	0.60120300
H	-5.68086600	0.89672700	-3.59989300
C	-5.25807100	0.56560700	-0.79980600
C	-7.34140300	2.80074900	3.25803700
H	-7.93527800	3.03639100	4.15738200
H	-4.27481100	-1.25496700	2.22634500
H	0.06971800	-7.47308800	-0.47673500
C	-5.45699700	1.06121400	1.56871600
O	1.00411400	-6.67854700	3.27157000
H	-7.54344400	3.57891300	2.50390900
H	-4.61248400	0.36628700	-1.65802100
H	-2.38786500	-2.42959400	3.78853900
H	0.48030000	-5.83518800	5.15892800
C	-4.65061900	0.80029100	0.45114200
C	-3.20086800	-1.08308800	2.22861700
H	0.26428300	-4.83284800	7.43137700
C	0.37520800	-4.76003100	5.28593500
C	0.77475300	-5.77235300	2.47161100
C	0.25800000	-4.18235700	6.55120300
C	-2.25330500	-1.67444300	3.01642600
C	0.84270600	-6.01429500	0.95513300
H	-4.97010200	1.26747100	2.52640100

H	-6.27767000	2.87138800	3.53485100
H	2.76045400	-7.04988000	1.09992600
C	0.36787400	-3.93424600	4.14209700
N	0.45974300	-4.46649000	2.83567700
C	0.13056000	-2.80339000	6.73094800
C	2.31782700	-6.20576900	0.54767300
C	-3.15875000	0.80281400	0.56412100
C	-2.51623700	-0.13615000	1.38138400
H	0.03889700	-2.35690800	7.71924500
H	0.44156300	-5.13689800	0.42031900
H	2.39457500	-6.41736600	-0.53119100
C	0.24713700	-2.52556900	4.29333400
H	0.30097500	-3.81285200	2.06308600
C	0.12477400	-1.97026600	5.59735500
C	-0.97704700	-1.14760600	2.60432900
H	-4.14164100	3.22082800	-0.58515100
H	-0.02358300	1.70236000	-7.41682800
N	-1.14358300	-0.19511800	1.60992500
O	-0.22214600	-0.20781000	7.97668400
C	0.24911100	-1.61083600	3.10320600
C	-2.44595400	1.84174200	-0.05622500
H	0.15308100	3.46171800	-7.67474800
C	-3.06816900	3.04709600	-0.55423400
H	2.91518400	-5.30423900	0.75682300
N	0.01658700	-0.56412100	5.69984700
C	0.21287900	2.65932000	-6.92343600
C	-0.14862100	0.22495500	6.82824900
H	1.25293400	2.60679500	-6.56246400
H	1.88026000	2.14510600	6.94037100
H	0.05276600	-0.06728400	4.81084000
H	-2.46978700	1.97241900	-6.76424000
H	-0.12229500	1.91526000	5.44823600
H	-2.38455900	3.74143400	-7.00072100
N	-1.06553700	1.94793300	-0.12413200

C	-0.24244700	1.73417800	6.53371300
C	-2.06178000	3.90602100	-0.89503800
C	1.46396300	-1.29646500	2.48218600
C	-2.23104900	2.92995300	-6.27291100
C	0.88411200	2.46626100	7.28589600
Co	0.24565300	0.59232900	0.47010000
C	-0.77407800	2.93435600	-5.77251700
C	-0.82040000	3.20771700	-0.66616500
H	-2.13648000	4.91974300	-1.28418500
H	2.88201500	-2.53498900	3.70779400
C	2.72981800	-1.88676400	2.84704300
N	1.61472700	-0.48104300	1.36626300
H	0.81535900	2.25439000	8.36378600
H	-0.65450100	2.14676300	-5.00836000
H	0.80613400	3.55579200	7.13951700
C	-0.45819500	4.31042600	-5.16057800
H	-2.94513100	3.07586400	-5.44593400
C	-1.62970600	2.24512600	6.96755700
H	-2.43874500	1.75602900	6.40094200
H	-0.06682300	3.35338500	-3.38577800
N	-0.08874800	4.27757400	-3.82074400
O	-0.53604800	5.33639100	-5.83437100
C	0.43217300	3.69560400	-1.05660000
C	3.63719800	-1.49148800	1.90648400
C	2.94640200	-0.60837100	0.99673200
H	-1.79017000	2.03678900	8.03651200
N	1.68261800	1.65825800	-0.36185700
H	-1.71119200	3.33267600	6.80871700
C	0.26786600	5.35995600	-2.98330700
H	3.95128600	5.49225700	2.59647300
C	1.58282300	2.89313300	-0.99414400
C	0.54232500	5.08578300	-1.61595100
H	4.69498800	-1.73695000	1.84244500
C	0.36912400	6.67966200	-3.46914600

C	2.97670200	1.21732500	-0.62470900
C	3.58626900	0.10929800	-0.02150800
C	3.32049300	6.00096100	3.34350500
H	0.14984200	6.87478500	-4.51674600
H	1.07122300	4.84942600	0.83351400
C	0.93024400	6.15044600	-0.75657100
H	3.49752700	5.52329200	4.32074500
N	1.19448400	5.83253100	0.59462700
H	5.15782200	-4.25842800	-1.10075700
H	3.64682700	7.05052500	3.40573000
H	4.35554500	-2.09608200	-1.31415200
C	0.74637600	7.70223500	-2.59651200
C	2.82054300	3.22309600	-1.65268300
C	1.03145600	7.46445900	-1.25045600
C	3.66577600	2.16364100	-1.46637100
C	1.82723800	5.93389000	2.96827800
C	1.61519400	6.65938000	1.62631300
H	1.53457300	4.87055300	2.87257500
C	6.22779400	-4.35526900	-1.34115300
C	5.21748500	-1.46906100	-1.06857200
C	4.98691100	-0.26421100	-0.39020700
H	4.85771100	-3.00113800	-3.35977600
H	6.36443500	-5.31080100	-1.87558800
H	0.82313100	8.72376000	-2.98166700
H	2.99560700	4.14091000	-2.21108800
H	6.78233100	-4.41675500	-0.39029000
H	1.32766800	8.26432500	-0.57442400
O	1.81791900	7.86635200	1.51159900
C	5.93689100	-3.13222100	-3.53406100
H	6.07311800	-4.07292100	-4.09439800
H	4.67958200	2.03712000	-1.83956700
C	6.73596900	-3.17539300	-2.20704500
C	6.52267600	-1.85331100	-1.44144500
C	6.07366800	0.56946600	-0.05438000

C	0.94850400	6.59489600	4.04562600
H	5.87079200	1.49174000	0.49478100
H	1.12644900	6.13289800	5.03016500
H	6.27743800	-2.30231200	-4.17497800
H	1.18453300	7.66754700	4.11669600
C	7.58000900	-0.99931500	-1.09198800
H	-0.12423500	6.49886100	3.81144300
C	7.38668300	0.21314500	-0.39319700
C	8.21866100	-3.42943300	-2.54623800
H	8.31537500	-4.38083900	-3.09422000
H	8.84400600	-3.50923300	-1.64159600
H	7.70065500	2.13828600	1.68853700
H	8.59868100	-1.28239400	-1.36694400
H	8.63902100	-2.63771700	-3.18842600
H	9.07634200	-0.03747100	1.80359800
C	8.20313500	2.36599800	0.73399400
H	7.53620600	3.01187700	0.13934200
C	8.60487900	1.08710000	-0.02872200
C	9.57128500	0.27427100	0.86930700
H	9.93717300	-0.63428800	0.36557600
H	9.10352600	2.95590100	0.97076200
C	9.34230500	1.50984700	-1.32431600
H	8.68181300	2.09656900	-1.98366600
H	9.70092600	0.64081900	-1.89817200
H	10.45113800	0.88353800	1.13751500
H	10.21969700	2.13297300	-1.08114900
C	-0.01544900	-2.95386900	-3.66537800
N	-0.63013500	-2.90775400	-2.31409300
S	0.28701700	-2.25395400	-1.04758400
N	-0.13205900	-0.54235300	-0.99935300
O	1.70445500	-2.51210300	-1.36621500
O	-0.29441400	-2.78156100	0.20581700
C	-2.09145300	-2.66473300	-2.25305400
C	-2.92390200	-3.93021900	-2.36600500

H	-2.31159700	-2.16802500	-1.29541600
H	-2.36865700	-1.95262700	-3.05260200
C	-3.94398800	-4.02885600	-3.32533300
C	-4.75837200	-5.16782000	-3.38995400
C	-2.72918500	-4.99379700	-1.46781500
C	-3.53717900	-6.13447300	-1.53378200
C	-4.55540400	-6.22488700	-2.49415000
H	-5.18729400	-7.11710100	-2.54329400
H	-3.37501300	-6.95586600	-0.82901400
H	-4.09790800	-3.20972100	-4.03671300
H	-5.54872500	-5.23058400	-4.14469300
H	-1.93986900	-4.91852100	-0.71405200
N	0.11336300	-0.05879700	-2.47885900
N	0.09901600	1.01620300	-2.89124300
C	-1.08281600	-3.11659600	-6.60933800
C	-0.86896600	-4.28633800	-5.67835600
C	-0.43053500	-4.19631200	-4.40602300
H	-0.26549800	-2.03251400	-4.22170800
H	1.07469800	-2.95893500	-3.51069200
H	-2.09801700	-3.14720600	-7.04449900
H	-0.95034900	-2.13648300	-6.12977100
H	-0.38217700	-3.16266100	-7.46289200
C	-1.18075100	-5.63428300	-6.28498500
H	-2.23641200	-5.68624000	-6.60823900
H	-1.00247300	-6.45769200	-5.57775800
H	-0.56929300	-5.81827800	-7.18730200
H	-0.31303000	-5.12088200	-3.82775700

Intermediate $C_{3.1c}$

C_{N2}:

G_corr: -0.013118 Hartree

H_corr: 0.00864 Hartree

SCF: -109.557996 Hartree

S: 45.794 Cal/Mol-Kelvin

H: -109.549356 Hartree

G: -109.571114 Hartree

Cartesian Coordinates:

N	0.00000000	0.00000000	0.55384100
N	0.00000000	0.00000000	-0.55384100

$C_{[Co(III)]3.1c}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.536966 Hartree

H_corr: 1.817971 Hartree

SCF: -6196.992441 Hartree

S: 591.424 Cal/Mol-Kelvin

H: -6195.17447 Hartree

G: -6195.455475 Hartree

Cartesian Coordinates:

H	8.54103900	-4.02697200	1.78189800
H	9.05893400	-2.75619300	0.65051400
C	8.17695400	-3.24125700	1.09826900
H	7.61570600	-3.73208800	0.28643100
H	10.08634100	0.15287600	-1.33042300
H	8.46949000	-2.34039200	3.70413100
C	9.83553200	1.19510600	-1.07308300
H	10.52723200	1.84536900	-1.63303300
H	8.98719400	-1.03635200	2.61059000
C	8.10711300	-1.57424000	2.99766800
H	8.79021900	-0.51043600	0.39398100
C	7.28236900	-2.23379400	1.86369200
H	8.36729700	0.28926000	-3.24413400
H	10.04108300	1.34505700	-0.00030900
H	6.51878500	-3.78112500	3.18966300
C	7.72742400	-0.33480800	0.21234300
C	6.11811900	-3.01489900	2.50578400

C	8.20185900	1.34263200	-2.96471000
H	8.92517400	1.96047400	-3.52366600
H	5.50112000	-3.53335300	1.75442000
C	6.78836100	-1.14335200	0.89065200
C	8.37976500	1.54864700	-1.43913200
H	7.49545000	-0.85261700	3.56351300
C	7.35332600	0.67805200	-0.68423900
H	1.92604900	-7.92703000	-0.37618100
H	2.69040200	-6.32224000	-0.22585200
H	7.19232800	1.62373700	-3.30408900
C	1.83666100	-6.93835900	0.10020500
H	5.45465500	-2.36102700	3.09433700
C	5.42608500	-0.91429100	0.64741200
C	8.14511200	3.04050700	-1.09288500
H	8.86813400	3.67851000	-1.62891200
H	4.58402600	-1.80962900	-2.04844700
H	1.91271300	-7.06990700	1.19204300
C	5.97444400	0.88609800	-0.89547500
O	0.42018100	-7.21199300	-2.49866100
H	8.26962600	3.22109500	-0.01247200
H	4.65131300	-1.50364200	1.14262400
H	2.65008100	-3.02315300	-3.53267000
H	0.13242400	-6.51898100	-4.46500500
C	5.01586600	0.10267000	-0.23886500
C	3.51074200	-1.63367700	-2.03823200
H	-0.11262900	-5.76227300	-6.82706100
C	0.05875500	-5.46105100	-4.70639800
C	0.38380800	-6.19847800	-1.80174200
C	-0.07727500	-5.01993100	-6.02355500
C	2.54316200	-2.23826900	-2.78661100
C	0.49182900	-6.28514400	-0.27182600
H	5.63341000	1.65600900	-1.59458300
H	7.13487200	3.37657200	-1.37564500
H	-0.69268900	-8.11692600	-0.18876200

C	0.10556000	-4.51790400	-3.65694700
N	0.23756900	-4.90707700	-2.30484100
C	-0.16746000	-3.66534200	-6.35066200
C	-0.69492000	-7.11187600	0.26118400
C	3.55169600	0.30828700	-0.46807100
C	2.85614900	-0.63237300	-1.23249800
H	-0.27042500	-3.32534700	-7.37940800
H	0.45236900	-5.27403600	0.16569000
H	-0.63310500	-7.21662600	1.35631900
C	0.01213200	-3.13195600	-3.95986400
H	0.24170700	-4.15586100	-1.60840400
C	-0.12115700	-2.71624200	-5.31369600
C	1.28563800	-1.64790800	-2.40053300
H	4.70035400	2.60857900	0.76232000
H	1.54982300	1.66226200	7.27758500
N	1.48576100	-0.64216800	-1.45923100
O	-0.44920300	-1.20255700	-7.86341000
C	0.04982200	-2.08750300	-2.88173600
C	2.91993500	1.45307700	0.02798900
H	1.80398100	3.42578400	7.43861000
C	3.62590100	2.57438600	0.59717300
H	-1.66044500	-6.63558400	0.02371800
N	-0.19493200	-1.32603900	-5.56371900
C	1.25762400	2.64877800	6.88357400
C	-0.34778300	-0.65487000	-6.76746800
H	0.18358500	2.79369100	7.08119500
H	-2.57827100	1.01198600	-6.55618700
H	-0.12563100	-0.73824900	-4.73437400
H	3.34523100	1.46306700	5.48230900
H	-0.27883900	1.16732300	-5.56830100
H	3.69937000	3.20619300	5.61676400
N	1.55747900	1.72237700	-0.04455300
C	-0.38340800	0.87964100	-6.63227800
C	2.69913100	3.54742100	0.84217000

C	-1.15886400	-1.59773700	-2.37116400
C	3.06714900	2.46123400	5.10706000
C	-1.73653200	1.39930900	-7.15309500
Co	0.12562800	0.43746600	-0.53410700
C	1.57344500	2.74427800	5.38461800
C	1.41172700	2.99594400	0.49600800
H	2.85350900	4.54465400	1.24965100
H	-2.59647000	-2.96148500	-3.42254100
C	-2.44397800	-2.15906700	-2.70342900
N	-1.30017600	-0.56521200	-1.45388300
H	-1.88537300	1.08047800	-8.19608600
H	0.96771900	1.99269300	4.84328000
H	-1.77082900	2.50037200	-7.11758600
C	1.23186400	4.15245300	4.86424300
H	3.30002500	2.49280300	4.03062100
C	0.79159200	1.48290300	-7.42458100
H	1.76437700	1.15413100	-7.02410800
H	0.68618800	3.25904800	3.09797600
N	0.76167300	4.16831100	3.55396100
O	1.40302900	5.16022500	5.54558400
C	0.20178800	3.63537900	0.79771600
C	-3.37053400	-1.50570300	-1.94188400
C	-2.66094300	-0.51597000	-1.16807100
H	0.73522900	1.16895900	-8.47810200
N	-1.24567700	1.75495200	0.05981700
H	0.76220600	2.58404000	-7.38739400
C	0.50104200	5.28000200	2.72190500
H	-2.95208300	5.91466800	-3.13710100
C	-1.03673700	2.99548900	0.64342900
C	0.22681200	5.03391700	1.34923000
H	-4.44813800	-1.65191300	-1.91712800
C	0.50349400	6.59993400	3.21529300
C	-2.60599000	1.51408900	0.19635900
C	-3.29557600	0.42404400	-0.34759400

C	-2.17584700	6.31857000	-3.80715200
H	0.71745200	6.77035600	4.26846100
H	-0.23105300	4.85684700	-1.12038000
C	-0.03277200	6.13245000	0.48452000
H	-2.32269300	5.87540000	-4.80540800
N	-0.27824300	5.84532300	-0.87706000
H	-5.71339200	-3.40500500	1.17461000
H	-2.32636200	7.40623300	-3.88372300
H	-4.62461400	-1.38222000	1.15959200
C	0.23925400	7.65505300	2.33950600
C	-2.27925300	3.54222800	1.13542100
C	-0.02748900	7.44837100	0.98432600
C	-3.24582600	2.60991600	0.88629800
C	-0.75938500	6.01887200	-3.28226600
C	-0.56795300	6.71301000	-1.92072000
H	-0.64843400	4.92355300	-3.16616600
C	-6.80983500	-3.31018600	1.21534200
C	-5.31304100	-0.69083200	0.66461400
C	-4.77689900	0.31703500	-0.14734300
H	-5.59832800	-1.78096000	3.21771100
H	-7.18933100	-4.12174500	1.85902400
H	0.24257600	8.67801500	2.72831600
H	-2.37762600	4.51037800	1.62284100
H	-7.19800000	-3.47624100	0.19711100
H	-0.22893800	8.27461700	0.30512300
O	-0.66728100	7.93245100	-1.80343100
C	-6.69902400	-1.74262600	3.19684600
H	-7.07493200	-2.53730300	3.86354300
H	-4.30577200	2.65671300	1.12607700
C	-7.25648200	-1.93160100	1.76364600
C	-6.70590600	-0.81471000	0.85260500
C	-5.64403600	1.21988600	-0.79679300
C	0.31912100	6.52349100	-4.25985700
H	-5.20574700	1.98744600	-1.43857000

H	0.17743400	6.07924500	-5.25839000
H	-7.00707800	-0.77139100	3.61743000
H	0.25824200	7.61843500	-4.35515200
C	-7.53648400	0.10163600	0.19010000
H	1.33423000	6.26853800	-3.91435200
C	-7.03440600	1.12600600	-0.64274200
C	-8.79660200	-1.92329900	1.84378500
H	-9.13771900	-2.73804900	2.50295400
H	-9.26382200	-2.08345300	0.85814700
H	-6.69611300	2.66770200	-3.01945600
H	-8.61815400	0.02115400	0.31892100
H	-9.18561100	-0.98014800	2.26173500
H	-8.39274900	0.72809000	-3.03843400
C	-7.28795700	3.13445400	-2.21489400
H	-6.61567600	3.77277900	-1.61815900
C	-8.01467900	2.08630300	-1.34781300
C	-8.96075000	1.27282500	-2.26669400
H	-9.55138000	0.53421800	-1.70206200
H	-8.02683900	3.79667600	-2.69454800
C	-8.85401100	2.83811400	-0.28404700
H	-8.20898400	3.43288300	0.38331400
H	-9.43968200	2.14842000	0.34409900
H	-9.67041600	1.94498000	-2.77818700
H	-9.56394000	3.52710800	-0.77219700
C	0.25392100	-1.60893500	3.95212800
N	-0.07990800	-2.39154500	2.73583300
S	0.67976500	-1.95209800	1.27153200
N	0.02998800	-0.43713900	1.04452300
O	0.24551200	-2.97915800	0.28534000
O	2.12522400	-1.85115100	1.59400500
C	-1.41682300	-3.00088500	2.68978400
C	-1.54025500	-4.14658300	3.68496100
H	-2.19454400	-2.24205900	2.89588900
H	-1.56925600	-3.37529000	1.66624400

C	-0.49084200	-5.06541600	3.86258500
C	-0.63108700	-6.14267200	4.74594500
C	-2.72718800	-4.32383800	4.41434600
C	-2.87339000	-5.40707800	5.29172200
C	-1.82451400	-6.31957800	5.46063500
H	-1.93385900	-7.16279200	6.14956200
H	-3.80601700	-5.53259200	5.85086100
H	0.44184700	-4.92024200	3.30892300
H	0.19491900	-6.84899700	4.87620700
H	-3.54686600	-3.60650700	4.29523100
C	-1.37158300	-1.14446400	6.60047200
C	-1.43238700	-0.28210900	5.36176700
C	-0.72148300	-0.49375900	4.23333400
H	0.30637800	-2.33138300	4.78274100
H	1.27547200	-1.22513700	3.80405600
H	-0.78177800	-2.06262700	6.47417100
H	-0.93902800	-0.58020600	7.44659000
H	-2.38716500	-1.44161900	6.91656100
C	-2.36846500	0.90039500	5.46682500
H	-3.40330000	0.56893100	5.66944000
H	-2.37812700	1.50562700	4.54816000
H	-2.08764100	1.55893800	6.30867000
H	-0.85173300	0.19352300	3.38664200

Transition State $TS2^{7}_{3.1c}$(1,7-HAA):

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -1438.8926 cm-1

G_corr: 1.536057 Hartree

H_corr: 1.811653 Hartree

SCF: -6196.955936 Hartree

S: 580.041 Cal/Mol-Kelvin

H: -6195.144282 Hartree

G: -6195.419879 Hartree

Cartesian Coordinates:

H	-9.70715700	-0.23725600	0.89031100
H	-9.43490100	0.98498700	-0.37317800
C	-8.92719300	0.31362700	0.33747500
H	-8.37896000	0.94162100	1.05857500
H	-8.84430000	3.11626500	-3.32399800
H	-9.56044800	-2.11369200	-0.84236900
C	-8.30967300	2.78106100	-4.22808600
H	-8.55896300	3.48790900	-5.03620200
H	-9.28727700	-0.92904800	-2.14009900
C	-8.78278700	-1.54063300	-1.37536000
H	-8.34538800	1.11535400	-2.39070900
C	-7.97236400	-0.67518600	-0.37781400
H	-6.77336500	4.52475300	-2.72024000
H	-8.70915000	1.79592500	-4.52037500
H	-8.16951000	-2.15951400	1.20142100
C	-7.28127100	1.01426400	-2.16545700
C	-7.36395400	-1.61113700	0.68607800
C	-6.31386300	4.18148600	-3.66166200
H	-6.59965800	4.89053200	-4.45713000
H	-6.80097000	-1.05424000	1.45259100
C	-6.89388600	0.11852700	-1.14391000
C	-6.78195700	2.74865400	-4.01996900
H	-8.13050500	-2.25930000	-1.89800100
C	-6.35921400	1.77669200	-2.89858800
H	0.33746000	3.51260500	7.36691000
H	-0.99466000	2.77845100	6.44591900
H	-5.22060200	4.24052000	-3.54156200
C	0.07850000	2.69179200	6.68140300
H	-6.68853800	-2.36005500	0.24132600
C	-5.52518300	-0.00751300	-0.86600300
C	-6.12309600	2.31171900	-5.35272400
H	-6.41053700	2.99822400	-6.16722000

H	-4.17544000	3.04387800	-0.27682300
H	0.24202100	1.73637900	7.20674600
C	-4.99258700	1.62912900	-2.58253600
O	0.90462500	5.19107000	5.43334000
H	-6.44026400	1.29503200	-5.63700100
H	-5.16592200	-0.67460700	-0.07972000
H	-2.25903500	4.63058900	0.82615000
H	0.58979300	6.77101300	3.98543200
C	-4.57060500	0.74443800	-1.58112200
C	-3.11044600	2.84845300	-0.17456800
H	0.48229300	8.61323900	2.30185600
C	0.51363300	6.55424300	2.92188900
C	0.79007700	4.16225100	4.77032300
C	0.45586600	7.57169400	1.96704200
C	-2.15128200	3.64165800	0.38462000
C	0.94813300	2.77398100	5.41650700
H	-4.23506200	2.19850700	-3.12977000
H	-5.02345600	2.31294600	-5.28943800
H	2.79520100	3.33575100	6.43185000
C	0.47991700	5.21190700	2.49551000
N	0.54928700	4.13129900	3.40410400
C	0.36942200	7.30367000	0.59909400
C	2.43891000	2.55134200	5.74603100
C	-3.11604100	0.59424200	-1.26147000
C	-2.45272000	1.64290200	-0.61905900
H	0.33488800	8.10009700	-0.14205200
H	0.62498600	1.99278000	4.70184600
H	2.58789100	1.57353400	6.23243000
C	0.37639000	4.90309100	1.11372500
H	0.48004000	3.20643500	2.97823300
C	0.33178900	5.96414800	0.16764900
C	-0.90304600	2.92560100	0.27424300
H	-4.14615000	-1.65681900	-2.64621100
H	-1.66767900	-6.34073400	4.22692800

N	-1.09538400	1.69059100	-0.33513300
O	0.25580400	7.66611800	-2.27801200
C	0.33157800	3.47685900	0.63869300
C	-2.47437300	-0.60511400	-1.57798600
H	-1.49430500	-7.72742500	3.11306000
C	-3.12951100	-1.69374700	-2.26176200
H	3.06551600	2.57966700	4.84011300
N	0.26518600	5.61571700	-1.19968300
C	-1.25120800	-6.66395300	3.25835100
C	0.23932000	6.43762300	-2.31749500
H	-0.15316100	-6.57693400	3.31159700
H	2.38519100	5.61059900	-3.89389500
H	0.24346400	4.61372700	-1.38431400
H	-3.78574000	-5.54514600	3.05479500
H	0.13194600	4.58764100	-3.46850300
H	-3.70929900	-6.92714700	1.92498100
N	-1.16223700	-0.94338300	-1.25940000
C	0.19759300	5.67653600	-3.65609200
C	-2.23796700	-2.72351900	-2.31950100
C	1.53684300	2.78015300	0.47920800
C	-3.37331900	-5.89150800	2.09281900
C	1.49416100	5.96441200	-4.43772700
Co	0.19894300	0.18238700	-0.36932900
C	-1.83155700	-5.82157400	2.10943600
C	-1.02723700	-2.26254800	-1.68656800
H	-2.36409900	-3.71120900	-2.75841300
H	2.98366400	4.40437700	1.04234400
C	2.82872200	3.37719500	0.71765400
N	1.67019900	1.46384900	0.05296900
H	1.60364800	7.04762400	-4.60090200
H	-1.53115100	-4.76898800	2.23259800
H	1.47417000	5.46520700	-5.42012900
C	-1.30559200	-6.35728700	0.76817300
H	-3.79776400	-5.25867200	1.29680800

C	-1.04483400	6.11656900	-4.45144400
H	-1.97718100	5.86552200	-3.92021800
H	-0.80725800	-4.42486300	0.26171500
N	-0.80450300	-5.38608500	-0.09565900
O	-1.36425200	-7.55843300	0.50453700
C	0.11840400	-3.05427100	-1.57227800
C	3.76151400	2.41849700	0.44709100
C	3.04180800	1.23100400	0.05086100
H	-1.02631900	7.20614900	-4.60604700
N	1.56267000	-1.22046800	-0.71791600
H	-1.06988700	5.62440800	-5.43723900
C	-0.33736700	-5.57225700	-1.41715000
H	3.88120900	-2.01450000	-5.52708600
C	1.32895500	-2.54150100	-1.08847700
C	0.10517100	-4.44070200	-2.15551700
H	4.84480500	2.49070500	0.51451300
C	-0.30353800	-6.84925000	-2.02013200
C	2.94282800	-1.14325800	-0.53772000
C	3.66754700	0.01224700	-0.22859400
C	3.19888900	-1.78501300	-6.36158300
H	-0.63559100	-7.70957200	-1.44400200
H	0.86545500	-2.58403400	-3.68734800
C	0.54786000	-4.61221600	-3.49901700
H	3.43026700	-0.76988700	-6.72344200
N	0.94651500	-3.45539900	-4.20878800
H	6.54215500	-0.70702800	3.53618900
H	3.40385800	-2.49951200	-7.17338500
H	5.29487100	-1.09751100	1.65115900
C	0.14914500	-6.98330500	-3.33278700
C	2.55762800	-3.29542900	-1.10305300
C	0.57229200	-5.88849700	-4.08862600
C	3.55938300	-2.42465400	-0.78382300
C	1.72390900	-1.88604400	-5.93232700
C	1.41752600	-3.33540700	-5.50746500

H	1.55418000	-1.19946300	-5.08079800
C	7.62514200	-0.66113200	3.34057300
C	5.86596000	-0.65602900	0.82895100
C	5.16710100	-0.04331300	-0.21905500
H	6.50229200	-2.97911800	2.25038100
H	8.13777900	-1.13310300	4.19588300
H	0.16847200	-7.97983900	-3.78508100
H	2.63013300	-4.34847500	-1.36746400
H	7.91520200	0.40198400	3.31502300
H	0.91719100	-5.99323200	-5.11562000
O	1.58186200	-4.27676600	-6.28124900
C	7.58744600	-2.86442700	2.10026500
H	8.09444200	-3.36319500	2.94367100
H	4.62909000	-2.61530200	-0.73153600
C	8.00850700	-1.37555000	2.02008300
C	7.27641700	-0.70016000	0.84156300
C	5.88534600	0.53782900	-1.28407900
C	0.77719900	-1.48907100	-7.08139100
H	5.32044300	1.00588900	-2.09340500
H	1.00285800	-0.47042300	-7.43695200
H	7.85658300	-3.40289300	1.17678000
H	0.89617900	-2.18585500	-7.92537700
C	7.95551600	-0.11389600	-0.23705500
H	-0.27867300	-1.51389100	-6.76627600
C	7.28693300	0.51041800	-1.31317100
C	9.54264200	-1.31851500	1.87281700
H	10.01650600	-1.81073300	2.73760700
H	9.91784800	-0.28235000	1.84017800
H	6.59505400	2.59234300	-3.13248000
H	9.04745300	-0.13859500	-0.24867400
H	9.89231800	-1.84159100	0.96752100
H	8.47187500	3.02849000	-1.41653700
C	7.20993400	1.77390300	-3.54188700
H	6.53678800	1.04028000	-4.01508800

C	8.10591200	1.12794300	-2.46562300
C	9.04661200	2.22218300	-1.90100500
H	9.75050800	1.81883100	-1.15599300
H	7.83805000	2.20345000	-4.33915900
C	8.95360100	0.02168600	-3.14303200
H	8.31119700	-0.77187700	-3.55833800
H	9.65529100	-0.45089600	-2.43763400
H	9.64355200	2.67139600	-2.71275100
H	9.54813900	0.44558600	-3.97005100
C	-0.61723200	-2.37733200	4.34510300
N	-1.13335900	-1.23287400	3.57255500
S	-1.27753000	-1.31490100	1.88488700
N	-0.11271300	-0.18622600	1.45061600
O	-2.60713300	-0.78164200	1.50439100
O	-0.96625500	-2.72828200	1.53137900
C	-1.87815300	-0.18459000	4.29295300
C	-3.04992200	-0.71226800	5.10916800
H	-1.17620600	0.34993200	4.95961400
H	-2.22957800	0.54014400	3.54405500
C	-4.11285800	-1.39012300	4.48312400
C	-5.19085700	-1.86515300	5.23826600
C	-3.08953400	-0.52422800	6.50045600
C	-4.17131000	-0.99613200	7.25784800
C	-5.22368600	-1.66995900	6.62749100
H	-6.06840700	-2.04254300	7.21518800
H	-4.18830500	-0.83896900	8.34089100
H	-4.08913200	-1.53235600	3.39824600
H	-6.01335600	-2.38791200	4.74007200
H	-2.26831600	0.00407600	6.99845300
C	1.80138600	-0.84506700	3.13992400
C	1.79459100	-2.27618900	3.40197300
C	0.72436600	-2.93299200	3.94425000
H	-0.57751200	-2.02434300	5.39463600
H	-1.35490300	-3.20056900	4.34532800

H	0.92811800	-0.55177000	2.13732900
H	1.29927700	-0.20560800	3.87636000
H	2.75123500	-0.42179800	2.78748400
C	3.01043000	-3.06757300	2.97156800
H	3.18704800	-2.95188000	1.88854500
H	2.89821400	-4.14246100	3.17772500
H	3.91778900	-2.71243700	3.49104100
H	0.81515800	-4.01430600	4.09779700

Intermediate $D_{3.1c}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.53411 Hartree

H_corr: 1.817136 Hartree

SCF: -6196.982763 Hartree

S: 595.679 Cal/Mol-Kelvin

H: -6195.165626 Hartree

G: -6195.448653 Hartree

Cartesian Coordinates:

H	-9.27874300	-0.82417200	2.35030000
H	-9.32936600	0.52190600	1.18897500
C	-8.65420500	-0.16485600	1.72370700
H	-8.02145900	0.44063100	2.39301000
H	-9.42698100	2.98366000	-1.53516200
H	-9.34379500	-2.52085400	0.43759500
C	-9.06662200	2.77688300	-2.55641200
H	-9.50860500	3.53825100	-3.21959000
H	-9.39163500	-1.20905600	-0.76256400
C	-8.71651200	-1.84322100	-0.16627700
H	-8.64855100	0.93855100	-0.94340000
C	-7.78975600	-1.00595300	0.75088600
H	-7.35325000	4.47507200	-1.19382400
H	-9.46443200	1.79811200	-2.87149000

H	-7.59200000	-2.62898300	2.18644100
C	-7.55695100	0.89644100	-0.93723500
C	-6.93399500	-1.97853100	1.58712200
C	-7.07380200	4.25773300	-2.23785700
H	-7.54990500	5.01673000	-2.88161300
H	-6.26904500	-1.44635000	2.28660900
C	-6.92738700	-0.06330000	-0.11364900
C	-7.52853200	2.83550200	-2.65142700
H	-8.12948700	-2.45920700	-0.86697900
C	-6.84097100	1.79371600	-1.74428300
H	-0.75645800	3.82216100	6.80779500
H	-1.70486400	3.15884100	5.45274500
H	-5.98327200	4.38492200	-2.32635300
C	-0.80134900	3.01010900	6.06583900
H	-6.31252600	-2.63267600	0.95436700
C	-5.52568300	-0.11491700	-0.11831100
C	-7.12615300	2.57684300	-4.12537600
H	-7.60518700	3.31551000	-4.79037600
H	-4.20219600	3.07564000	0.37214100
H	-0.91065500	2.05414900	6.60309900
C	-5.43315000	1.71924300	-1.71190600
O	0.77412500	5.41148600	5.17277100
H	-7.44024400	1.57179500	-4.45139100
H	-4.98185300	-0.83038300	0.50195700
H	-2.15443800	4.75700700	0.99391700
H	0.77168400	6.98264700	3.66150400
C	-4.77448200	0.77536200	-0.91217000
C	-3.13310500	2.91250400	0.25646100
H	0.82525600	8.78503100	1.93043800
C	0.70230400	6.74542100	2.60160700
C	0.61458700	4.38205300	4.51991300
C	0.73101000	7.73967400	1.62061800
C	-2.10705500	3.75507700	0.57128200
C	0.47741000	3.01058800	5.20567000

H	-4.83065900	2.39340300	-2.32838300
H	-6.03747500	2.65162800	-4.27516300
H	1.86169800	3.55638700	6.79465000
C	0.58144400	5.39894900	2.20590700
N	0.53121700	4.33663500	3.13581800
C	0.64095100	7.44520100	0.25794700
C	1.72880900	2.74555400	6.06230300
C	-3.28014700	0.69505800	-0.89956300
C	-2.54089000	1.72251300	-0.30852900
H	0.66272000	8.22471600	-0.50145500
H	0.39164500	2.21484900	4.44121300
H	1.63183500	1.79406500	6.61007700
C	0.49519000	5.06464100	0.82925800
H	0.40224800	3.41219600	2.72436200
C	0.52080300	6.10046000	-0.14207700
C	-0.88477400	3.06491300	0.23365700
H	-4.44388200	-1.33138300	-2.51088600
H	-1.50007300	-6.73995700	2.92141300
N	-1.15457600	1.80957900	-0.29741400
O	0.54374500	7.73484700	-2.63198400
C	0.38594200	3.62964700	0.39332600
C	-2.66090100	-0.39301700	-1.52040800
H	-1.45843400	-7.93922600	1.59684300
C	-3.37492200	-1.36461200	-2.31245600
H	2.64085300	2.69399700	5.44541400
N	0.42619200	5.71873500	-1.49879000
C	-1.19699200	-6.90649800	1.87459000
C	0.43949200	6.51014600	-2.63851400
H	-0.10030300	-6.80792700	1.81835700
H	2.48102200	5.57098400	-4.29551000
H	0.33318400	4.71556100	-1.65343300
H	-3.73868000	-5.82843700	2.12949100
H	0.21950100	4.63864400	-3.73767600
H	-3.78654100	-7.00492100	0.78435900

N	-1.30170900	-0.68486100	-1.49055500
C	0.31199300	5.72020000	-3.95467700
C	-2.45817700	-2.27473900	-2.75020800
C	1.56305100	2.90519800	0.16520700
C	-3.43728700	-6.00440500	1.08389200
C	1.57761000	5.94635800	-4.80320600
Co	0.13631400	0.34363800	-0.62033000
C	-1.90547300	-5.90710100	0.94096700
C	-1.18390800	-1.87709300	-2.20465900
H	-2.61264000	-3.15241200	-3.37473100
H	3.08130700	4.49825800	0.61261200
C	2.88027400	3.45880800	0.36059900
N	1.63977100	1.56277900	-0.19333100
H	1.71683500	7.02171100	-4.99282500
H	-1.58599300	-4.88428800	1.19770200
H	1.49232200	5.43015400	-5.77321600
C	-1.52428600	-6.22252900	-0.51428800
H	-3.95027900	-5.25964800	0.45385600
C	-0.95325100	6.18318100	-4.70091700
H	-1.86672500	5.97874400	-4.11909900
H	-0.81630100	-4.29760100	-0.67754200
N	-0.94341500	-5.16472500	-1.20943400
O	-1.74083900	-7.33403600	-0.99663000
C	-0.02861700	-2.65345600	-2.31864800
C	3.76846200	2.43796000	0.18059900
C	2.99754500	1.26003200	-0.13737900
H	-0.90531500	7.26700500	-4.88703700
N	1.45150800	-1.02879200	-1.16573200
H	-1.04366500	5.66664700	-5.67025400
C	-0.52860700	-5.14830100	-2.56081100
H	3.69107900	-1.05527200	-6.31518300
C	1.18662600	-2.26533200	-1.74094800
C	-0.07443300	-3.92284400	-3.12050800
H	4.85392300	2.46874800	0.24136000

C	-0.54902200	-6.31075500	-3.36192600
C	2.80341200	-1.08199900	-0.82346300
C	3.56464800	-0.00092400	-0.36460200
C	2.93951100	-0.67041000	-7.02334200
H	-0.90182400	-7.24265000	-2.92616000
H	0.72265600	-1.86529000	-4.33610200
C	0.34336000	-3.88549400	-4.48060700
H	3.17120400	0.38791000	-7.22595200
N	0.76262600	-2.63804800	-4.99905300
H	6.18881000	1.40358700	3.37363200
H	3.03953300	-1.23587700	-7.96222200
H	4.98044200	0.09078700	1.94609300
C	-0.12723400	-6.24065300	-4.69037500
C	2.36040400	-3.10101600	-1.72944100
C	0.31842100	-5.05022500	-5.26845100
C	3.35626800	-2.37711400	-1.13982100
C	1.51123000	-0.81859500	-6.47074200
C	1.18980200	-2.31345100	-6.27760900
H	1.44902000	-0.29156900	-5.49919000
C	7.27656000	1.24768300	3.29845300
C	5.62944400	-0.08006900	1.08182100
C	5.04283900	-0.16742800	-0.18828100
H	5.94168100	-1.18510100	3.63423200
H	7.69416600	1.32484800	4.31660800
H	-0.14832800	-7.15002800	-5.29913800
H	2.39781100	-4.11422700	-2.12478800
H	7.69214500	2.07393600	2.69868900
H	0.64079200	-4.99743900	-6.30668300
O	1.29963100	-3.11678500	-7.20189700
C	7.03768400	-1.25708400	3.55216000
H	7.45304900	-1.20787100	4.57307300
H	4.38463200	-2.67484100	-0.94763100
C	7.62754700	-0.12581000	2.67332800
C	7.02264000	-0.21554100	1.25665900

C	5.86283100	-0.38881400	-1.31475800
C	0.47246400	-0.20491000	-7.43045300
H	5.38831400	-0.43841500	-2.29715500
H	0.69739700	0.85755300	-7.61901500
H	7.27684800	-2.24879100	3.13462000
H	0.48726200	-0.73821600	-8.39356500
C	7.80404400	-0.43229000	0.11173700
H	-0.54904800	-0.26966000	-7.02156800
C	7.25239600	-0.52008300	-1.18555100
C	9.16281300	-0.27204400	2.67041800
H	9.54424600	-0.19609000	3.70164100
H	9.65348200	0.52008800	2.08115300
H	6.86544100	0.12442600	-3.93774200
H	8.88563600	-0.53563600	0.22361100
H	9.48606700	-1.24858200	2.27382600
H	8.68787100	1.38274800	-2.61993600
C	7.40604600	-0.81304300	-3.72714900
H	6.67895000	-1.64153500	-3.74353800
C	8.18165900	-0.74765300	-2.39586700
C	9.20075300	0.41606200	-2.48760600
H	9.82646300	0.49001400	-1.58411700
H	8.10933800	-0.97896600	-4.55923400
C	8.94400500	-2.08457600	-2.21499300
H	8.24536200	-2.93488700	-2.15235200
H	9.55990400	-2.08940600	-1.30179700
H	9.87525400	0.26851700	-3.34800300
H	9.61723200	-2.26113900	-3.07088300
C	0.38907200	-2.94008700	3.67471500
N	-0.45875200	-1.82291000	3.20782400
S	-0.86091200	-1.62386900	1.57970300
N	0.08786500	-0.28474700	1.19488900
O	-2.27117400	-1.20151000	1.49078100
O	-0.44465500	-2.88744400	0.90962400
C	-1.05885800	-0.92549900	4.21163400

C	-2.04362400	-1.63469000	5.12969500
H	-0.24565000	-0.47647100	4.80880100
H	-1.55712500	-0.10929700	3.66847400
C	-3.19984600	-2.24046000	4.60307500
C	-4.11412200	-2.87558000	5.45109700
C	-1.81975400	-1.68441400	6.51511900
C	-2.73748100	-2.31730400	7.36626500
C	-3.88671500	-2.91454300	6.83519700
H	-4.60401400	-3.41082700	7.49631900
H	-2.54996900	-2.34676900	8.44423900
H	-3.37603000	-2.20322500	3.52352900
H	-5.01194700	-3.33965500	5.03100200
H	-0.91511400	-1.22936500	6.93291500
C	1.41430700	-3.69130100	6.48117300
C	2.10749700	-2.84427200	5.61985500
C	1.64241800	-2.46590600	4.35025900
H	-0.22068700	-3.57708000	4.33738000
H	0.62677900	-3.54808900	2.78609000
H	1.05473000	-0.59198300	1.39158300
H	0.44043200	-4.11818300	6.23476500
H	1.82830200	-3.95439600	7.45767100
C	3.46606600	-2.31664700	6.05954800
H	3.55652400	-2.29439200	7.15620400
H	3.64579200	-1.29640100	5.68564700
H	4.27900100	-2.95519900	5.67427800
H	2.26068700	-1.77663900	3.76102800

Transition State TS3[5] (Radical Substitution for 5-member ring):

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -155.8669 cm-1

G_corr: 1.541246 Hartree

H_corr: 1.816452 Hartree

SCF: -6196.975316 Hartree

S: 579.22 Cal/Mol-Kelvin

H: -6195.158864 Hartree

G: -6195.43407 Hartree

Cartesian Coordinates:

H	-9.12724800	-3.13112800	-0.88915700
H	-9.36173100	-1.74076500	0.19524800
C	-8.59889000	-2.36023800	-0.30264000
H	-8.01729300	-2.87069000	0.48228000
H	-9.81050800	1.39912900	2.05276700
H	-9.05775200	-1.58140600	-2.92432800
C	-9.46699000	2.38117700	1.68801000
H	-10.01079200	3.15085300	2.25968200
H	-9.29497500	-0.16168000	-1.87936400
C	-8.53238800	-0.82825000	-2.31255400
H	-8.79911200	0.47010200	0.25347800
C	-7.67654600	-1.52053600	-1.22194100
H	-7.89161100	1.45387600	3.77204200
H	-9.76954700	2.48262900	0.63265200
H	-7.25263800	-3.22426400	-2.50809000
C	-7.70964900	0.51604100	0.32052900
C	-6.69127100	-2.47909100	-1.92069700
C	-7.63186100	2.45430900	3.38899000
H	-8.21076400	3.19875400	3.96175600
H	-6.06664700	-3.03005300	-1.19937600
C	-6.95271100	-0.44796300	-0.38178100
C	-7.94813000	2.57073500	1.87654300
H	-7.90227500	-0.22346900	-2.98516300
C	-7.12170100	1.52452800	1.09950300
H	-3.69276400	-7.23125300	0.93410000
H	-3.94538500	-5.46767400	0.84198100
H	-6.56516600	2.62716000	3.60215200
C	-3.40566900	-6.31673100	0.39197300
H	-6.01980500	-1.94816200	-2.61484900

C	-5.55473600	-0.38520900	-0.28421200
C	-7.57505700	3.99129800	1.38298000
H	-8.15175400	4.75421200	1.93313500
H	-4.56317300	-1.13549300	2.45926000
H	-3.73924500	-6.41307900	-0.65434400
C	-5.71314300	1.56195600	1.16383700
O	-1.59300900	-7.02971500	2.66872500
H	-7.79586600	4.10842400	0.30920900
H	-4.91517000	-1.10055000	-0.80532100
H	-2.66617400	-2.55248100	3.80268000
H	-0.74933500	-6.42760500	4.50173900
C	-4.93120100	0.62017000	0.48201100
C	-3.48404500	-1.12353400	2.32199900
H	0.04648000	-5.73067200	6.75866500
C	-0.42594800	-5.40593400	4.68737700
C	-1.44869000	-6.05566700	1.93019500
C	0.01970700	-4.99855500	5.94547000
C	-2.53375000	-1.83015100	2.99955800
C	-1.87876700	-6.11444700	0.45558200
H	-5.20794800	2.32515000	1.76389000
H	-6.50635700	4.21275500	1.53182800
H	-1.34086900	-8.22094400	0.28098200
C	-0.46683900	-4.47502200	3.62712700
N	-0.90944200	-4.83721500	2.33410800
C	0.42950900	-3.68858900	6.20082300
C	-1.13588000	-7.27186200	-0.23790700
C	-3.43590100	0.65108800	0.56057300
C	-2.78971200	-0.28476900	1.37420600
H	0.77206200	-3.37224200	7.18423200
H	-1.62420600	-5.16747700	-0.04755800
H	-1.46071400	-7.36901800	-1.28661400
C	-0.04858200	-3.13470700	3.85372400
H	-0.85161600	-4.11324900	1.61206200
C	0.39422200	-2.75253700	5.15150700

C	-1.25797800	-1.46391400	2.43184800
H	-4.43130000	2.91259600	-0.86093400
H	-0.98655600	1.90306300	-7.44731800
N	-1.41809300	-0.47983000	1.45920100
O	1.45888300	-1.33827600	7.55331600
C	-0.05898100	-2.10411900	2.76021200
C	-2.72686100	1.64862500	-0.11559000
H	-0.78775500	3.66872700	-7.64911700
C	-3.35751900	2.78942700	-0.73873800
H	-0.04466000	-7.11415400	-0.23534500
N	0.77806300	-1.40430300	5.33910800
C	-0.58946500	2.81832900	-6.97964200
C	1.27178100	-0.77975100	6.47386000
H	0.50378700	2.70963800	-6.89145100
H	3.70672900	0.40325300	5.80120900
H	0.68047500	-0.81409000	4.51421100
H	-3.17950100	2.20166600	-6.19081000
H	1.34088800	1.02492200	5.24854100
H	-3.07921200	3.97387500	-6.38204600
N	-1.34428700	1.78455400	-0.13095200
C	1.58370500	0.71713400	6.28374400
C	-2.36104100	3.66234500	-1.06840700
C	1.14565800	-1.80635500	2.10566200
C	-2.78827200	3.12804400	-5.73974100
C	3.08627500	0.95167400	6.52851600
Co	-0.01074000	0.42326700	0.41121200
C	-1.25163100	3.06171200	-5.61392600
C	-1.11316700	3.02603500	-0.71253500
H	-2.44694300	4.65219400	-1.51295100
H	2.46410900	-3.40167800	2.97539100
C	2.36621200	-2.54825100	2.30712300
N	1.34792700	-0.76363500	1.21214600
H	3.36101300	0.60694500	7.53719500
H	-0.99424600	2.22615400	-4.93509400

H	3.33181700	2.02312200	6.44774800
C	-0.74895900	4.39082300	-5.02047600
H	-3.27351700	3.25908100	-4.75918900
C	0.72178600	1.53941600	7.25984000
H	-0.35429900	1.41724600	7.05511200
H	-0.42964600	3.39254900	-3.25424500
N	-0.35338400	4.31101300	-3.69056500
O	-0.73980200	5.42396500	-5.68592700
C	0.14273000	3.60326100	-0.94985500
C	3.31931300	-1.96830100	1.51962000
C	2.69350300	-0.84615100	0.85954600
H	0.90925400	1.21210000	8.29394500
N	1.45207900	1.61648500	-0.21247300
H	0.96375200	2.61210500	7.18514000
C	-0.00016600	5.35665800	-2.80547600
H	3.29842900	5.48905300	3.20141300
C	1.34066200	2.90460900	-0.72541500
C	0.22206500	5.02357300	-1.44184300
H	4.36805400	-2.23926500	1.41861600
C	0.12146600	6.69070200	-3.24100200
C	2.80690600	1.30997300	-0.30264700
C	3.40103500	0.11417800	0.12436900
C	2.52361000	5.92468700	3.85298400
H	-0.04577700	6.92198400	-4.29102000
H	0.57581700	4.71402300	1.03290000
C	0.53471200	6.06314600	-0.52187800
H	2.59400200	5.43835700	4.83937600
N	0.71019000	5.70430400	0.83303200
H	5.47328500	-3.68488200	-1.89683000
H	2.74662300	6.99545800	3.97631100
H	4.56286000	-1.57537700	-1.63670400
C	0.44702600	7.68223000	-2.31327000
C	2.63810100	3.41864900	-1.09437400
C	0.65032500	7.39547100	-0.96217600

C	3.54127700	2.42057800	-0.86039900
C	1.11468600	5.74600300	3.25797500
C	1.03193900	6.50444700	1.92017400
H	0.93339100	4.66683600	3.09153100
C	6.57342800	-3.68121500	-1.95176200
C	5.31068000	-1.02693200	-1.05564300
C	4.86792700	-0.09866000	-0.10462800
H	5.48012700	-1.81963000	-3.72365100
H	6.87312600	-4.43267700	-2.70200700
H	0.54042400	8.71745100	-2.65557000
H	2.81517600	4.40965100	-1.50803900
H	6.95712700	-4.00925400	-0.97194400
H	0.89410700	8.17223800	-0.23978200
O	1.23473100	7.71529800	1.85684900
C	6.58055700	-1.87145800	-3.71733100
H	6.88530600	-2.60157300	-4.48642100
H	4.61423400	2.42719600	-1.03943000
C	7.13164800	-2.28616500	-2.32999300
C	6.68622200	-1.25428900	-1.27268300
C	5.81428200	0.61975200	0.65451100
C	0.03082500	6.28750400	4.20989000
H	5.44781600	1.32740000	1.40156000
H	0.09437000	5.79333400	5.19284200
H	6.96442700	-0.88237500	-4.01645100
H	0.16453900	7.37036300	4.35604200
C	7.59731800	-0.51898500	-0.49988000
H	-0.98275900	6.12101400	3.81025400
C	7.19042700	0.42261800	0.47122200
C	8.66607500	-2.39675800	-2.43820900
H	8.93134900	-3.14265500	-3.20507900
H	9.12581700	-2.72447600	-1.49136700
H	6.99298000	1.65763600	3.03704900
H	8.66717900	-0.68032300	-0.64994200
H	9.13053900	-1.44214800	-2.73560000

H	8.49594900	-0.41985300	2.77786300
C	7.62758300	2.16977700	2.29527300
H	7.01924400	2.94147300	1.79535100
C	8.25463200	1.18334600	1.28920800
C	9.11618600	0.16816600	2.08184500
H	9.63671900	-0.53962800	1.41747800
H	8.42440700	2.69051400	2.85072700
C	9.16491500	1.98831500	0.32763700
H	8.58135200	2.72567700	-0.24764500
H	9.68417400	1.33684200	-0.39293900
H	9.88400000	0.69539600	2.67307100
H	9.93582000	2.53511800	0.89660200
C	-0.79282800	-1.75712600	-3.91323800
N	-0.65366500	-2.76196100	-2.82449900
S	-1.01680400	-2.04339000	-1.30856400
N	0.01714700	-0.67038100	-1.26522200
O	-0.68120800	-3.06465200	-0.28670200
O	-2.39002700	-1.53252800	-1.42546200
C	0.51193200	-3.66522500	-2.86469400
C	0.40207000	-4.67111200	-3.99949800
H	1.46938500	-3.11218400	-2.94443000
H	0.52533700	-4.19624700	-1.89981400
C	-0.83909100	-5.22379500	-4.36291800
C	-0.91683400	-6.19003600	-5.37305500
C	1.56020400	-5.10347800	-4.66872000
C	1.48364100	-6.07591900	-5.67503600
C	0.24366900	-6.62034200	-6.03160300
H	0.18093300	-7.37583900	-6.82065800
H	2.39501900	-6.40405800	-6.18446000
H	-1.74217500	-4.88385400	-3.84776900
H	-1.88924300	-6.61193000	-5.64577000
H	2.53408400	-4.68295500	-4.39343300
C	2.04517600	-1.26942700	-4.88116200
C	1.35201300	-0.30361500	-4.18999900

C	0.01777200	-0.49463000	-3.71024800
H	-0.52176100	-2.27818200	-4.84528300
H	-1.86037600	-1.50566300	-3.97778800
H	0.97495300	-1.06399200	-1.28334400
H	1.62144800	-2.24571700	-5.12834900
H	3.04732300	-1.06627100	-5.26788400
C	1.97991900	1.05673700	-3.96583500
H	1.90886300	1.35956900	-2.91142200
H	1.46647000	1.83032200	-4.56172300
H	3.04149000	1.06972900	-4.25153400
H	-0.54251800	0.39877800	-3.42975300

Transition State TS3[7] (Radical Substitution for 7-member ring):

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -154.4719 cm-1

G_corr: 1.537674 Hartree

H_corr: 1.815555 Hartree

SCF: -6196.965023 Hartree

S: 584.849 Cal/Mol-Kelvin

H: -6195.149469 Hartree

G: -6195.427349 Hartree

Cartesian Coordinates:

H	-9.66655700	-0.27118800	0.71300900
H	-9.38538100	1.02736100	-0.46990300
C	-8.88285400	0.31564300	0.20429600
H	-8.34637900	0.90046100	0.96930800
H	-8.77110600	3.34750000	-3.26295100
H	-9.49032200	-2.03844600	-1.12691000
C	-8.22790600	3.07197000	-4.18196900
H	-8.47205200	3.82865800	-4.94530900
H	-9.20856800	-0.77617600	-2.34758000
C	-8.70970300	-1.43079200	-1.61544100

H	-8.27528900	1.29225400	-2.45519000
C	-7.91475700	-0.62387600	-0.55812400
H	-6.71025000	4.71848500	-2.55224500
H	-8.62246200	2.10681800	-4.54017900
H	-8.12259300	-2.19987100	0.92845200
C	-7.21288000	1.17888700	-2.22756400
C	-7.31397100	-1.61991200	0.45423800
C	-6.24093100	4.43719700	-3.50929900
H	-6.52125400	5.19513800	-4.26039900
H	-6.75979700	-1.11001200	1.25880100
C	-6.83204900	0.21972800	-1.26264400
C	-6.70192200	3.02928500	-3.96296600
H	-8.04800700	-2.11385100	-2.17280100
C	-6.28632600	1.98806300	-2.90268200
H	-0.08287500	3.42134700	7.41435100
H	-1.27729200	2.70083700	6.31237600
H	-5.14899900	4.49088000	-3.37524700
C	-0.24172900	2.61666400	6.68097000
H	-6.63186500	-2.33936600	-0.02724000
C	-5.46526200	0.07745100	-0.98300800
C	-6.03053000	2.68045800	-5.31527200
H	-6.31277400	3.41730400	-6.08647000
H	-4.11224600	3.11243300	-0.22380100
H	-0.13510900	1.64825200	7.19621100
C	-4.92190300	1.82288800	-2.58534100
O	0.68493900	5.15878700	5.58365000
H	-6.34260000	1.68351800	-5.66705600
H	-5.11071200	-0.64342900	-0.24321900
H	-2.19503400	4.64867300	0.94552800
H	0.59782600	6.76092600	4.11166500
C	-4.50633400	0.87614900	-1.63969900
C	-3.05136400	2.90051100	-0.11122900
H	0.55205200	8.61094300	2.43166100
C	0.55257200	6.54940500	3.04512500

C	0.66337000	4.13905000	4.89789900
C	0.52702800	7.57071900	2.09275900
C	-2.09101000	3.66997000	0.48076900
C	0.77928900	2.74286500	5.53829400
H	-4.16113100	2.42727100	-3.08880700
H	-4.93150800	2.67986800	-5.24239500
H	2.47059300	3.32721000	6.78310000
C	0.52075000	5.21010300	2.61093000
N	0.55928100	4.12400200	3.51518400
C	0.47633500	7.30759000	0.72210700
C	2.22130400	2.54576900	6.04856800
C	-3.05465600	0.70367300	-1.31519100
C	-2.40005500	1.70536900	-0.59088700
H	0.46688900	8.10690600	-0.01669600
H	0.56562500	1.96484900	4.77840500
H	2.33068000	1.56410300	6.53738400
C	0.44996700	4.90475200	1.22649100
H	0.57357100	3.20637600	3.07124800
C	0.44009500	5.96989100	0.28395600
C	-0.84762400	2.94791000	0.36262500
H	-4.07317800	-1.44688000	-2.86737100
H	-1.57633200	-6.40165700	3.94712300
N	-1.04585500	1.72484200	-0.27653100
O	0.42922700	7.68172800	-2.15436100
C	0.39403000	3.48152100	0.74021100
C	-2.41253400	-0.47312200	-1.70805200
H	-1.43567700	-7.75381300	2.78643900
C	-3.06581800	-1.51576800	-2.46340500
H	2.95578000	2.60153300	5.22906100
N	0.40420200	5.62688700	-1.08525500
C	-1.20091500	-6.69114600	2.95157700
C	0.40748300	6.45359000	-2.20019200
H	-0.10314000	-6.58667100	2.95679800
H	2.58317400	5.62639100	-3.73540600

H	0.38290800	4.62548000	-1.27372600
H	-3.75900700	-5.63392000	2.90018000
H	0.31850700	4.60902500	-3.36092700
H	-3.70751600	-6.96062700	1.70488000
N	-1.11215900	-0.84387800	-1.38233900
C	0.39137300	5.69843300	-3.54242800
C	-2.18839500	-2.55557200	-2.54774200
C	1.59265700	2.77350500	0.57443400
C	-3.38549400	-5.92650500	1.90488100
C	1.70469700	5.98556500	-4.29585600
Co	0.23713100	0.21528600	-0.39710500
C	-1.84720900	-5.82391600	1.85601500
C	-0.98768400	-2.14327200	-1.86139500
H	-2.31901800	-3.52062600	-3.03335800
H	3.05789900	4.35734000	1.20526600
C	2.89011000	3.34050900	0.85499900
N	1.70998000	1.46249700	0.12162500
H	1.82095800	7.06909300	-4.45209200
H	-1.55630000	-4.77243000	2.00523500
H	1.70326100	5.49055800	-5.28054600
C	-1.36867000	-6.31242800	0.47903200
H	-3.85924800	-5.26878600	1.15813700
C	-0.83309400	6.14575500	-4.36134300
H	-1.77693500	5.89616900	-3.85010800
H	-0.77345000	-4.38626500	0.06484200
N	-0.82143300	-5.32739100	-0.33963800
O	-1.49341400	-7.49410700	0.15640000
C	0.13981300	-2.96249300	-1.73806100
C	3.80933800	2.36772600	0.58849400
C	3.07619300	1.20356300	0.14787200
H	-0.80763400	7.23576400	-4.51191700
N	1.58421500	-1.19493100	-0.76003600
H	-0.83974100	5.65687700	-5.34902700
C	-0.35323800	-5.47656600	-1.66610600

H	3.98431900	-1.88298100	-5.59216500
C	1.34371400	-2.49157000	-1.19886700
C	0.11450800	-4.32964600	-2.36429100
H	4.89182700	2.41653300	0.68454700
C	-0.33987000	-6.73308900	-2.31149600
C	2.95599700	-1.14911400	-0.53059600
C	3.68768200	-0.01916100	-0.15064300
C	3.32315400	-1.60688200	-6.42959800
H	-0.69658100	-7.60491300	-1.76837400
H	0.93835900	-2.44121100	-3.81989300
C	0.57000800	-4.46620100	-3.70722000
H	3.58629100	-0.58582200	-6.75084300
N	1.00251400	-3.29491800	-4.37213600
H	6.40379200	-0.83663600	3.70662400
H	3.52502400	-2.29722200	-7.26283500
H	5.22314600	-1.18093200	1.77312400
C	0.12161700	-6.83258200	-3.62423200
C	2.56133000	-3.26718000	-1.20632700
C	0.57523200	-5.72244800	-4.33889200
C	3.56359800	-2.42954700	-0.81201900
C	1.83850700	-1.68538800	-6.02961700
C	1.48937200	-3.14053700	-5.66102600
H	1.67053600	-1.02471400	-5.15754100
C	7.49413600	-0.81050100	3.55271400
C	5.83267000	-0.74211800	0.97741900
C	5.18524000	-0.10512100	-0.08878600
H	6.36945300	-3.09345300	2.39329600
H	7.96428100	-1.30215400	4.42127800
H	0.12479900	-7.81372600	-4.10941100
H	2.62672800	-4.30818600	-1.51667400
H	7.80621000	0.24670100	3.55068400
H	0.92918100	-5.80024400	-5.36522300
O	1.63743100	-4.05730400	-6.46711300
C	7.46170200	-2.99886100	2.28638500

H	7.92587300	-3.51660500	3.14290100
H	4.62748300	-2.64071400	-0.72884900
C	7.91392000	-1.51778100	2.23942100
C	7.24045600	-0.81556900	1.04177100
C	5.95398600	0.47047700	-1.12084400
C	0.92281900	-1.22496400	-7.17997400
H	5.42886200	0.95788900	-1.94540800
H	1.18052300	-0.20095700	-7.49624300
H	7.75518400	-3.53267500	1.36766700
H	1.03895200	-1.89547100	-8.04536200
C	7.97076800	-0.23305500	-0.00493500
H	-0.13869700	-1.23313100	-6.88352400
C	7.35496000	0.41444500	-1.09874900
C	9.45336400	-1.48928800	2.15102700
H	9.88448300	-1.99954600	3.02766000
H	9.84924200	-0.46033100	2.14390600
H	6.77052300	2.52142400	-2.92798500
H	9.06168700	-0.27994900	0.02354100
H	9.82708200	-2.00974100	1.25386700
H	8.58597600	2.91198100	-1.13812800
C	7.38503700	1.69392800	-3.31935300
H	6.71647700	0.97571900	-3.82178000
C	8.22806100	1.02527200	-2.21445300
C	9.16504500	2.09933300	-1.60660500
H	9.83345200	1.67894700	-0.83867300
H	8.05026100	2.11608100	-4.09004400
C	9.08199100	-0.09072000	-2.86753900
H	8.44242400	-0.86995400	-3.31323100
H	9.74799800	-0.58048700	-2.13964500
H	9.79963400	2.54386900	-2.39197100
H	9.71494000	0.32867600	-3.66794300
C	-0.54010900	-1.79339600	4.48574200
N	-1.60601600	-1.48233000	3.48293900
S	-1.32363000	-1.47309800	1.79077000

N	-0.13659800	-0.29428500	1.47845500
O	-2.65178900	-1.15458300	1.22207400
O	-0.69629600	-2.76773500	1.44923500
C	-2.59815800	-0.51531700	4.00082400
C	-3.49677600	-1.14909700	5.05001900
H	-2.08878100	0.37054200	4.43414600
H	-3.20538300	-0.17599600	3.14956900
C	-4.22946200	-2.30961900	4.74016900
C	-5.08733200	-2.87919800	5.68709300
C	-3.63711600	-0.57440300	6.32312800
C	-4.49946900	-1.14200400	7.27212500
C	-5.22556800	-2.29628800	6.95592200
H	-5.89743600	-2.74280300	7.69538800
H	-4.59930100	-0.68273700	8.26052500
H	-4.11829700	-2.76178600	3.74991800
H	-5.65519400	-3.77985500	5.43360200
H	-3.06949600	0.32834500	6.57562400
C	1.91532800	-0.91805900	3.12588000
C	1.69160000	-2.27936900	3.37458400
C	0.54495700	-2.71320300	4.02754600
H	-1.08202300	-2.23947100	5.33658000
H	-0.11370000	-0.83830300	4.85331800
H	-0.52750200	0.56975800	1.89748000
H	2.72902200	-0.58543000	2.47910000
H	1.36035100	-0.13386300	3.63985200
C	2.66371300	-3.30163900	2.82213300
H	2.65385800	-3.28908100	1.72033600
H	2.40502100	-4.32019200	3.14724900
H	3.69656800	-3.09567300	3.14800500
H	0.37880400	-3.78676800	4.15505300

Intermediate $E^5_{3.1c}$:

$E_{3.6c}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.214509 Hartree

H_corr: 0.278469 Hartree

SCF: -1125.170135 Hartree

S: 134.616 Cal/Mol-Kelvin

H: -1124.891665 Hartree

G: -1124.955626 Hartree

Cartesian Coordinates:

H	-4.66389700	1.95064500	-1.40094100
C	-4.16064700	1.21289800	-0.76824400
H	-2.44833000	1.04241800	-2.08369900
C	-2.91165200	0.70257800	-1.15031800
H	-5.73121400	1.18109900	0.72442100
C	-4.75789000	0.78249000	0.42221500
C	-2.25188100	-0.24741700	-0.35367700
C	-4.10129300	-0.15991900	1.22798800
H	-0.56663000	-0.31433600	-1.70649900
H	-1.03878600	-1.89499800	-1.05905100
C	-0.92326200	-0.83293700	-0.79315900
C	-2.85770800	-0.67192200	0.84356800
H	-4.56309100	-0.49927900	2.16043900
H	2.74879900	4.13529600	0.43397400
H	2.55808600	-0.58412900	-1.67927000
H	1.17200200	3.41288600	0.82433800
C	2.02120900	3.37347400	0.11838100
H	1.24583600	1.23943800	-1.36732500
H	-2.33853200	-1.39924900	1.47465000
C	1.73290500	0.89615500	-0.43181400
N	0.06190800	-0.77905500	0.31965300
N	2.42666300	-0.38686700	-0.68440500
C	2.65141200	2.00167000	0.06503800
O	1.28035900	-2.72837800	-1.01925900
H	1.62226400	3.67402100	-0.86794600

C	0.59797700	0.56357100	0.60903300
S	1.51008500	-1.69746700	0.00580100
H	-0.22215100	1.29285800	0.56935500
C	3.91746600	1.75978800	0.43438800
H	4.56057500	2.56309200	0.80664600
H	1.02163200	0.56047700	1.62477200
O	2.09290800	-2.03091700	1.30538500
H	4.33613300	0.75248200	0.37718100

Intermediate $E^{7}_{3.1c}$:

$Product_{3.2c}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.218324 Hartree

H_corr: 0.279663 Hartree

SCF: -1125.178866 Hartree

S: 129.1 Cal/Mol-Kelvin

H: -1124.899202 Hartree

G: -1124.960542 Hartree

Cartesian Coordinates:

C	0.36685000	0.42232300	1.28630700
N	0.16165600	-0.65147900	0.27382400
S	1.59321900	-1.51504800	-0.10525800
N	2.75306000	-0.44092900	-0.74789200
O	1.25870000	-2.43041700	-1.20118900
O	2.14239100	-1.95192300	1.18329800
C	-0.68325100	-0.27855800	-0.88277500
C	-2.11888100	-0.03735100	-0.45134400
H	-0.64131800	-1.12010800	-1.59069600
H	-0.29247700	0.62046500	-1.40146500
C	-2.79568600	1.13127700	-0.83580500
C	-4.13486000	1.33439400	-0.47294100
C	-2.80203500	-0.99985500	0.31466300

C	-4.13644700	-0.79612000	0.68205400
C	-4.80785700	0.37097200	0.28762700
H	-5.85215200	0.52811300	0.57479700
H	-4.65775200	-1.55323700	1.27625500
H	-2.27138900	1.88892300	-1.42935100
H	-4.65002900	2.24942400	-0.78180000
H	-2.27303000	-1.90584200	0.62576300
C	3.18897100	0.67166500	0.12797300
C	2.22360900	1.84708500	0.25721600
C	0.98096400	1.70943300	0.76894600
H	0.96679800	-0.02488700	2.09477400
H	-0.62781000	0.62911700	1.70983000
H	3.40571700	0.22005200	1.11009100
H	4.15660700	1.01591600	-0.27240300
H	2.46240100	-0.14056600	-1.68362500
C	2.74285500	3.18100700	-0.22207800
H	3.02921300	3.14495400	-1.28935800
H	3.65472800	3.47230700	0.33064400
H	2.00116300	3.98374400	-0.09522600
H	0.34069100	2.60033500	0.80844800

3.5 REFERENCES

1. (a) Nechab, M.; Mondal, S.; Bertrand, M. P. 1,n-Hydrogen-Atom Transfer (HAT) Reactions in Which n≠5: An Updated Inventory. *Chem. Eur. J.* **2014,** *20*, 16034-16059. (b) Sarkar, S.; Cheung, K. P. S.; Gevorgyan, V. C–H Functionalization Reactions Enabled by Hydrogen Atom Transfer to Carbon-centered Radicals. *Chem. Sci.* **2020,** *11*, 12974-12993.

2. Huang, X. L.; Dannenberg, J. J. Molecular Orbital Estimation of the Activation Enthalpies for Intramolecular Hydrogen Transfer as Functions of Size of the Cyclic Transition State and Carbon-Hydrogen-Carbon Angle. *J. Org. Chem.* **1991,** *56*, 5421-5424.

3. (a) Dorigo, A. E.; Houk, K. N. Transition Structures for Intramolecular Hydrogen-atom Transfers: the Energetic Advantage of Seven-membered over Six-membered Transition Structures. *J. Am. Chem. Soc.* **1987,** *109*, 2195-2197. (b) Dorigo, A. E.; Houk, K. N. The Relationship between Proximity and Reactivity. An Ab Initio Study of the Flexibility of the OH.bul. + CH4 Hydrogen Abstraction Transition State and a Force-field Model for the Transition States of Intramolecular Hydrogen Abstractions. *J. Org. Chem.* **1988,** *53*, 1650-1664. (c) Dorigo, A. E.; McCarrick, M. A.; Loncharich, R. J.; Houk, K. N. Transition Structures for Hydrogen Atom Transfers to Oxygen. Comparisons of Intermolecular and Intramolecular Processes, and Open- and Closed-shell Systems. *J. Am. Chem. Soc.* **1990,** *112*, 7508-7514. (d) Moran, D.; Jacob, R.; Wood, G. P. F.; Coote, M. L.; Davies, M. J.; O'Hair, R. A. J.; Easton, C. J.; Radom, L. Rearrangements in Model Peptide-Type Radicals via Intramolecular Hydrogen-Atom Transfer. *Helv. Chim. Acta* **2006,** *89*, 2254-2272. (e) Kuwata, K. T.; Dibble, T. S.; Sliz, E.; Petersen, E. B. Computational Studies of Intramolecular Hydrogen Atom Transfers in the β-Hydroxyethylperoxy and β-Hydroxyethoxy Radicals. *J. Phys. Chem. A* **2007,** *111*, 5032-5042.

4. (a) Hofmann, A. W. Ueber die Einwirkung des Broms in alkalischer Lösung auf die Amine. *Berichte der deutschen chemischen Gesellschaft* **1883,** *16*, 558-560. (b) Löffler, K.; Freytag, C. Über eine neue Bildungsweise von N-alkylierten Pyrrolidinen. *Berichte der deutschen chemischen Gesellschaft* **1909,** *42*, 3427-3431. (c) Barton, D. H. R.; Beaton, J. M.; Geller, L. E.; Pechet, M. M. A New Photochemical Reaction1. *J. Am. Chem. Soc.* **1961,** *83*, 4076-4083.

5. Chu, J. C. K.; Rovis, T. Complementary Strategies for Directed C(sp3)−H Functionalization: A Comparison of Transition-Metal-Catalyzed Activation, Hydrogen Atom Transfer, and Carbene/Nitrene Transfer. *Angew. Chem., Int. Ed.* **2018,** *57*, 62-101.

6. Li, C.; Lang, K.; Lu, H.; Hu, Y.; Cui, X.; Wojtas, L.; Zhang, X. P. Catalytic Radical Process for Enantioselective Amination of C(sp^3)−H Bonds. *Angew. Chem., Int. Ed.* **2018,** *57*, 16837-16841.

7. (a) Zhang, W.; Wang, F.; McCann, S. D.; Wang, D.; Chen, P.; Stahl, S. S.; Liu, G. Enantioselective Cyanation of Benzylic C–H bonds via Copper-Catalyzed Radical Relay. *Science* **2016,** *353*, 1014-1018. (b) Nakafuku, K. M.; Zhang, Z.; Wappes, E. A.; Stateman, L. M.; Chen, A. D.; Nagib, D. A. Enantioselective Radical C–H Amination for the Synthesis of β-Amino Alcohols. *Nature Chem.* **2020,** *12*, 697-704.

8. Chen, H.; Sanjaya, S.; Wang, Y.-F.; Chiba, S. Copper-Catalyzed Aliphatic C–H Amination with an Amidine Moiety. *Org. Lett.* **2013,** *15*, 212-215.

9. Xiong, T.; Zhang, Q. New Amination Strategies Based on Nitrogen-Centered Radical Chemistry. *Chem. Soc. Rev.* **2016,** *45*, 3069-3087.

10. Lang, K.; Torker, S.; Wojtas, L.; Zhang, X. P. Asymmetric Induction and Enantiodivergence in Catalytic Radical C–H Amination via Enantiodifferentiative H-Atom Abstraction and Stereoretentive Radical Substitution. *J. Am. Chem. Soc.* **2019,** *141*, 12388-12396.

11. Hu, Y.; Lang, K.; Li, C.; Gill, J. B.; Kim, I.; Lu, H.; Fields, K. B.; Marshall, M.; Cheng, Q.; Cui, X.; Wojtas, L.; Zhang, X. P. Enantioselective Radical Construction of 5-Membered Cyclic Sulfonamides by Metalloradical C–H Amination. *J. Am. Chem. Soc.* **2019,** *141*, 18160-18169.

12. (a) Hopmann, K. H.; Ghosh, A. Mechanism of Cobalt-Porphyrin–Catalyzed Aziridination. *ACS Catal.* **2011,** *1*, 597-600. (b) Lyaskovskyy, V.; Suarez, A. I. O.; Lu, H.; Jiang, H.; Zhang, X. P.; de Bruin, B. Mechanism of Cobalt(II) Porphyrin-Catalyzed C–H Amination with Organic Azides: Radical Nature and H-Atom Abstraction Ability of the Key Cobalt(III)–Nitrene Intermediates. *J. Am. Chem. Soc.* **2011,** *133*, 12264-12273. (c) Olivos Suarez, A. I.; Jiang, H.; Zhang, X. P.; de Bruin, B. The Radical Mechanism of Cobalt(II) Porphyrin-catalyzed Olefin Aziridination and the Importance of Cooperative H-bonding. *Dalton Transactions* **2011,** *40*, 5697-5705. (d) Goswami, M.; Lyaskovskyy, V.; Domingos, S. R.; Buma, W. J.; Woutersen, S.; Troeppner, O.; Ivanović-Burmazović, I.; Lu, H.; Cui, X.; Zhang, X. P.; Reijerse, E. J.; DeBeer, S.; van Schooneveld, M. M.; Pfaff, F. F.; Ray, K.; de Bruin, B. Characterization of Porphyrin-Co(III)-'Nitrene Radical' Species Relevant in Catalytic Nitrene Transfer Reactions. *J. Am. Chem. Soc.* **2015,** *137*, 5468-5479.

13. (a) Jiang, H.; Lang, K.; Lu, H.; Wojtas, L.; Zhang, X. P. Asymmetric Radical Bicyclization of Allyl Azidoformates via Cobalt(II)-Based Metalloradical Catalysis. *J. Am. Chem. Soc.* **2017,** *139*, 9164-9167. (b) Jin, L.-M.; Xu, P.; Xie, J.; Zhang, X. P. Enantioselective Intermolecular Radical C–H Amination. *J. Am. Chem. Soc.* **2020,** *142*, 20828-20836. (c) Riart-Ferrer, X.; Sang, P.; Tao, J.; Xu, H.; Jin, L.-M.; Lu, H.; Cui, X.; Wojtas, L.; Zhang, X. P. Metalloradical Activation of Carbonyl Azides for Enantioselective Radical Aziridination. *Chem* **2021,** *7*, 1120-1134. (d) Lang, K.; Hu, Y.; Lee, W.-C. C.; Zhang, X. P. Combined Radical and Ionic Approach for the Enantioselective Synthesis of β-Functionalized Amines from Alcohols. *Nature Synthesis* **2022,** *1*, 548-557.

14. Dudev, T.; Lim, C. Ring Strain Energies from ab Initio Calculations. *J. Am. Chem. Soc.* **1998,** *120*, 4450-4458.

15. Ruppel, J. V.; Jones, J. E.; Huff, C. A.; Kamble, R. M.; Chen, Y.; Zhang, X. P. A Highly Effective Cobalt Catalyst for Olefin Aziridination with Azides: Hydrogen Bonding Guided Catalyst Design. *Org. Lett.* **2008,** *10*, 1995-1998.

16. Chen, Y.; Fields, K. B.; Zhang, X. P. Bromoporphyrins as Versatile Synthons for Modular Construction of Chiral Porphyrins: Cobalt-Catalyzed Highly Enantioselective and Diastereoselective Cyclopropanation. *J. Am. Chem. Soc.* **2004,** *126*, 14718-14719.

17. Lang, K.; Li, C.; Kim, I.; Zhang, X. P. Enantioconvergent Amination of Racemic Tertiary C–H Bonds. *J. Am. Chem. Soc.* **2020,** *142*, 20902-20911.

18. (a) Raymo, F. M.; Bartberger, M. D.; Houk, K. N.; Stoddart, J. F. The Magnitude of [C−H···O] Hydrogen Bonding in Molecular and Supramolecular Assemblies. *J. Am. Chem. Soc.* **2001,** *123*, 9264-9267. (b) Niebel, C.; Lokshin, V.; Sigalov, M.; Krief, P.; Khodorkovsky, V. Intra- and Intermolecular C(sp2)–H···O Hydrogen Bonds in a Series of Isobenzofuranone Derivatives: Manifestation and Energetics. *Eur. J. Org. Chem.* **2008,** *2008*, 3689-3699. (c) Reep, C.; Sun, S.; Takenaka, N. C(sp2)−H Hydrogen-Bond Donor Groups in Chiral Small-Molecule Organocatalysts. *Asian J. Org. Chem.* **2019,** *8*, 1306-1316.

19. Bruker. *APEX2.* Bruker AXS Inc., Madison, Wisconsin, USA, 2012.

20. Bruker. SAINT. Data Reduction Software, 2013.

21. Sheldrick, G. M. *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany, 1996.

22. Farrugia, L. J. WinGX suite for small-molecule single-crystal crystallography. *J. Appl. Cryst.* **1999**, 837-838.

23. Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16, Revision A.03*. Gaussian, Inc., Wallingford CT, 2016.

24. (a) Schultz, N. E.; Zhao Y Fau - Truhlar, D. G.; Truhlar, D. G. Density Functionals for Inorganometallic and Organometallic Chemistry. (b) Dzik, W. I.; Xu, X.; Zhang, X. P.; Reek, J. N. H.; de Bruin, B. 'Carbene Radicals' in CoII(por)-Catalyzed Olefin Cyclopropanation. *J. Am. Chem. Soc.* **2010,** *132*, 10891-10902.

25. Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. Auxiliary Basis Sets for Main Row Atoms and Transition Metals and Their Use to Approximate Coulomb Potentials. *Theor. Chem. Acc.* **1997,** *97*, 119-124.

26. Legault, C. Y. *CYLview, 1.0b*, Université de Sherbrooke: 2020.

27. Humphrey, W., Dalke, A. and Schulten, K. VMD - Visual Molecular Dynamics. *J. Mol. Graph.* **1996,** *14*, 33-38.

CHAPTER 4 - METALLORADICAL ACTIVATION OF ALKYL HYDROPEROXIDES FOR CATALYTIC RADICAL C–H HYDROXYLATION

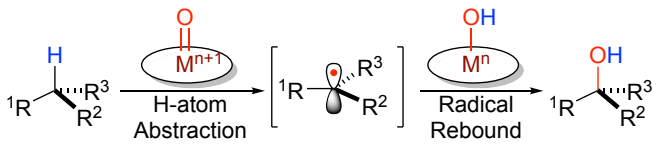
4.1 INTRODUCTION

Introducing an oxygen atom or hydroxyl group by replacing a C−H bond in a molecule can significantly alter a molecule's physical and biological properties.[1] For example, the meticulous positioning of oxygen functionality in a compound of interest can serve as effective hydrogen bond donors and acceptors, allowing small molecules to bind to specific protein sites and afford varying physiological responses.[2] Thus, selective hydroxylation of C(sp^3)−H bonds has been receiving extensive attention from synthetic chemists due to the promise of impressive improvements in efficient synthesis and optimization of drugs.[3] In this context, catalytic oxygen-atom-transfer C(sp^3)−H hydroxylation, in which a metal-oxo or an organic oxidant is deployed, has been actively examined and has demonstrated substantial promise for this purpose.[4] Among the research efforts of developing metal-catalyzed C(sp^3)−H hydroxylation reactions from several groups, the deployment of bioinspired Fe, Mn, and other metal complexes on catalytic access to high-valent metal-oxo species have been extensively conducted to hydroxylate C−H bonds.[4]

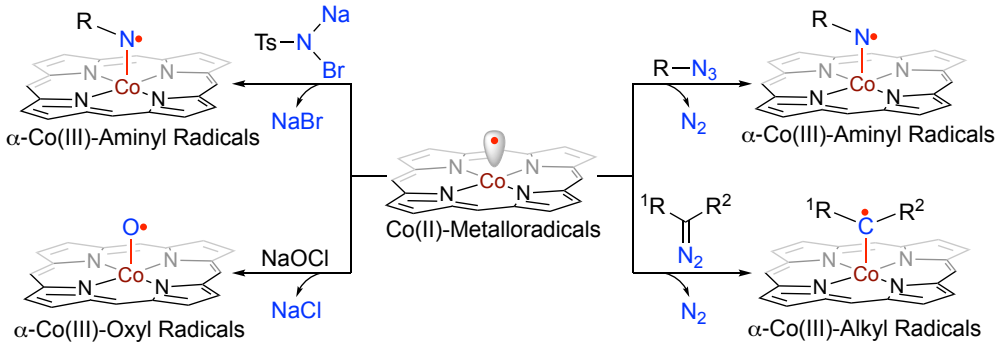
High-valent terminal oxo complexes (M^{n+1}=O) of transition metals have been postulated as vital reactive intermediates in many biological[5] and chemical oxidation

processes.[6] They are often recognized to be capable of hydrogen atom abstraction (HAA) from C(sp^3)–H bonds for the generation of metal hydroxide complexes (M^n–OH) and associated alkyl radicals, which undergo subsequent radical rebound in achieving C–H hydroxylation (Scheme 4.1).[7] However, the tunability in electronic and steric properties of the metal oxo unit formed on a given metal complex is not straightforward[8] and is limited by the fact that the O atom in the metal oxo cannot bear any tuning substituents. The reactivity bias among C–H bonds with similar bond dissociation energies is defined by their electronic properties. Due to the electrophilic character of high-valent metal-oxo species, the electron-rich C–H bonds are generally preferred in HAA step.[9] Thus, the hydroxylation of the electron-deficient C–H bonds is generally not executable with the same metal-oxo species.[9] Accordingly, the catalytic C–H hydroxylation based on this classic mechanism is limited in altering the chemoselectivity bias, the regioselectivity bias and the reactivity bias for different substrates. Regarding this issue, it is essential to develop a general approach of C–H hydroxylation with switchable chemoselectivity, regioselectivity and reactivity.

Scheme 4.1 Catalytic C-H Hydroxylation through Metal-oxo Intermediates



Scheme 4.2 Metalloradical Activation of Radical Precursors via Co(II)-based MRC

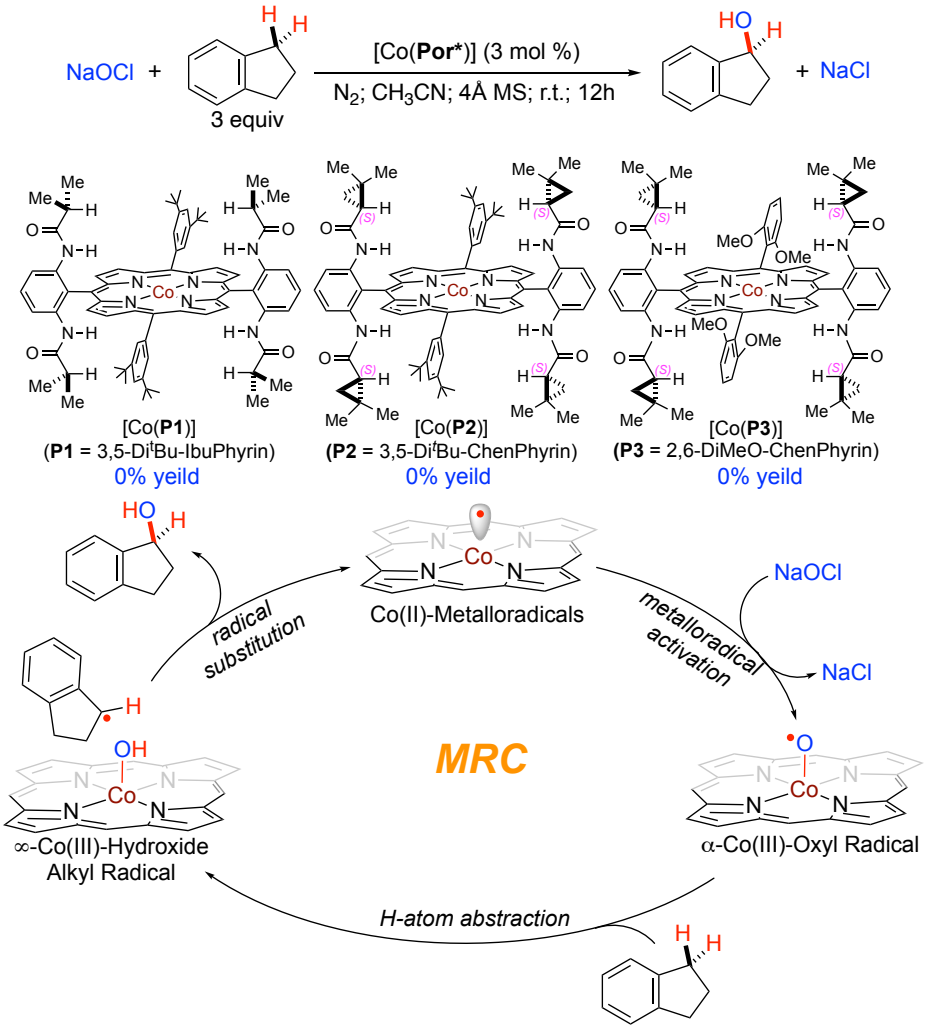


In the past two decades, metalloradical catalysis (MRC) has presented a conceptually different approach based on catalytic generation of metal-supported organic radicals as key intermediates from metalloradical activation of radical precursors and further control of the subsequent homolytic radical reactions.[10] As stable 15e-metalloradicals, Co(II)-based porphyrin catalysts have a unique capability to conduct homolytic cleavage of strong bonds in azides and diazos reagents, and weak bonds in Bromamine-T and NaOCl, and to afford α-Co(III)-organic radicals and outgoing species (Scheme 4.2). [10a,10b,11a,10c-t,11b] And the outgoing species are not radicals. Various α-Co(III)-alkyl radicals and α-Co(III)-aminyl radicals from different precursors hold different reactivity and selectivity, attributed to their organic substitutions (Scheme 4.2; –R/R^1/R^2 group) that can alter the electronic and steric properties of these radicals.[12]

In contrast to α-Co(III)-alkyl radicals and α-Co(III)-aminyl radicals, the reactivity and selectivity of α-Co(III)-oxyl radicals might be less tunable due to the lack of organic substitutions (i.e. R, R1 and R2 groups). It might then seem that, similarly to the metal-oxo species, α-Co(III)-oxyl radicals might not be sufficiently tunable to preform highly

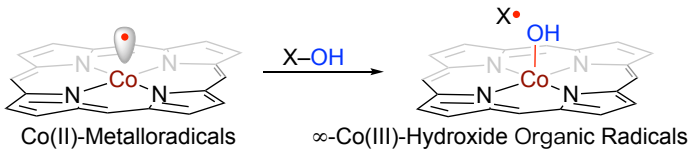
selective C–H hydroxylation reactions. Indeed, our preliminary results has demonstrated α-Co(III)-oxyl radicals was not able to perform C–H hydroxylation of indane (Table 4.1).

Table 4.1 C–H hydroxylation Reactions via α-Co(III)-Oxyl Radicals[a]



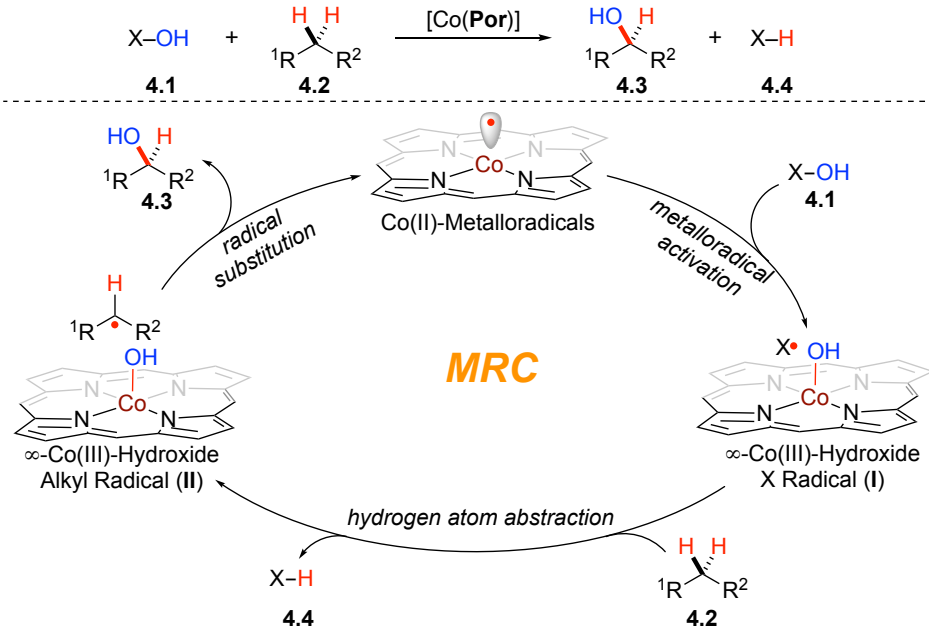
[a]Carried out with NaOCl (0.10 mmol) in the presence of 4 Å molecular sieves and indane (3 equiv) by [Co(**Por***)] (3 mol %) in acetonitrile (0.5 mL) at room temperature for 12 h; NMR yields; Full recovery of starting material indane.

Scheme 4.3 Generation of ∞-Co(III)-Hydroxide Organic Radicals via MRC



However, if non-radical α-Co(III)-hydroxide complexes with outgoing organic radicals can be formed through metalloradical activation (Scheme 4.3), the precursors with different electronic and steric properties could allow outgoing organic radicals to proceed highly selective HAA with various C–H bonds depending on the electronic and steric properties. (The non-radical α-Co(III)-hydroxide complexes with outgoing organic radicals together is termed as ∞-Co(III)-hydroxide organic radicals. Note: ∞ symbol represents no covalent bond connecting two species.) It could be a great approach for C–H hydroxylation to deploy the outgoing organic radicals for C–H activation through HAA (Scheme 4.4). The subsequent alkyl radicals from HAA can undergo radical substitution on –OH group from α-Co(III)-hydroxide complexes, affording alcohols through the formation of C–O bond and translocating the radical to Co(II)-based porphyrins. As the electronic and steric properties of organic radicals can be easily altered by their substituents, this strategy would be extremely valuable for achieving highly selective C–H hydroxylation reactions. Meanwhile, switchable chemoselectivity, regioselectivity and reactivity among different C–H bonds could be realized under Co(II)-based catalysis.

Scheme 4.4 Metalloradical C–H Hydroxylation via ∞-Co(III)-Hydroxide Organic Radicals



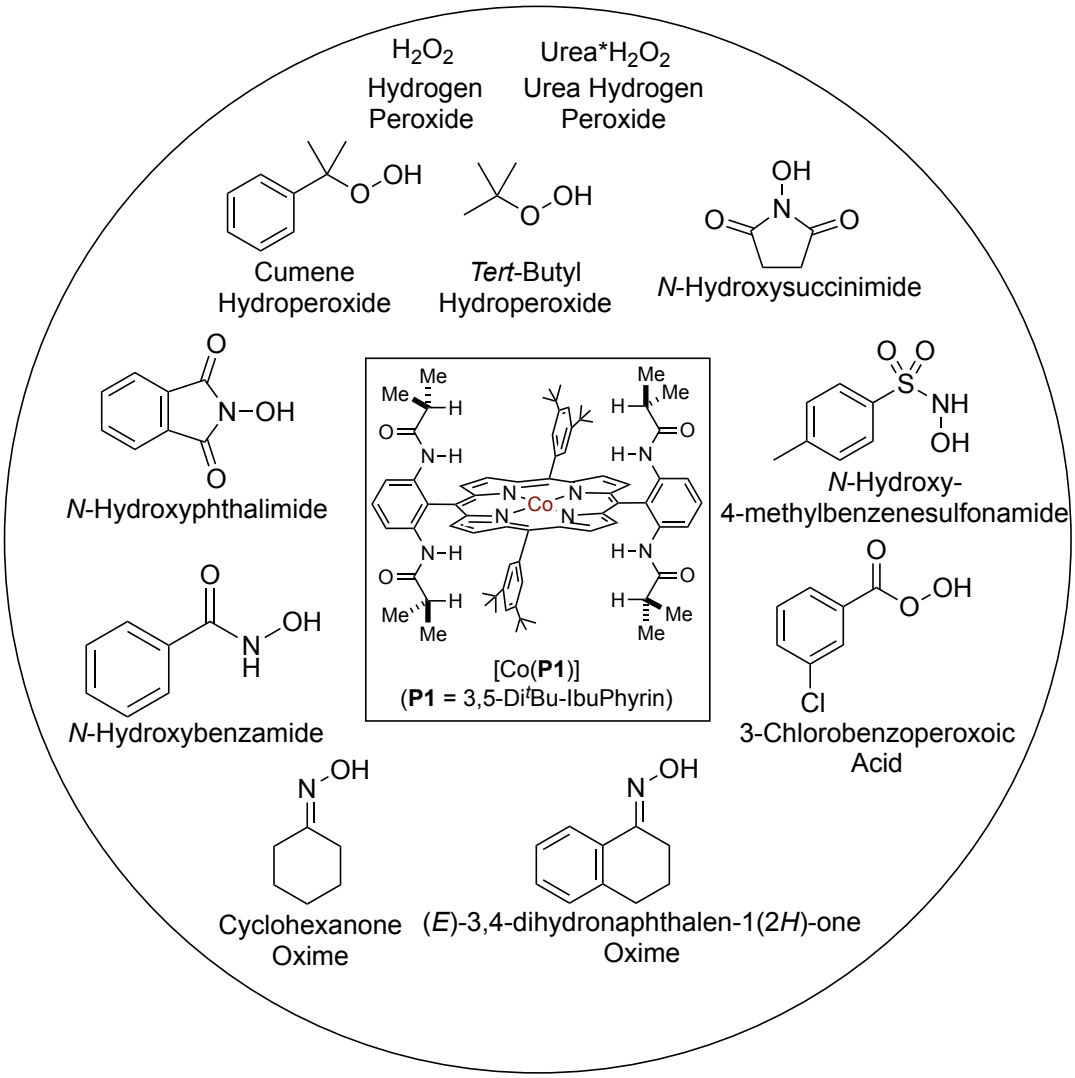
Therefore, as a new direction of metalloradical catalysis (MRC) for controlling homolytic radical reaction, we hope to develop a fundamentally different catalytic mechanism for C–H hydroxylation that involves metalloradical activation of radical precursors by Co(II)-based porphyrin catalysts for facile generation of α-Co(III)-hydroxide complexes along with closely associated organic radicals (∞-Co(III)-hydroxide organic radicals).

4.2 RESULTS AND DISCUSSION

4.2.1 Examination on Metalloradical Activation of Oxidants via UV-Vis Spectroscopy

At the outset of our investigation, we focused our efforts on identifying suitable –OH group containing oxidants as potential radical precursors that could be homolytically activated by Co(II)-metalloradicals [Co(**Por**)] for the generation of the proposed ∞-Co(III)-hydroxide organic radicals (Scheme 4.3). The ∞-Co(III)-hydroxide organic radicals were proposed to consist of two individual species, α-Co(III)-hydroxide and organic radical, which may interact with each other through some interactions. An effective approach to examine the formation of α-Co(III)-hydroxide from Co(II)-metalloradicals is to measure the absorbance via UV-Vis (ultraviolet-visible spectroscopy). As reported, the maximum absorption of [Co^{II}(**Por**)] generally lies in the range from 415 nm to 425 nm in various solvents, and the maximum absorption of [Co^{III}(**Por**)] typically lies in the range from 435 nm to 445 nm in the same solvents.[13,14] Some common –OH group containing oxidants (Table 4.2), such as hydrogen peroxides, alkyl hydroperoxides, peroxide acids, *N*-hydroxyamides, *N*-hydroxyimides and oximes, were proposed to serve as the precursors of ∞-Co(III)-hydroxide organic radicals. UV-Vis experiments were conducted with Co(II)-metalloradical [Co(**P1**)] (**P1** = 3,5-Di^{t}Bu-IbuPhyrin) in the presence of these oxidants in benzene at room temperature under a N_2 atmosphere.

Table 4.2 Common Oxidants with –OH Group



UV-Vis experiments revealed that the signal for [Co^{III}(**P1**)] only appeared with cumene hydroperoxide, *N*-hydroxy-4-methylbenzenesulfonamide and 3-chloroperoxybenzoic acid under this particular condition (Table 4.3). However, the peak of [Co^{III}(**P1**)] fades away rapidly on the spectra of *N*-hydroxy-4-methylbenzenesulfonamide and 3-chloroperoxybenzoic acid (See Spectra on Section 4.4.2). While *N*-hydroxy-4-methylbenzenesulfonamide and 3-chloroperoxybenzoic acid completely turned [Co^{II}(**P1**)] to [Co^{III}(**P1**)], but the disappearance of the [Co^{III}(**P1**)]

corresponding peak could be caused by further reactions and denied the possibility of being a suitable precursor of ∞-Co(III)-hydroxide organic radicals. The rest of the attempted oxidants, hydrogen peroxide, urea hydrogen peroxide, ^{t}butyl hydroperoxide, *N*-hydroxyphthalimide, *N*-hydroxybenzamide, *N*-hydroxy-4-methylbenzenesulfonamide, cyclohexanone oxime, (*E*)-3,4-dihydronaphthalen-1(2H)-one oxime, were suggested not to be effective to oxidize [Co^{II}(**P1**)] to [Co^{III}(**P1**)] at room temperature in benzene. Thus, UV-Vis studies suggest that only cumene hydroperoxide could serve as a potential precursor of ∞-Co(III)-hydroxide organic radicals, as it can effectively and steadily oxidize [Co^{II}(**P1**)] to [Co^{III}(**P1**)].

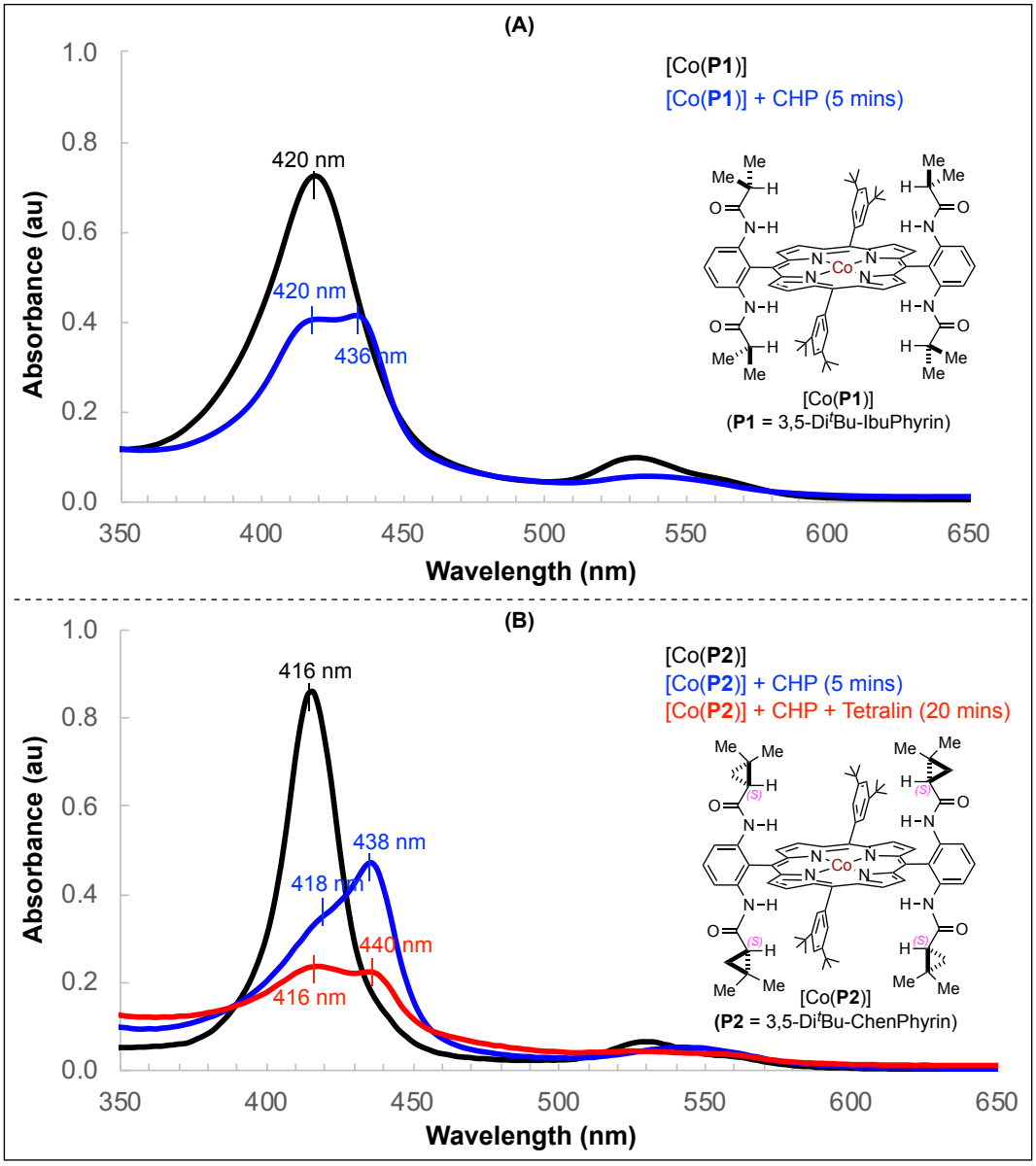
Table 4.3 Examination on Metalloradical Activation of Oxidants via UV-Vis[a]

Oxidants	[Co^{II}(P1)]	[Co^{III}(P1)]
Hydrogen Peroxide	+	–
Urea Hydrogen Peroxide	+	–
Cumene Hydroperoxide	+	+
Tert-Butyl Hydroperoxide	+	–
N-Hydroxysuccinimide	+	–
N-Hydroxyphthalimide	+	–
N-Hydroxybenzamide	+	–
N-Hydroxy-4-methylbenzenesulfonamide	–	–
Cyclohexanone Oxime	+	–
(*E*)-3,4-dihydronaphthalen-1(2*H*)-one Oxime	+	–
3-Chloroperoxybenzoic acid	–	–

[a]The maximum absorption of [Co^{II}(**P1**)] lies in the range from 415 nm to 425 nm; The maximum absorption of [Co^{III}(**P1**)] peak lies in the range from 435 nm to 445 nm; +

represents the presence of the signal on the spectra after 60 mins; – represents the absence of the signal on the spectra after 60 mins.

Scheme 4.5 UV-Vis Studies on Metalloradical Activation of Cumene Hydroperoxide



When cumene hydroperoxide (CHP) was added into a solution of Co(II)-metalloradical [Co(**P1**)] (**P1** = 3,5-Di^{t}Bu-IbuPhyrin) in benzene at room temperature, significant bathochromic shift of the Soret band (from 420 nm to 436 nm) was observed in

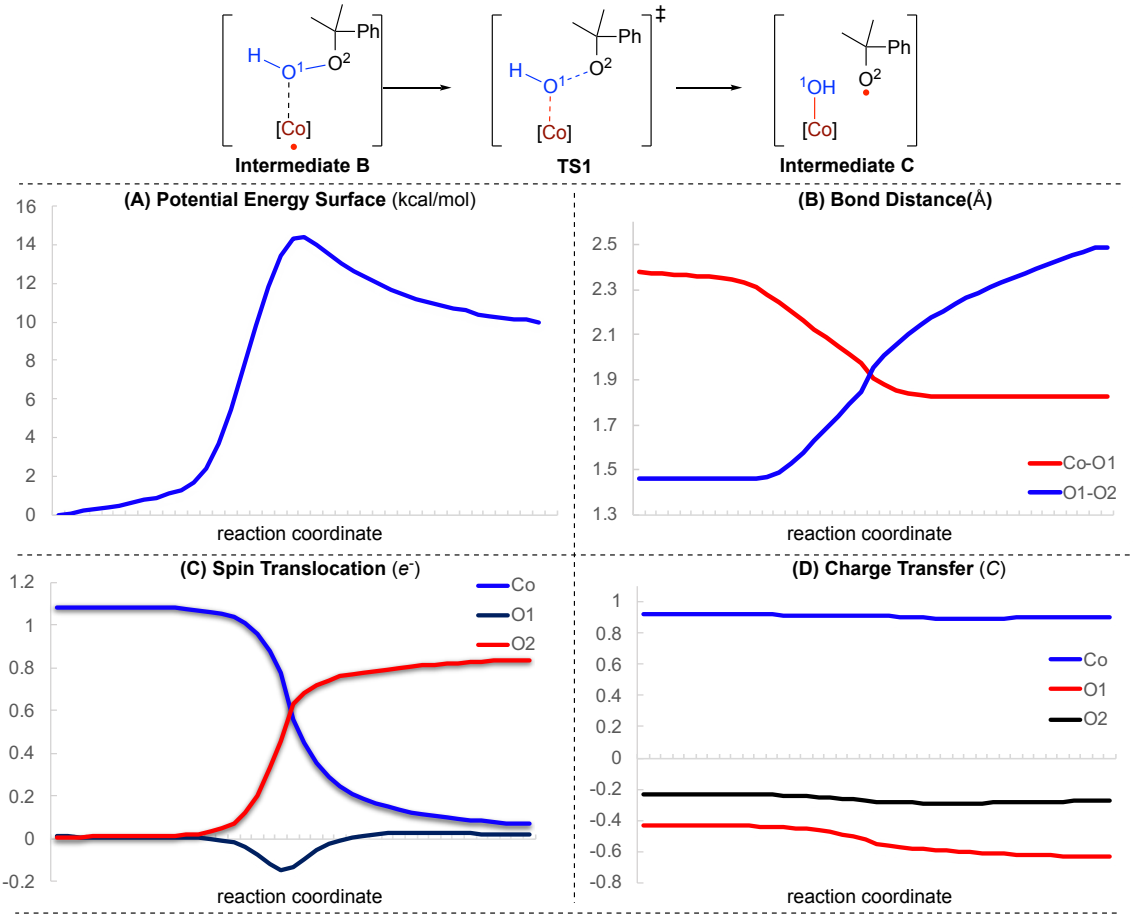
5 mins by UV-Vis (Scheme 4.5 A). Similar fast bathochromic shifts of Soret (from 416 nm to 438 nm) and other bands were observed by UV-Vis with the use of Co(II) complex of D_2-symmetric chiral amidoporphyrin [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-ChenPhyrin) (Scheme 4.5 B). Importantly, when [Co(**P2**)] was exposed to air for 8 h without CHP, there was no bathochromic shifts of Soret band. This characteristic change in the optical absorption spectra is in agreement with the reported redshifts associated with one-electron oxidation of Co(II) to Co(III) in the metalloporphyrins. When tetralin was added as C–H source in the reaction, the peak of Co(III) complex was shifting back to the one of Co(II) complex after 20 mins, indicating the turnover of the catalysts possibly from the C–H hydroxylation reaction (Scheme 4.5 B). Additionally, on account of the commercially availability of CHP at low cost and the stability and safety at room temperature, it was selected as the radical precursor of choice for further studies regarding the metalloradical activation and C–H hydroxylation.

4.2.2 Computational Investigation on Metalloradical Activation of CHP

While UV-Vis studies suggest CHP could serve as a potential precursor of ∞-Co(III)-hydroxide organic radicals, the mechanism of metalloradical activation of CHP remains unexplored. CHP was proposed to initially form an adduct with Co(II)-metalloradicals (Scheme 4.6; Intermediate **B**) and then get activated through the homolytic cleavage of O^1–O^2 bond (Scheme 4.6; **TS1**), affording ∞-Co(III)-hydroxide cumyloxyl radical (Scheme 4.6; Intermediate **C**). If so, this metalloradical activation process should involve spin translocation from the [Co(**Por**)] to the oxygen atom (O^2) of CHP (Scheme 4.6). To

shed light on this metalloradical activation process, DFT calculations were conducted to investigate spin translocation, charge variation, bond distance change of all participant atoms along the minimal energy reaction path (Scheme 4.6).

Scheme 4.6 Quantitative Analysis on Metalloradical Activation of CHP[a]

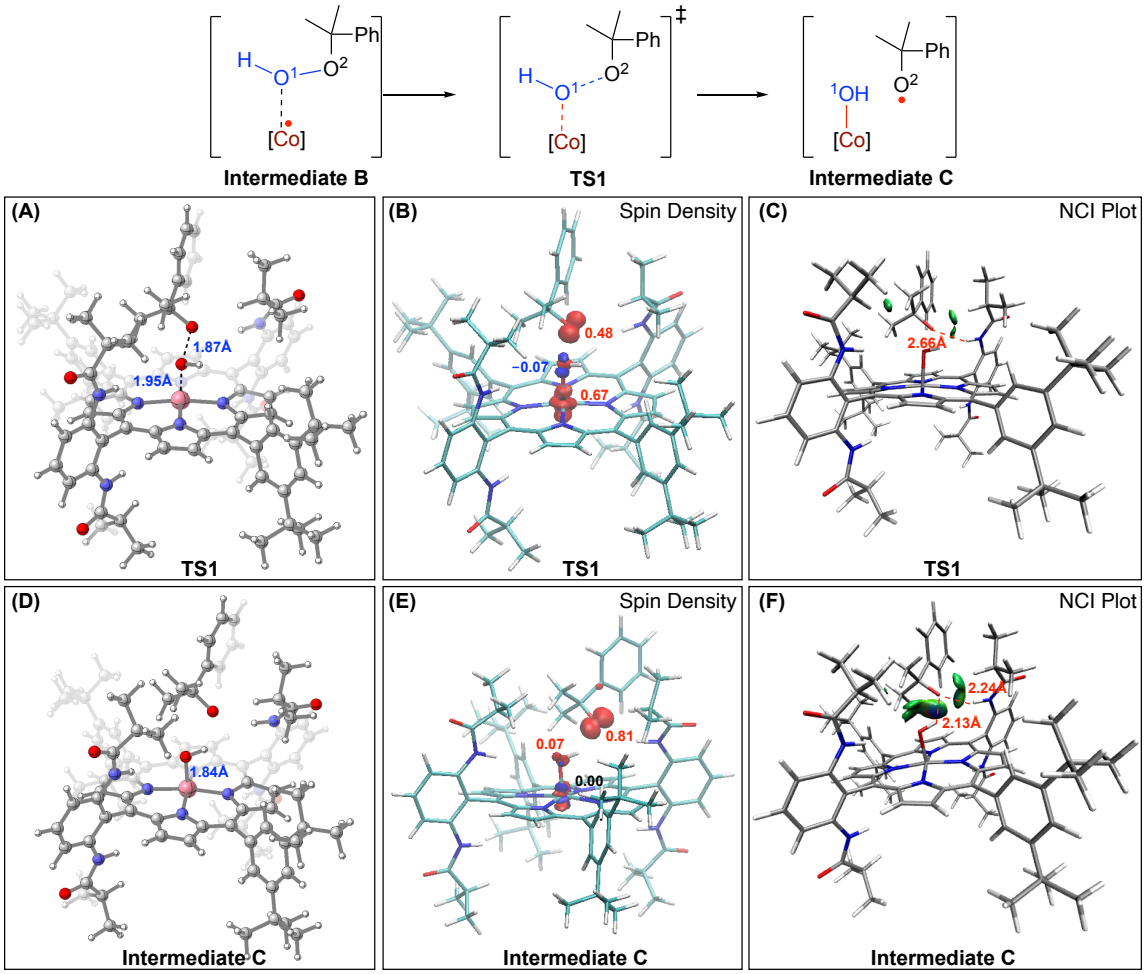


[a]Applied B3LYP/6-311G(d)$_{C, O, H, N}$/def2-svp$_{Co}$ level of theory for the geometry optimization and the energy calculations.

Firstly, the potential energy surface displays an accessible activation barrier (about 14 kcal/mol in terms of internal energy) of this metalloradical activation process (Scheme 4.6.A). Secondly, the formation of the Co–O^1 bond accompanies the cleavage of the O^1–

O^2 bond mediated by spin translocation along the reaction path (Scheme 4.6.B). Thirdly, the spin density on the Co center goes from its original +1 to zero as the reaction proceeds. With the same X-axes variation of reaction coordinate, the spin density on O^2 atom increases from original zero to +1, and only trace amount of spin density locates on the O^1 atom in intermediate **C** (Scheme 4.6.C). These changes of spin density are consistent with the postulated spin translocation from the cobalt center to the oxygen atom (O^2) as the O^1–O^2 bond is cleaved and the Co–O^1 bond is formed (Scheme 4.6). Lastly, the analysis of the Mulliken charge suggests slightly change in charge occurs for cobalt and O^1 (Scheme 4.6.D).

Scheme 4.7 Conformational Investigation on Metalloradical Activation of CHP[a]



[a]Applied B3LYP/6-311G(d)$_{\_C,\ O,\ H,\ N}$/def2-svp$_{_Co}$ level of theory for the geometry optimization and the energy calculations; Green solid surface indicates attractive interactions in NCI plots; Spin density unit: e^-.

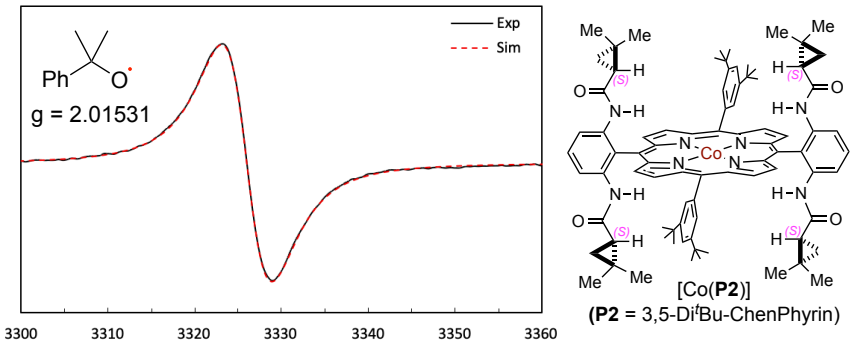
In addition to the quantitative analysis of metalloradical activation of CHP, the structural information, spin density plots, non-covalent interactions plots of intermediate **C** and **TS1** was visualized to shed light on this process and the nature of ∞-Co(III)-hydroxide cumyloxyl radical (Scheme 4.7). In the NCI plots of **TS1**, a weak H-bonding interaction O^2--(2.66Å)--H–N was displayed (Scheme 4.7.C), potentially reducing the

energy barrier of metalloradical activation. Along the reaction occurring, this H-bonding gets stronger, indicated by its distance O^2--(2.24Å)--H–N in intermediate **C** (Scheme 4.7.F). Beyond this H-bonding, there is additional one formed among O^2 and α-Co(III)-hydroxide, O^2--(2.13Å)--H–O^1 in intermediate **C** (Scheme 4.7.F). While ∞-Co(III)-hydroxide cumyloxyl radical intermediate **C** was considered as two individual components (α-Co(III)-hydroxide and cumyloxyl radical), the cumyloxyl radical is tightly bonded in the cavity of the catalyst with the support of two strong H-bondings. This nature of ∞-Co(III)-hydroxide cumyloxyl radical could be very beneficial for potential asymmetric induction and the fast turn-over of the catalytic cycle.

4.2.3 Characterization of ∞-Co(III)-Hydroxide Cumyloxyl Radicals

While UV-Vis experiments and DFT calculations hint at a positive interaction between the Co(II) porphyrin and the radical precursor CHP, they do not provide enough information about the exact nature of the new radical species, termed ∞-Co(III)-hydroxide alkoxyl radical. A series of Electron Paramagnetic Resonance (EPR) experiments were conducted to explore the nature of ∞-Co(III)-hydroxide cumyloxyl radical.

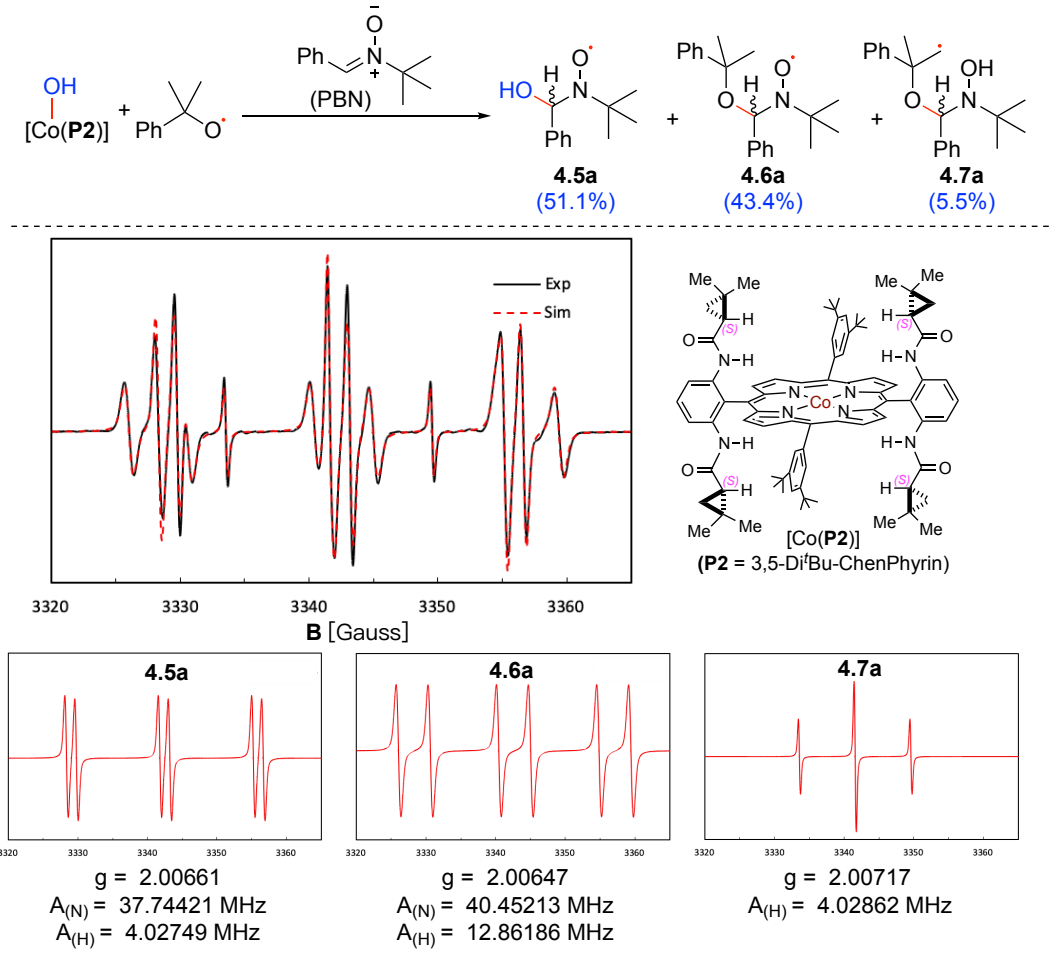
Scheme 4.8 EPR Experiment of [Co(P2)] and CHP



While [Co(**P2**)] are EPR silent at room temperature, the EPR spectrum of the reaction mixture between [Co(**P2**)] and CHP displayed a diagnostic peak. The presence of EPR signal documents the formation of a new radical species, possibly corresponding to ∞-Co(III)-hydroxide alkoxyl radical (Scheme 4.8). It is worth mentioning that control experiments in the absence of [Co(**P2**)] showed no EPR signal, and when [Co(**P2**)] was exposed to oxygen in the absence of other species under the same reaction conditions, no signal was observed either. The observed diagnostic peak was then simulated with the proposed cumyloxyl radical using SpinFit software, which matches the experimental result well. Thus, this EPR experiment suggests the existence of cumyloxyl radical.

To investigate the nature of the newly formed radical, we utilized the spin trapping reagent *N*-tert-butyl-α-phenylnitrone (PBN) for spin trapping experiments. The simple diagnostic signal (a simple antisymmetric peak) associated with ∞-Co(III)-hydroxide alkoxyl radicals (Scheme 4.8), varied drastically upon the addition of trapping reagent PBN (Scheme 4.9). These changes are coherently attributed to the trapping of ∞-Co(III)-hydroxide alkoxyl radicals.

Scheme 4.9 Spin Trapping EPR Experiment with PBN

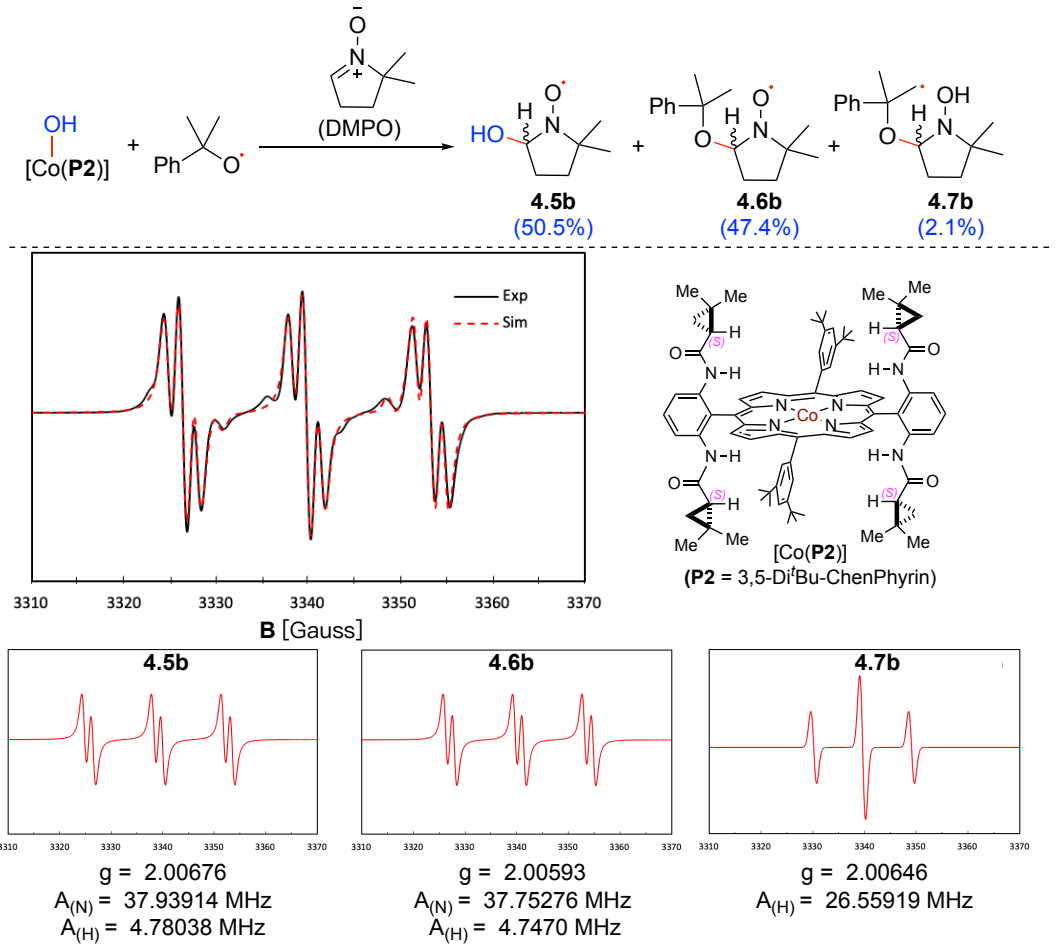


As ∞-Co(III)-hydroxide alkoxyl radicals are proposed to consist of two separated species, α-Co(III)-hydroxide complex and cumyloxyl radical species, both the hydroxyl substituent on Co(III) and cumyloxyl radical could be trapped by PBN, resulting in the formation of radical **4.5a** and radical **4.6a** (See more details on Section 4.4.6). Initially, radical **4.5a** and radical **4.6a** were taken for the simulation of the new signals observed upon the addition of PBN using SpinFit software. While the simulation roughly matched the texture of the experimental EPR spectrum, there are still some details lacking. Thus, radical **4.7a** was proposed to be afforded from radical **4.6a** through intramolecular 1,6-

HAA and deployed into the simulation along with radical **4.5a** and radical **4.6a**. An immaculate match between simulated and observed EPR spectrum was then uncovered with the composition of radical **4.5a**, **4.6a**, and **4.7a** in 51.1%, 43.4%, and 5.5%, respectively. Theoretically, radical **4.5a** and radical **4.6a** were formed in equal amounts. It is noted that some of radical **4.6a** was turned to radical **4.7a**, cutting down the amount of radical **4.6a**. However, the total amount of radical **4.6a** and **4.7a** occupies 48.9%, which is almost identical to the amount of radical **4.5a**. All these information strongly support the hypothesis that ∞-Co(III)-hydroxide alkoxyl radical was formed, and it consists of two individual species, α-Co(III)-hydroxide complex and cumyloxyl radical species.

Continuously, an additional spin trapping reagent 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO) was deployed in the examination of ∞-Co(III)-hydroxide alkoxyl radicals (Scheme 4.10; See more details on Section 4.4.6). As expected, similar spectacles were observed that radical **4.5b**, **4.6b**, and **4.7b** species were observed in 50.5%, 47.4%, 2.1% yield , supporting the hypothesis that ∞-Co(III)-hydroxide alkoxyl radical was formed to consist of two individual species, α-Co(III)-hydroxide complex and cumyloxyl radical species.

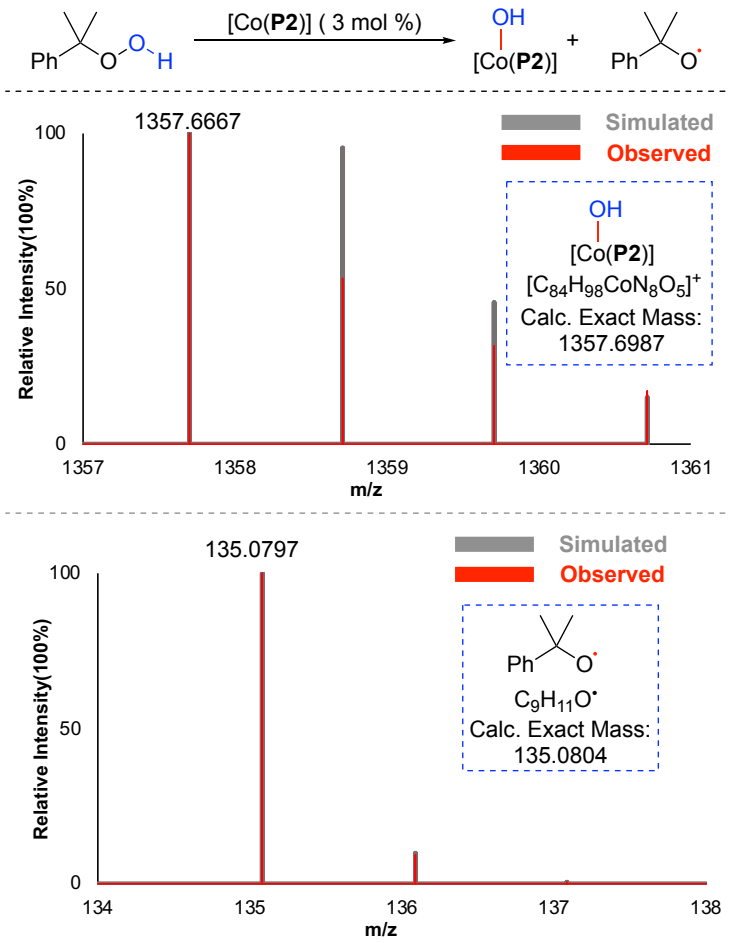
Scheme 4.10 Spin Trapping EPR Experiment with DMPO



While UV-Vis experiments, EPR experiments and DFT calculations has successfully probed ∞-Co(III)-hydroxide cumyloxyl radical, they do not provide direct evidence about its existence. While this putative reactive ∞-Co(III)-hydroxide alkoxyl radical intermediate was less likely isolatable, we could read its existence by high-resolution mass spectrometry (HRMS) (Scheme 4.11). Consistently, HRMS experiments reveal that the proposed ∞-Co(III)-hydroxide alkoxyl radical intermediate was observed as two separated species, α-Co(III)-hydroxide complex and cumyloxyl radical species, indicated by the characteristic peak in the DART-TOF analysis of the in situ-generated mixture of CHP and [Co(**P2**)],

and its observed isotopic distribution matched with the simulations. The HRMS experiments give the direct and strong support to the hypothesis that ∞-Co(III)-hydroxide alkoxyl radical were formed, and it consists of two individual species, α-Co(III)-hydroxide complex and cumyloxyl radical species.

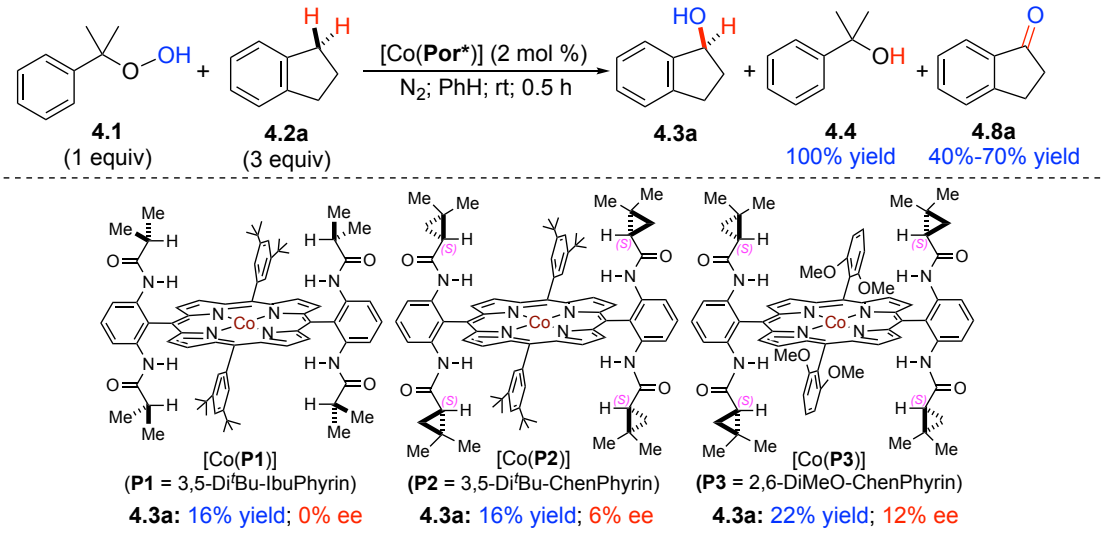
Scheme 4.11 HRMS Experiments of ∞-Co(III)-Hydroxide Alkoxyl Radicals



4.2.4 Metalloradical C–H Hydroxylation via ∞-Co(III)-Hydroxide Cumyloxyl Radicals

Encouraged by the obtained data on the characterization of ∞-Co(III)-hydroxide alkoxyl radical, we anticipated that if it could partake in catalytic radical C–H hydroxylation via the proposed catalytic cycle in the presence of C–H substrates (Scheme 4.4). To probe the idea, we proceeded with the [Co(**Por**)]-catalyzed C–H hydroxylation in the presence of CHP **4.1** and indane **4.2a** as a proof-of-concept model reaction (Table 4.4). The reactions were conducted in benzene, under the protection of N_2 and at room temperature for 0.5 h.

Table 4.4 Metalloradical C–H Hydroxylation with CHP[a]



[a]Carried out with CHP (**4.1**; 0.2 mmol) and indane (**4.2a**; 0.6 mmol) using [Co(**Por***)] (2 mol %) under N_2 atmosphere in benzene (0.5 mL) at room temperature for 0.5 h; NMR yield; Enantiomeric excess (ee) determined by chiral HPLC.

When achiral Co(II)-based amidoporphyrin [Co(**P1**)] (**P1** = 3,5-Di^{t}Bu-IbuPhyrin) was employed, it afforded 1-indanol **4.3a** in 16% yield. It is important to note that no **4.3a** was observed in the absence of any [Co(**P1**)] under identical reaction conditions. Despite the magnitude of the yield, these results support the involvement of the [Co(**P1**)] in the C–H hydroxylation reaction and hence, further support the hypothesis instigated by EPR, UV-Vis, and HRMS characterization studies. It demonstrated that the new species ∞-Co(III)-hydroxide cumyloxyl radical is essential to this catalytic C–H hydroxylation of **4.3a**.

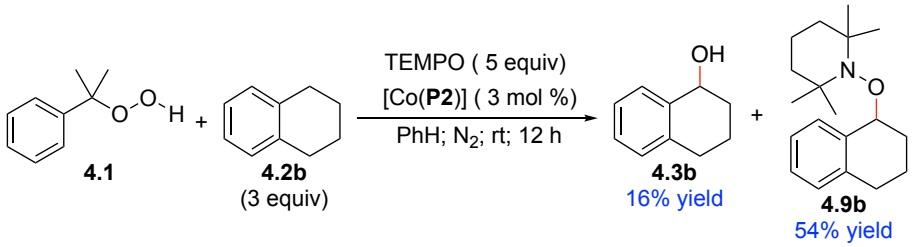
To ascertain the possibility of asymmetric induction in this metalloradical C–H hydroxylation system, chiral amidoporphyrins were deployed into the reaction (Table 4.4). When chiral amidoporphyrin [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-ChenPhyrin) was exposed to CHP in the presence of indane, the corresponding alcohol **4.3a** was obtained in 16% yield but with a noticeable degree of enantioselectivity (6% ee). When another chiral amidoporphyrin [Co(**P3**)] (**P3** = 2,6-DiMeO-ChenPhyrin) was treated with CHP in the presence of indane, the corresponding alcohol **4.3a** was obtained in a higher yield of 22%, and with a higher enantioselectivity of 12% ee.

In addition to the product **4.3a** formed from C–H hydroxylation, the overoxidation of **4.3a** occurred simultaneously under the catalyzation of [Co(**Por***)], affording 1-indanone **4.8a** in 40%-70% yield (if **4.8a** was oxidized from **4.3a** by another **CHP**). Therefore, the overoxidation is responsible for the low yield of C–H hydroxylation.

4.2.5 Mechanistic Studies of Metalloradical C–H Hydroxylation via ∞-Co(III)-Hydroxide Cumyloxyl Radicals

To shed light into the mechanism of this metalloradical catalytic C–H hydroxylation reaction, we explored the radical C–H hydroxylation with substrate **4.2b** in presence of excess amount of TEMPO (5 equiv) using [Co(**P2**)] (Scheme 4.11). In addition to the generation of C–H hydroxylation product **4.3b** (16% yield), TEMPO trapping product **4.9b** was obtained in 54% yield, resulting from the facile radical recombination of TEMPO and benzyl radical generate after intermolecular HAA from **4.2b**. And it is worth to mention that there was no reaction occurring without [Co(**P2**)]. The observation is in good agreement with the putative stepwise radical mechanism proposed (Scheme 4.3).

Scheme 4.12 TEMPO Trapping Experiment[a]

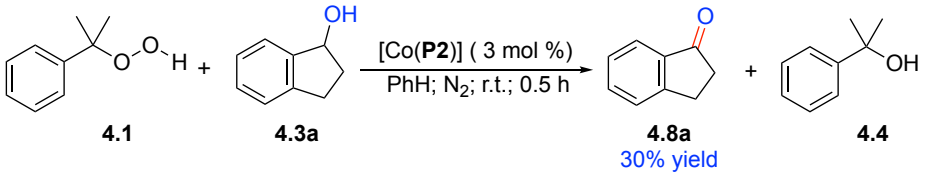


[a]Carried out with CHP (**4.1**; 0.2 mmol) and alkane (**4.2b**; 0.6 mmol) using [Co(**P2**)] (3 mol %) at presence of TEMPO (5 equiv) under N_2 atmosphere in benzene (0.5 mL) at room temperature for 12 h; NMR yield.

To understand the generation of side product **4.8a** in the C–H hydroxylation of indane, 1-indanol **4.3a** was treated with CHP and [Co(**P2**)] under the same reaction condition for 0.5 h (Scheme 4.12). 1-Indanone **4.8a** was afforded in 30% NMR yield. It gave us some clues that **4.8a** might be generated from **4.3a**, as benzylic C–H bond in **4.3a**

is more activated than the one in **4.2a**. Additionally, there was no reaction occurring without [Co(**P2**)].

Scheme 4.13 Overoxidation Experiment[a]

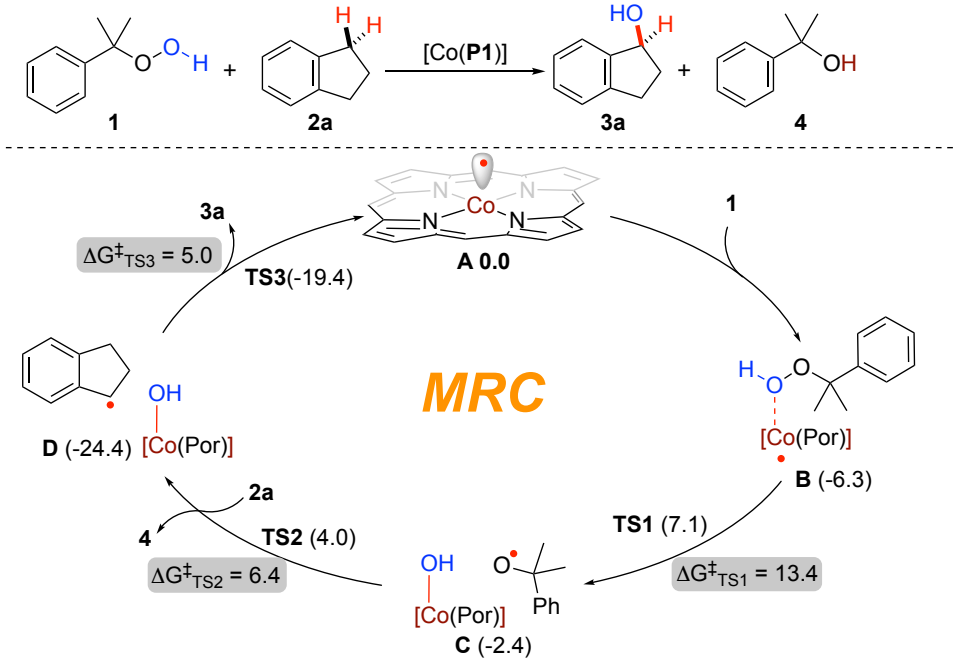


[a]Carried out with CHP (**4.1**; 0.2 mmol) and alcohol (**4.3a**; 0.6 mmol) using [Co(**P2**)] (3 mol %) under N_2 atmosphere in benzene (0.5 mL) for 0.5 h at room temperature; NMR yield.

To examine the energy profiles of C–H hydroxylation and overoxidation, we then carried out DFT study on the catalytic pathway by [Co(**P1**)] (**P1** = 3,5-Di^{t}Bu-IbuPhyrin) for the C–H hydroxylation reaction of indane with CHP (Scheme 4.13; see Experimental Section for more details). The DFT calculations indicate the formation of intermediate **B** adduct upon the weak interaction of the **CHP** to the cobalt center of the catalyst, which is exergonic by −6.3 kcal/mol. Upon further activation, the adduct **B** undergoes the elimination of cumyl alcohol to generate ∞-Co(III)-hydroxide alkoxyl radical **C**. The metalloradical activation step, which is slightly endergonic by +3.9 kcal/mol, has a reasonable activation energy ($\Delta G^{\ddagger}_{TS1}$ = 13.4 kcal/mol). According to the DFT calculations, the subsequent hydrogen atom abstraction of ∞-Co(III)-hydroxide alkoxyl radical **C** to indane is associated with an accessible activation barrier ($\Delta G^{\ddagger}_{TS2}$ = 6.4 kcal/mol), leading to the formation of ∞-Co(III)-hydroxide alkyl radical intermediate **D**. The final radical

substitution is an almost barrierless process, resulting in the formation of 1-indanol **4.3a** and the regeneration of the metalloradical catalyst [Co(**P1**)].

Scheme 4.14 Energy Profiles of Metalloradical C–H Hydroxylation with CHP[a]



[a]Applied B3LYP/6-311G(d)_C, O, H, N/def2-svp_Co//def2tzvp level of theory along with Grimme's dispersion correction (D3-BJ).; Energy unit: kcal/mol.

4.3 CONCLUSIONS

In summary, we have demonstrated, for the first time, the generation and characterization of ∞-Co(III)-hydroxide alkoxyl radical via the reaction of common oxidant CHP with Co(II)-based amidoporphyrins. The reactive ∞-Co(III)-hydroxide alkoxyl radical has been observed as two individual species, α-Co(III)-hydroxide complex and cumyloxyl radical species, and well characterized via UV-Vis, EPR, and HRMS. DFT studies reveal the mechanism of metalloradical activation of CHP that the single electron radical translocates from Co to O^2 atom via inner phase electron transfer.

Furthermore, these ∞-Co(III)-hydroxide alkoxyl radicals have been demonstrated to be competent intermediates for the enantioselective radical C–H hydroxylation. Further mechanistic studies on the C–H hydroxylation reaction agrees with the proposed stepwise radical mechanism inherent of MRC (Scheme 4.3). We envision that these findings can have potential implications in the design of selective oxidation reactions and can open new reactivity modes via Co(II)-metalloradical C–H hydroxylation and oxidation.

4.4 EXPERIMENTAL SECTION

4.4.1 General Considerations

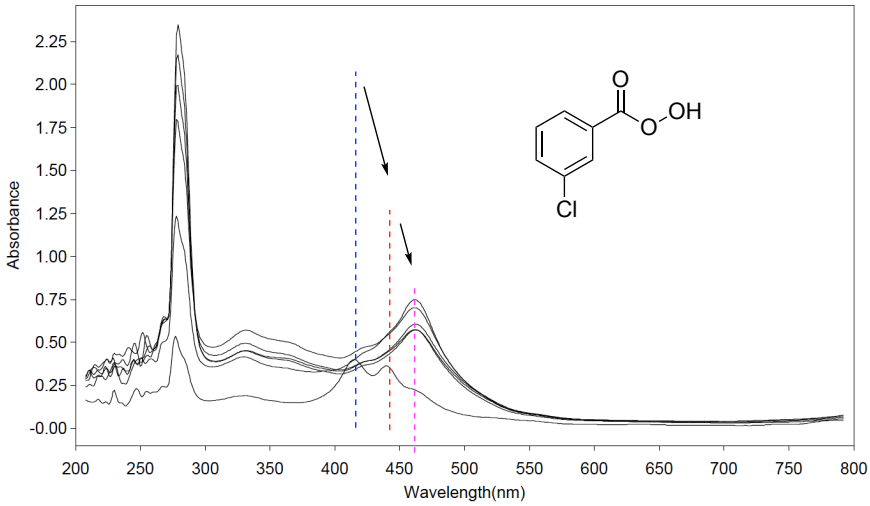
All C–H hydroxylation reactions were performed under a nitrogen atmosphere in an oven-dried glassware following standard Schlenk techniques. Gas tight syringes were used to transfer liquid reagents and solvents in catalytic reactions. Anhydrous solvents were purchased from Sigma-Aldrich and used without further purification. Thin layer chromatography was performed on Merck TLC plates (silica gel 60 F254). Flash column chromatography was performed with silica gel (60 Å, 230-4mesh, 32-63 μm). ^{1}H NMR and ^{13}C NMR were recorded on Varian/Agilent 400, Varian/Agilent 500, Varian/Agilent 600, and Bruker 5instruments with chemical shifts reported relative to residual solvent, and data is reported as: s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, sext. = sextet, sept. = septet, m = multiplet. Infrared spectra were measured with a Nicolet Avatar 320 spectrometer with a Smart Miracle accessory. HRMS data was obtained on an Agilent 11LC/MS/TOF mass spectrometer. HPLC measurements were carried out on a Shimadzu HPLC system with Chiralcel IC, IA and OD-H columns. Optical rotations were recorded on the Rudolph Research Analytical, Autopol® IV, Automatic Polarimeter.

4.4.2 General Procedure for Preparation of UV-Vis Detection

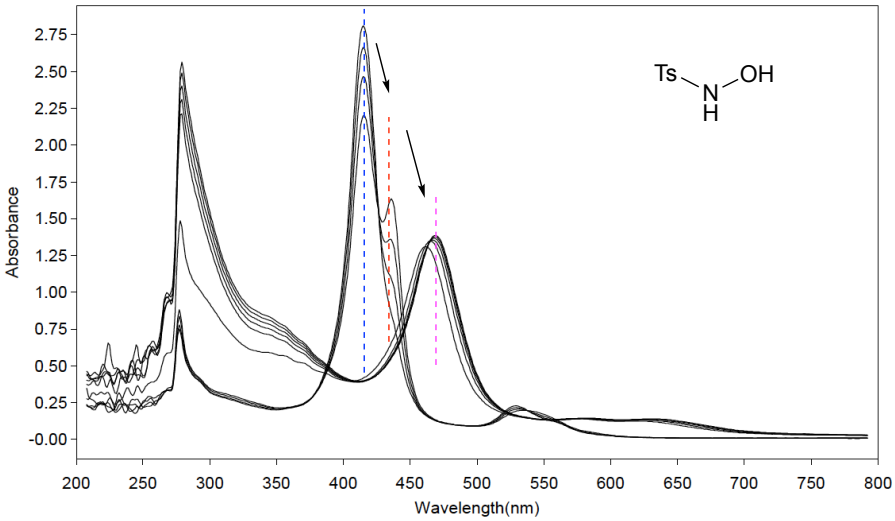
An UV-Vis cuvette with solvents was babbled with nitrogen several times. Under nitrogen atmosphere, catalyst [Co(**Por**)](1 mol %), cumene hydroperoxide or other oxidants (0.05 mmol) or alkane (0.15 mmol) were added quickly and sequentially. The

cuvette was then capped with its cap. The absorption spectrum of reaction mixture was carried out from 200 nm to 800 nm for 60 mins at room temperature. After the completion of the experiment, the cuvette was cleaned and dried for next usage.

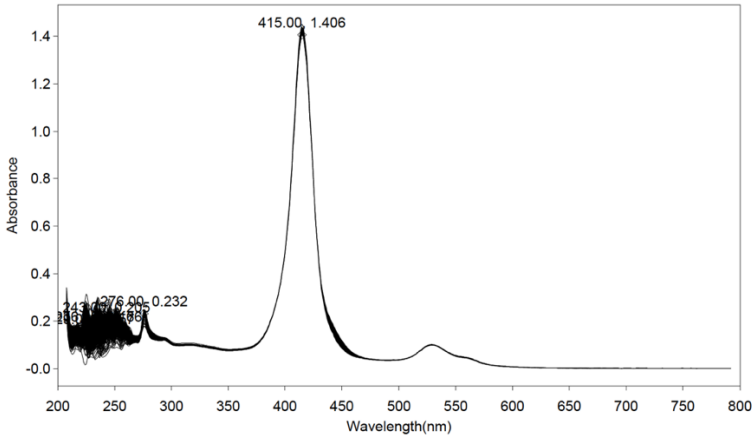
[Co(**P1**)] with 3-Chloroperoxybenzoic acid:



[Co(**P1**)] with *N*-Hydroxy-4-methylbenzenesulfonamide:

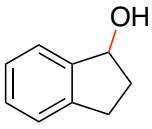


[Co(**P2**)] Exposed to Air in Benzene After 8 h Spectrum:



4.4.3 General Procedure for [Co(Por)]-Catalyzed C–H Amination

An oven dried Schlenk tube was charged with catalyst [Co(**Por**)](2 mol %). This reaction vessel was evacuated and backfilled with nitrogen several times. Under nitrogen atmosphere, cumene hydroperoxide (0.1 mmol) and alkane (0.3 mmol) was added followed by the addition of 0.5 mL of benzene. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at room temperature for 0.5 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum, and purified by flash column chromatography. The fractions containing product were collected and concentrated by rotary evaporation to obtain the target compound.

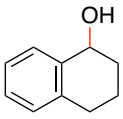


2,3-dihydro-1*H*-inden-1-ol 4.3a was obtained with catalyst **[Co(P3)]** through the general procedure. Colorless oil. Yield: 22%. R_f = 0.4 (5:1 Hexanes/EtOAc).

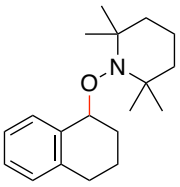
$[\alpha]_D^{20}$ = +1.6(*c* = 0.5, $CHCl_3$).^{1}H NMR (5MHz, $CDCl_3$): δ 7.44 – 7.39 (m, 1H), 7.26 – 7.23 (m, 3H), 5.24 (t, *J* = 6.1 Hz, 1H), 3.00–3.12 (m, 1H), 2.78–2.88 (m, 1H), 2.55–2.44 (m, 1H), 2.00–1.89 (m, 1H), 1.88–1.78 (m, 1H); HPLC analysis: *ee* = 12%. ODH (96% hexanes: 4% isopropanol, 0.8 mL/min): t_{major} = 13.280 min, t_{minor} = 14.957 min. This is a comercial available compound.

4.4.4 General Procedure for TEMPO Trapping Experiment

An oven dried Schlenk tube was charged with catalyst [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-ChenPhyrin) (3 mol %). This reaction vessel was evacuated and backfilled with nitrogen several times. Under nitrogen atmosphere, cumene hydroperoxide (0.1 mmol), Tetralin **1b** (0.3 mmol) and TEMPO (10 equiv, 3 mmol) was added followed by the addition of 0.5 mL of PhH. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at room temperature for 0.5 h. After the completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum, and purified by flash column chromatography. The fractions containing product were collected and afford **4.3b** (16% yield), **4.9b** (54% yield).



1,2,3,4-tetrahydronaphthalen-1-ol 4.9b was obtained with catalyst **[Co(P1)]** through the general procedure. Colorless oil. Yield: 16%. R_f = 0.4 (5:1 Hexanes/EtOAc).^{1}H NMR (5MHz, $CDCl_3$): δ 7.46–7.33 (m, 1H), 7.24–7.13 (m, 2H), 7.12–7.04 (m, 1H), 4.78 (br, 1H), 2.85–2.66 (m, 2H), 2.00–1.70 (m, 5H). This is a comercial available compound.



2,2,6,6-tetramethyl-1-((1,2,3,4-tetrahydronaphthalen-1-yl)oxy) piperidine 4.9b was obtained with catalyst **[Co(P7)]** through the general procedure. White solid. Yield: 54%. R_f = 0.5 (5:1 Hexanes/EtOAc). ^{1}H NMR (5MHz, $CDCl_3$): δ 7.67 – 7.60 (m, 1H), 7.20 – 7.10 (m, 1H), 7.09 – 7.04 (m, 1H), 4.95 – 4.81(m, 1H), 2.92 – 2.64 (m, 2H), 2.13 – 1.91 (m, 3H), 1.78 – 1.64 (m, 1H), 1.61 –1.29(m, 6H), 1.26 (s, 3H), 1.18 – 1.08 (m, 6H), 0.72 (s, 3H). This is a known compound.[15]

4.4.5 General Procedure for Overoxidation Experiment

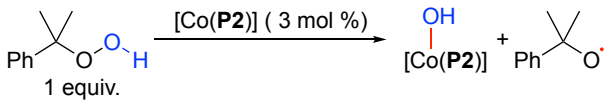
An oven dried Schlenk tube was charged with catalyst [Co(**P2**)] (**P2** = 3,5-Di^{t}Bu-ChenPhyrin) (3 mol %). This reaction vessel was evacuated and backfilled with nitrogen several times. Under nitrogen atmosphere, CHP **4.1** (0.1 mmol) and 2,3-dihydro-1*H*-inden-1-ol **4.3a** (1 equiv) were added followed by the addition of 0.5 mL of PhH. The Schlenk tube was then purged with nitrogen for 2 minutes and sealed with a Teflon screw cap. The reaction mixture was stirred at room temperature for 0.5 h. After the completion of the reaction, it afforded **4.8a** in 30% NMR yield. (**4.8a** is a commercially available compound.)

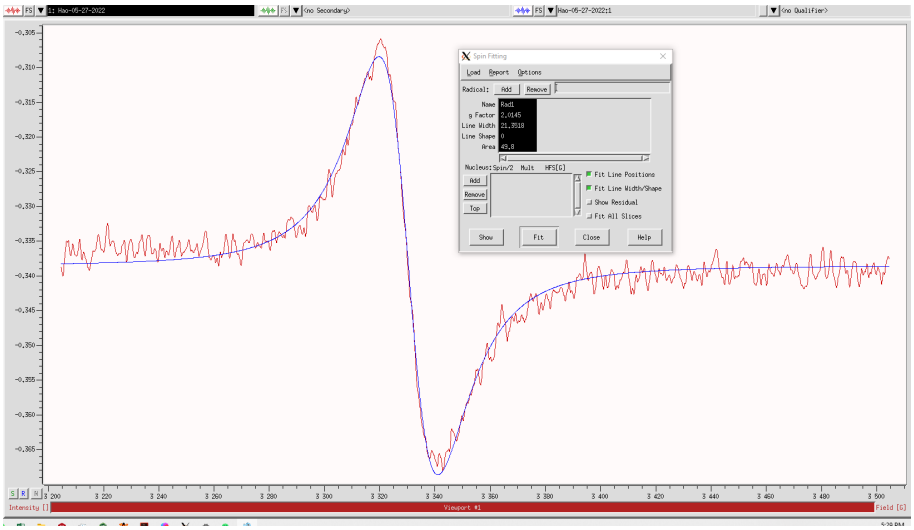
4.4.6 General Procedure for EPR Experiments

General Procedure for EPR Experiments: To an oven dried EPR tube, [Co(**P2**)] (3 mol %) were added and the tube was then degassed with argon. After 10-15 times cumene hydroperoxide **4.1** (0.2 mmol), other additives were weighed out and quickly transferred

with benzene (0.5 ml) into the tube. Then the tube was capped with a rubber cap and further wrapped with parafilm. The sample was then carried out for EPR experiment at room temperature (EPR settings: T = 298 K; microwave frequency: 9.37762 GHz; power: 20 mW; modulation amplitude: 1.0 G). [The simulation of the EPR spectra was performed by iteration of the isotropic g-values and line widths using the EPR simulation program SpinFit Xenon]

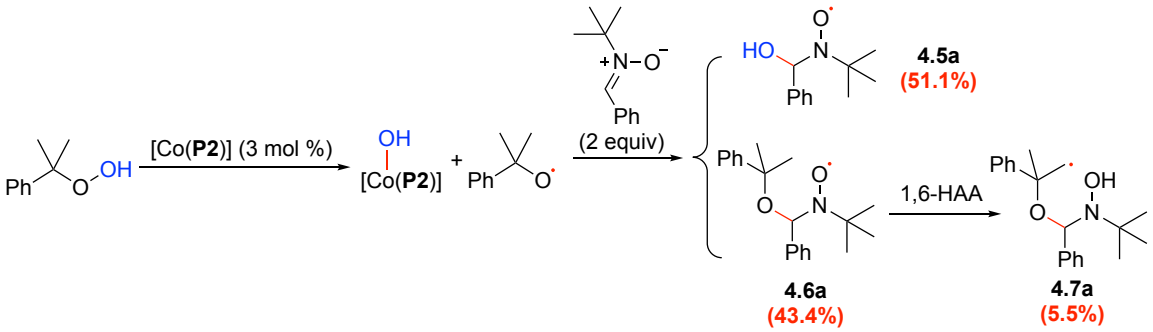
- Metalloradical Activation of Cumene Hydroperoxide EPR

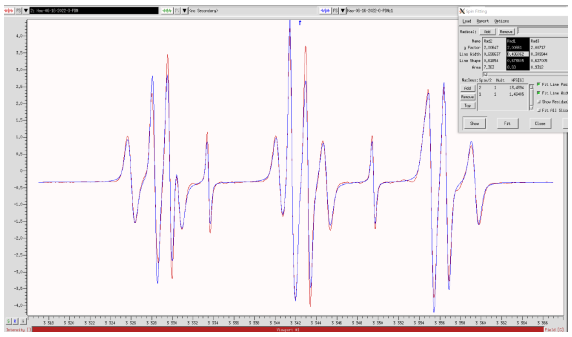


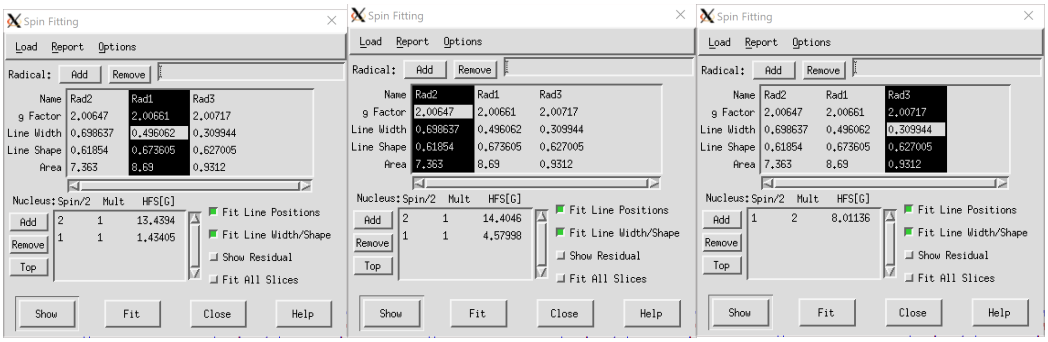


- EPR Experiment on Metalloradical Activation with PBN Trapping

Experimental Procedure: The additive *N*-tertbutyl-α-phenylnitrone (PBN, 2 equiv) was added to carry out the EPR.



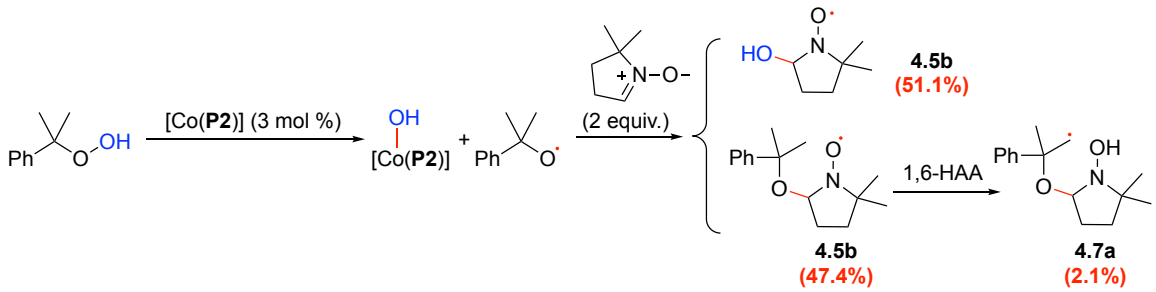


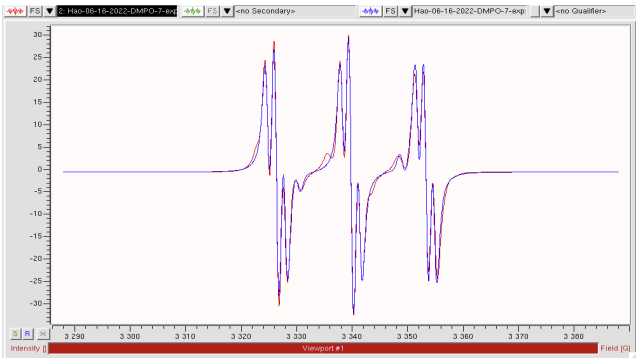


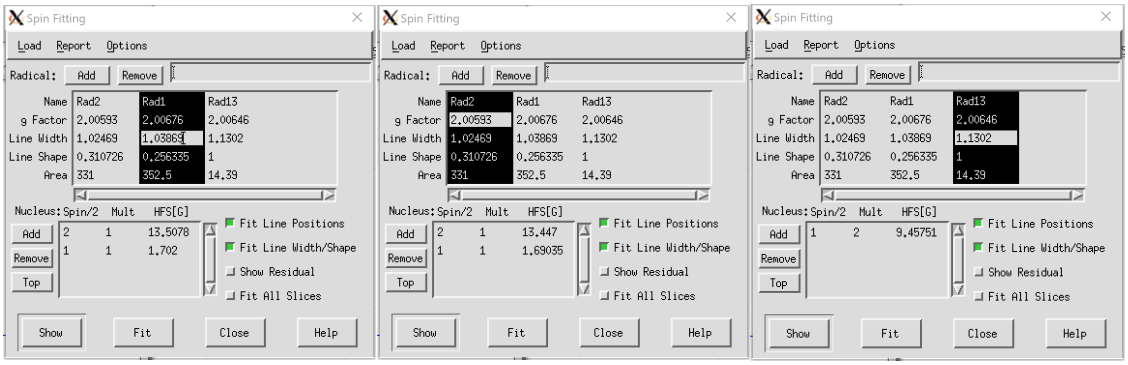
4.5a			**4.6a**			**4.7a**		
	g	2.00661		g	2.00647		g	2.00717
	HFS	A		HFS	A		HFS	A
N	13.4394	37.74421	N	14.4046	40.4521269	H	1.43405	4.0286166
H	1.43405	4.02749262	H	4.57998	12.8618589			

- EPR Experiment on Metalloradical Activation with DMPO Trapping

Experimental Procedure: The additive 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO, 2 equiv) was added to carry out the EPR.







4.5b			4.6b			4.7b		
	g	2.00676		g	2.00593		g	2.00646
	HFS	A		HFS	A		HFS	A
N	13.5078	37.9391455	N	13.447	37.7527564	H	9.45751	26.5591886
H	1.702	4.78038064	H	1.69035	4.74569582			

4.4.7 Details on DFT Calculations

In the investigation of C–H hydroxylation reaction, catalyst [Co(**P1**)] was modeled for the DFT calculations. The geometry optimizations were performed with the Gaussian 16[16] at the B3LYP[17]/def2-svp$_{Co}$[18]//6-311G*$_{H, C, N, O}$ level of theory in the gas phase at room temperature. Gas-phase Hessian matrix calculations were applied to the characterization of all minima (without imaginary frequency) and transition states (with only one imaginary frequency). Thermochemical parameters such as internal energy, enthalpy, entropy, Gibbs free energy and thermal corrections were obtained from these calculations. To better estimate the weak interactions and further improve the accuracy of energies, single point energies were carried out at the B3LYP/def2-tzvp[18] level of theory along with Grimme's dispersion correction[19] (D3-BJ). In addition**,** Reaction pathway analysis of metalloradical activation were carried out by extracting 40 data points of the structures from each step on the coordinates change and followed by single point energy calculation of all extracted structures to obtain their energy, charges, spin density and so on. The structures were displayed by CYLview[20] and VMD[21].

Intermediate A

$A_{[Co(II)(\mathbf{P1})]}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.344631 Hartree

H_corr: 1.581728 Hartree

SCF: -5072.884220 Hartree

S: 499.012 Cal/Mol-Kelvin

H: -5071.302492 Hartree

G: -5071.539589 Hartree

Cartesian Coordinates:

H	-9.31654800	-0.71726100	-3.68509000
H	-9.44651500	-1.00752800	-1.95054400
C	-8.73756200	-0.84294100	-2.76508700
H	-8.13487200	-1.74942800	-2.86848100
H	-9.68023400	-1.15075300	1.71860900
H	-9.31394200	1.80696800	-3.29664900
C	-9.32076500	-0.35857900	2.38104600
H	-9.79815200	-0.50751400	3.35308300
H	-9.44204800	1.56437600	-1.55458600
C	-8.73411800	1.64961700	-2.38207400
H	-8.79596900	0.00760000	-0.01201900
C	-7.84376900	0.39339800	-2.51687500
H	-7.67760900	-2.57663900	2.46953300
H	-9.67313600	0.59984400	1.99011100
H	-7.55337900	0.71852300	-4.64033200
C	-7.71409700	0.00465500	-0.00303400
C	-6.93848400	0.58106600	-3.74704000
C	-7.40178100	-1.76058500	3.14314500
H	-7.91680300	-1.92207800	4.09499700
H	-6.29926100	-0.28837600	-3.92305200
C	-7.03733800	0.19316500	-1.22017900
C	-7.79105800	-0.38991100	2.54418600
H	-8.12900500	2.54400700	-2.21004700
C	-7.05055400	-0.18517700	1.20943200
H	-1.19462500	-5.27338300	-6.12659700
H	-2.06603200	-4.17876600	-5.04673200
H	-6.32868800	-1.83594400	3.33291800
C	-1.15192400	-4.29974200	-5.63466000
H	-6.29759100	1.46215900	-3.65516000
C	-5.64303300	0.18923900	-1.19478500
C	-7.39219800	0.73112300	3.53072300
H	-7.90859000	0.60062300	4.48661000

H	-4.52366600	-2.62237100	-0.06697900
H	-1.14142800	-3.52370800	-6.40480300
C	-5.64718000	-0.18520800	1.18806600
O	0.08746300	-6.50470600	-4.05821900
H	-7.65900300	1.71541500	3.13618600
H	-5.07286800	0.32919100	-2.10430500
H	-2.62060000	-4.52453100	-0.06486400
H	0.04829700	-7.58985600	-2.15377500
C	-4.94187500	0.00041800	0.00314300
C	-3.45282800	-2.49487000	-0.04575900
H	-0.00008000	-8.81495900	0.00004700
C	0.02738100	-7.05803400	-1.21575800
C	0.08114900	-5.33562800	-3.71761900
C	-0.00007100	-7.72968900	0.00004000
C	-2.49560400	-3.45286900	-0.04577200
C	0.10309500	-4.20450400	-4.75426000
H	-5.08702000	-0.32790400	2.10571800
H	-6.31907100	0.73583400	3.73451800
H	1.43917300	-5.28284600	-6.08145800
C	0.02755900	-5.65820100	-1.21769000
N	0.05388100	-4.90407400	-2.40946100
C	-0.02751100	-7.05801800	1.21583000
C	1.38658500	-4.30880400	-5.59133400
C	-3.44172100	-0.00051900	0.00439300
C	-2.77580500	-1.22346200	-0.01364400
H	-0.04843600	-7.58982900	2.15385300
H	0.09778900	-3.23342400	-4.24349800
H	1.40788200	-3.53288500	-6.36138100
C	-0.00004600	-4.94505400	0.00002300
H	0.05176300	-3.90444900	-2.27618400
C	-0.02766400	-5.65818600	1.21774500
C	-1.22557900	-2.77315000	-0.01718200
H	-4.52333000	2.62099400	0.07914700
H	1.09978000	3.52743500	-6.41609900

N	-1.40781300	-1.40607600	-0.00266500
O	-0.08761300	-6.50465500	4.05828300
C	-0.00003400	-3.44124100	0.00001400
C	-2.77547400	1.22237000	0.02078300
H	1.14983100	5.27718600	-6.13780000
C	-3.45252300	2.49367100	0.05469900
H	2.28095100	-4.19439000	-4.97250800
N	-0.05397300	-4.90404300	2.40950600
C	1.11504100	4.30325900	-5.64582200
C	-0.08125500	-5.33558100	3.71766900
H	2.03510700	4.18518000	-5.06667500
H	2.06589700	-4.17875500	5.04686700
H	-0.05183600	-3.90442000	2.27621600
H	-1.44892100	3.52751100	-6.34832900
H	-0.09786400	-3.23337000	4.24352200
H	-1.48355700	5.27735800	-6.06807300
N	-1.40762500	1.40503100	0.00653900
C	-0.10321700	-4.20444300	4.75429600
C	-2.49539600	3.45177200	0.05269700
C	1.22552300	-2.77317100	0.01719900
C	-1.42297200	4.30349200	-5.57850000
C	1.15175900	-4.29970300	5.63475400
Co	-0.00000400	-0.00054100	0.00000200
C	-0.13122400	4.20357800	-4.75361500
C	-1.22543300	2.77214500	0.02079000
H	-2.62037100	4.52342200	0.07268000
H	2.62051500	-4.52457500	0.06488300
C	2.49553700	-3.45291100	0.04578100
N	1.40778100	-1.40609900	0.00266700
H	1.19441300	-5.27334000	6.12670200
H	-0.11780600	3.23246900	-4.24306200
H	1.14124600	-3.52366100	6.40488900
C	-0.10361700	5.33465600	-3.71707000
H	-2.31101400	4.18584800	-4.95123000

C	-1.38674900	-4.30870100	5.59131300
H	-2.28108400	-4.19427400	4.97244500
H	-0.06260600	3.90343600	-2.27596000
N	-0.06680900	4.90306500	-2.40914200
O	-0.11405600	6.50375600	-4.05749800
C	0.00002500	3.44023900	0.00002000
C	3.45277800	-2.49492900	0.04574700
C	2.77577600	-1.22350900	0.01363000
H	-1.43938200	-5.28273500	6.08144800
N	1.40764100	1.40500700	-0.00653200
H	-1.40806200	-3.53277000	6.36134800
C	-0.03421700	5.65717700	-1.21752200
H	2.31124000	4.18599800	4.95123700
C	1.22547200	2.77212400	-0.02076300
C	0.00003800	4.94404200	0.00003300
H	4.52361400	-2.62244800	0.06695500
C	-0.03407400	7.05701200	-1.21557500
C	2.77548700	1.22232300	-0.02079200
C	3.44171300	-0.00057800	-0.00441600
C	1.42319700	4.30353500	5.57852500
H	-0.06021100	7.58883700	-2.15345900
H	0.06267900	3.90339300	2.27600700
C	0.03430400	5.65715400	1.21760200
H	1.44924800	3.52754700	6.34834500
N	0.06688100	4.90302100	2.40920800
H	6.32859300	-1.83603100	-3.33299500
H	1.48368300	5.27740200	6.06810800
H	5.08697500	-0.32798100	-2.10576600
C	0.00006100	7.72865900	0.00005900
C	2.49544700	3.45173000	-0.05267400
C	0.03418400	7.05698900	1.21568000
C	3.45255700	2.49361200	-0.05470000
C	0.13144500	4.20348800	4.75366300
C	0.10367200	5.33458600	3.71714500

H	0.11813000	3.23238900	4.24308900
C	7.40169000	-1.76069700	-3.14323700
C	5.64715200	-0.18530000	-1.18812200
C	4.94186700	0.00033200	-0.00318800
H	6.31902600	0.73574900	-3.73457900
H	7.91669600	-1.92219400	-4.09509800
H	0.00006900	8.81393000	0.00006800
H	2.62044000	4.52337800	-0.07264300
H	7.67751100	-2.57676100	-2.46963500
H	0.06032700	7.58879700	2.15357300
O	0.11427600	6.50368000	4.05759000
C	7.39215600	0.73101400	-3.53079900
H	7.90853200	0.60051000	-4.48669400
H	4.52336600	2.62091700	-0.07915900
C	7.79100600	-0.39003500	-2.54427400
C	7.05052500	-0.18529400	-1.20950900
C	5.64304600	0.18913400	1.19473100
C	-1.11481500	4.30300400	5.64589700
H	5.07289600	0.32909100	2.10426000
H	-1.09945300	3.52715600	6.41614800
H	7.65898700	1.71529800	-3.13625800
H	-1.14970400	5.27691100	6.13790800
C	7.71408900	0.00451900	0.00294900
H	-2.03487900	4.18484100	5.06676300
C	7.03735100	0.19303300	1.22010500
C	9.32071600	-0.35873700	-2.38115600
H	9.79808600	-0.50767300	-3.35320100
H	9.68017700	-1.15092400	-1.71873100
H	6.29928900	-0.28847400	3.92298400
H	8.79596100	0.00744500	0.01191800
H	9.67311300	0.59967600	-1.99021800
H	8.13484900	-1.74958700	2.86839800
C	6.93854100	0.58094500	3.74696600
H	6.29767900	1.46206100	3.65509500

C	7.84380400	0.39324700	2.51679000
C	8.73756400	-0.84311700	2.76499500
H	9.44650400	-1.00772800	1.95044400
H	7.55345200	0.71837900	4.64025100
C	8.73418900	1.64943800	2.38197300
H	8.12910000	2.54384600	2.20995200
H	9.44210400	1.56417500	1.55447400
H	9.31656400	-0.71745200	3.68499100
H	9.31403200	1.80677500	3.29653900

CHP:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.155632 Hartree

H_corr: 0.20369 Hartree

SCF: -500.775336 Hartree

S: 101.149 Cal/Mol-Kelvin

H: -500.571646 Hartree

G: -500.619704 Hartree

Cartesian Coordinates:

C	1.62945900	1.61113200	-0.37222500
C	1.10459300	0.27961000	0.16850500
H	2.71997300	1.59549400	-0.36338300
H	1.31146600	2.45422300	0.24450700
H	1.28830400	1.77970100	-1.39623900
C	1.54093000	0.06476400	1.62477400
H	1.20984000	-0.91143700	1.98307100
H	1.10128600	0.83116100	2.26776900
H	2.62710800	0.11485400	1.70994100
C	-0.41005700	0.10888600	0.03372600
C	-0.97012600	-1.17421000	0.10152200
C	-1.26906100	1.20135800	-0.11511200
C	-2.34720200	-1.35567100	0.02058000

C	-2.64986400	1.02055500	-0.18641300
C	-3.19443400	-0.25810400	-0.12085700
H	-0.31806500	-2.03316900	0.20123600
H	-2.75953600	-2.35872500	0.06827700
H	-4.26890500	-0.39937000	-0.18067800
H	-3.29802500	1.88415600	-0.29817900
H	-0.87104100	2.20744600	-0.17539400
O	1.60969200	-0.80462800	-0.66522700
O	3.05596700	-0.88155500	-0.52923200
H	3.32689600	-0.66479300	-1.43225700

Intermediate B:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.524921 Hartree

H_corr: 1.787471 Hartree

SCF: -5573.694231 Hartree

S: 552.584 Cal/Mol-Kelvin

H: -5571.906760 Hartree

G: -5572.169310 Hartree

Cartesian Coordinates:

C	0.04715800	-0.55210600	-4.84410600
C	-1.00049800	-0.94179200	-3.80161200
H	0.66368100	0.25840400	-4.45307100
H	-0.41788200	-0.19083100	-5.76343800
H	0.69495800	-1.39588300	-5.09072100
C	-1.93745100	0.23185400	-3.49138700
H	-2.62743800	-0.03023800	-2.68884400
H	-2.52131100	0.48395200	-4.37956100
H	-1.37227600	1.11194400	-3.18324500
C	-1.81180500	-2.18735100	-4.16290600
C	-2.55490300	-2.84067500	-3.16932900
C	-1.87987000	-2.67103200	-5.47275600

C	-3.33858100	-3.94777600	-3.48046600
C	-2.67649100	-3.77167300	-5.78607100
C	-3.40629400	-4.41574700	-4.79164600
H	-2.51165400	-2.48956500	-2.14570300
H	-3.89774500	-4.44433900	-2.69424300
H	-4.02107000	-5.27625700	-5.03462400
H	-2.71913500	-4.12725600	-6.81053700
H	-1.31730400	-2.19275600	-6.26558800
O	-0.31639200	-1.37169400	-2.57865300
O	0.37132100	-0.22586800	-1.98608100
H	1.29108500	-0.52789100	-2.01073800
H	-8.96455700	1.75090700	4.25300200
H	-9.14327000	1.91652900	2.50633200
C	-8.41475200	1.77051200	3.30706200
H	-7.75590200	2.64308100	3.31915900
H	-9.50155000	1.80948200	-1.15610300
H	-9.12581200	-0.79085200	4.06246600
C	-9.22212800	0.94350400	-1.76244100
H	-9.72680700	1.04609500	-2.72670700
H	-9.30659300	-0.67318900	2.31220200
C	-8.57341400	-0.73920600	3.11926800
H	-8.62956300	0.71551200	0.63216300
C	-7.60573600	0.46603500	3.12579200
H	-7.44238400	3.02769600	-2.10002700
H	-9.62175600	0.04656700	-1.28145000
H	-7.25436200	0.28303800	5.25703200
C	-7.55036800	0.65396300	0.58655400
C	-6.66687800	0.31615600	4.33575700
C	-7.24811200	2.14050100	-2.70910000
H	-7.79005400	2.25573500	-3.65273500
H	-5.97232700	1.15606400	4.42311200
C	-6.83916900	0.51783100	1.79101500
C	-7.70134500	0.85545400	-1.97969600
H	-8.02929300	-1.67980000	2.99705300

C	-6.92337600	0.71303600	-0.65816400
H	-0.91387400	6.17711700	5.56191600
H	-1.75245200	4.97617200	4.57200600
H	-6.18118800	2.12610300	-2.94264000
C	-0.86791100	5.15136500	5.19068300
H	-6.08178800	-0.60638600	4.29033200
C	-5.44912400	0.43695000	1.71843200
C	-7.41619800	-0.37024600	-2.87721300
H	-7.95750500	-0.28487800	-3.82446800
H	-4.22452700	3.08083100	0.14693500
H	-0.91540500	4.47234400	6.04636200
C	-5.52237000	0.63389600	-0.68364100
O	0.53662000	7.12827100	3.42960200
H	-7.73518800	-1.29595100	-2.39030500
H	-4.85393400	0.33365700	2.61669100
H	-2.22620300	4.83966300	-0.23068700
H	0.58830100	7.97211400	1.40998400
C	-4.78246900	0.49550700	0.48703500
C	-3.16484500	2.88528000	0.09996000
H	0.61641700	8.93143000	-0.87549900
C	0.54475500	7.33375100	0.54179000
C	0.48190400	5.92780700	3.23191400
C	0.55972400	7.85545500	-0.74545900
C	-2.15900000	3.77199500	-0.08870800
C	0.42939300	4.93097200	4.39734800
H	-4.99206400	0.67613900	-1.62854500
H	-6.35427800	-0.46991100	-3.11234100
H	1.71889400	6.14384300	5.65142500
C	0.47114300	5.94624500	0.71082500
N	0.45424200	5.34218900	1.98526900
C	0.50544900	7.04448200	-1.87187500
C	1.66907300	5.11727000	5.28367700
C	-3.28572100	0.41184000	0.43990800
C	-2.55787600	1.58409700	0.24062200

H	0.52073300	7.46046000	-2.86661600
H	0.42912000	3.90527400	4.00797700
H	1.63236100	4.44289100	6.14353000
C	0.41177700	5.09290100	-0.41301700
H	0.40673000	4.33491600	1.97406400
C	0.43218000	5.65616300	-1.70638300
C	-0.92873100	3.01920400	-0.05990400
H	-4.49967300	-2.13699700	0.78715100
H	-0.02805800	-1.86058500	7.51711900
N	-1.18619800	1.68237200	0.14916600
O	0.52312100	6.16287500	-4.62306800
C	0.33075900	3.60273400	-0.22123900
C	-2.68293900	-0.83397600	0.61675500
H	-0.11261000	-3.62843200	7.61920500
C	-3.42377600	-2.05941400	0.79300200
H	2.59142700	4.91193500	4.73321700
N	0.37766900	4.76800500	-2.80199100
C	0.06562100	-2.78806900	6.94569900
C	0.43815100	5.04386500	-4.14994600
H	1.09536700	-2.85883900	6.58451100
H	2.57957900	3.49263300	-4.96152800
H	0.31522800	3.79280000	-2.55077500
H	-2.48574200	-1.71127800	6.85567900
H	0.20376600	2.91155900	-4.44551000
H	-2.65510500	-3.47318600	6.94673200
N	-1.32916300	-1.08232500	0.66296600
C	0.41232000	3.80221500	-5.05084000
C	-2.51423400	-3.04966200	0.96073100
C	1.52167600	2.87346600	-0.16743000
C	-2.38324000	-2.64267000	6.29219200
C	1.79238100	3.63373600	-5.70751300
Co	0.14726800	0.20847000	0.31692300
C	-0.94208000	-2.81365400	5.78764200
C	-1.21115200	-2.43531000	0.88872300

H	-2.69247900	-4.10130400	1.12468400
H	3.00243900	4.51303400	-0.54388400
C	2.82347300	3.46891200	-0.33794000
N	1.63772700	1.52380000	0.08401100
H	2.04129300	4.51927100	-6.29598400
H	-0.71179000	-1.98589800	5.10542600
H	1.79916900	2.76627300	-6.37332500
C	-0.82609300	-4.14909400	5.04053100
H	-3.09805800	-2.61671900	5.46492400
C	-0.69536400	3.95157300	-6.10157600
H	-1.68377700	4.01245300	-5.63790300
H	-0.41575700	-3.08082100	3.36328600
N	-0.52420900	-4.02420800	3.70253000
O	-0.99900700	-5.20979200	5.61369300
C	-0.01906600	-3.14091200	1.07435800
C	3.73257300	2.47636400	-0.18339600
C	2.99446900	1.26997100	0.09711800
H	-0.54205600	4.86223100	-6.68310900
N	1.49582600	-1.22845200	0.66528500
H	-0.69507300	3.09922300	-6.78668600
C	-0.35765600	-5.02666000	2.72353400
H	3.11107200	-4.27615800	-2.31285100
C	1.24054500	-2.54182000	0.99520100
C	-0.09569500	-4.60646800	1.40024700
H	4.80754900	2.54328500	-0.24169500
C	-0.42901600	-6.38974600	3.03192300
C	2.87046700	-1.11110100	0.66920800
C	3.59720300	0.04343100	0.37593000
C	2.75719700	-4.77652500	-3.21887400
H	-0.63041800	-6.69422900	4.04674100
H	0.27444500	-4.13062400	-1.05553300
C	0.10408200	-5.57774900	0.39525600
H	3.05412400	-4.16904700	-4.07869400
N	0.37345800	-5.12517500	-0.91391600

H	6.59008200	2.59500500	3.07646600
H	3.26688800	-5.74016100	-3.29217200
H	5.26730500	0.86819300	2.31247200
C	-0.23503400	-7.31993600	2.01859600
C	2.47287000	-3.25091800	1.23210700
C	0.03015100	-6.94051300	0.70927500
C	3.47986000	-2.36751400	1.02807000
C	1.23027400	-4.97695500	-3.20148100
C	0.86910600	-5.83933600	-1.98582500
H	0.75084800	-3.99605100	-3.10991600
C	7.65716300	2.41401300	2.92910400
C	5.81544900	0.44358600	1.47863700
C	5.09512000	-0.03391600	0.38763600
H	6.44686000	0.24622600	4.18906400
H	8.18234200	2.81104700	3.80311400
H	-0.29100500	-8.37703400	2.25808000
H	2.54214100	-4.28850800	1.52032400
H	7.97416500	2.99142000	2.05619500
H	0.19069600	-7.67227400	-0.06620800
O	1.05320700	-7.04301600	-1.98111800
C	7.51785900	0.13726400	4.00417500
H	8.04431500	0.50527000	4.89008000
H	4.54150200	-2.53519500	1.11938900
C	7.97180100	0.91187100	2.74600500
C	7.21668200	0.37684600	1.51497600
C	5.78205300	-0.59120600	-0.69881600
C	0.74009400	-5.65023700	-4.48738200
H	5.20329600	-0.95571100	-1.53805300
H	1.06029800	-5.08156500	-5.36482300
H	7.73035500	-0.93087800	3.90631700
H	1.14431100	-6.66122700	-4.56213300
C	7.86486400	-0.18242200	0.41333700
H	-0.34990300	-5.71700900	-4.51183600
C	7.17415300	-0.67298200	-0.70773100

C	9.49715900	0.75706000	2.61587500
H	9.98507100	1.14992500	3.51172000
H	9.89545100	1.31026200	1.76091000
H	6.45658700	-0.92900800	-3.44642200
H	8.94504100	-0.24349800	0.41770100
H	9.79743800	-0.28955200	2.51564800
H	8.37529700	0.66525000	-2.81968500
C	7.04555200	-1.74873200	-3.02564700
H	6.35629400	-2.53213400	-2.69910900
C	7.96372200	-1.27358500	-1.88578100
C	8.92553800	-0.20856600	-2.45995900
H	9.64673700	0.13747200	-1.71617700
H	7.64894300	-2.16485400	-3.83663500
C	8.78169100	-2.48880600	-1.39263000
H	8.12731900	-3.26439900	-0.98538000
H	9.49503800	-2.21388600	-0.61243900
H	9.49201800	-0.61936200	-3.30126400
H	9.34969100	-2.92792500	-2.21847700

Transition State TS1:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -519.8977 cm-1

G_corr: 1.525031 Hartree

H_corr: 1.785016 Hartree

SCF: -5573.672970 Hartree

S: 547.183 Cal/Mol-Kelvin

H: -5571.887954 Hartree

G: -5572.147939 Hartree

Cartesian Coordinates:

C	0.41832300	-0.45366800	4.67582900
C	1.30302200	-1.17530000	3.65321900
H	-0.09175400	0.36429000	4.16569000

H	0.99571600	-0.02949700	5.50121100
H	-0.33972600	-1.12447900	5.08577600
C	2.38486200	-0.22330300	3.11720400
H	2.98124600	-0.71317500	2.34721900
H	3.05180800	0.08760100	3.92594300
H	1.91978300	0.66075300	2.68006200
C	1.96275800	-2.45675700	4.20549400
C	2.63013600	-3.31789900	3.32200400
C	1.94117200	-2.78379800	5.56458300
C	3.26519700	-4.46449100	3.78751600
C	2.58791200	-3.92747300	6.03247700
C	3.24959400	-4.77317100	5.14710900
H	2.64246700	-3.08991600	2.26305300
H	3.77098000	-5.12020600	3.08598500
H	3.74593500	-5.66681000	5.51141000
H	2.56770700	-4.15731000	7.09315300
H	1.42913100	-2.14604000	6.27459500
O	0.50043400	-1.69005100	2.60324400
O	-0.19400900	-0.23608300	1.65296100
H	-1.08193700	-0.58114900	1.81900300
H	8.65095200	1.85894800	-4.80315700
H	8.93118700	2.10437600	-3.07938900
C	8.15992300	1.90298400	-3.82624200
H	7.47416700	2.75464200	-3.83268600
H	9.53044400	2.13909700	0.55461300
H	8.90416900	-0.66651900	-4.51967500
C	9.30723000	1.29554000	1.21361300
H	9.86743000	1.45037600	2.13940500
H	9.18897200	-0.46916200	-2.79072500
C	8.40971300	-0.59083800	-3.54646500
H	8.57324000	0.96351100	-1.12880600
C	7.40568000	0.58428200	-3.54135100
H	7.50579200	3.35827800	1.56812100
H	9.69610300	0.38585700	0.74793400

H	6.92953800	0.29947700	-5.63682700
C	7.50109300	0.87614200	-1.01318900
C	6.39918300	0.35531500	-4.68262200
C	7.36792500	2.49606500	2.22657500
H	7.96289200	2.66474200	3.12925400
H	5.67453000	1.17036900	-4.76080500
C	6.72150500	0.67116500	-2.16430100
C	7.80492200	1.18810600	1.52862400
H	7.90455100	-1.54094100	-3.35198400
C	6.95100600	0.97092800	0.26544800
H	0.67132600	6.53376300	-5.22124900
H	1.57951200	5.30441200	-4.33309400
H	6.31765600	2.47116900	2.52563200
C	0.66977400	5.48674300	-4.91187900
H	5.84743800	-0.58100600	-4.56253500
C	5.34149000	0.55674000	-2.00161400
C	7.60226700	-0.00044700	2.49577700
H	8.20083700	0.13755400	3.40133900
H	4.14440300	3.20547600	-0.23349400
H	0.70983300	4.86189900	-5.80821500
C	5.55725100	0.85787900	0.38244400
O	-0.72366900	7.30947600	-2.99385600
H	7.90823200	-0.94181200	2.03111400
H	4.69552300	0.40011600	-2.85604300
H	2.13663500	4.87104800	0.41778300
H	-0.75205400	8.02908900	-0.92943700
C	4.75120300	0.65175600	-0.73393400
C	3.09770600	2.97345200	-0.11760100
H	-0.76396400	8.85250700	1.40882800
C	-0.68294000	7.34229500	-0.10082800
C	-0.64001100	6.10111800	-2.86939700
C	-0.68846200	7.78737600	1.21491300
C	2.08709300	3.81334200	0.21006400
C	-0.59265600	5.17653700	-4.09312600

H	5.08447400	0.92250000	1.35603100
H	6.55980000	-0.10705700	2.80356500
H	-1.96029500	6.41596400	-5.23392100
C	-0.58526300	5.96909500	-0.35146300
N	-0.57569300	5.44280300	-1.66034800
C	-0.60132700	6.91367400	2.29064200
C	-1.86657500	5.37236300	-4.92777000
C	3.26508000	0.52690400	-0.59055400
C	2.51873300	1.66574800	-0.29571800
H	-0.60941800	7.27117300	3.30771400
H	-0.54702700	4.13028900	-3.76599700
H	-1.83757200	4.74961800	-5.82599300
C	-0.49230600	5.05281400	0.72051300
H	-0.50701400	4.43832200	-1.71282400
C	-0.50365000	5.53808700	2.04529400
C	0.87726100	3.03103100	0.20972000
H	4.52941600	-1.99765700	-0.90602500
H	0.32397800	-2.54427100	-7.47411200
N	1.15327200	1.71790900	-0.10489300
O	-0.54859200	5.89336700	4.97981200
C	-0.38695700	3.57938800	0.43530000
C	2.68723800	-0.73469500	-0.72870300
H	0.43618200	-4.31104900	-7.38199600
C	3.45269700	-1.94849900	-0.86555200
H	-2.76333700	5.10595700	-4.36139200
N	-0.41627900	4.59278900	3.08894900
C	0.22090300	-3.40663100	-6.80989500
C	-0.45366700	4.80004300	4.45212200
H	-0.82095400	-3.45627500	-6.48137500
H	-2.55092000	3.18908900	5.26494000
H	-0.33828900	3.63234000	2.78911300
H	2.75271500	-2.28551000	-6.74537800
H	-0.19110600	2.65984500	4.63642800
H	2.94833500	-4.04360900	-6.63503200

N	1.34101100	-1.01869700	-0.70656000
C	-0.38493600	3.51823500	5.28948100
C	2.56560400	-2.97209100	-0.90545600
C	-1.56430700	2.84032000	0.30815500
C	2.64081700	-3.15101200	-6.08667600
C	-1.73796800	3.30373500	5.98748100
Co	-0.15172000	0.21533500	-0.23870500
C	1.18385200	-3.29014800	-5.61955600
C	1.25086400	-2.38798100	-0.82053700
H	2.76673200	-4.02833200	-0.99640100
H	-3.07345800	4.43591700	0.73971200
C	-2.87692600	3.41274200	0.45878300
N	-1.65770700	1.51459400	-0.06039100
H	-1.97321500	4.15697000	6.62710300
H	0.91725900	-2.39719700	-5.04053400
H	-1.71113700	2.40456200	6.60884100
C	1.05529600	-4.53877900	-4.73666100
H	3.32292100	-3.02224700	-5.24155900
C	0.75951900	3.62866000	6.30550800
H	1.72941700	3.72526300	5.80982500
H	0.54778600	-3.30379100	-3.20845600
N	0.68675700	-4.27618500	-3.43546200
O	1.27345300	-5.65119600	-5.18173100
C	0.07318400	-3.12927200	-0.92760700
C	-3.76897000	2.43617900	0.16395500
C	-3.01054200	1.25670200	-0.16190800
H	0.61808400	4.50583300	6.93934600
N	-1.47109600	-1.21230100	-0.68804400
H	0.79371300	2.74170100	6.94390000
C	0.48450200	-5.17114100	-2.36242100
H	-3.23395700	-3.75962600	2.35418200
C	-1.19269800	-2.54076300	-0.92265300
C	0.16652300	-4.61758700	-1.10094600
H	-4.84598600	2.49536600	0.16087300

C	0.56540500	-6.55796800	-2.52540600
C	-2.84388400	-1.10358900	-0.77760000
C	-3.59147600	0.04615300	-0.53230100
C	-2.98974400	-4.23967000	3.30647000
H	0.81001900	-6.96506600	-3.49366500
H	-0.20519000	-3.92552700	1.35419900
C	-0.08634800	-5.47864300	-0.01067300
H	-3.29849200	-3.56750500	4.11222900
N	-0.41839000	-4.90685100	1.23697700
H	-6.35588800	2.52252200	-3.52656000
H	-3.57950100	-5.15632000	3.38249100
H	-5.10617500	0.81473300	-2.61019800
C	0.32265000	-7.37915800	-1.43128600
C	-2.40571900	-3.26784300	-1.19333400
C	-0.00175200	-6.86623800	-0.18282600
C	-3.42433100	-2.37720800	-1.11647900
C	-1.48662700	-4.55558500	3.41652400
C	-1.10825200	-5.50498400	2.27572400
H	-0.92567900	-3.62157700	3.31704300
C	-7.43229200	2.35317500	-3.44957800
C	-5.71744300	0.41943400	-1.80629400
C	-5.08471900	-0.02743100	-0.65039300
H	-6.15215300	0.13764000	-4.54804000
H	-7.89084800	2.72522100	-4.37077400
H	0.38629400	-8.45521900	-1.55752700
H	-2.45393800	-4.32140200	-1.42112500
H	-7.80515300	2.96032800	-2.62006400
H	-0.20702800	-7.51658200	0.65215100
O	-1.43581400	-6.67776700	2.28778600
C	-7.23479700	0.04205500	-4.43871400
H	-7.69176200	0.38523300	-5.37187100
H	-4.47754100	-2.55360600	-1.26839600
C	-7.77213000	0.85967300	-3.24213100
C	-7.11298700	0.36000900	-1.94305100

C	-5.85221300	-0.54414100	0.40146700
C	-1.15030800	-5.20032300	4.76594800
H	-5.33894800	-0.88326100	1.29225500
H	-1.48222500	-4.56109700	5.58902900
H	-7.46382100	-1.02089100	-4.32331900
H	-1.64593800	-6.16858300	4.85788700
C	-7.84408300	-0.15894800	-0.87421500
H	-0.07477500	-5.35588600	4.87681000
C	-7.24190400	-0.61651900	0.31027500
C	-9.30415100	0.71855900	-3.21825100
H	-9.72262600	1.08503800	-4.15925300
H	-9.75855700	1.30163800	-2.41257600
H	-6.72704300	-0.78864200	3.10072900
H	-8.92151500	-0.21357800	-0.95557900
H	-9.61969000	-0.32236700	-3.10666100
H	-8.57785700	0.80000100	2.28674300
C	-7.29313400	-1.61637800	2.66474400
H	-6.59062000	-2.41620800	2.41572900
C	-8.12119900	-1.17134800	1.44639700
C	-9.11018400	-0.07935300	1.91380200
H	-9.77015100	0.24978700	1.10802300
H	-7.95836300	-1.99993400	3.44269400
C	-8.91460300	-2.39487000	0.93399900
H	-8.24107900	-3.18869100	0.59968700
H	-9.56768000	-2.13946000	0.09644600
H	-9.74219700	-0.45788800	2.72287300
H	-9.54457200	-2.80227700	1.73052000

Intermediate C

$C_{Co(III)}$:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.523025 Hartree

H_corr: 1.785732 Hartree

SCF: -5573.686134 Hartree

S: 552.913 Cal/Mol-Kelvin

H: -5571.900402 Hartree

G: -5572.163109 Hartree

Cartesian Coordinates:

C	-0.75961400	-1.55719700	-4.45827800
C	-1.50610200	-2.30821400	-3.34918700
H	-0.38091000	-0.62680800	-4.03344200
H	-1.40976100	-1.31040000	-5.30151900
H	0.09095800	-2.13564800	-4.82502800
C	-2.68991300	-1.46391300	-2.83934900
H	-3.21069100	-1.96954500	-2.02641700
H	-3.39935500	-1.28066700	-3.65107000
H	-2.30480000	-0.51429300	-2.46665600
C	-1.98675500	-3.72395200	-3.76751700
C	-2.57044100	-4.56045000	-2.80499700
C	-1.85878600	-4.19515100	-5.07744900
C	-3.04004300	-5.82269100	-3.15154300
C	-2.34185300	-5.45560100	-5.42608000
C	-2.93087600	-6.27422300	-4.46602500
H	-2.65073100	-4.22064700	-1.77974400
H	-3.48694000	-6.45656000	-2.39258900
H	-3.29702700	-7.25881500	-4.73804600
H	-2.25114400	-5.79768700	-6.45209900
H	-1.39900600	-3.57956600	-5.84011400
O	-0.63548300	-2.60353100	-2.29757100
O	0.16256900	-0.13824600	-1.56308800
H	0.59510100	-1.00076100	-1.63659500
H	-8.69177300	2.99790200	4.17078300
H	-8.95772900	2.81269800	2.43730600
C	-8.19224800	2.80507000	3.21648100
H	-7.51050100	3.63702100	3.01973200
H	-9.52437700	1.95873600	-1.09688800

H	-8.93040000	0.47834500	4.51224100
C	-9.29310200	0.98166800	-1.52988100
H	-9.84612200	0.90462100	-2.46962000
H	-9.20129000	0.24519500	2.78548100
C	-8.42802400	0.31698800	3.55363200
H	-8.57743500	1.23515900	0.82716700
C	-7.42947800	1.46174700	3.26833000
H	-7.49459000	2.90670500	-2.35809300
H	-9.68294000	0.21015100	-0.86024400
H	-6.97013600	1.70250500	5.37298900
C	-7.50416100	1.12654000	0.74469600
C	-6.43177600	1.52566200	4.43820100
C	-7.34869200	1.91186300	-2.78809900
H	-7.93645100	1.85499100	-3.70928300
H	-5.71103500	2.33929300	4.31942100
C	-6.73402000	1.21345200	1.91684700
C	-7.78791200	0.80877100	-1.79850300
H	-7.91679700	-0.64846100	3.60091600
C	-6.94382400	0.90716400	-0.51409700
H	-1.48814800	7.95543900	3.40081300
H	-2.16468200	6.42632000	2.82622700
H	-6.29578600	1.82081500	-3.06411700
C	-1.37136200	6.87035500	3.43399500
H	-5.87548500	0.59169100	4.55560900
C	-5.35200200	1.07046800	1.79707900
C	-7.57392800	-0.57681700	-2.44920300
H	-8.16568700	-0.66409900	-3.36547500
H	-4.13941800	3.26686400	-0.40749200
H	-1.51308200	6.53975000	4.46650700
C	-5.54876500	0.77305000	-0.58937900
O	0.21646800	8.17822200	1.24540700
H	-7.88067400	-1.38006800	-1.77356900
H	-4.71240600	1.13063700	2.66841500
H	-2.11193200	4.80065200	-1.29025500

H	0.54200400	8.24772900	-0.92326600
C	-4.75297900	0.85279100	0.54954600
C	-3.08644800	3.03458400	-0.42706300
H	0.83359400	8.32213100	-3.38355700
C	0.58823500	7.33909800	-1.50233600
C	0.20021300	6.98568300	1.49075900
C	0.75196900	7.36319600	-2.88190800
C	-2.06659900	3.80702100	-0.87206700
C	0.02223400	6.46985300	2.92492000
H	-5.06685900	0.59925800	-1.54507500
H	-6.52860400	-0.74874800	-2.71511200
H	1.11218700	8.13498200	3.78804600
C	0.48170300	6.10300000	-0.85476900
N	0.32513100	5.99265900	0.54345200
C	0.81785700	6.20142400	-3.64050900
C	1.13268600	7.04399000	3.81587700
C	-3.26359000	0.70696600	0.45435000
C	-2.50940800	1.79184900	0.01808700
H	0.95213400	6.23380600	-4.70995200
H	0.09524200	5.37517600	2.93689400
H	0.99999700	6.72141300	4.85210300
C	0.53643200	4.90466100	-1.59798400
H	0.29016600	5.04708900	0.89216200
C	0.71281700	4.96165400	-2.99772700
C	-0.85430100	3.05928900	-0.65907300
H	-4.54727300	-1.72813500	1.11434200
H	-0.70238600	-1.32177800	7.66728600
N	-1.13719000	1.83086900	-0.10587700
O	1.22864100	4.39705300	-5.85327600
C	0.41685700	3.57089500	-0.91843800
C	-2.69379300	-0.52455200	0.76539800
H	-0.87602600	-3.07839900	7.83143900
C	-3.47020900	-1.69937400	1.06297200
H	2.12272900	6.71774600	3.48535900

N	0.78052900	3.73911500	-3.69682100
C	-0.58246500	-2.27763400	7.15015700
C	1.05287800	3.51647000	-5.03051200
H	0.47875400	-2.40484500	6.91897700
H	3.27289200	1.87273500	-4.92034800
H	0.65960500	2.91085100	-3.13203200
H	-3.05558100	-1.11054100	6.71194200
H	0.84822700	1.41399200	-4.55991600
H	-3.31172400	-2.85869100	6.85056700
N	-1.34763300	-0.82304400	0.78438300
C	1.14506600	2.03475800	-5.41293600
C	-2.59501700	-2.72005500	1.23314200
C	1.58341500	2.89848000	-0.55815300
C	-2.92799400	-2.06904800	6.20149600
C	2.60400400	1.70355000	-5.76872400
Co	0.15448000	0.35243000	0.20792500
C	-1.44594000	-2.31765700	5.88128500
C	-1.27486700	-2.17016500	1.07194900
H	-2.80816600	-3.75230000	1.46387900
H	3.10845300	4.43439000	-1.12832600
C	2.89957100	3.46209100	-0.70952600
N	1.65650200	1.65022400	0.01901600
H	2.94400900	2.32774600	-6.59791500
H	-1.10094000	-1.53108500	5.19868300
H	2.69713800	0.65535500	-6.06546300
C	-1.30014900	-3.68923000	5.20854700
H	-3.53732900	-2.05178800	5.29350600
C	0.20238200	1.74768300	-6.58879000
H	-0.84201000	1.92831800	-6.31960200
H	-0.65820900	-2.71351900	3.54989500
N	-0.83905900	-3.63692500	3.91127400
O	-1.58383900	-4.71528000	5.80006300
C	-0.10688500	-2.90189200	1.28481400
C	3.77467400	2.54989000	-0.22238300

C	3.00091300	1.41424100	0.20823600
H	0.44716500	2.39186500	-7.43529500
N	1.44107800	-1.02038400	0.84643200
H	0.29248700	0.70584500	-6.90761800
C	-0.59617800	-4.68979600	3.00241100
H	3.42423300	-3.94161600	-1.71733400
C	1.15870600	-2.32113800	1.21346400
C	-0.21290200	-4.34547200	1.68382800
H	4.84957900	2.61904000	-0.16753800
C	-0.69248800	-6.03194800	3.38324700
C	2.81148200	-0.89446300	0.97722900
C	3.56695800	0.23974100	0.69451900
C	3.25709000	-4.63962800	-2.54276600
H	-0.98962700	-6.27660000	4.39072600
H	0.21112900	-4.12524500	-0.89232700
C	0.09993300	-5.37273000	0.76776900
H	3.58208600	-4.15266300	-3.46654000
N	0.51263700	-5.02417000	-0.53831500
H	6.20112600	3.10778300	3.44083800
H	3.88755700	-5.51623400	-2.37702700
H	4.99066500	1.28880000	2.71159400
C	-0.39614200	-7.02054400	2.45307100
C	2.36354700	-3.00922800	1.59116200
C	-0.00019600	-6.71348500	1.15917300
C	3.38125900	-2.12530400	1.45676300
C	1.77854300	-5.05329200	-2.64499600
C	1.37537400	-5.74773800	-1.34119800
H	1.17229600	-4.15388200	-2.78282800
C	7.27962000	2.93433000	3.43589000
C	5.63535200	0.78944300	1.99659400
C	5.05235200	0.18522500	0.88681300
H	5.94970100	0.88300600	4.76830700
H	7.69682200	3.42947600	4.31800500
H	-0.47199600	-8.06180800	2.74939900

H	2.40668100	-4.03246800	1.93023000
H	7.69065800	3.42541600	2.54951200
H	0.25292500	-7.49070600	0.45581600
O	1.82111000	-6.84112300	-1.04190800
C	7.03583200	0.77742000	4.71943600
H	7.45308700	1.24481500	5.61657500
H	4.42821600	-2.27809300	1.66534000
C	7.62594400	1.42805300	3.44760100
C	7.02330200	0.75382800	2.20100100
C	5.86359400	-0.46809000	-0.05028400
C	1.54532600	-6.00031500	-3.82913600
H	5.38845700	-0.92527700	-0.90877700
H	1.88915000	-5.54078700	-4.76029200
H	7.26704900	-0.29059000	4.75817600
H	2.09265600	-6.93341600	-3.68183300
C	7.79894000	0.09603400	1.24609600
H	0.48600000	-6.24138200	-3.94628000
C	7.24772600	-0.52149300	0.11027400
C	9.15738000	1.29185500	3.50965800
H	9.53496300	1.78519700	4.40909300
H	9.64740000	1.76148600	2.65239500
H	6.85269000	-1.07655100	-2.65001900
H	8.87172200	0.05737600	1.38064500
H	9.47592700	0.24686400	3.55503500
H	8.66784700	0.61865700	-1.98171600
C	7.39850500	-1.83376900	-2.08063200
H	6.68474200	-2.59479500	-1.75415900
C	8.17427500	-1.22214700	-0.90077700
C	9.18322500	-0.19926200	-1.47079800
H	9.80946800	0.23944600	-0.69062500
H	8.09596100	-2.31766600	-2.76928400
C	8.94398600	-2.36011000	-0.19250400
H	8.25616400	-3.10478700	0.21729500
H	9.56040200	-1.98976300	0.62982000

H	9.84791100	-0.68143700	-2.19397900
H	9.60762800	-2.86889800	-0.89820200

C_{2a}:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.133025 Hartree

H_corr: 0.171930 Hartree

SCF: -349.148690 Hartree

S: 81.883 Cal/Mol-Kelvin

H: -348.976760 Hartree

G: -349.015665 Hartree

Cartesian Coordinates:

C	-1.56538900	1.22890000	0.12779200
C	-0.14879700	0.69983100	0.05149300
C	-0.14878400	-0.69989100	0.05149900
C	1.05060900	1.40367400	0.00457100
C	1.05062600	-1.40369500	0.00438100
C	2.25380600	0.69771200	-0.04662200
C	2.25380900	-0.69769900	-0.04677200
H	1.05570200	-2.49022700	0.00094400
H	3.19495500	-1.23691200	-0.09230600
H	3.19496100	1.23692900	-0.09195300
H	1.05563500	2.49020700	0.00131200
C	-2.42175600	-0.00003100	-0.26396600
H	-1.79383800	1.55524000	1.15102500
H	-1.74002700	2.09109500	-0.52213100
C	-1.56545700	-1.22886300	0.12809500
H	-1.79371000	-1.55449800	1.15161100
H	-1.74025900	-2.09136000	-0.52134300
H	-2.57814200	-0.00013200	-1.34714500
H	-3.40727600	0.00003700	0.20716300

Transition State TS2 (HAA):

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -1346.9266 cm-1

G_corr: 1.671044 Hartree

H_corr: 1.953888 Hartree

SCF: -5922.839654 Hartree

S: 595.294 Cal/Mol-Kelvin

H: -5920.885766 Hartree

G: -5921.168610 Hartree

Cartesian Coordinates:

C	4.16282200	-2.17528700	-1.50539500
C	4.69449200	-3.30248400	-2.36069900
C	3.95998900	-3.39145100	-3.55915400
C	5.73629500	-4.18636700	-2.11004500
C	4.26398900	-4.37828700	-4.50230600
C	6.04113600	-5.16627500	-3.05785600
C	5.30928200	-5.26076800	-4.24585500
H	3.69865900	-4.45305000	-5.42616300
H	5.56211700	-6.02551600	-4.97319000
H	6.85490900	-5.86008500	-2.87242400
H	6.31149600	-4.12024600	-1.19113500
C	3.29860000	-1.35113100	-2.49108200
H	3.54582200	-2.57690000	-0.69272400
H	4.95208600	-1.58588000	-1.03178400
C	2.91447100	-2.35178900	-3.58479500
H	1.84753500	-2.88726100	-3.19829800
H	2.64006400	-1.93839900	-4.55654300
H	3.90588400	-0.55393800	-2.93901800
H	2.43417700	-0.87354000	-2.02648900
C	0.16175500	-4.23275000	-4.90555300
C	-0.30750200	-3.43147700	-3.68139700
H	1.00005000	-3.71631600	-5.37782800

H	-0.62527400	-4.33091700	-5.65798500
H	0.50402700	-5.22809700	-4.61681800
C	-0.71518000	-2.00766200	-4.10862500
H	-0.90058300	-1.37906700	-3.23677500
H	-1.61038800	-2.02489400	-4.73688700
H	0.09021200	-1.54452100	-4.68634500
C	-1.46951900	-4.11770600	-2.93652700
C	-1.96068000	-3.53472900	-1.75880000
C	-2.04783300	-5.31295800	-3.37420400
C	-2.99467500	-4.13308000	-1.04449900
C	-3.09198500	-5.90694100	-2.66537500
C	-3.56558000	-5.32380500	-1.49454800
H	-1.53204800	-2.60453900	-1.40331900
H	-3.35048800	-3.66921300	-0.13109900
H	-4.36990400	-5.79114300	-0.93545900
H	-3.52744500	-6.83258600	-3.02887600
H	-1.69308100	-5.79686900	-4.27557000
O	0.72210300	-3.39336300	-2.69981100
O	0.00310600	-0.39936600	-1.11039400
H	0.38933800	-1.25249300	-0.86906500
H	-9.99654700	2.84429800	1.42545800
H	-9.86947500	1.73810600	0.05797600
C	-9.28855100	2.30366600	0.78992900
H	-8.69576300	3.04245200	0.24361700
H	-9.53595000	-0.85805400	-2.51757800
H	-9.96961400	0.88285500	3.06030600
C	-9.13028000	-1.85147400	-2.30665600
H	-9.46200500	-2.51487500	-3.10961100
H	-9.84221800	-0.26087100	1.72402400
C	-9.26207500	0.36659600	2.40436500
H	-8.95740800	-0.30944700	-0.38282900
C	-8.38433400	1.38858100	1.64662500
H	-7.37554900	-0.35984100	-3.83464100
H	-9.58200900	-2.21547300	-1.37976000

H	-8.40864600	2.77455300	3.31330200
C	-7.88576100	-0.20837800	-0.27442100
C	-7.66923700	2.26662500	2.68863000
C	-7.05761400	-1.38277400	-3.61413900
H	-7.43668800	-2.03126500	-4.40972900
H	-7.05307900	3.03955100	2.22121000
C	-7.39610900	0.63975800	0.73329000
C	-7.59285800	-1.84788800	-2.24074200
H	-8.64999800	-0.29425200	3.02432800
C	-7.05171800	-0.92044900	-1.13679200
H	-3.63286700	7.89752900	1.98416400
H	-3.98594600	6.22004000	1.55289700
H	-5.96703200	-1.41032900	-3.66133900
C	-3.34926600	6.85979200	2.17040600
H	-7.03140400	1.67803700	3.35370600
C	-6.01327000	0.76711600	0.85683200
C	-7.12001400	-3.29420700	-1.97131900
H	-7.49528600	-3.96881800	-2.74706200
H	-4.80290200	2.08343500	-1.67230100
H	-3.55528000	6.62886400	3.21905900
C	-5.66481700	-0.77083200	-0.97178200
O	-1.76209200	8.16212500	-0.01248100
H	-7.49003200	-3.65371100	-1.00672500
H	-5.58255400	1.41333900	1.61116600
H	-3.01215400	3.88092100	-2.57595100
H	-1.23229800	8.03524700	-2.13285200
C	-5.14452900	0.06708700	0.00939100
C	-3.75206200	2.15550200	-1.44040100
H	-0.66141100	7.88602700	-4.54043400
C	-0.93959600	7.09604000	-2.57470500
C	-1.60114800	7.02352500	0.38763200
C	-0.61610900	6.99539900	-3.92192800
C	-2.85261800	3.05906400	-1.89517300
C	-1.86037600	6.65064300	1.85334000

H	-4.97558200	-1.30713700	-1.61456300
H	-6.03146900	-3.37707700	-1.96324900
H	-1.15750400	8.56613000	2.59038600
C	-0.88150700	5.94792500	-1.77681100
N	-1.18903400	5.97022200	-0.39990500
C	-0.23709000	5.79279800	-4.50416700
C	-0.96627700	7.50538300	2.76284200
C	-3.66207300	0.24563300	0.15799400
C	-3.04478300	1.27207200	-0.54845900
H	0.01341400	5.72879400	-5.55086000
H	-1.61522100	5.59355600	2.01594000
H	-1.16485300	7.28464300	3.81511200
C	-0.49872000	4.70990800	-2.33802700
H	-1.10171800	5.08162100	0.06836700
C	-0.17670100	4.64035600	-3.71041200
C	-1.58990700	2.73261900	-1.28267900
H	-4.66098500	-1.81418000	1.81968300
H	-0.12087100	2.51247300	7.39312300
N	-1.71946200	1.63675500	-0.45949800
O	0.72611300	3.86931900	-6.41492400
C	-0.43056200	3.48091200	-1.47604300
C	-2.96583000	-0.59279500	1.02225800
H	-0.07440400	1.07401000	8.42817600
C	-3.60097000	-1.61391900	1.81330800
H	0.09466400	7.31961900	2.57381500
N	0.19364400	3.38354700	-4.23262600
C	0.03122200	1.42975300	7.40165900
C	0.61957200	3.06630600	-5.50554500
H	1.05765200	1.23074800	7.08101300
H	3.06831300	1.83902400	-5.09792500
H	0.15796600	2.61672400	-3.57704400
H	-2.59310400	2.15248200	6.88410500
H	0.72799500	1.02102100	-4.80054700
H	-2.63127300	0.70964600	7.91231800

N	-1.60533000	-0.58002400	1.25587200
C	0.97836000	1.58906500	-5.70400500
C	-2.62431700	-2.23714100	2.51561800
C	0.78746800	3.14531200	-0.88639700
C	-2.43167000	1.07120300	6.90164100
C	2.49125100	1.47488400	-5.95255400
Co	-0.25020000	0.60376600	0.40152900
C	-0.98996800	0.73287100	6.49154000
C	-1.38273500	-1.60535200	2.15319500
H	-2.71617700	-3.05530600	3.21300400
H	2.03466000	4.86687800	-1.58571500
C	1.97918400	3.93787800	-1.03972700
N	1.03914700	2.03901500	-0.10416400
H	2.77678400	2.06178900	-6.82801600
H	-0.83171800	1.07618700	5.46140800
H	2.77470900	0.43380500	-6.13040800
C	-0.78888400	-0.78680100	6.56896700
H	-3.16012400	0.61056700	6.22853100
C	0.17267500	1.02340300	-6.88156700
H	-0.90206300	1.05184100	-6.68306800
H	-0.50006900	-0.76368500	4.56185600
N	-0.53099500	-1.38501100	5.35482700
O	-0.86542900	-1.37943000	7.62986500
C	-0.14549700	-2.00706100	2.65512300
C	2.96515300	3.29525500	-0.37059900
C	2.38581900	2.09930100	0.18666200
H	0.36438300	1.60591100	-7.78451000
N	1.17059300	-0.26053900	1.49152000
H	0.45011800	-0.01633900	-7.07443000
C	-0.31504200	-2.74725900	5.05267900
H	3.05968800	-5.10757500	0.27431700
C	1.04723400	-1.38158600	2.29122700
C	-0.10845300	-3.09192200	3.69646100
H	3.99323200	3.59696600	-0.25110500

C	-0.29792800	-3.73301400	6.04447500
C	2.52034300	0.03982800	1.49359800
C	3.11389200	1.15974800	0.91360500
C	2.56933100	-5.93785000	-0.24249600
H	-0.45938700	-3.45388700	7.07351900
H	0.26543000	-3.98477500	1.35272200
C	0.12702200	-4.44147300	3.35374600
H	2.82364800	-5.86488500	-1.30182800
N	0.35160900	-4.75484600	1.99849500
H	5.15120000	3.49650000	4.52019600
H	2.98073100	-6.87003100	0.15231800
H	4.37115700	1.78385200	3.19940800
C	-0.07304200	-5.05276600	5.67452000
C	2.33511700	-1.80120100	2.77175000
C	0.13956800	-5.42370900	4.35415300
C	3.24543700	-0.93311700	2.26722800
C	1.04194600	-5.90085500	-0.05679600
C	0.73587100	-5.96362800	1.44071800
H	0.66867100	-4.96543600	-0.48603200
C	6.23743300	3.60457400	4.48019000
C	5.07260600	1.71051100	2.37589600
C	4.58096300	1.38941200	1.11264400
H	5.51535800	0.97027000	5.03000600
H	6.57846600	3.87475600	5.48415100
H	-0.06176400	-5.81931900	6.44276000
H	2.50392000	-2.65065300	3.41529100
H	6.46317200	4.44021300	3.81209600
H	0.31932600	-6.45082300	4.08129400
O	0.86512400	-6.99297100	2.07786700
C	6.59027800	1.15761100	4.97741000
H	6.93196200	1.39691400	5.98890100
H	4.31397500	-0.93421000	2.41063400
C	6.93327100	2.30882600	4.00481100
C	6.43781800	1.95013800	2.59131400

C	5.47030900	1.30683100	0.03141400
C	0.36608900	-7.07128300	-0.77931400
H	5.06913500	1.06074400	-0.94298900
H	0.63570500	-7.06562200	-1.83804400
H	7.07538700	0.22651600	4.67136100
H	0.68057500	-8.02086700	-0.34196500
C	7.29072700	1.85388500	1.49162500
H	-0.72247300	-7.00736800	-0.71297800
C	6.83548500	1.53628800	0.20068800
C	8.45387500	2.53854200	4.05571200
H	8.75467700	2.78791900	5.07655400
H	8.76656300	3.36690900	3.41415900
H	6.42916700	1.87521700	-2.59070800
H	8.34812500	2.03373500	1.63274300
H	9.01492700	1.64742100	3.76119600
H	7.84724000	3.61685600	-1.33251800
C	7.16827700	1.12241400	-2.30336100
H	6.67394600	0.14750200	-2.28490700
C	7.84322600	1.45696300	-0.96158700
C	8.56105400	2.81726500	-1.11608500
H	9.11014400	3.09820900	-0.21465900
H	7.92023900	1.08725700	-3.09582000
C	8.88875700	0.35833900	-0.66351600
H	8.41183400	-0.61962600	-0.55502400
H	9.44517900	0.55962500	0.25474500
H	9.27997200	2.77737200	-1.93991000
H	9.61380900	0.28935800	-1.48005000

Intermediate D:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.670405 Hartree

H_corr: 1.958858 Hartree

SCF: -5922.884168 Hartree

S: 607.099 Cal/Mol-Kelvin

H: -5920.925310 Hartree

G: -5921.213763 Hartree

Cartesian Coordinates:

C	3.97327100	1.34095500	-3.40258200
C	5.26399000	0.74222900	-3.91793300
C	5.04798300	-0.61580300	-4.30064200
C	6.51679800	1.31372300	-4.03066800
C	6.13299100	-1.38095000	-4.79231800
C	7.58350500	0.54646000	-4.52483000
C	7.38317400	-0.78989600	-4.89887300
H	5.98411400	-2.41496600	-5.08769300
H	8.21963200	-1.36755300	-5.28037700
H	8.56892100	0.99044900	-4.62055400
H	6.68186500	2.34874900	-3.74362100
C	2.90803500	0.22696300	-3.62813400
H	4.05687300	1.59427300	-2.34062600
H	3.71865400	2.27107000	-3.92037500
C	3.69752200	-0.95738300	-4.11095200
H	-0.62436800	-1.81148700	-1.64822000
H	3.26098700	-1.92585500	-4.32303000
H	2.17129300	0.53289800	-4.38595600
H	2.32722700	0.00998100	-2.72375900
C	-0.44885300	-2.24042900	-4.22327900
C	-1.53812500	-2.63871100	-3.21542400
H	0.04029800	-1.32513800	-3.88159200
H	-0.85218800	-2.04725000	-5.22041300
H	0.31317600	-3.01798000	-4.30281600
C	-2.66392700	-1.58494500	-3.21320300
H	-3.40598600	-1.82751300	-2.45093400
H	-3.16600200	-1.54234200	-4.18335200
H	-2.26080300	-0.59211300	-2.99178000
C	-2.14884000	-4.01214300	-3.50610200

C	-2.76834900	-4.72728400	-2.47414700
C	-2.16422000	-4.56395400	-4.79090500
C	-3.37252700	-5.95771500	-2.71559900
C	-2.77244000	-5.79469100	-5.03694800
C	-3.37729700	-6.49851800	-4.00005700
H	-2.76698200	-4.31512300	-1.47317500
H	-3.83641100	-6.49741000	-1.89583600
H	-3.84557300	-7.45920000	-4.18923600
H	-2.76598800	-6.20397500	-6.04246800
H	-1.69489100	-4.04222700	-5.61705000
O	-0.95021200	-2.70606700	-1.90384700
O	-0.03982900	-0.18560800	-1.20315100
H	-0.46728500	0.48801100	-1.74715300
H	-9.69632000	3.10334500	2.83072300
H	-9.59245000	3.04222100	1.07155500
C	-9.00992600	2.95558800	1.99150400
H	-8.28423200	3.77345700	2.00293700
H	-9.40355500	2.45768300	-2.55541700
H	-10.05754000	0.57688600	2.93015700
C	-9.10959500	1.50258200	-2.99933700
H	-9.45062900	1.50934400	-4.03782000
H	-9.95816200	0.46787100	1.17298400
C	-9.36557600	0.46075800	2.09056500
H	-8.90866100	1.56762000	-0.53233100
C	-8.30486100	1.58490400	2.10651600
H	-7.12716100	3.40418300	-3.28690000
H	-9.65285000	0.70499700	-2.48528300
H	-8.29999100	1.67073600	4.27236800
C	-7.84550600	1.42335900	-0.39352000
C	-7.57863800	1.53552000	3.46233300
C	-6.91868700	2.43444300	-3.74736800
H	-7.29781200	2.46167700	-4.77335100
H	-6.83128300	2.32804100	3.55724600
C	-7.34250600	1.40071300	0.91850100

C	-7.58661900	1.28740500	-2.95546300
H	-8.89725000	-0.52367800	2.17536700
C	-7.03446500	1.26789400	-1.51797400
H	-0.68391900	7.19604900	5.18054900
H	-1.73395100	6.03196000	4.36485600
H	-5.83380300	2.31893300	-3.80145300
C	-0.81525800	6.13746100	4.94862000
H	-7.08124600	0.57598400	3.62797000
C	-5.97110900	1.21031500	1.08406100
C	-7.27331500	-0.06039100	-3.64411800
H	-7.65700600	-0.06390400	-4.66882500
H	-4.29007200	3.52530600	-0.51292600
H	-0.94771000	5.59197900	5.88681000
C	-5.65911500	1.08522400	-1.30571300
O	0.79405000	7.62456300	2.93739900
H	-7.73771200	-0.89312900	-3.10894900
H	-5.53181800	1.18587300	2.07316700
H	-2.10766000	5.08254800	-0.75539900
H	0.94789500	8.18271500	0.83011700
C	-5.12442200	1.05404700	-0.02129600
C	-3.25594700	3.24993400	-0.37967400
H	1.14179900	8.81910500	-1.55705600
C	0.86704300	7.44038400	0.05203200
C	0.59433000	6.42439700	2.89878200
C	0.97209200	7.78092500	-1.29054600
C	-2.15744300	4.03511100	-0.50118400
C	0.40554500	5.60639000	4.18292600
H	-4.98906000	0.95655500	-2.14856300
H	-6.20007900	-0.25705200	-3.69392500
H	1.90710800	6.73643200	5.26905500
C	0.64840600	6.10206900	0.39815100
N	0.51889700	5.68280300	1.73861900
C	0.86729700	6.83597300	-2.30295600
C	1.68335400	5.69478100	5.03100000

C	-3.65300400	0.85667800	0.18685800
C	-2.79888300	1.93654500	-0.01657500
H	0.94412200	7.11375700	-3.34203200
H	0.22779800	4.55373100	3.92949200
H	1.56157600	5.14486800	5.96805300
C	0.53836300	5.11580500	-0.60767000
H	0.35072400	4.69628900	1.86078400
C	0.64817400	5.49589100	-1.96254600
C	-1.01850000	3.20996500	-0.20728300
H	-5.11802700	-1.54046500	0.53593700
H	-2.42102400	-1.26494200	7.76838900
N	-1.42102100	1.92394000	0.10402600
O	0.45110000	5.66172300	-4.90826700
C	0.29389900	3.68139700	-0.22906100
C	-3.19511500	-0.39873300	0.57201600
H	-2.68939700	-3.01292300	7.88910400
C	-4.05369100	-1.54453500	0.71010500
H	2.54575100	5.27679900	4.50420500
N	0.53570900	4.48250500	-2.93804700
C	-2.26531100	-2.22341500	7.26580800
C	0.40999600	4.60457400	-4.30729600
H	-1.18770500	-2.39459200	7.19296400
H	2.12738700	3.18629200	-6.00073400
H	0.47412900	3.54491300	-2.57183300
H	-4.59898400	-0.95716500	6.48077700
H	0.40361700	2.44150800	-4.36481800
H	-4.94043700	-2.69464500	6.55889500
N	-1.88979200	-0.73752800	0.86954900
C	0.16711000	3.27680600	-5.03617600
C	-3.26745000	-2.58604700	1.07225400
C	1.38092100	2.88639600	0.13066300
C	-4.43453600	-1.91695600	5.98348400
C	1.06846000	3.18387300	-6.27221900
Co	-0.25932700	0.36637800	0.55289400

C	-2.93274100	-2.22352700	5.88268800
C	-1.92379000	-2.08250300	1.17179500
H	-3.55693200	-3.60749900	1.26323000
H	3.04773300	4.33973000	-0.20310400
C	2.74006300	3.35569800	0.11528600
N	1.32246700	1.58664100	0.59473200
H	0.89237500	4.03509400	-6.93174600
H	-2.45966500	-1.44862200	5.26650700
H	0.86556100	2.26503800	-6.82858600
C	-2.74118700	-3.59760600	5.22644900
H	-4.90189100	-1.87006600	4.99581100
C	-1.32144900	3.18861200	-5.41815700
H	-1.96946600	3.23086200	-4.53807600
H	-1.76465700	-2.65012800	3.72257800
N	-2.05410300	-3.56423700	4.03296600
O	-3.17649600	-4.60989800	5.74499300
C	-0.84240500	-2.86314600	1.57662000
C	3.51141200	2.33846200	0.57009100
C	2.62977800	1.24061500	0.86705200
H	-1.59320400	4.01723000	-6.07587500
N	0.85346700	-1.07744800	1.34368400
H	-1.52746100	2.25283000	-5.94455900
C	-1.70128600	-4.62637600	3.17078900
H	3.20453700	-4.07687800	-1.01838300
C	0.44760100	-2.34990600	1.68722800
C	-1.07960500	-4.29853700	1.94131900
H	4.58217500	2.31815300	0.69602800
C	-1.91685500	-5.96309300	3.51798100
C	2.20882600	-1.04717400	1.60342000
C	3.07007700	0.02145200	1.37545400
C	3.06908800	-4.83923700	-1.79081400
H	-2.39390400	-6.19618200	4.45677800
H	-0.32083600	-4.18644400	-0.64422700
C	-0.66062900	-5.33485400	1.08124900

H	3.50698100	-4.45740600	-2.71742200
N	-0.01825600	-5.01616700	-0.13805200
H	5.70398500	2.84646600	4.16683900
H	3.62393800	-5.72980000	-1.48824300
H	4.40184500	1.08800200	3.44125200
C	-1.50492200	-6.96351400	2.64502400
C	1.55360600	-3.10898900	2.20783000
C	-0.88154200	-6.66953300	1.44148000
C	2.63909300	-2.30248400	2.16277600
C	1.58397400	-5.17595000	-1.99300500
C	1.02011100	-5.74185800	-0.68767300
H	1.04379500	-4.26195900	-2.25070300
C	6.75844600	2.58146000	4.27350900
C	5.05914900	0.48862100	2.82079700
C	4.52357800	-0.14095200	1.70010400
H	5.13424700	0.74954700	5.60000200
H	7.14013000	3.10018200	5.15814400
H	-1.67335700	-8.00078500	2.91604300
H	1.48976600	-4.12657800	2.55995600
H	7.28907200	2.97199300	3.40071000
H	-0.54540700	-7.45701400	0.78470600
O	1.48052300	-6.75143400	-0.18252600
C	6.20636400	0.54880000	5.66003100
H	6.58382800	1.04084900	6.56162300
H	3.64611800	-2.52214300	2.47915300
C	6.96299900	1.05567700	4.41117000
C	6.41372500	0.34920100	3.15762800
C	5.35050700	-0.92829900	0.88751700
C	1.39166900	-6.20575200	-3.11688000
H	4.91624000	-1.40178500	0.01636500
H	1.83268700	-5.84215400	-4.04986500
H	6.33487300	-0.52962200	5.78661300
H	1.87539100	-7.14922500	-2.85456800
C	7.20621800	-0.44112200	2.32494000

H	0.33305500	-6.40382500	-3.30290300
C	6.70345400	-1.09154500	1.18510400
C	8.46415100	0.79407300	4.62509700
H	8.80486900	1.31611300	5.52308900
H	9.06833500	1.15768400	3.78948600
H	6.49866000	-1.86747600	-1.55391500
H	8.25451600	-0.56298700	2.56267500
H	8.68037000	-0.26838900	4.76583700
H	8.37402100	-0.25965800	-0.87307900
C	6.92166400	-2.60404600	-0.86686100
H	6.11872800	-3.27037500	-0.53976400
C	7.64741000	-1.94697800	0.31986300
C	8.77816100	-1.05563600	-0.24238500
H	9.36661000	-0.58916700	0.55151100
H	7.62948100	-3.20775500	-1.44079900
C	8.26266500	-3.06991900	1.18603000
H	7.48591800	-3.72069100	1.59700800
H	8.84321200	-2.67569500	2.02338000
H	9.46256800	-1.65114700	-0.85410400
H	8.93389000	-3.68922700	0.58356400

Transition State TS3 (Radical Substitution):

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -159.7451 cm-1

G_corr: 1.680639 Hartree

H_corr: 1.957922 Hartree

SCF: -5922.886450 Hartree

S: 583.592 Cal/Mol-Kelvin

H: -5920.928528 Hartree

G: -5921.205811 Hartree

Cartesian Coordinates:

C	1.79144200	1.98461700	-5.00197600

C	3.07567800	1.43472700	-4.43602300
C	2.81433800	0.23113000	-3.72010900
C	4.36432300	1.92594700	-4.53891700
C	3.87521600	-0.45714100	-3.08941100
C	5.40763000	1.22701600	-3.92067500
C	5.15937400	0.04845800	-3.20089800
H	3.67771500	-1.36833600	-2.53675800
H	5.98451300	-0.46580500	-2.72130700
H	6.42325100	1.60147000	-3.99709000
H	4.57078900	2.83743900	-5.09161800
C	0.75950300	0.85390000	-4.74728300
H	1.50896400	2.90438900	-4.47846500
H	1.87805600	2.24314700	-6.06075800
C	1.45509600	-0.11381600	-3.83422300
H	-1.00234900	-1.60379000	-2.06081600
H	1.01052300	-1.02290900	-3.46419500
H	0.49090800	0.34863200	-5.68566900
H	-0.18450400	1.22371400	-4.33757900
C	-1.84393800	-1.83276300	-4.61498300
C	-2.43285900	-2.33182900	-3.28875400
H	-1.32283700	-0.89087400	-4.44137600
H	-2.61395100	-1.64293100	-5.36680800
H	-1.12803300	-2.54969200	-5.02209600
C	-3.45676400	-1.30773400	-2.76319400
H	-3.85578900	-1.62387100	-1.79932400
H	-4.29087000	-1.19399400	-3.46085300
H	-2.98439300	-0.32942100	-2.62880800
C	-3.11100700	-3.70011400	-3.42186500
C	-3.40555700	-4.43455200	-2.26668500
C	-3.49561000	-4.23611900	-4.65459700
C	-4.05315900	-5.66353900	-2.33918200
C	-4.14923900	-5.46660000	-4.73186600
C	-4.42941400	-6.18668000	-3.57531900
H	-3.11444500	-4.03822900	-1.30257900

H	-4.25778000	-6.21663800	-1.42794000
H	-4.93257800	-7.14651700	-3.63476700
H	-4.43310100	-5.86183000	-5.70239300
H	-3.28544900	-3.70465300	-5.57516900
O	-1.36664300	-2.48254000	-2.33151400
O	-0.09749100	-0.10930500	-1.56899600
H	-0.57018200	0.66053700	-1.91118700
H	-8.33736600	3.01252900	5.18816400
H	-8.66305200	3.24235300	3.47038200
C	-7.88728500	2.97503600	4.19144300
H	-7.11113800	3.74381800	4.14393000
H	-9.39686400	3.27121900	-0.13197500
H	-8.88497700	0.52594600	4.99175900
C	-9.30162400	2.39266100	-0.77594800
H	-9.87875800	2.59129600	-1.68285100
H	-9.21666600	0.70755900	3.26918900
C	-8.42566800	0.51895500	3.99858000
H	-8.51292900	2.03232000	1.54336300
C	-7.29772200	1.57260700	3.91810100
H	-7.28809200	4.22084900	-1.25367800
H	-9.77354100	1.54576100	-0.27045500
H	-6.76814000	1.29392900	6.00149700
C	-7.46454900	1.81469800	1.38839500
C	-6.27583500	1.26221000	5.02599100
C	-7.28012400	3.33492400	-1.89471400
H	-7.88888800	3.55369300	-2.77733000
H	-5.46106200	1.99103700	5.04895500
C	-6.66689200	1.54476200	2.51343700
C	-7.83666700	2.10232800	-1.14654600
H	-8.03823700	-0.48693300	3.81503100
C	-6.96144600	1.81274400	0.08727000
H	1.53774200	6.23782700	5.48325400
H	0.29415600	5.22512600	4.73853300
H	-6.25317300	3.18025700	-2.23357400

C	1.30899800	5.22462500	5.14592100
H	-5.83885300	0.26610900	4.91531200
C	-5.31862500	1.26080100	2.29983000
C	-7.81565200	0.87840900	-2.09020200
H	-8.43175900	1.06702400	-2.97474600
H	-3.86100800	3.73467900	0.67529000
H	1.32184900	4.56182400	6.01533600
C	-5.59705100	1.52974700	-0.08075500
O	2.72031800	6.87673800	3.01700900
H	-8.20914900	-0.01063200	-1.58999200
H	-4.66028200	1.04644100	3.13196000
H	-1.67250000	5.18411100	0.08801900
H	2.30010300	7.73999900	1.06414100
C	-4.77530200	1.25293500	1.00802100
C	-2.85810600	3.38204200	0.49289100
H	1.79580800	8.75282500	-1.14145900
C	1.84075100	7.15843600	0.28071300
C	2.31003000	5.73494100	2.91237400
C	1.54687900	7.71263000	-0.95770100
C	-1.75498400	4.11339000	0.19634500
C	2.33993100	4.76521700	4.10121900
H	-5.16125700	1.51378200	-1.07359100
H	-6.80632000	0.64329800	-2.43527500
H	4.07119200	5.71813700	4.99306800
C	1.52781400	5.81483400	0.51648600
N	1.76790600	5.20107100	1.76313000
C	0.93177100	6.98000400	-1.96416300
C	3.75428100	4.71790600	4.69278800
C	-3.32060100	0.94863800	0.81057300
C	-2.44819100	2.00293500	0.54529600
H	0.68866100	7.42671500	-2.91472200
H	2.06645000	3.75797400	3.76339200
H	3.78289500	4.06646600	5.57039100
C	0.93152100	5.02831100	-0.49799200

H	1.47809300	4.23720900	1.82325200
C	0.60788100	5.63853700	-1.73033400
C	-0.66079300	3.18637300	0.06878600
H	-4.86981000	-1.40509700	1.18304200
H	-0.86632600	-2.18264200	7.58868600
N	-1.09330900	1.89716100	0.30099200
O	-0.61852700	6.39334900	-4.31551800
C	0.64686400	3.57331100	-0.24160900
C	-2.89850300	-0.37634500	0.90492100
H	-1.14227800	-3.93353600	7.56532600
C	-3.79748900	-1.48607000	1.09823900
H	4.48075900	4.34055600	3.96770900
N	-0.06145600	4.85519200	-2.69914000
C	-0.85058800	-3.07510700	6.95712900
C	-0.70349200	5.27293900	-3.84861900
H	0.17860600	-3.23312300	6.62296800
H	-0.40699700	3.97711800	-6.31440800
H	-0.25374800	3.90855800	-2.40765300
H	-3.27087800	-1.73542800	6.87372700
H	-1.31654600	3.21590300	-4.11845100
H	-3.62697600	-3.47123000	6.82146900
N	-1.59682000	-0.82146400	0.83967700
C	-1.59806700	4.20700400	-4.49557800
C	-3.03723100	-2.60687000	1.13728600
C	1.72157900	2.67874700	-0.22028200
C	-3.24486900	-2.62807300	6.24274100
C	-1.42938800	4.22561300	-6.01789300
Co	0.03032800	0.23776800	0.35455800
C	-1.81206100	-2.91468500	5.77006600
C	-1.66639800	-2.18750000	0.98988300
H	-3.36015000	-3.62710400	1.27482600
H	3.38897600	4.02572500	-0.87402800
C	3.08094900	3.05876500	-0.50740100
N	1.67011700	1.36677800	0.20404100

H	-1.65405900	5.21904200	-6.40876900
H	-1.47187600	-2.07106100	5.15682500
H	-2.10387800	3.50586800	-6.48941600
C	-1.80280900	-4.20147700	4.93359900
H	-3.92053400	-2.46458200	5.39847100
C	-3.05829000	4.47924400	-4.08915800
H	-3.19354200	4.43255300	-3.00534300
H	-1.12818000	-3.08695500	3.37871800
N	-1.37414800	-4.02999000	3.63660500
O	-2.15228200	-5.26612400	5.41184100
C	-0.57838000	-3.05444700	1.10214800
C	3.85692900	1.98774200	-0.21405000
C	2.97736700	0.94020800	0.24205700
H	-3.36660200	5.47129100	-4.42693500
N	1.17137400	-1.32905400	0.81338600
H	-3.72551700	3.74228100	-4.54438800
C	-1.23054100	-4.98374200	2.60468700
H	2.78374000	-4.02135800	-2.42443600
C	0.74325800	-2.60699000	1.09107900
C	-0.82761700	-4.51651400	1.33014100
H	4.92682000	1.89852800	-0.30941700
C	-1.43688600	-6.34888600	2.82434000
C	2.54211300	-1.36023900	0.95980300
C	3.42119000	-0.31167500	0.68069500
C	2.45185800	-4.67307000	-3.23839900
H	-1.74467500	-6.68760500	3.80099100
H	-0.55692400	-4.09019200	-1.30678100
C	-0.61515400	-5.44604900	0.29129700
H	2.70118600	-4.18521900	-4.18532900
N	-0.20049700	-4.98564800	-0.98096400
H	6.50806800	2.75185100	2.62167500
H	3.01692500	-5.60516100	-3.17186000
H	5.02501800	0.99830500	2.36991900
C	-1.23013800	-7.24057700	1.77797800

C	1.85724900	-3.44543600	1.45201100
C	-0.82224100	-6.81126900	0.52372300
C	2.96411800	-2.66858200	1.40027800
C	0.94374400	-4.95308200	-3.15299700
C	0.64382100	-5.66746400	-1.83180100
H	0.39960400	-4.00604900	-3.18137600
C	7.54687900	2.42273600	2.69847600
C	5.57768000	0.24780500	1.81647700
C	4.88880100	-0.52629700	0.88329000
H	5.93015900	1.01662200	4.47679600
H	8.04127500	3.06281300	3.43540500
H	-1.38960600	-8.30025000	1.95009600
H	1.78327500	-4.48534500	1.72935800
H	8.02253800	2.59763400	1.72936400
H	-0.64253600	-7.51698400	-0.27248300
O	1.13992000	-6.75113900	-1.57301400
C	6.98612100	0.73765000	4.48938700
H	7.48029500	1.35309100	5.24728600
H	3.97693900	-2.94628100	1.64186900
C	7.65655900	0.93746500	3.11115400
C	6.94561500	0.06109900	2.06287100
C	5.58955800	-1.51511000	0.17428800
C	0.47357900	-5.83192800	-4.32203800
H	5.04594500	-2.11046100	-0.54684000
H	0.72278700	-5.36328300	-5.27900200
H	7.04925600	-0.30594800	4.80953500
H	0.95880000	-6.80956200	-4.28220200
C	7.60217700	-0.93332800	1.33833200
H	-0.60810200	-5.98653800	-4.29617600
C	6.94856500	-1.73814000	0.38972600
C	9.14924100	0.59211200	3.25395100
H	9.60700800	1.24040400	4.00565600
H	9.69754300	0.74171200	2.31977400
H	6.45495300	-2.97902400	-2.13299400

H	8.65665300	-1.09964100	1.51391100
H	9.30332800	-0.44042300	3.57903000
H	8.52912900	-1.46693400	-1.88323600
C	6.87201000	-3.61743100	-1.34930300
H	6.04427000	-4.13252000	-0.85508600
C	7.74261700	-2.82842900	-0.35550300
C	8.90351900	-2.17992500	-1.14306700
H	9.59542200	-1.64418500	-0.48928700
H	7.47725800	-4.38075600	-1.84494300
C	8.32088400	-3.83148300	0.66909300
H	7.52331200	-4.31318300	1.24114500
H	8.99481700	-3.34953500	1.38087800
H	9.47807300	-2.94383900	-1.67549000
H	8.88725200	-4.61565600	0.15770700

Byproduct 4.4

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.153977 Hartree

H_corr: 0.199039 Hartree

SCF: -425.612814 Hartree

S: 94.842 Cal/Mol-Kelvin

H: -425.413775 Hartree

G: -425.458837 Hartree

Cartesian Coordinates:

C	2.00361200	0.64681700	-1.26846400
C	1.45392900	-0.02790200	-0.00000700
H	3.09914300	0.61405000	-1.27223000
H	1.70500000	1.69511000	-1.34064500
H	1.64135000	0.12352600	-2.15516800
C	2.00361400	0.64716700	1.26827600
H	1.64133100	0.12407700	2.15509800
H	1.70495800	1.69546000	1.34021500

H	3.09914000	0.61441700	1.27209500
C	-0.07435100	-0.01845900	0.00002300
C	-0.80545300	-1.20901200	0.00002500
C	-0.77455500	1.19425400	-0.00000900
C	-2.19970200	-1.18605300	0.00001400
C	-2.16619800	1.21763800	-0.00002500
C	-2.88633000	0.02451400	-0.00000900
H	-0.27416100	-2.15125000	0.00004600
H	-2.74940700	-2.12239100	0.00001100
H	-3.97164700	0.04039400	-0.00000700
H	-2.68800400	2.16967900	-0.00006100
H	-0.23467400	2.13634300	-0.00001700
O	1.85956100	-1.40564900	0.00019600
H	2.82308600	-1.42799900	0.00013900

Product 4.3a:

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.135433 Hartree

H_corr: 0.177403 Hartree

SCF: -424.398932 Hartree

S: 88.333 Cal/Mol-Kelvin

H: -424.221529 Hartree

G: -424.263499 Hartree

Cartesian Coordinates:

O	2.23349100	-1.47779900	-0.41318700
C	1.57500100	-0.46735100	0.34688500
C	0.06661600	-0.40598400	0.17761900
C	-0.35615300	0.91828900	0.04339500
C	-0.84974100	-1.45127200	0.15270900
C	-1.70843200	1.21026100	-0.11087800
C	-2.20490400	-1.16054300	-0.00494500
C	-2.63070100	0.16313100	-0.13388500

H	-2.04551300	2.23697100	-0.22340900
H	-3.68720200	0.37779100	-0.26129400
H	-2.93194600	-1.96603700	-0.03469900
H	-0.52084000	-2.48374700	0.23737500
C	2.03210100	0.91782500	-0.14152100
C	0.82948200	1.85897700	0.09780000
H	0.89583000	2.33581200	1.08391700
H	0.77012300	2.66645500	-0.63719300
H	2.22833600	0.82274500	-1.21353000
H	2.95418000	1.25141800	0.33819600
H	1.81856300	-0.59749500	1.41352600
H	2.13092200	-2.32152200	0.03952500

4.5 REFERENCES

1. (a) Weber, J. M.; Leung, J. O.; Swanson, S. J.; Idler, K. B.; McAlpine, J. B. An Erythromycin Derivative Produced by Targeted Gene Disruption in Saccharopolyspora Erythraea. *Science* **1991,** *252*, 114-117. (b) Zambias, R. A.; Hammond, M. L.; Heck, J. V.; Bartizal, K.; Trainor, C.; Abruzzo, G.; Schmatz, D. M.; Nollstadt, K. M. Preparation and Structure-Activity Relationships of Simplified Analogs of the Antifungal Agent Cilofungin: A Total Synthesis Approach. *J. Med. Chem.* **1992,** *35*, 2843-2855. (c) Davies, N. M. Clinical Pharmacokinetics of Ibuprofen. *Clinical Pharmacokinetics* **1998,** *34*, 101-154. (d) Xu, L.; Liu, H.; Hong, A.; Vivian, R.; Murray, B. P.; Callebaut, C.; Choi, Y.-C.; Lee, M. S.; Chau, J.; Tsai, L. K.; Stray, K. M.; Strickley, R. G.; Wang, J.; Tong, L.; Swaminathan, S.; Rhodes, G. R.; Desai, M. C. Structure–Activity Relationships of Diamine Inhibitors of Cytochrome P450 (CYP) 3A as Novel Pharmacoenhancers. Part II: P2/P3 Region and Discovery of Cobicistat (GS-9350). *Bioorg. Med. Chem. Lett.* **2014,** *24*, 995-999.

2. (a) McDonald, I. K.; Thornton, J. M. Satisfying Hydrogen Bonding Potential in Proteins. *J. Mol. Biol.* **1994,** *238*, 777-793. (b) Petukhov, M.; Rychkov, G.; Firsov, L.; Serrano, L. H-bonding in Protein Hydration Revisited. *Protein Sci.* **2004,** *13*, 2120-2129. (c) White, M. C.; Zhao, J. Aliphatic C–H Oxidations for Late-Stage Functionalization. *J. Am. Chem. Soc.* **2018,** *140*, 13988-14009.

3. Serrano-Plana, J.; Rumo, C.; Rebelein, J. G.; Peterson, R. L.; Barnet, M.; Ward, T. R. Enantioselective Hydroxylation of Benzylic C(sp3)–H Bonds by an Artificial Iron Hydroxylase Based on the Biotin–Streptavidin Technology. *J. Am. Chem. Soc.* **2020,** *142*, 10617-10623.

4. (a) Bigi, M. A.; Reed, S. A.; White, M. C. Directed Metal (Oxo) Aliphatic C–H Hydroxylations: Overriding Substrate Bias. *J. Am. Chem. Soc.* **2012,** *134*, 9721-9726. (b) Guo, M.; Corona, T.; Ray, K.; Nam, W. Heme and Nonheme High-Valent Iron and Manganese Oxo Cores in Biological and Abiological Oxidation Reactions. *ACS Cent. Sci.* **2019,** *5*, 13-28. (c) Goetz, M. K.; Schneider, J. E.; Filatov, A. S.; Jesse, K. A.; Anderson, J. S. Enzyme-Like Hydroxylation of Aliphatic C–H Bonds From an Isolable Co-Oxo Complex. *J. Am. Chem. Soc.* **2021,** *143*, 20849-20862.

5. (a) Denisov, I. G.; Makris, T. M.; Sligar, S. G.; Schlichting, I. Structure and Chemistry of Cytochrome P450. *Chem. Rev.* **2005,** *105*, 2253-2278. (b) Ortiz de Montellano, P. R. Hydrocarbon Hydroxylation by Cytochrome P450 Enzymes. *Chem. Rev.* **2010,** *110*, 932-948. (c) Monti, D.; Ottolina, G.; Carrea, G.; Riva, S. Redox Reactions Catalyzed by Isolated Enzymes. *Chem. Rev.* **2011,** *111*, 4111-4140. (d) Oloo, W. N.; Que, L. Bioinspired Nonheme Iron Catalysts for C–H and C═C Bond Oxidation: Insights into the Nature of the Metal-Based Oxidants. *Acc. Chem. Res.* **2015,** *48*, 2612-2621. (e) Rudolf, J. D.; Chang, C.-Y.; Ma, M.; Shen, B. Cytochromes P450 for Natural Product Biosynthesis in Streptomyces: Sequence, Structure, and Function. *Nat. Prod. Rep.* **2017,** *34*, 1141-1172.

6. (a) Epoxides and Aziridines in Click Chemistry. In *Aziridines and Epoxides in Organic Synthesis*, pp 443-477. (b) Que Jr, L.; Tolman, W. B. Biologically Inspired Oxidation Catalysis. *Nature* **2008,** *455*, 333. (c) Newhouse, T.; Baran, P. S. If C–H Bonds Could Talk: Selective C–H Bond Oxidation. *Angew. Chem., Int. Ed.* **2011,** *50*, 3362-3374. (d) Qiu, Y.; Gao, S. Trends in Applying C–H Oxidation to the Total Synthesis of Natural Products. *Nat. Prod. Rep.* **2016,** *33*, 562-581.

7. (a) Jones, R. D.; Summerville, D. A.; Basolo, F. Synthetic Oxygen Carriers Related to Biological Systems. *Chem. Rev.* **1979,** *79*, 139-179. (b) Punniyamurthy, T.; Velusamy, S.; Iqbal, J. Recent Advances in Transition Metal Catalyzed Oxidation of Organic Substrates with Molecular Oxygen. *Chem. Rev.* **2005,** *105*, 2329-2364. (c) Wang, C.-C.; Chang, H.-C.; Lai, Y.-C.; Fang, H.; Li, C.-C.; Hsu, H.-K.; Li, Z.-Y.; Lin, T.-S.; Kuo, T.-S.; Neese, F.; Ye, S.; Chiang, Y.-W.; Tsai, M.-L.; Liaw,

W.-F.; Lee, W.-Z. A Structurally Characterized Nonheme Cobalt–Hydroperoxo Complex Derived from Its Superoxo Intermediate via Hydrogen Atom Abstraction. *J. Am. Chem. Soc.* **2016,** *138*, 14186-14189.

8. (a) Smeltz, J. L.; Lilly, C. P.; Boyle, P. D.; Ison, E. A. The Electronic Nature of Terminal Oxo Ligands in Transition-Metal Complexes: Ambiphilic Reactivity of Oxorhenium Species. *J. Am. Chem. Soc.* **2013,** *135*, 9433-9441. (b) Halbach, R. L.; Gygi, D.; Bloch, E. D.; Anderson, B. L.; Nocera, D. G. Structurally Characterized Terminal Manganese(iv) Oxo Tris(alkoxide) Complex. *Chem. Sci.* **2018,** *9*, 4524-4528. (c) Shimoyama, Y.; Kojima, T. Metal–Oxyl Species and Their Possible Roles in Chemical Oxidations. *Inorg. Chem.* **2019,** *58*, 9517-9542. (d) Schneider, J. E.; Goetz, M. K.; Anderson, J. S. Statistical Analysis of C–H Activation by Oxo Complexes Supports Diverse Thermodynamic Control over Reactivity. *Chem. Sci.* **2021,** *12*, 4173-4183.

9. (a) Dantignana, V. Bioinspired Metal-based Oxidants: Selectivity in Catalytic Hydroxylation of Aliphatic C−H bonds and Insight into the Reactivity of Oxoiron Species. Ph.D. Dissertation, University of Girona, 2020. (b) Kal, S.; Xu, S.; Que Jr, L. Bio-inspired Nonheme Iron Oxidation Catalysis: Involvement of Oxoiron(V) Oxidants in Cleaving Strong C−H Bonds. *Angew. Chem., Int. Ed.* **2020,** *59*, 7332-7349.

10. (a) Wayland, B. B.; Poszmik, G.; Mukerjee, S. L.; Fryd, M. Living Radical Polymerization of Acrylates by Organocobalt Porphyrin Complexes. *J. Am. Chem. Soc.* **1994,** *116*, 7943-7944. (b) Zhang, X.-X.; Wayland, B. B. Rhodium(II) Porphyrin Bimetalloradical Complexes: Preparation and Enhanced Reactivity with CH4 and H2. *J. Am. Chem. Soc.* **1994,** *116*, 7897-7898. (c) Chan, K. S.; Li, X. Z.; Dzik, W. I.; de Bruin, B. Carbon−Carbon Bond Activation of 2,2,6,6-Tetramethyl-piperidine-1-oxyl by a RhII Metalloradical: A Combined Experimental and Theoretical Study. *J. Am. Chem. Soc.* **2008,** *130*, 2051-2061. (d) Doyle, M. P. Exceptional Selectivity in Cyclopropanation Reactions Catalyzed by Chiral Cobalt(II)–Porphyrin Catalysts. *Angew. Chem., Int. Ed.* **2009,** *48*, 850-852. (e) Fantauzzi, S.; Caselli, A.; Gallo, E. Nitrene Transfer Reactions Mediated by Metallo-Porphyrin Complexes. *Dalton Trans.* **2009,** *28*, 5434-5443. (f) Chan, Y. W.; Chan, K. S. Metalloradical-Catalyzed Aliphatic Carbon−Carbon Activation of Cyclooctane. *J. Am. Chem. Soc.* **2010,** *132*, 6920-6922. (g) Driver, T. G. Recent Advances in Transition Metal-Catalyzed N-Atom Transfer Reactions of Azides. *Organic & Biomolecular Chemistry* **2010,** *8*, 3831-3846. (h) Che, C.-M.; Lo, V. K.-Y.; Zhou, C.-Y.; Huang, J.-S. Selective Functionalisation of Saturated C–H Bonds with Metalloporphyrin Catalysts. *Chem. Soc. Rev.* **2011,** *40*, 1950-1975. (i) Lu, H.; Zhang, X. P. Catalytic C–H Functionalization by Metalloporphyrins: Recent Developments and Future Directions. *Chem. Soc. Rev.* **2011,** *40*, 1899–1909. (j) Li, G.; Han, A.; Pulling, M. E.; Estes, D. P.; Norton, J. R. Evidence for Formation of a Co–H Bond from (H2O)2Co(dmgBF2)2 under H2: Application to Radical Cyclizations. *J. Am. Chem. Soc.* **2012,** *134*, 14662-14665. (k) Pellissier, H.; Clavier, H. Enantioselective Cobalt-Catalyzed Transformations. *Chem. Rev.* **2014,** *114*, 2775–2823. (l) Kuo, J. L.; Hartung, J.; Han, A.; Norton, J. R. Direct Generation of Oxygen-Stabilized Radicals by H• Transfer from Transition Metal Hydrides. *J. Am. Chem. Soc.* **2015,** *137*, 1036-1039. (m) Reddy, A. R.; Hao, F.; Wu, K.; Zhou, C.-Y.; Che, C.-M. Cobalt(II) Porphyrin-Catalyzed Intramolecular Cyclopropanation of N-Alkyl Indoles/Pyrroles with Alkylcarbene: Efficient Synthesis of Polycyclic N-Heterocycles. *Angew. Chem., Int. Ed.* **2016,** *55*, 1810-1815. (n) Chirila, A.; Gopal Das, B.; Paul, N. D.; de Bruin, B. Diastereoselective Radical-Type Cyclopropanation of Electron-Deficient Alkenes Mediated by the Highly Active Cobalt(II) Tetramethyltetraaza[14]annulene Catalyst. *ChemCatChem* **2017,** *9*, 1413-1421. (o) Gu, Z.-Y.; Liu, Y.; Wang, F.; Bao, X.; Wang, S.-Y.; Ji, S.-J. Cobalt(II)-Catalyzed Synthesis of Sulfonyl Guanidines via Nitrene Radical Coupling with Isonitriles: A Combined Experimental and Computational Study. *ACS Catal.* **2017,** *7*, 3893-3899. (p) Kuijpers, P. F.; Tiekink, M. J.; Breukelaar, W. B.; Broere, D. L. J.; van Leest, N. P.; van der Vlugt, J. I.; Reek, J. N. H.; de Bruin, B. Cobalt-Porphyrin-Catalysed Intramolecular Ring-Closing C−H Amination of Aliphatic Azides: A Nitrene-Radical Approach to

Saturated Heterocycles. *Chemistry – A European Journal* **2017,** *23*, 7945-7952. (q) Roy, S.; Das, S. K.; Chattopadhyay, B. Cobalt(II)-based Metalloradical Activation of 2-(Diazomethyl)pyridines for Radical Transannulation and Cyclopropanation. *Angew. Chem., Int. Ed.* **2018,** *57*, 2238-2243. (r) Demarteau, J.; Debuigne, A.; Detrembleur, C. Organocobalt Complexes as Sources of Carbon-Centered Radicals for Organic and Polymer Chemistries. *Chem. Rev.* **2019,** *119*, 6906–6955. (s) Huang, H.-M.; Garduño-Castro, M. H.; Morrill, C.; Procter, D. J. Catalytic cascade reactions by radical relay. *Chem. Soc. Rev.* **2019,** *48*, 4626–4638. (t) Singh, R.; Mukherjee, A. Metalloporphyrin Catalyzed C–H Amination. *ACS Catal.* **2019,** *9*, 3604–3617.

11. (a) Harden, J. D.; Ruppel, J. V.; Gao, G.-Y.; Zhang, X. P. Cobalt-catalyzed Intermolecular C–H Amination with Bromamine-T as Nitrene Source. *Chem. Commun.* **2007**, 4644-4646. (b) Riart-Ferrer, X. Enantioselective Radical Strategy for the Stereoselective Synthesis of Three-Membered Heterocycles via Co(II)-Based Metalloradical Catalysis. Ph.D. Dissertation, Boston College, 2021.

12. (a) Lu, H.; Zhang, X. P. Catalytic C–H Functionalization by Metalloporphyrins: Recent Developments and Future Directions. *Chem. Soc. Rev.* **2011,** *40*, 1899-1909. (b) Jiang, H.; Zhang, X. P. In *Oxidation: C-N Bond Formation by Oxidation (Aziridines)*, Elsevier B.V.: 2012; pp 168-182. (c) Pellissier, H.; Clavier, H. Enantioselective Cobalt-Catalyzed Transformations. *Chem. Rev.* **2014,** *114*, 2775-2823. (d) Zhang, X. P.; Cui, X. In *Asymmetric C-H Functionalization by Transition Metal-Catalyzed Carbene Transfer Reactions*, Elsevier B.V.: 2014; pp 86-120. (e) Demarteau, J.; Debuigne, A.; Detrembleur, C. Organocobalt Complexes as Sources of Carbon-Centered Radicals for Organic and Polymer Chemistries. *Chem. Rev.* **2019,** *119*, 6906-6955. (f) Lee, W.-C. C.; Zhang, X. P. Asymmetric Radical Cyclopropanation of Alkenes. *Trends Chem.* **2022,** *4*, 850-851. (g) Wang, X.; Zhang, X. P., Catalytic Radical Approach for Selective Carbene Transfers via Cobalt(II)-Based Metalloradical Catalysis. In *Transition Metal-Catalyzed Carbene Transformations*, 2022; pp 25-66.

13. Goswami, M.; Lyaskovskyy, V.; Domingos, S. R.; Buma, W. J.; Woutersen, S.; Troeppner, O.; Ivanović-Burmazović, I.; Lu, H.; Cui, X.; Zhang, X. P.; Reijerse, E. J.; DeBeer, S.; van Schooneveld, M. M.; Pfaff, F. F.; Ray, K.; de Bruin, B. Characterization of Porphyrin-Co(III)-'Nitrene Radical' Species Relevant in Catalytic Nitrene Transfer Reactions. *J. Am. Chem. Soc.* **2015,** *137*, 5468-5479.

14. (a) Mu, X. H.; Kadish, K. M. Oxidative Electrochemistry of Cobalt Tetraphenylporphyrin under a CO Aatmosphere. Interaction between Carbon Monoxide and Electrogenerated [(TPP)Co]+ in Nonbonding Media. *Inorg. Chem.* **1989,** *28*, 3743-3747. (b) Campo Dall' Orto, V.; Carballo, R.; Hurst, J. A.; Rezzano, I. UV–vis Spectroscopic Study of Co(II)/Co(III) Oxidation in Poly[M-protoporphyrins] Films and their Interaction with Axial Ligands. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2005,** *61*, 2089-2093.

15. Zheng, C.; Wang, Y.; Xu, Y.; Chen, Z.; Chen, G.; Liang, S. H. Ru-Photoredox-Catalyzed Decarboxylative Oxygenation of Aliphatic Carboxylic Acids through N-(acyloxy)phthalimide. *Org. Lett.* **2018,** *20*, 4824-4827.

16. Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi,

J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16, Revision A.03*. Gaussian, Inc., Wallingford CT, 2016.

17. Tirado-Rives, J.; Jorgensen, W. L. Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. *J. Chem. Theory Comput.* **2008,** *4*, 297-306.

18. Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. Auxiliary Basis Sets for Main Row Atoms and Transition Metals and Their Use to Approximate Coulomb Potentials. *Theor. Chem. Acc.* **1997,** *97*, 119-124.

19. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *The Journal of Chemical Physics* **2010,** *132*, 154104.

20. Legault, C. Y. *CYLview, 1.0b*, Université de Sherbrooke: 2020.

21. Humphrey, W., Dalke, A. and Schulten, K. VMD - Visual Molecular Dynamics. *J. Mol. Graph.* **1996,** *14*, 33-38.

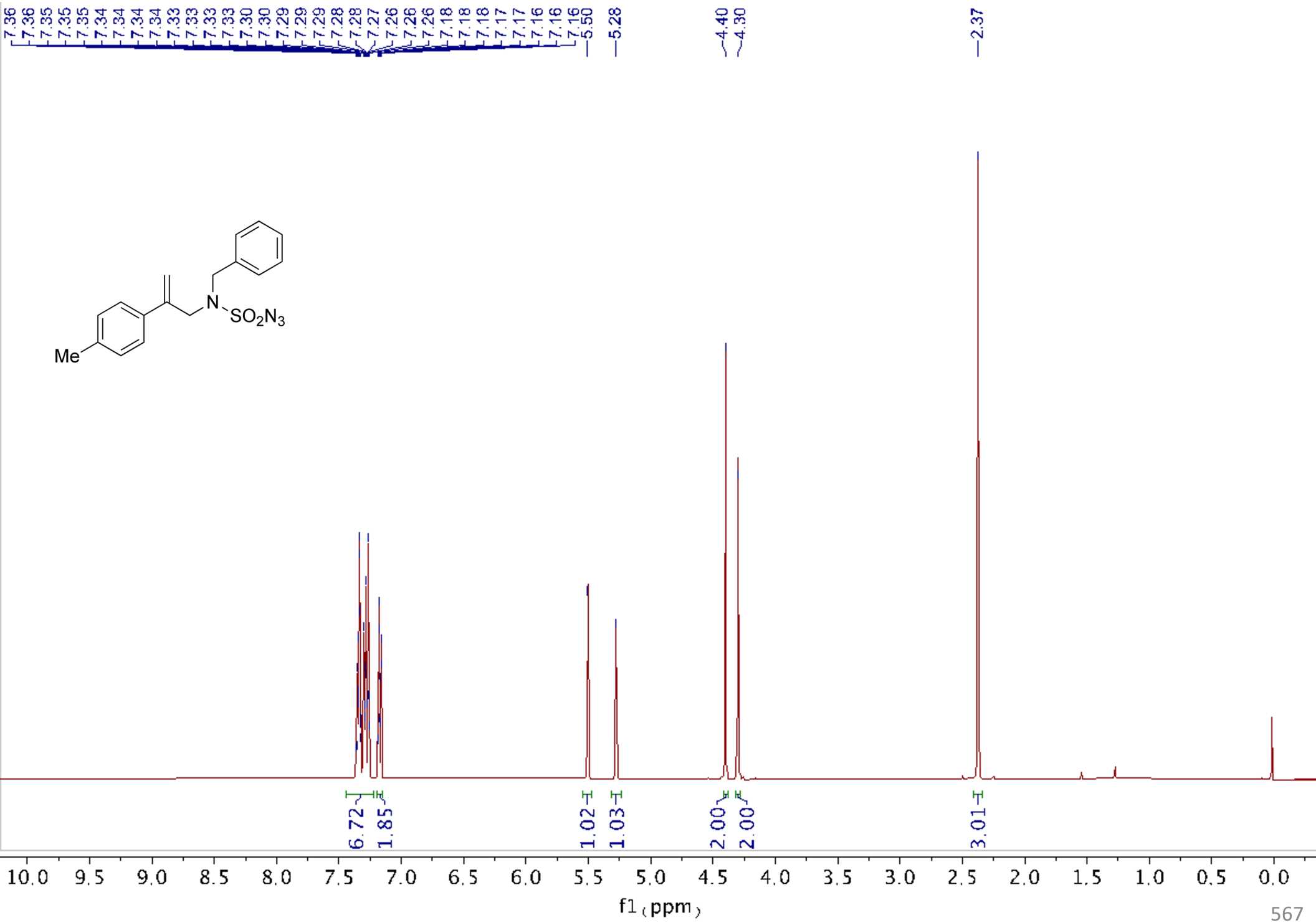
CHAPTER 5 – SPECTRA

- **Chapter 2: Enantioselective Radical *N*-Heterobicyclization with A New Mode of Asymmetric Induction.** Please see the page 566 to page 776 for spectra.
- **Chapter 3: Catalytic Radical *N*-Heterocyclization by Metalloradical C–H Amination involving 1,7-Hydrogen Atom Abstraction.** Please see the page 777 to page 797 for spectra.
- **Chapter 4: Metalloradical Activation of Alkyl Hydroperoxides for Catalytic Radical C−H Hydroxylation.** Please see the page 798 to page 800 for spectra.

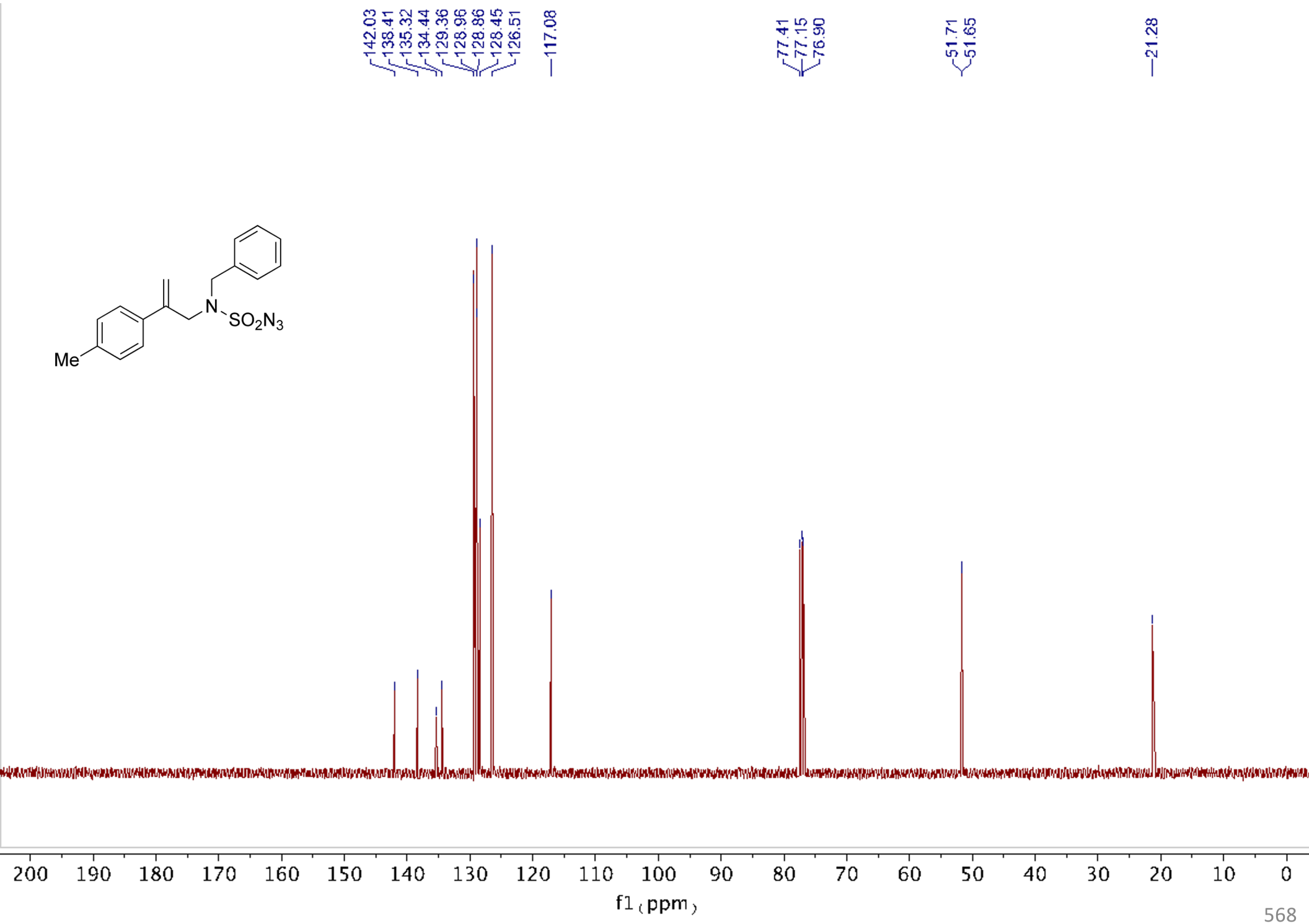
CHAPTER 2

Enantioselective Radical *N*-Heterobicyclization with A New Mode of Asymmetric Induction

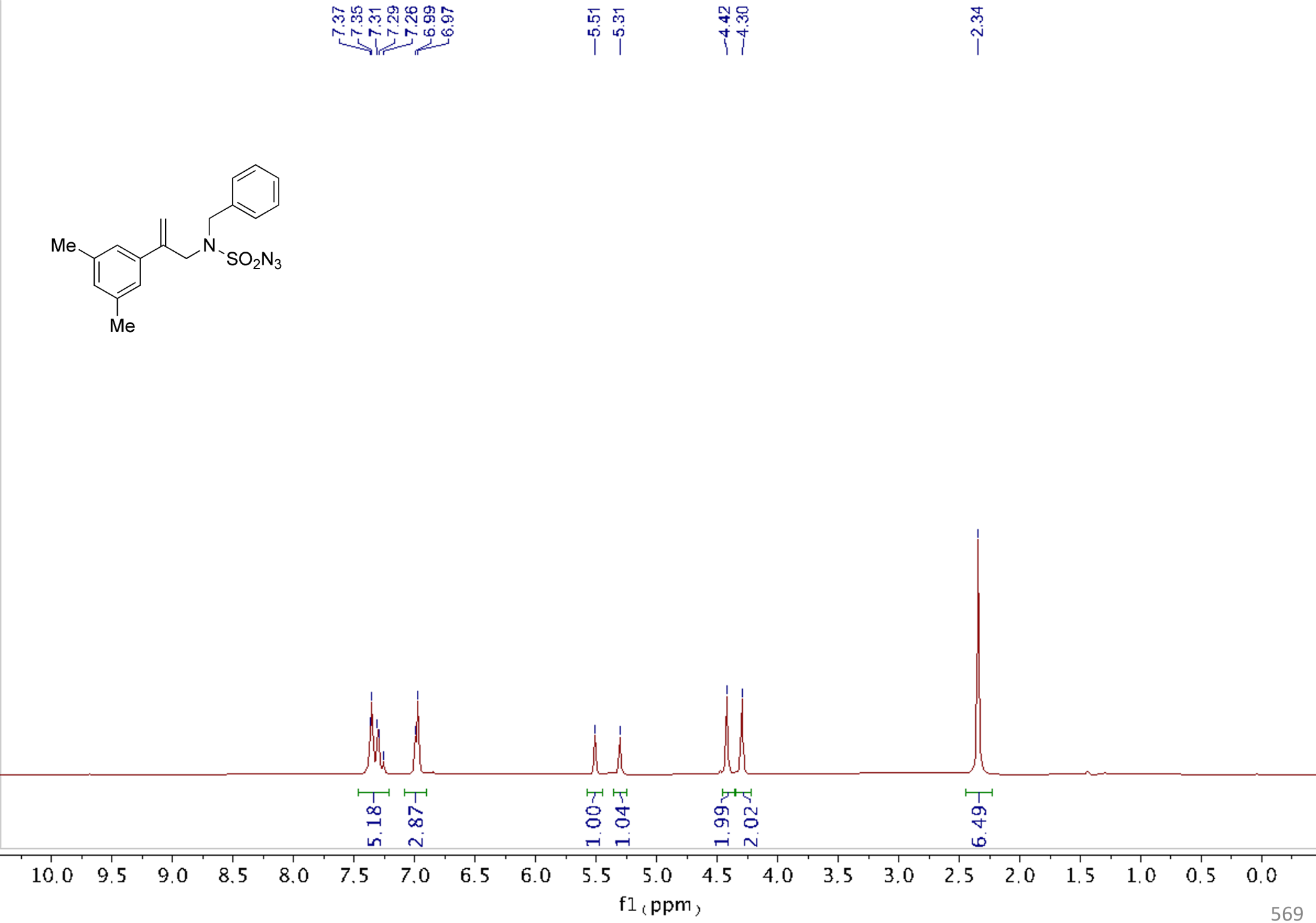
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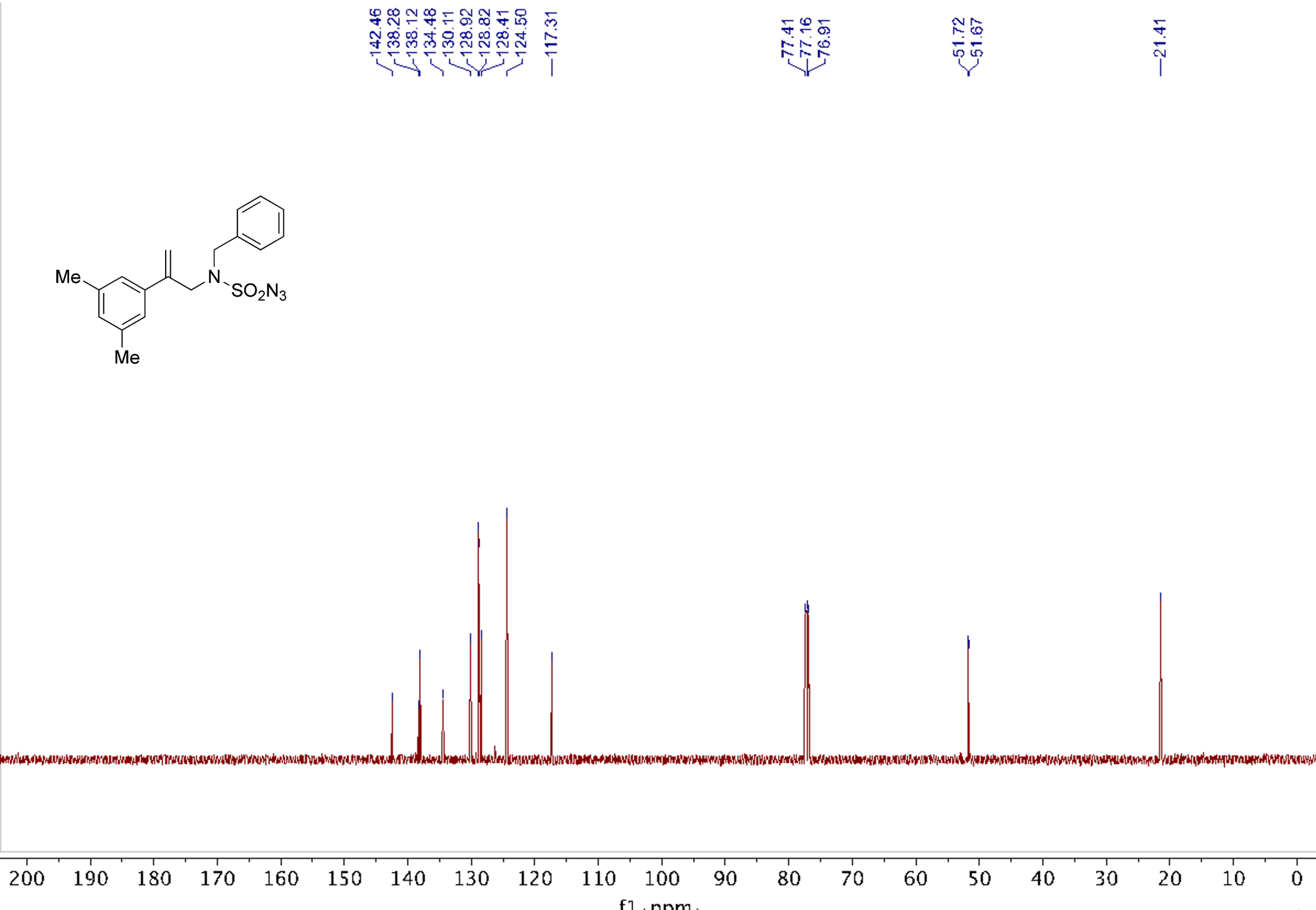
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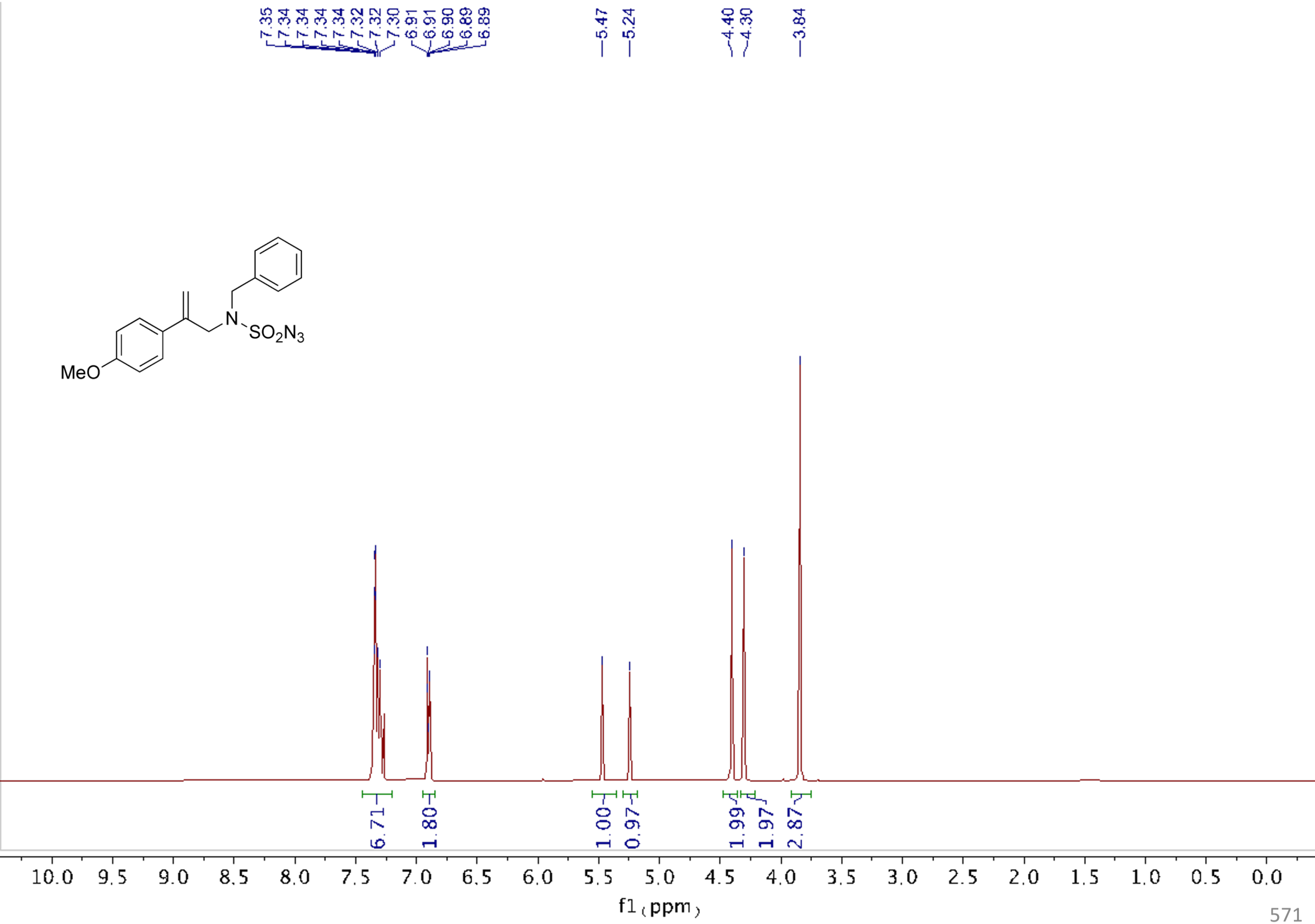
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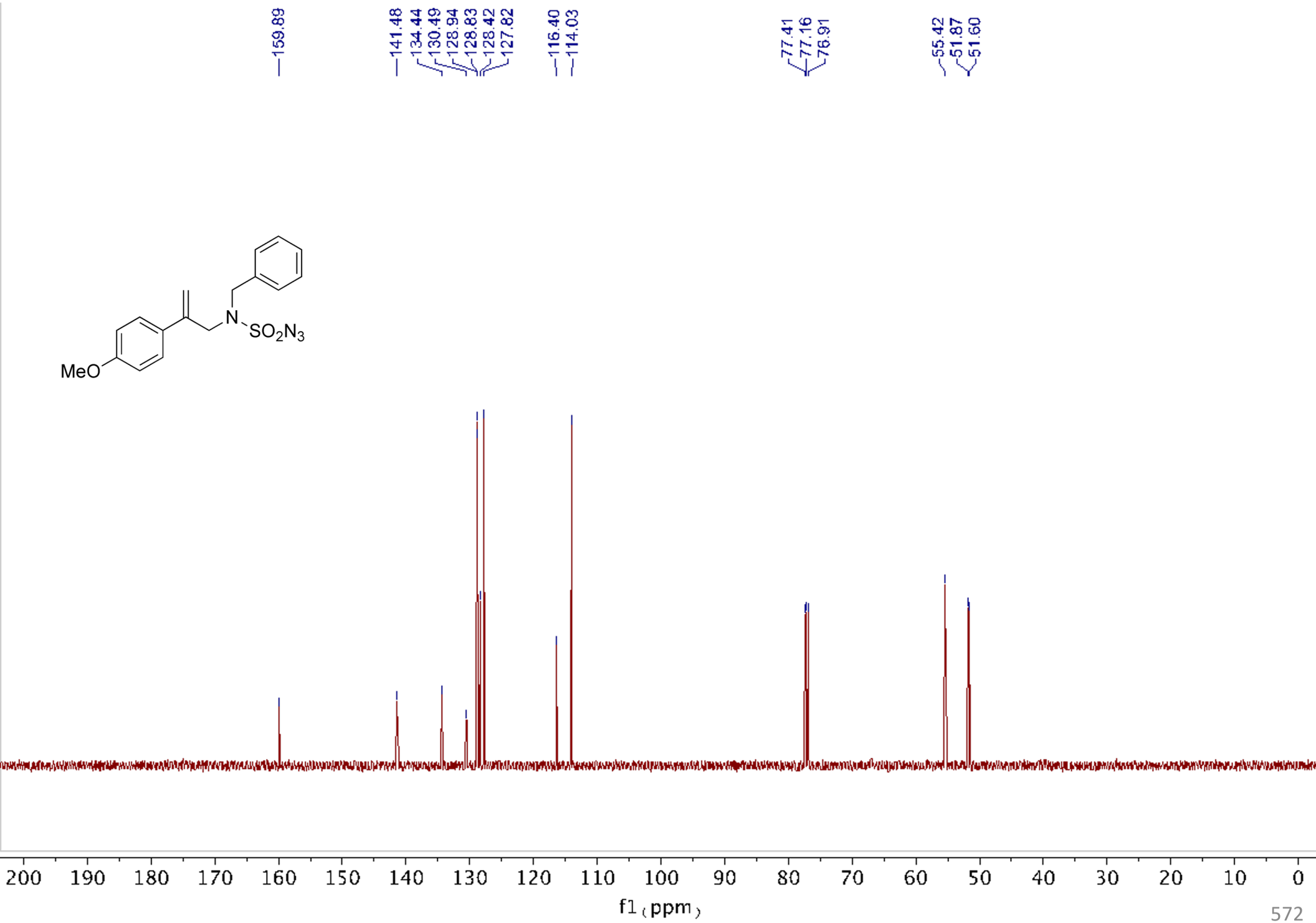
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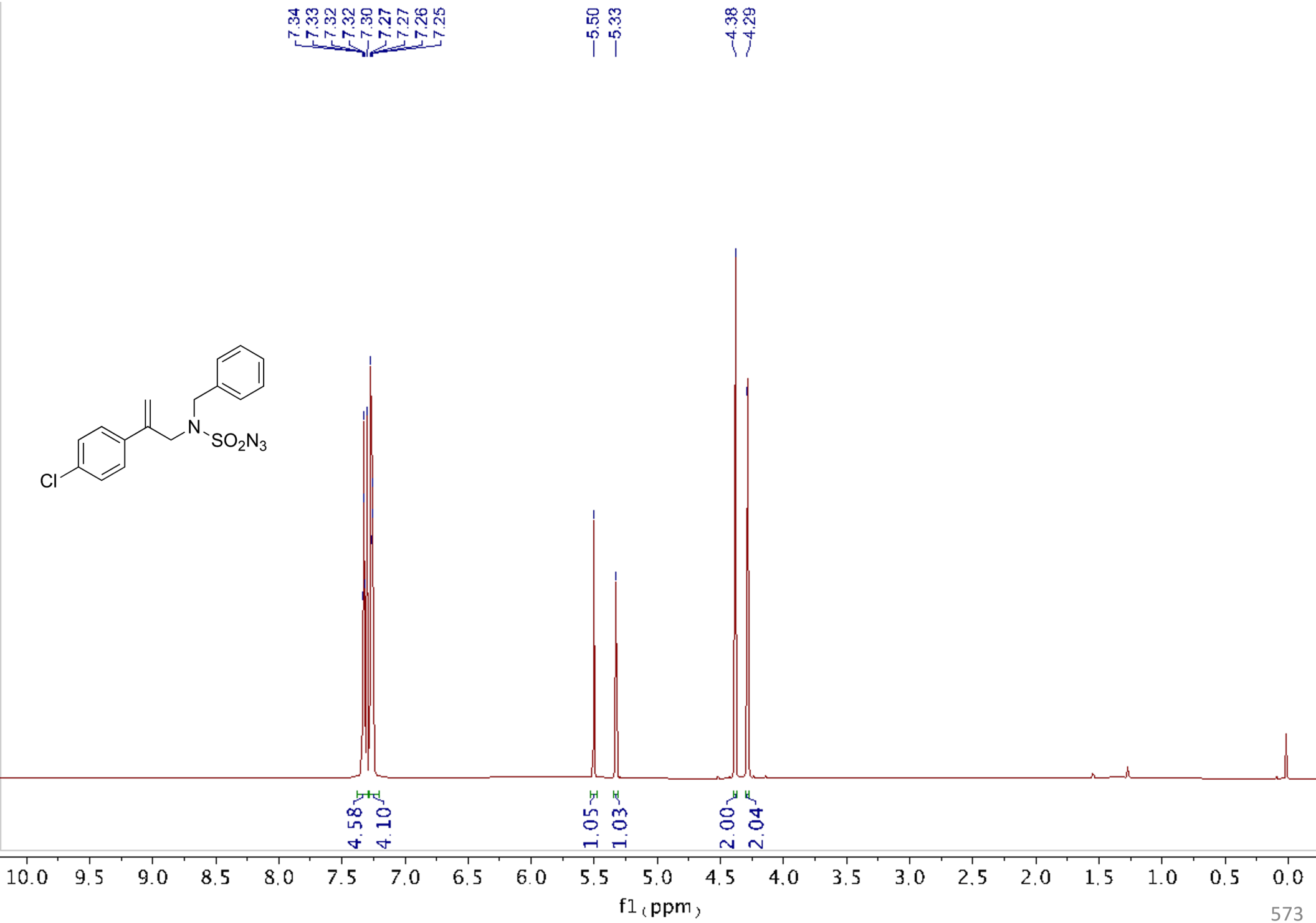
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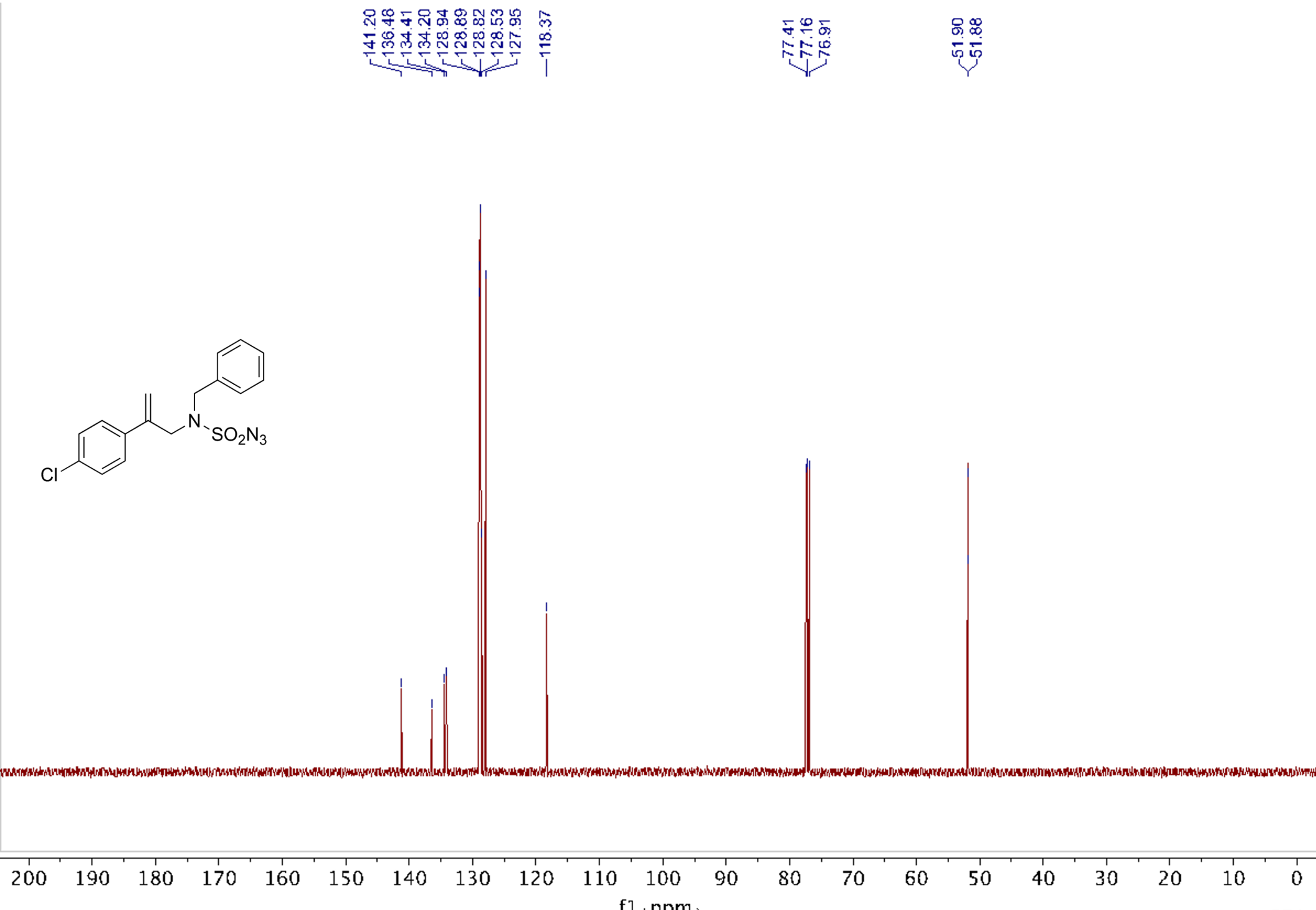
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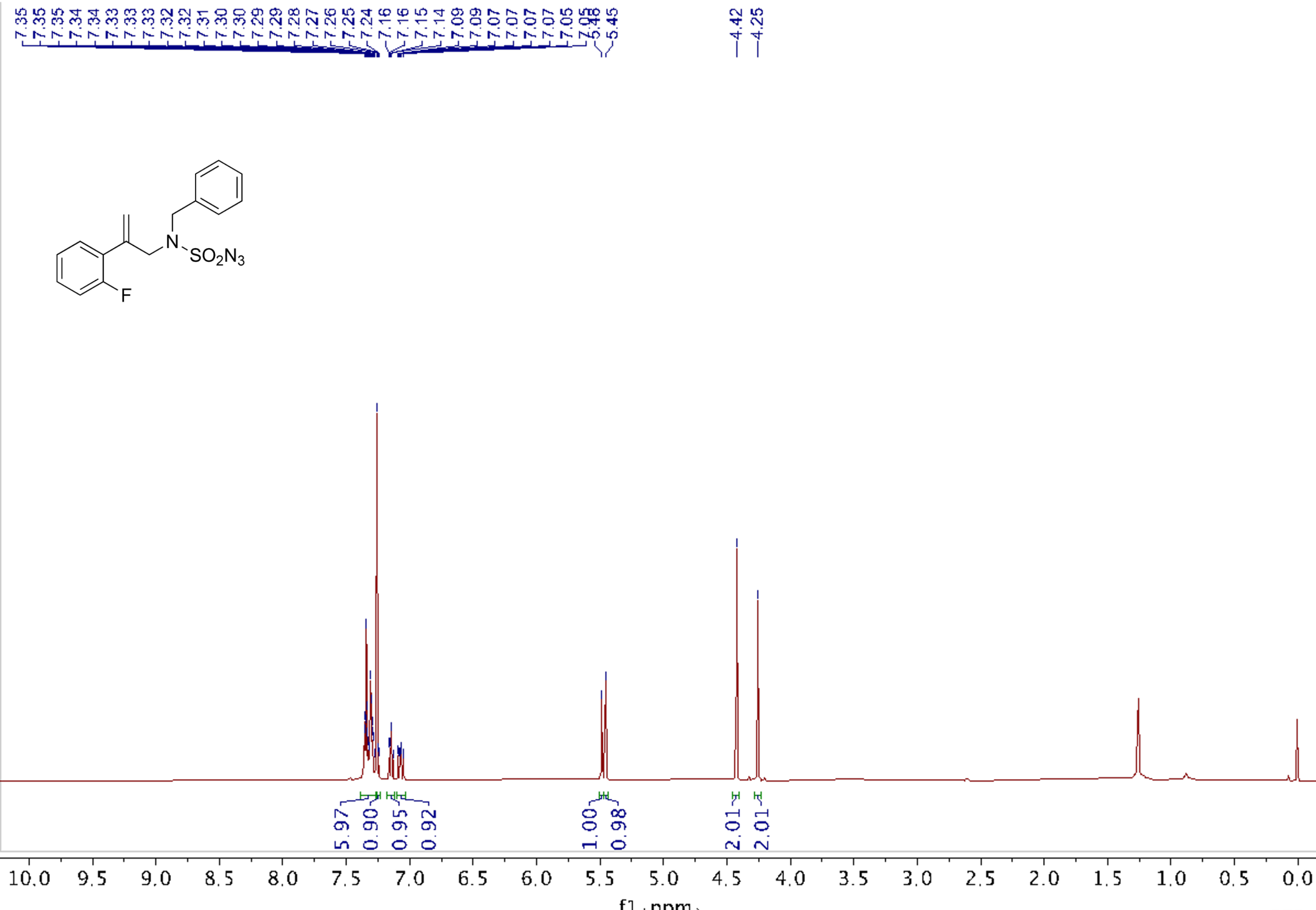
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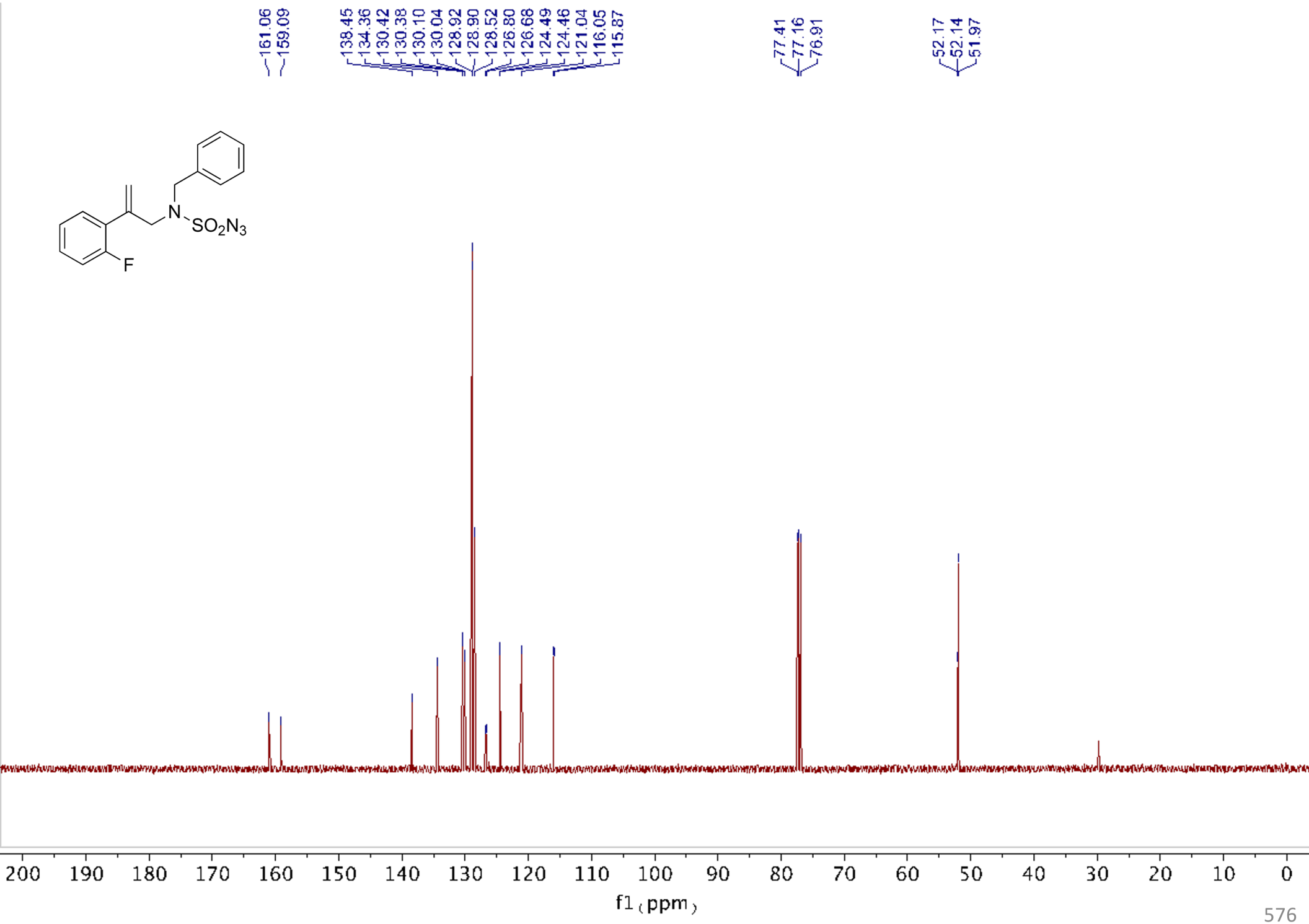
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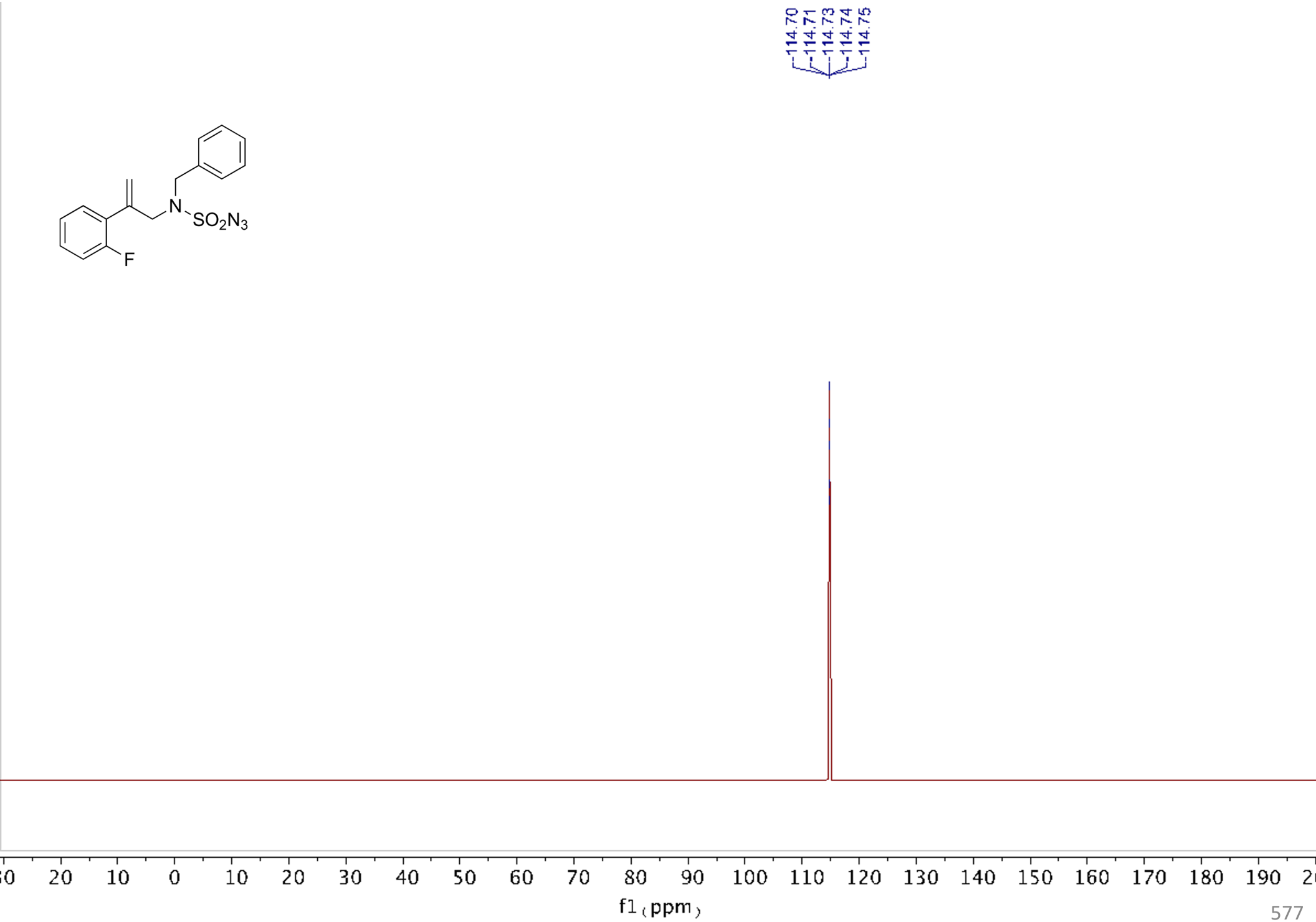
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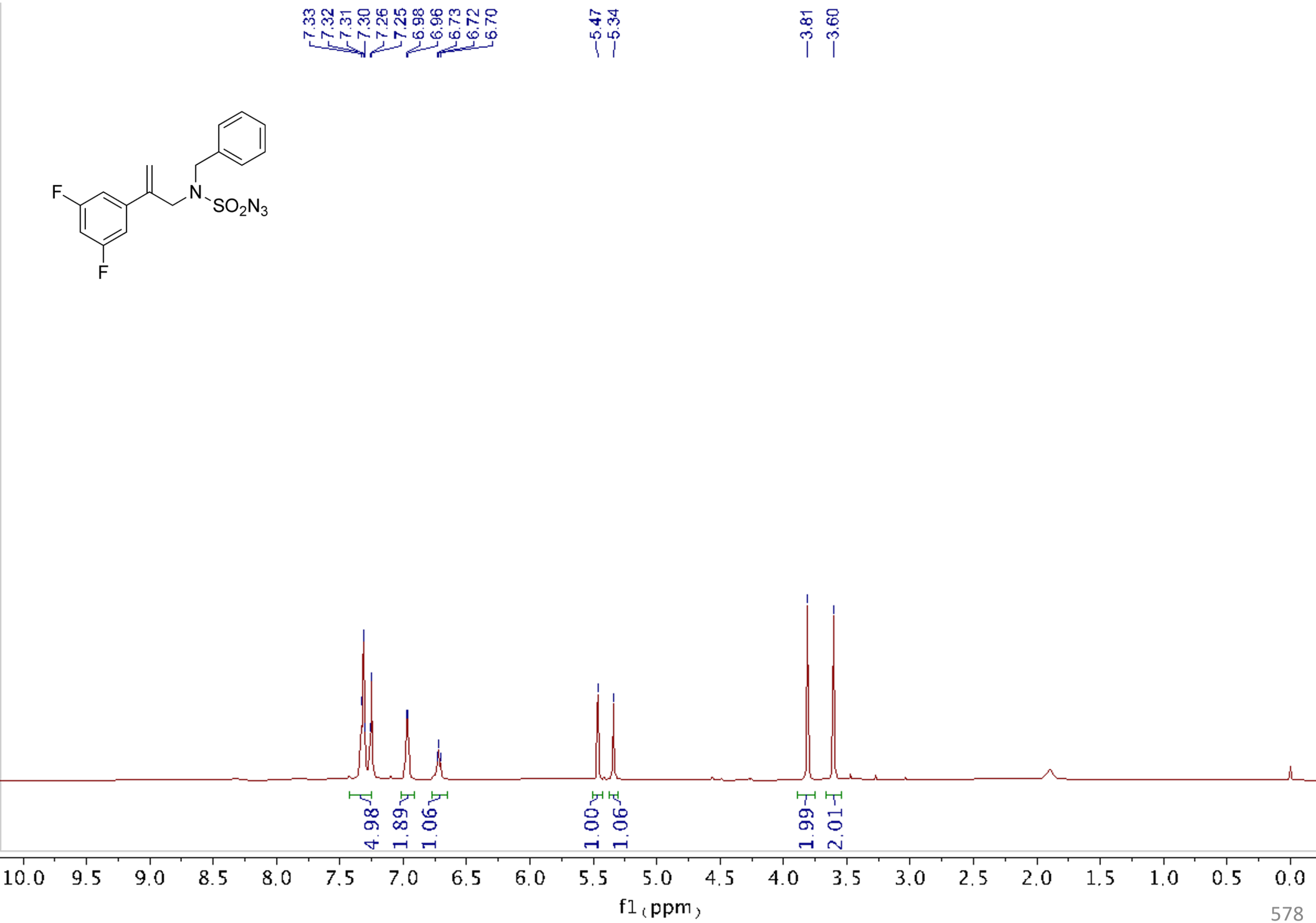
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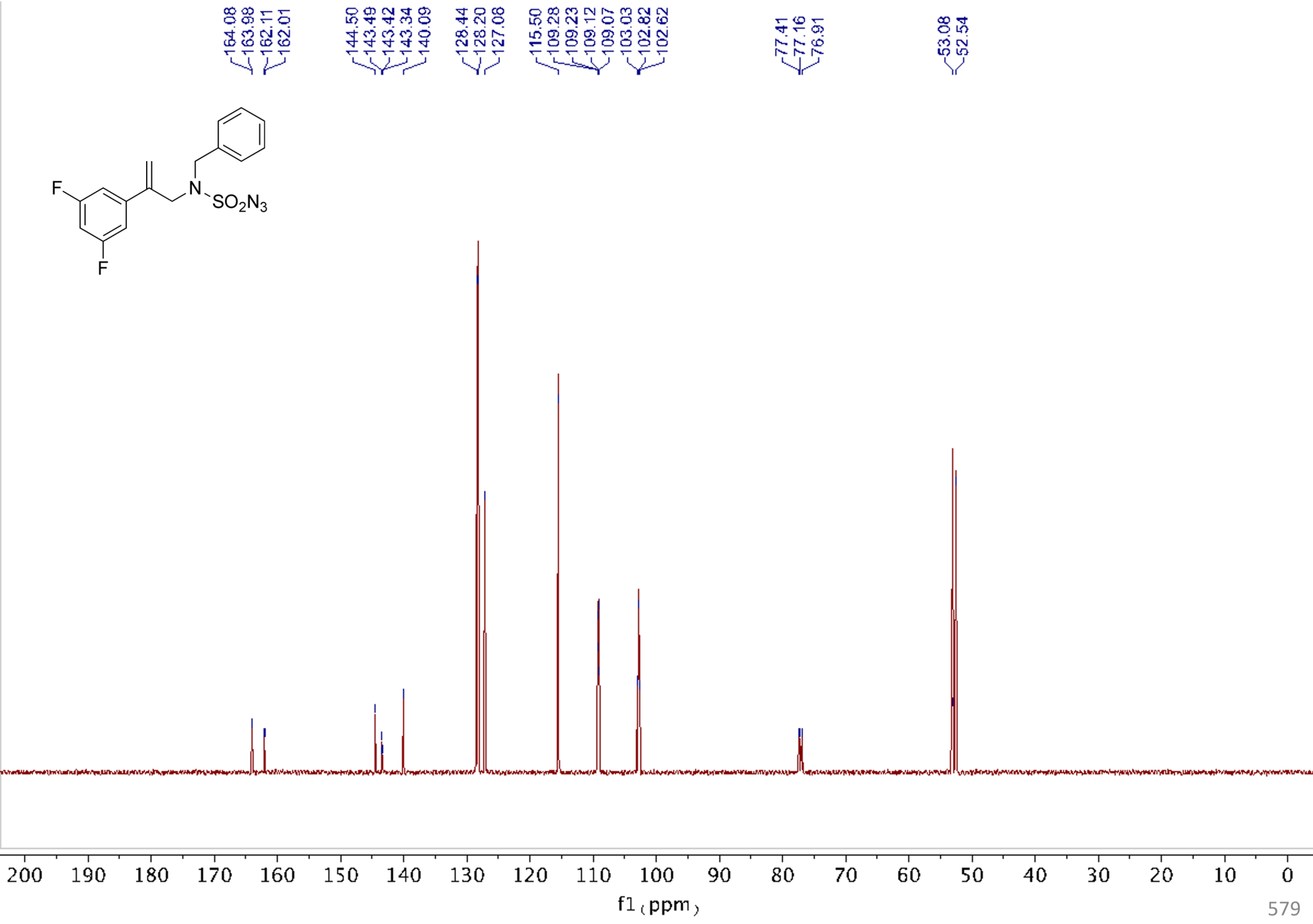
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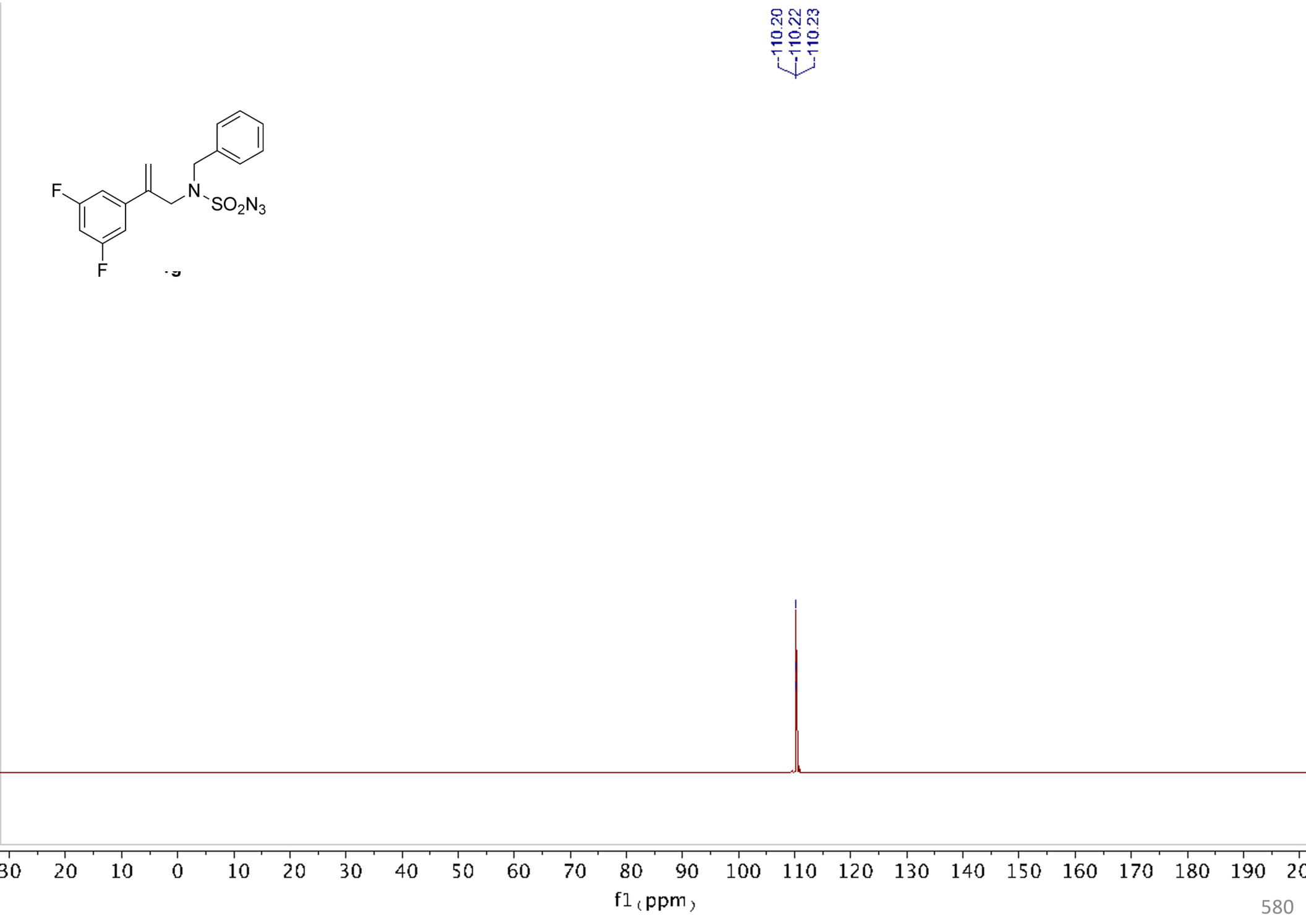
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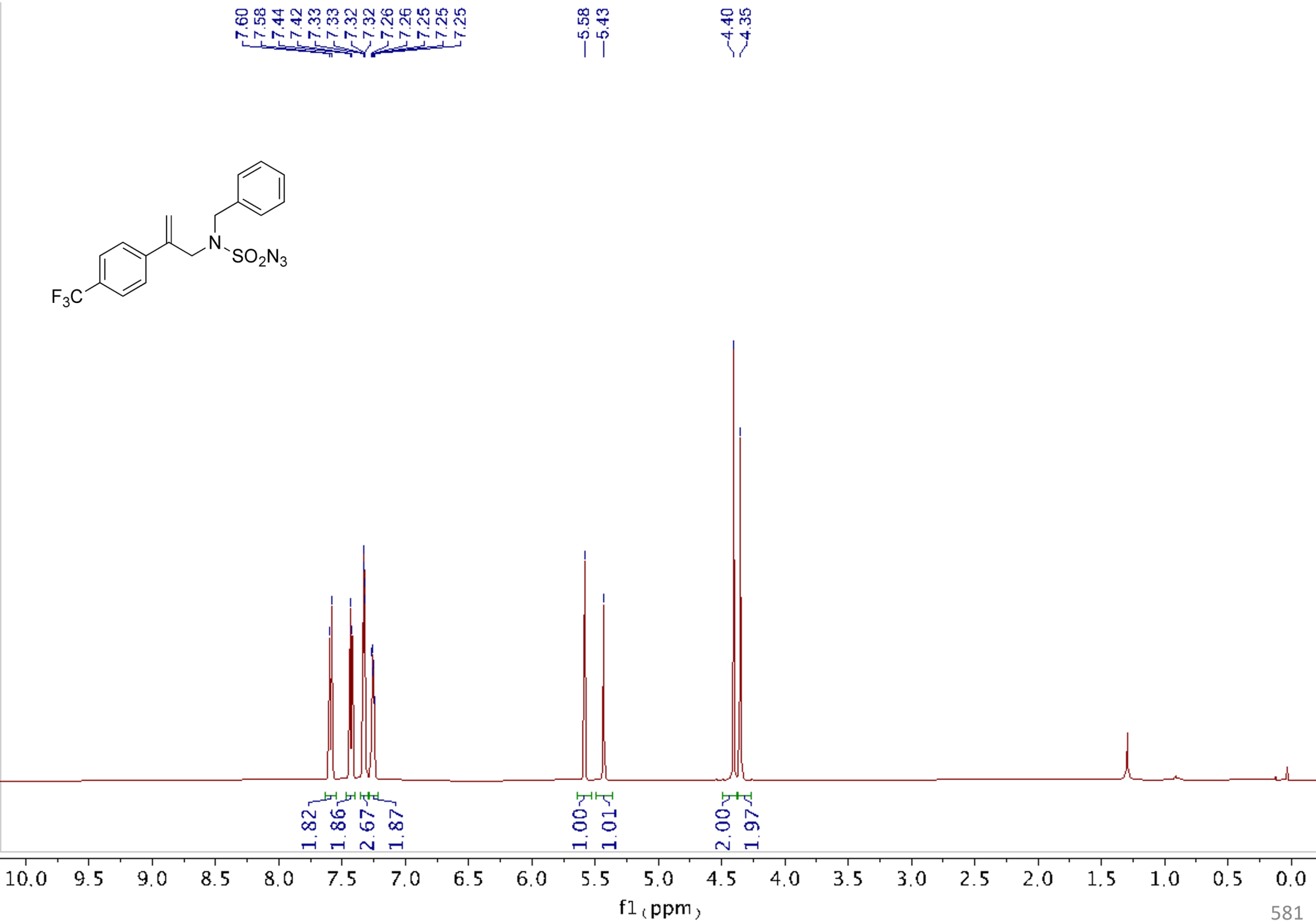
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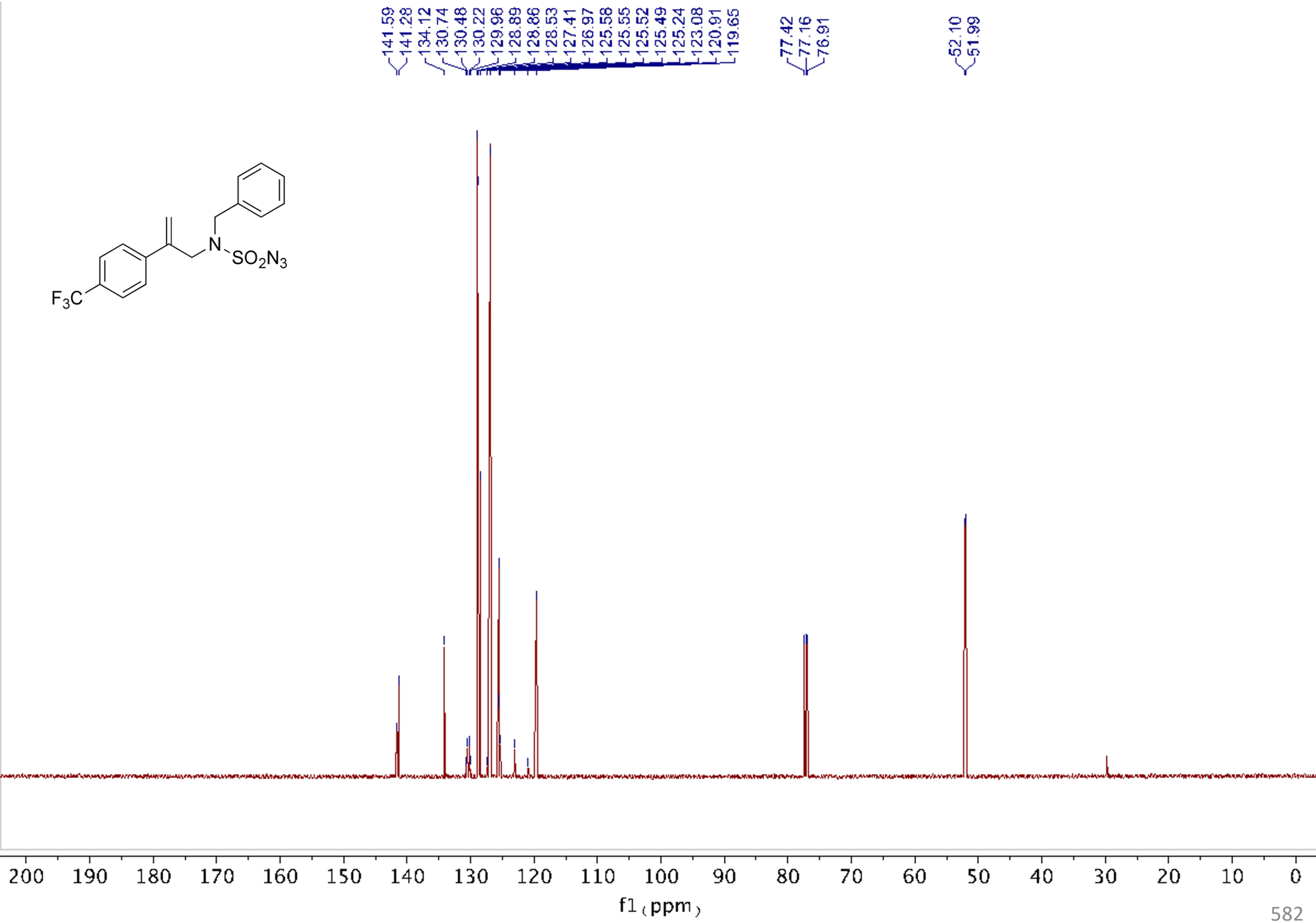
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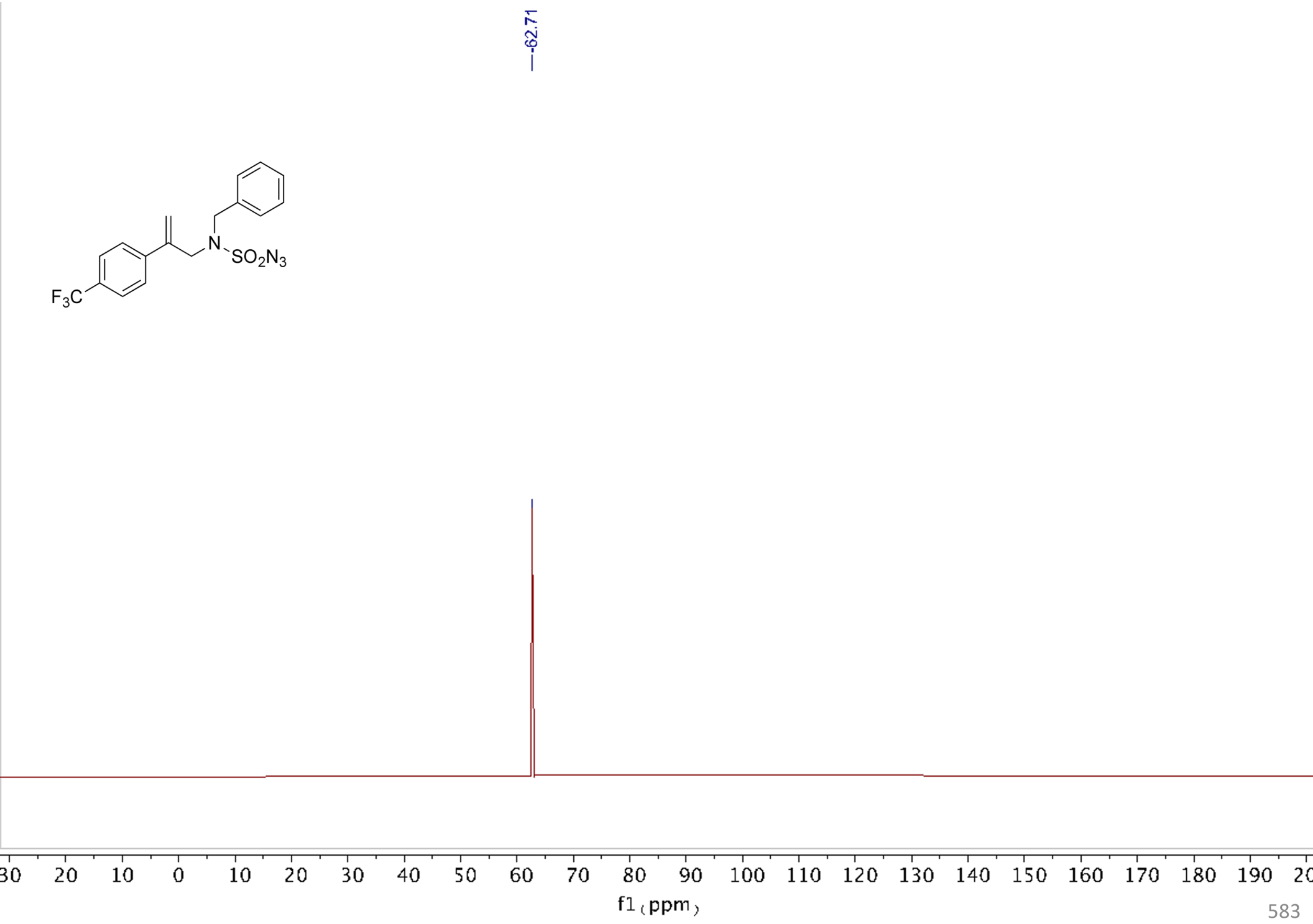
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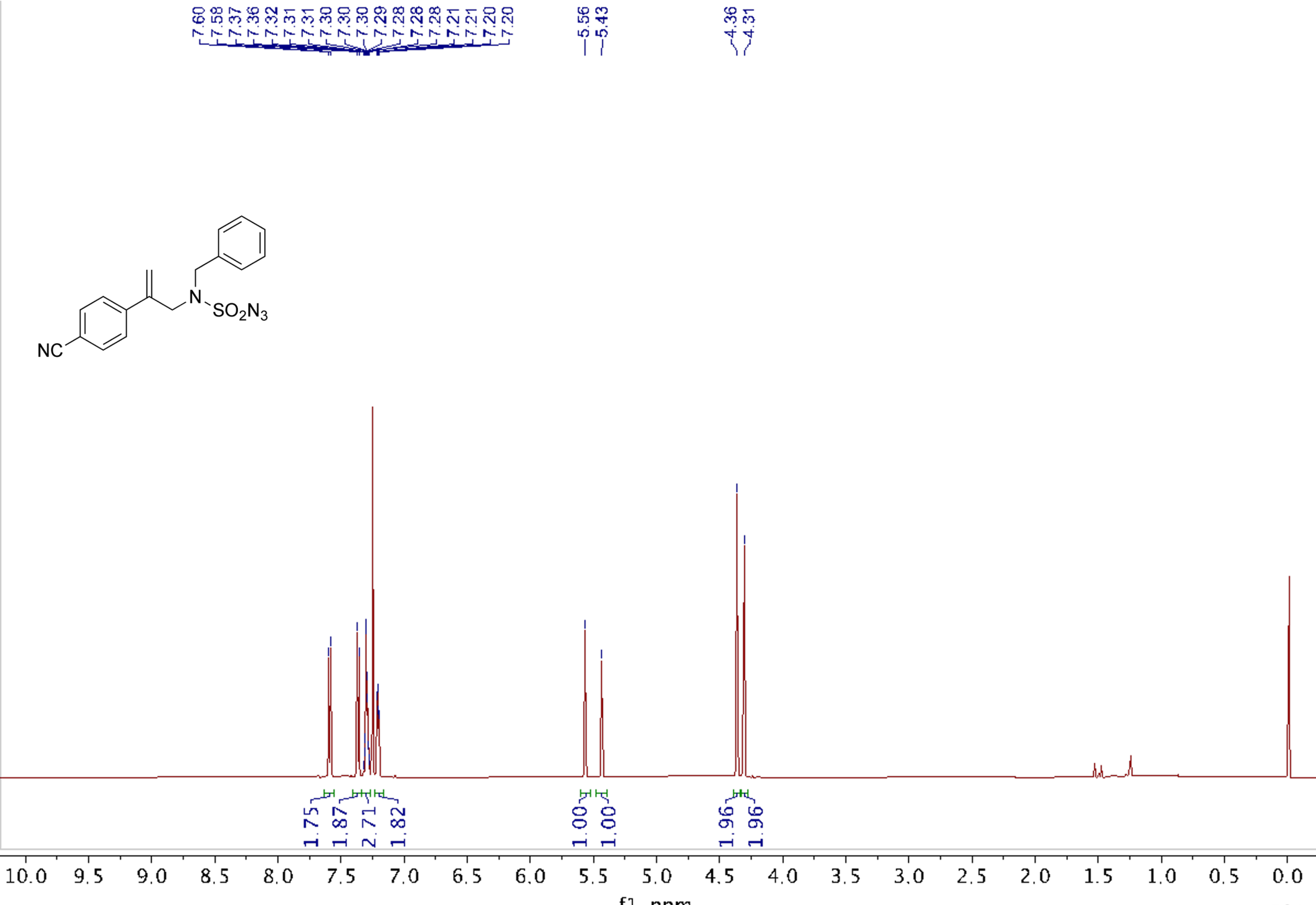
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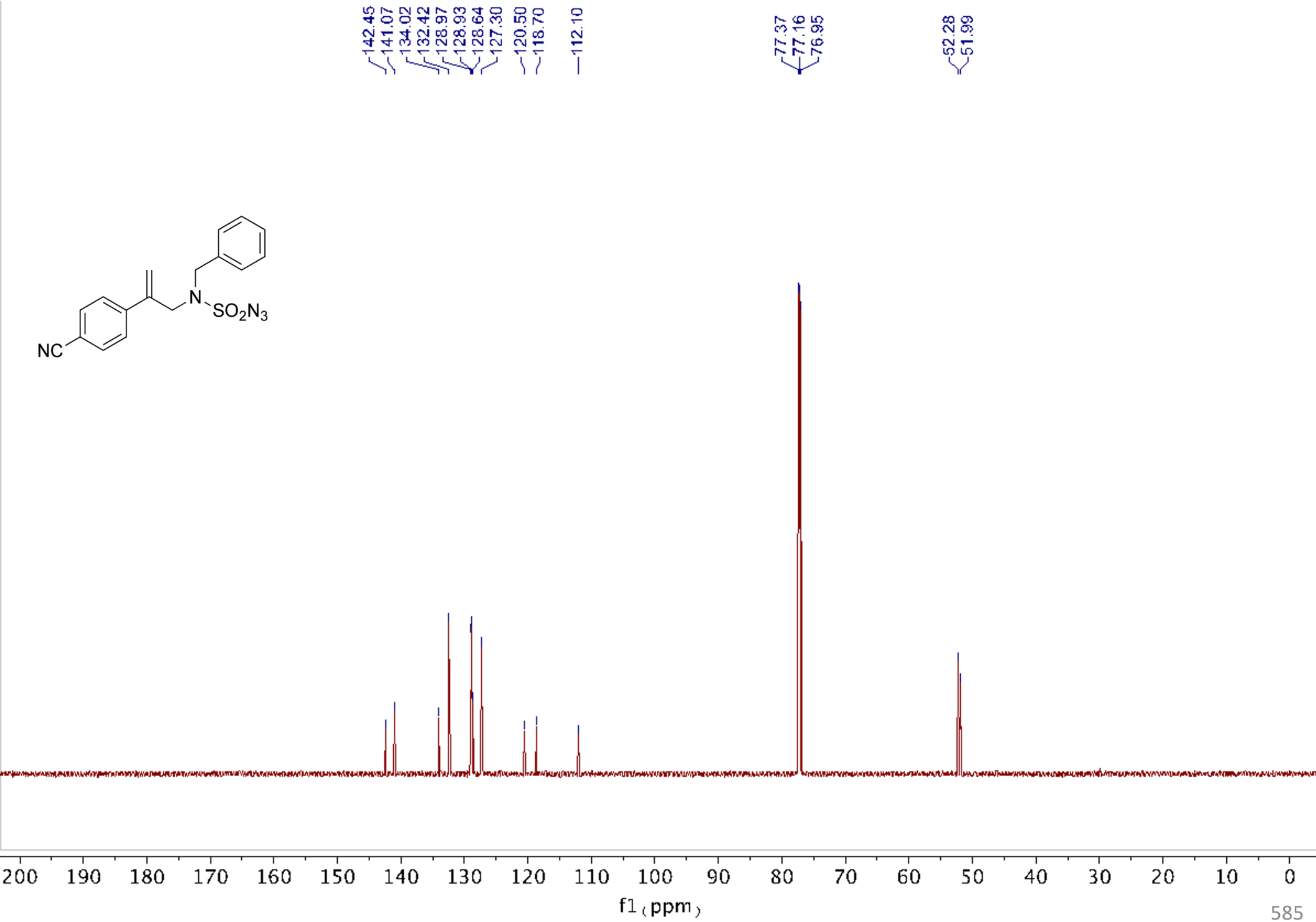
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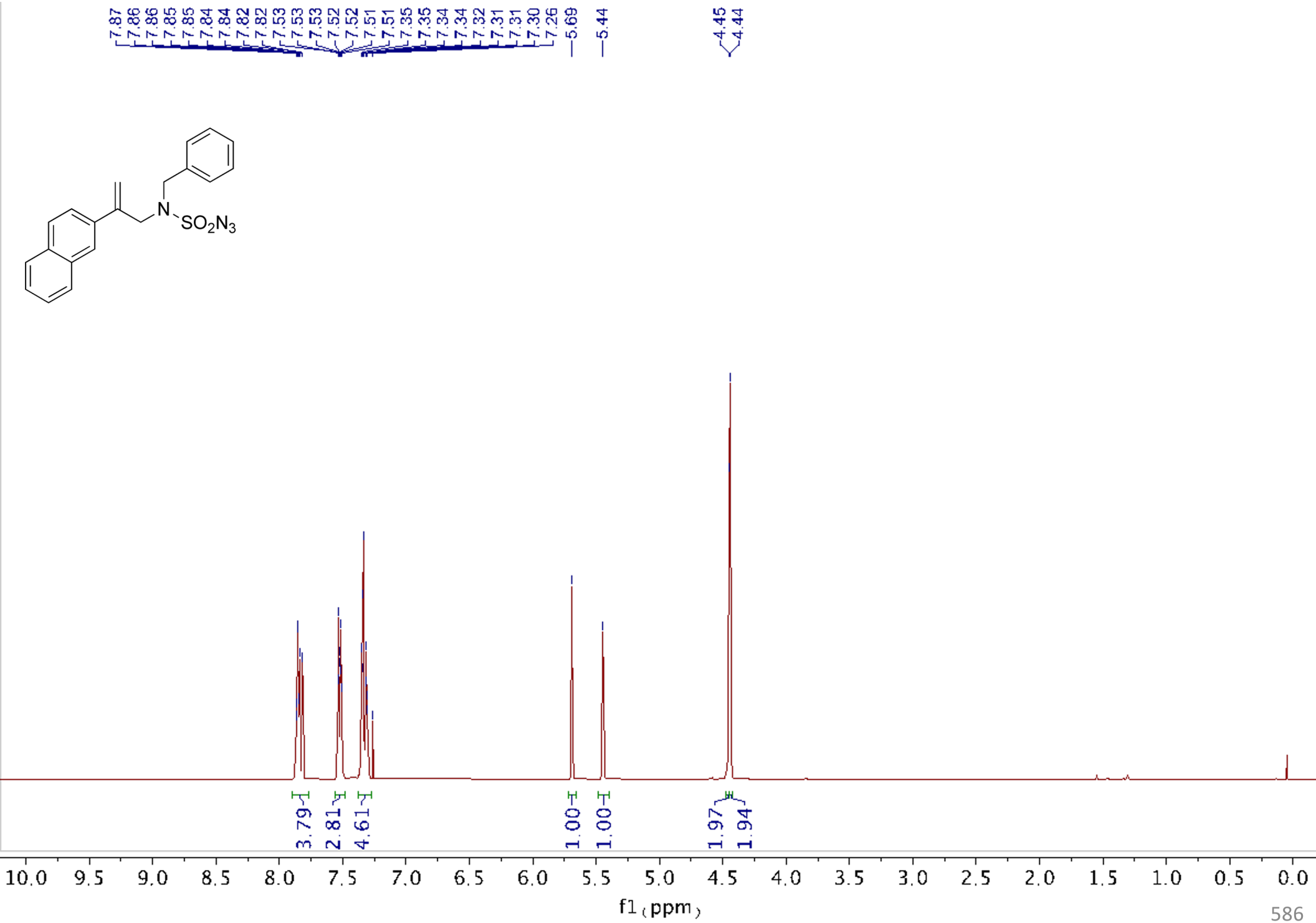
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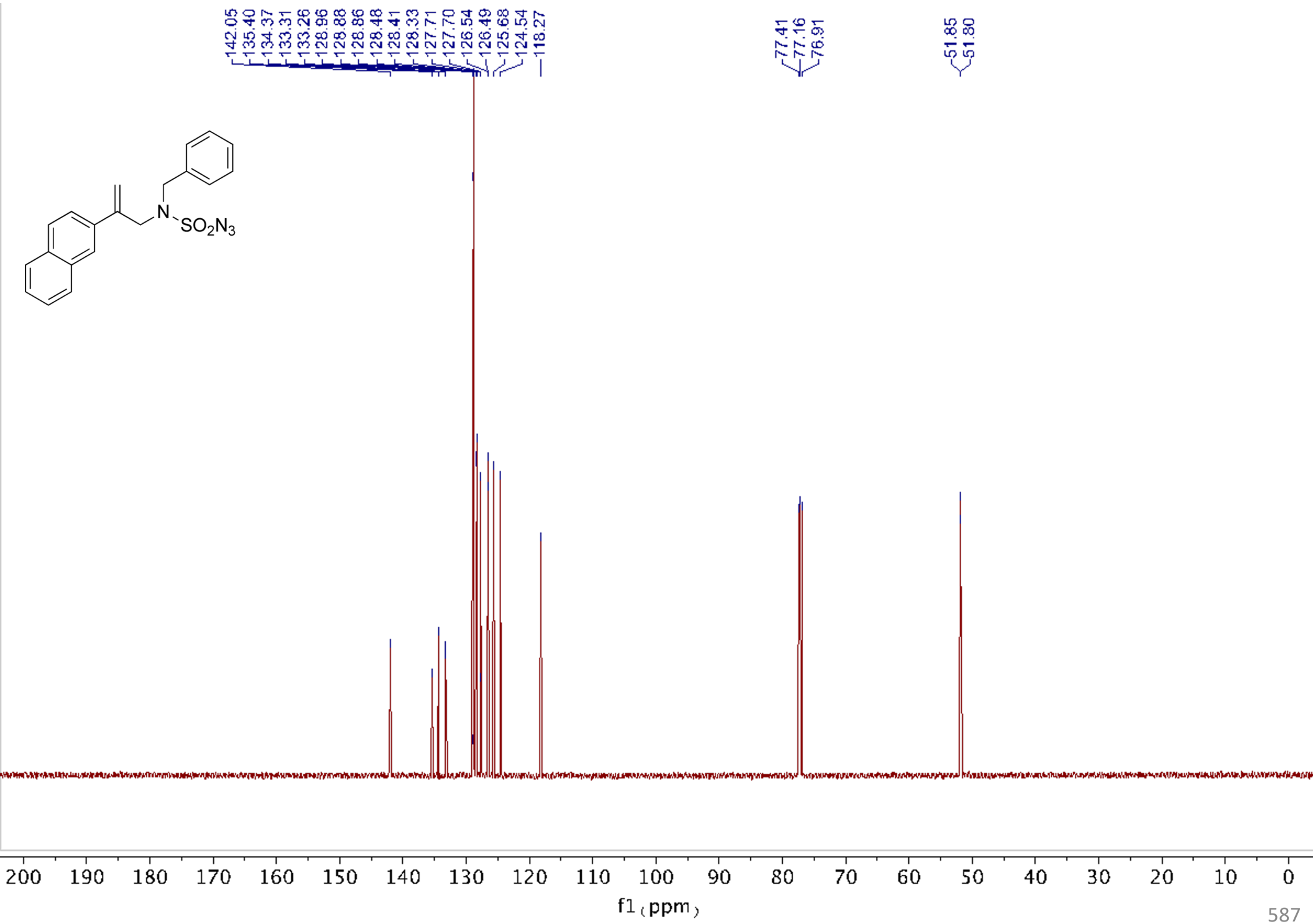
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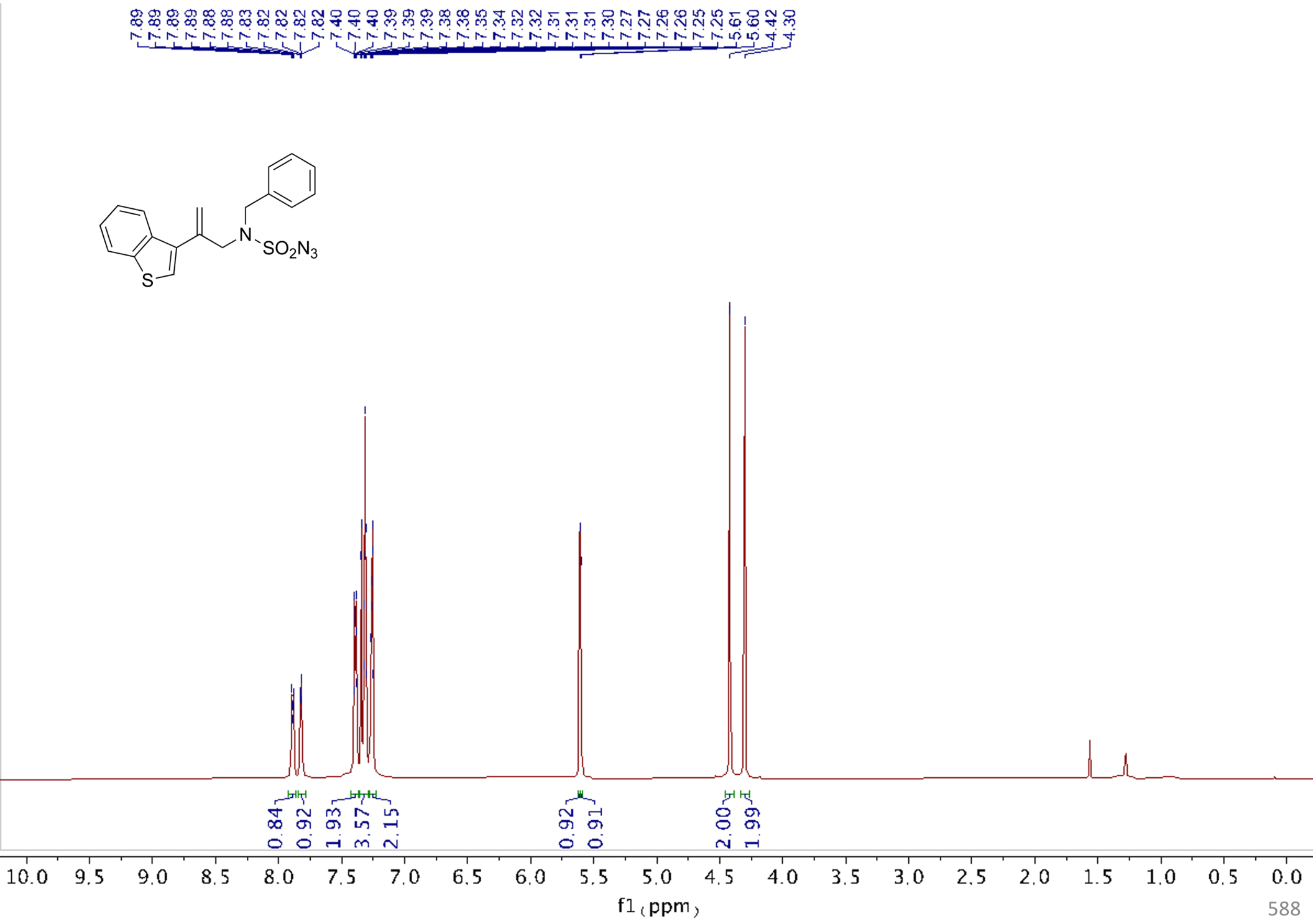
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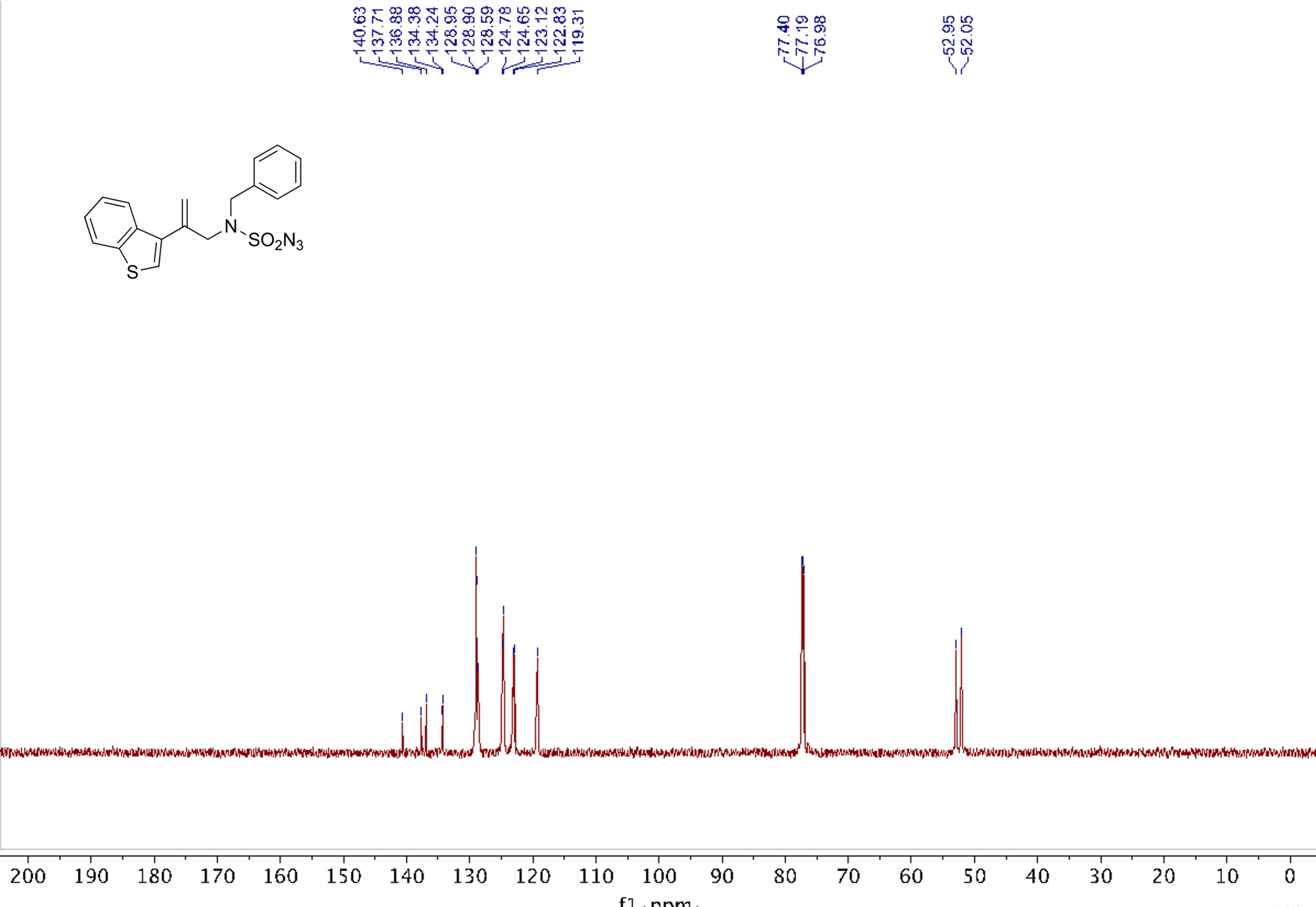
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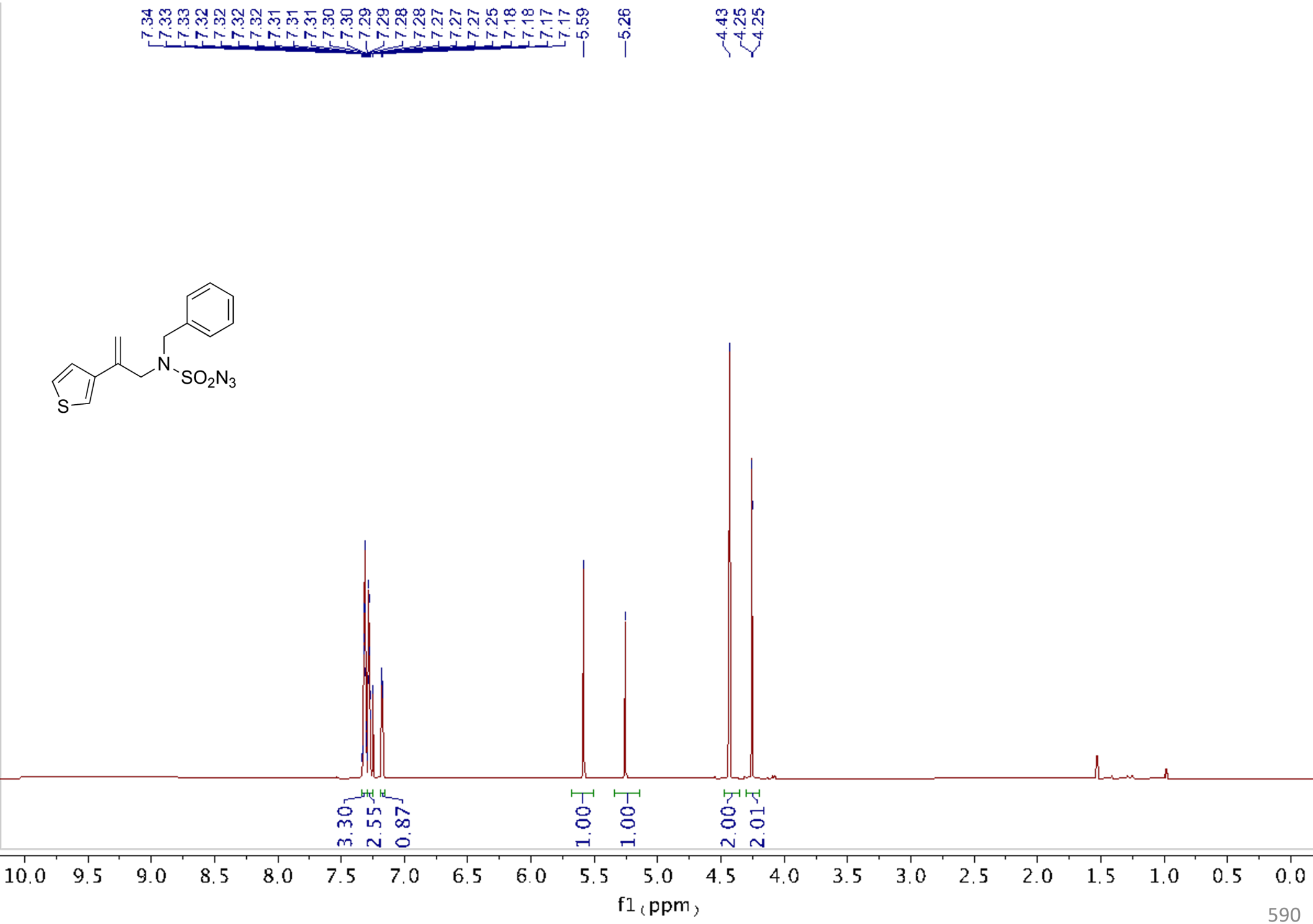
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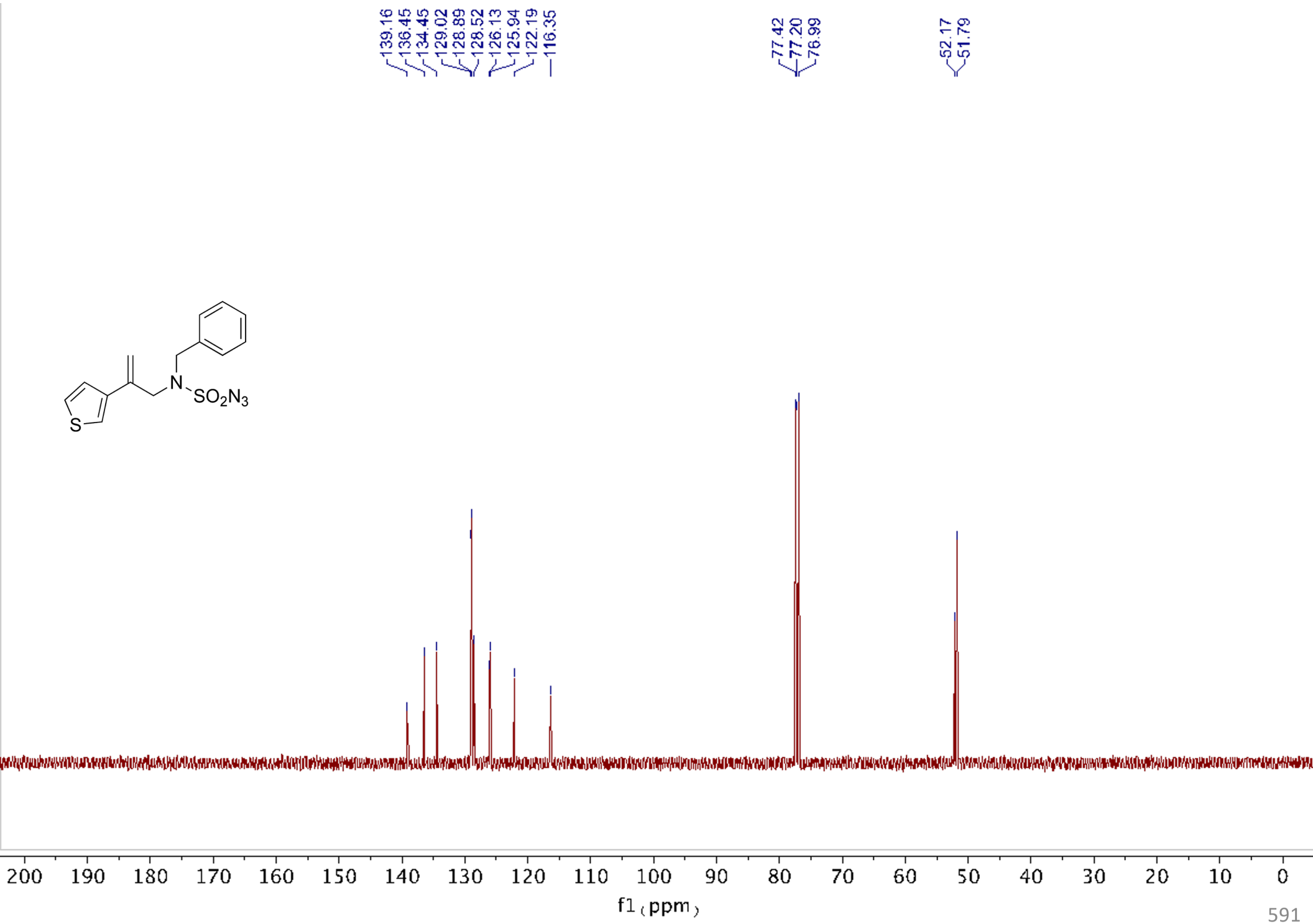
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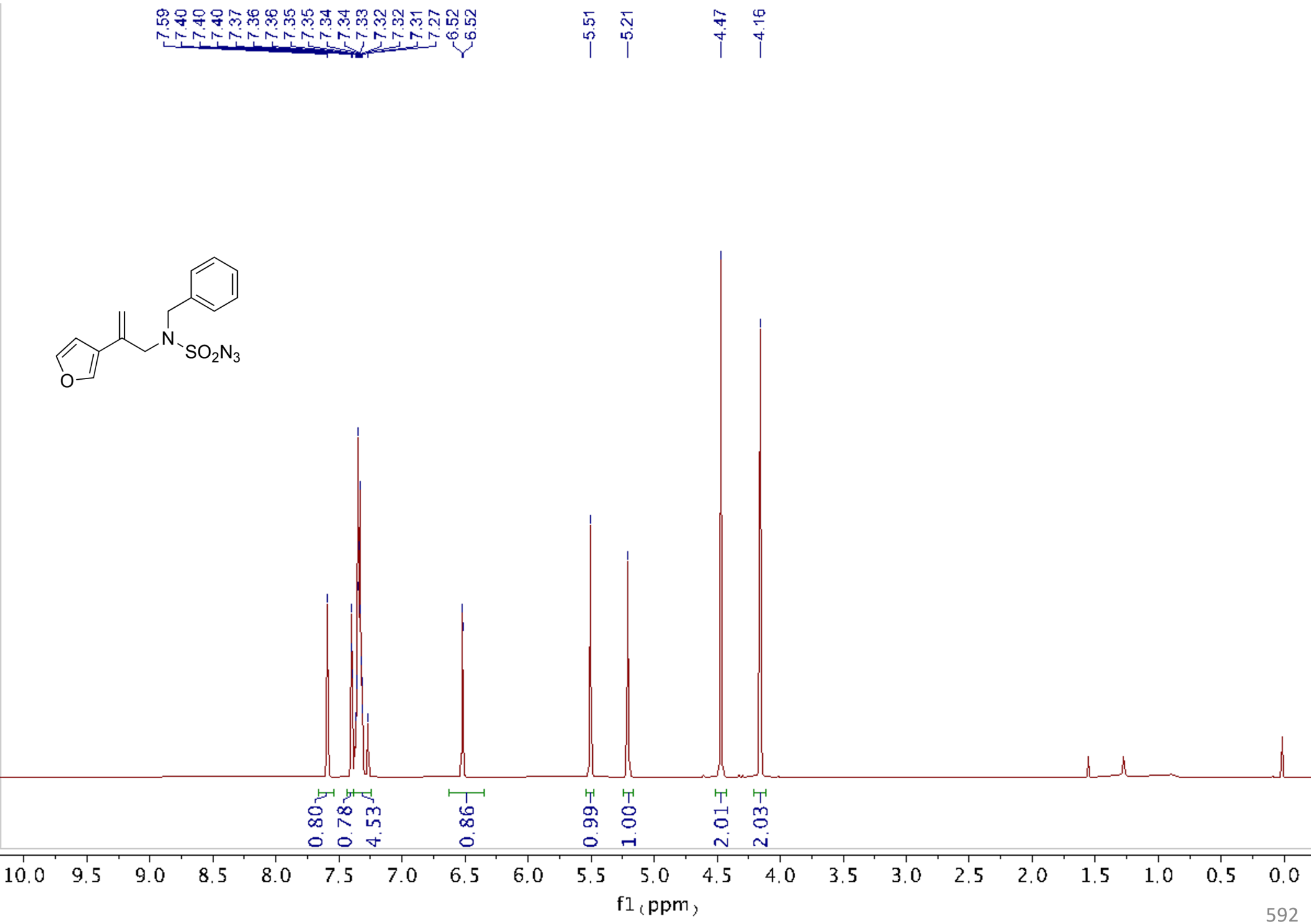
^{1}H NMR 3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)thiophene 2.11



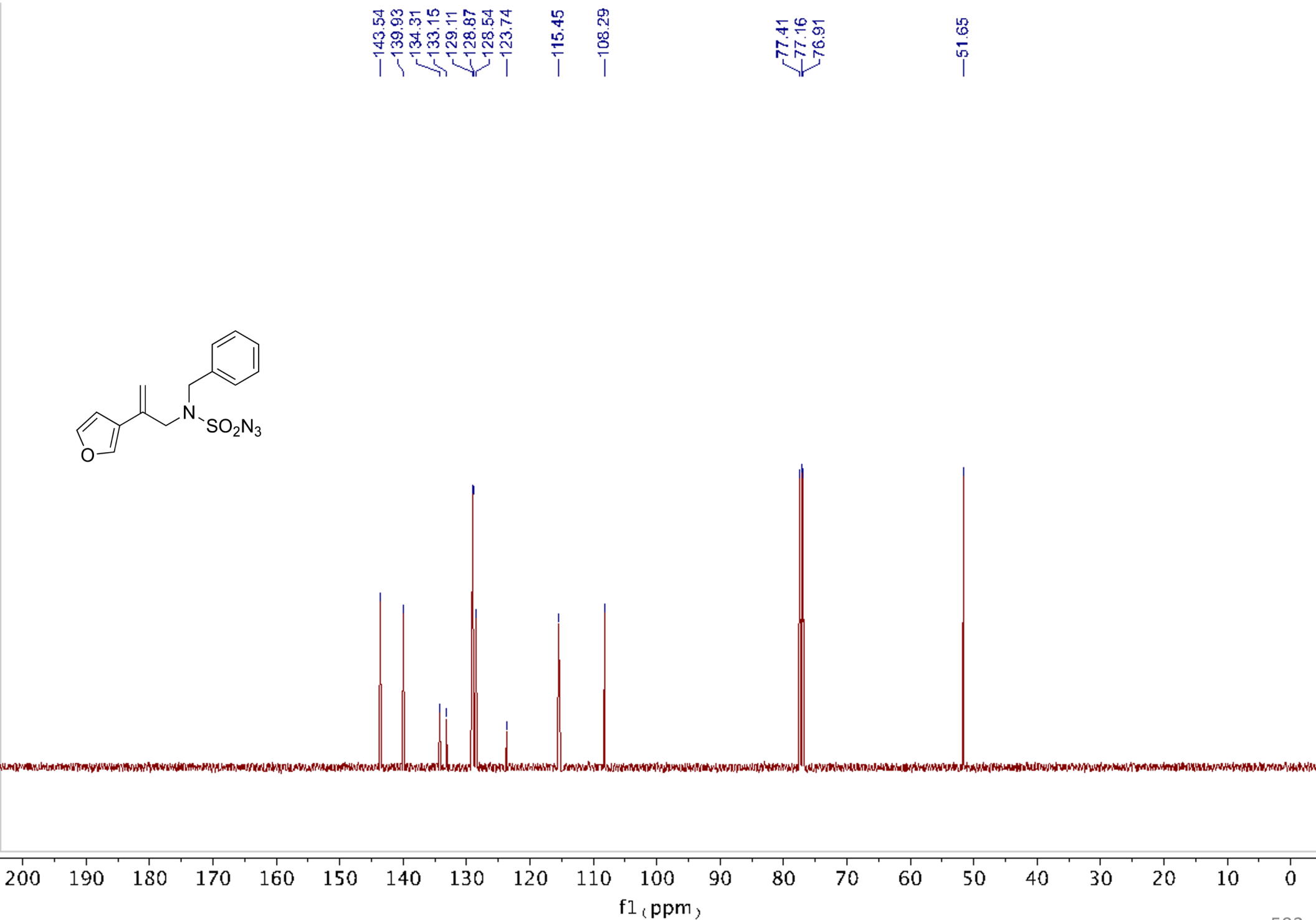
^{13}C NMR 3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)thiophene 2.11



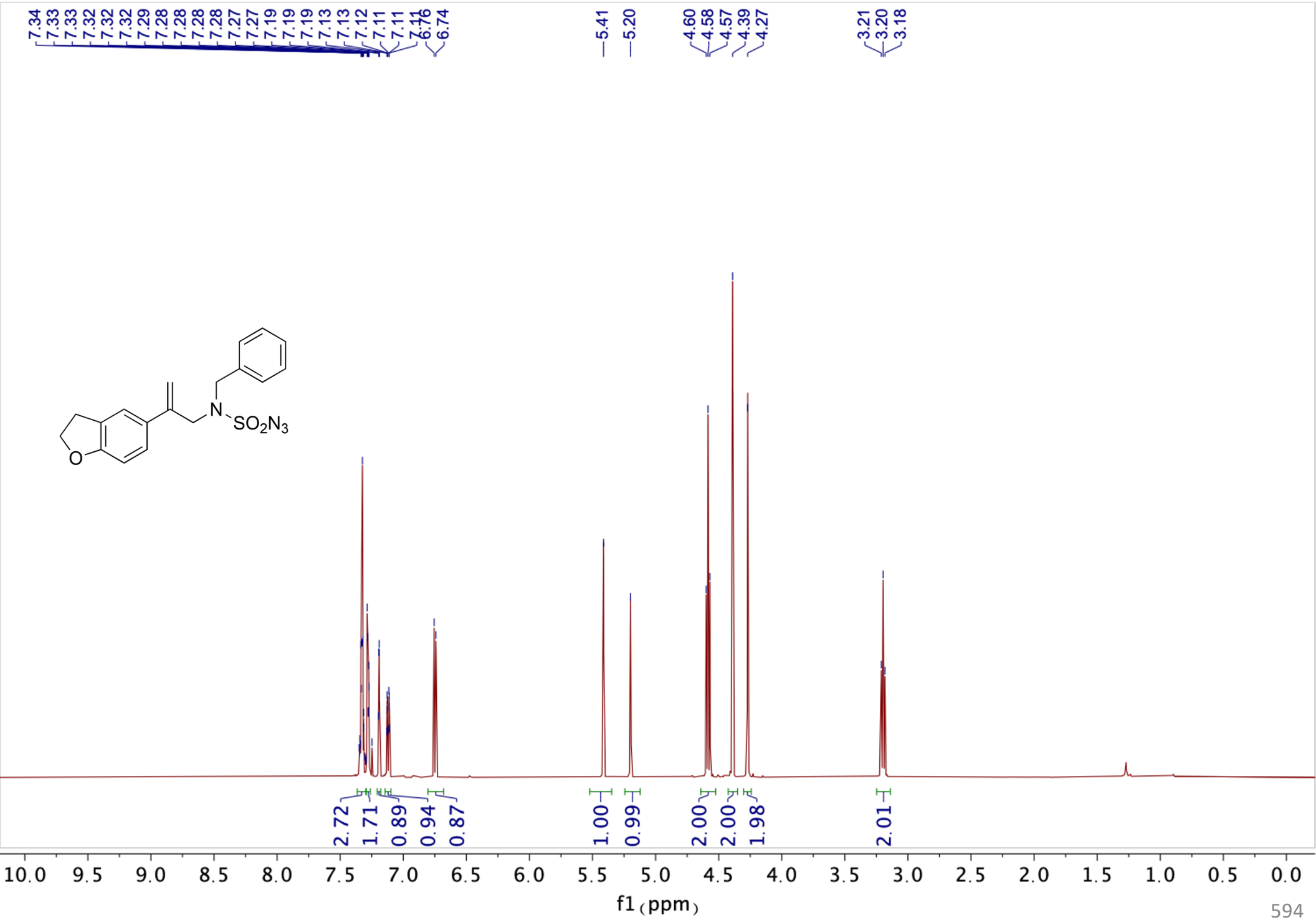
^{1}H NMR 3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)furan 2.1m



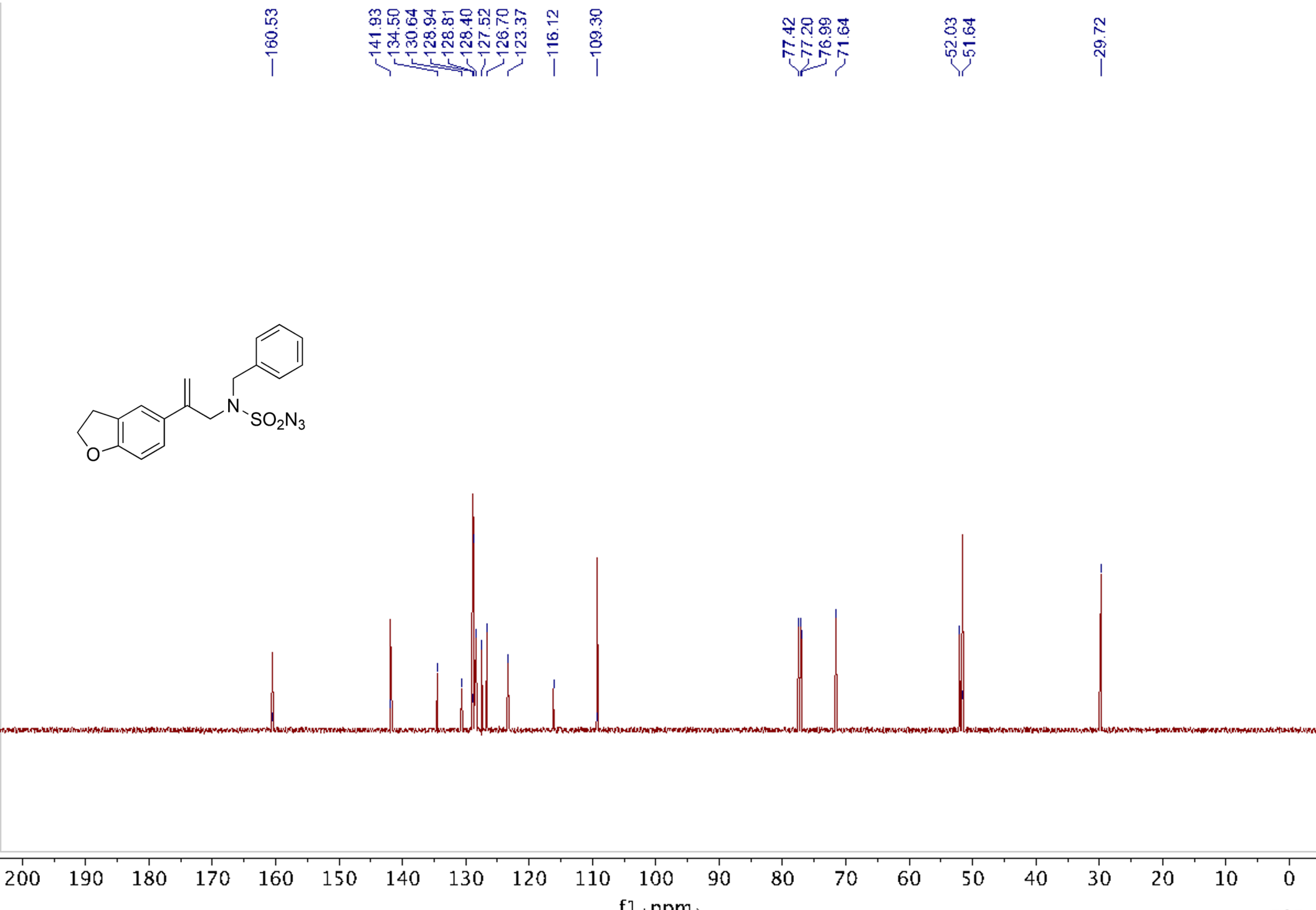
^{13}C NMR 3-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)furan 2.1m



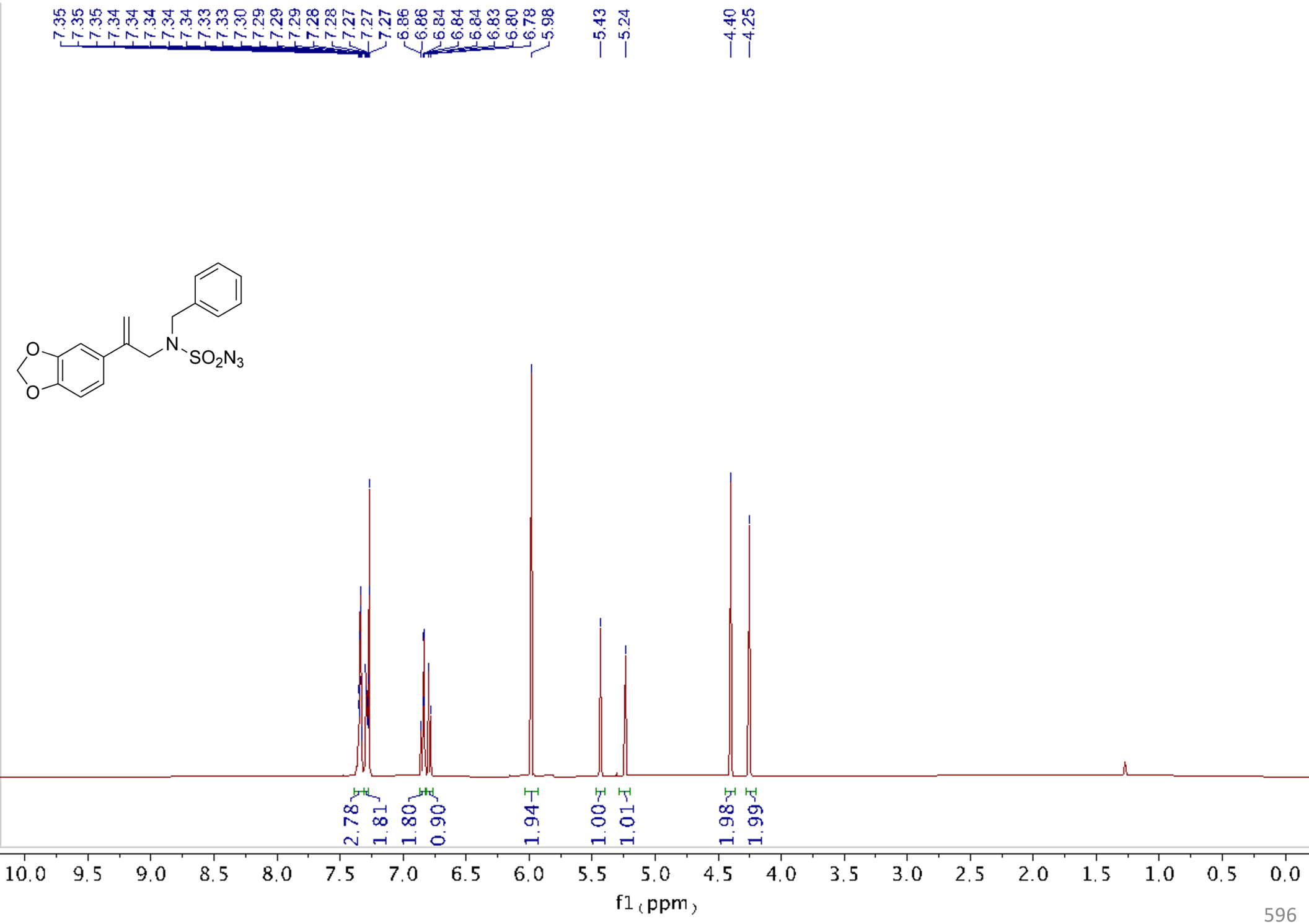
^{1}H NMR 5-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2,3-dihydrobenzofuran 2.1n



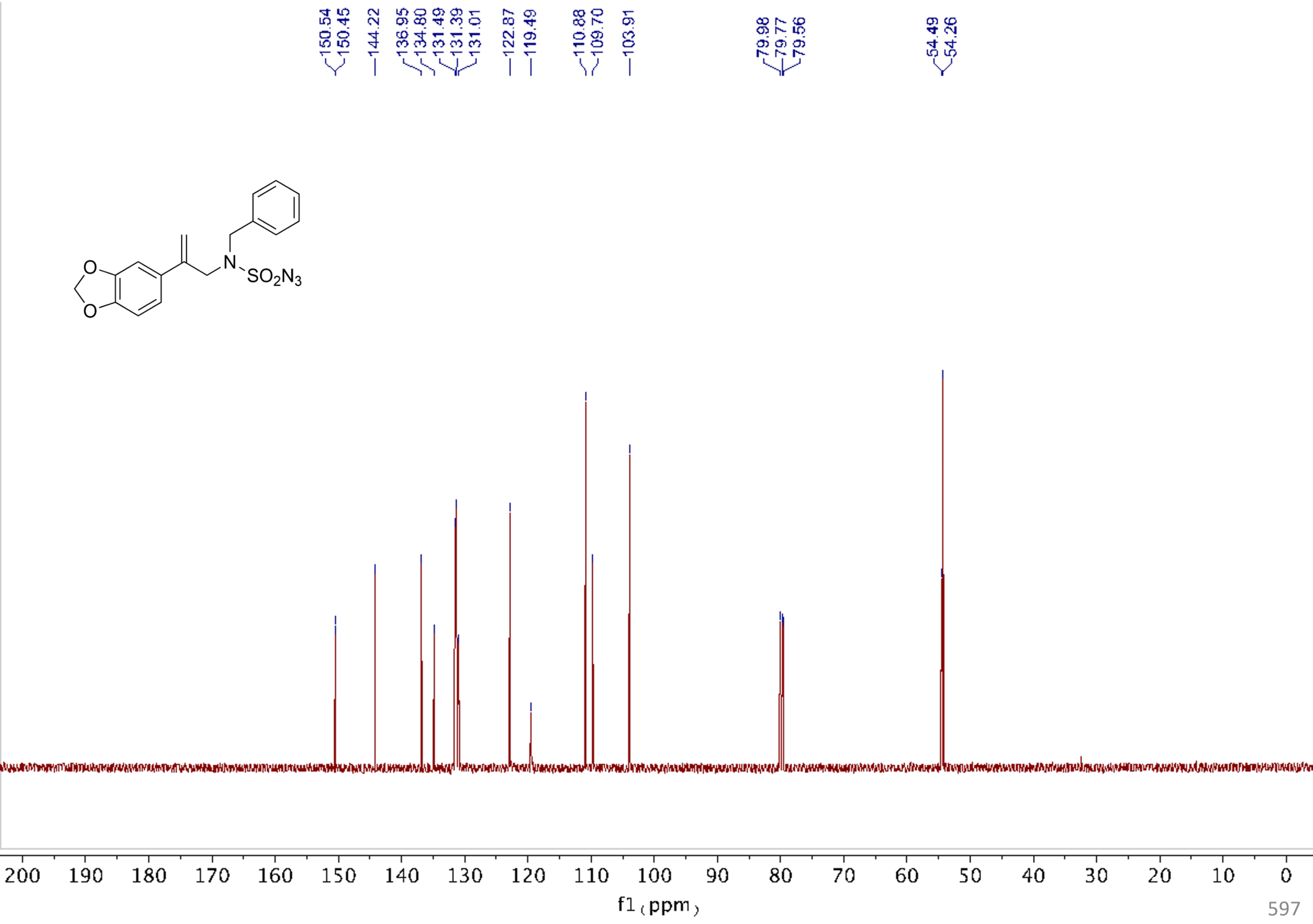
^{13}C NMR 5-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2,3-dihydrobenzofuran 2.1n



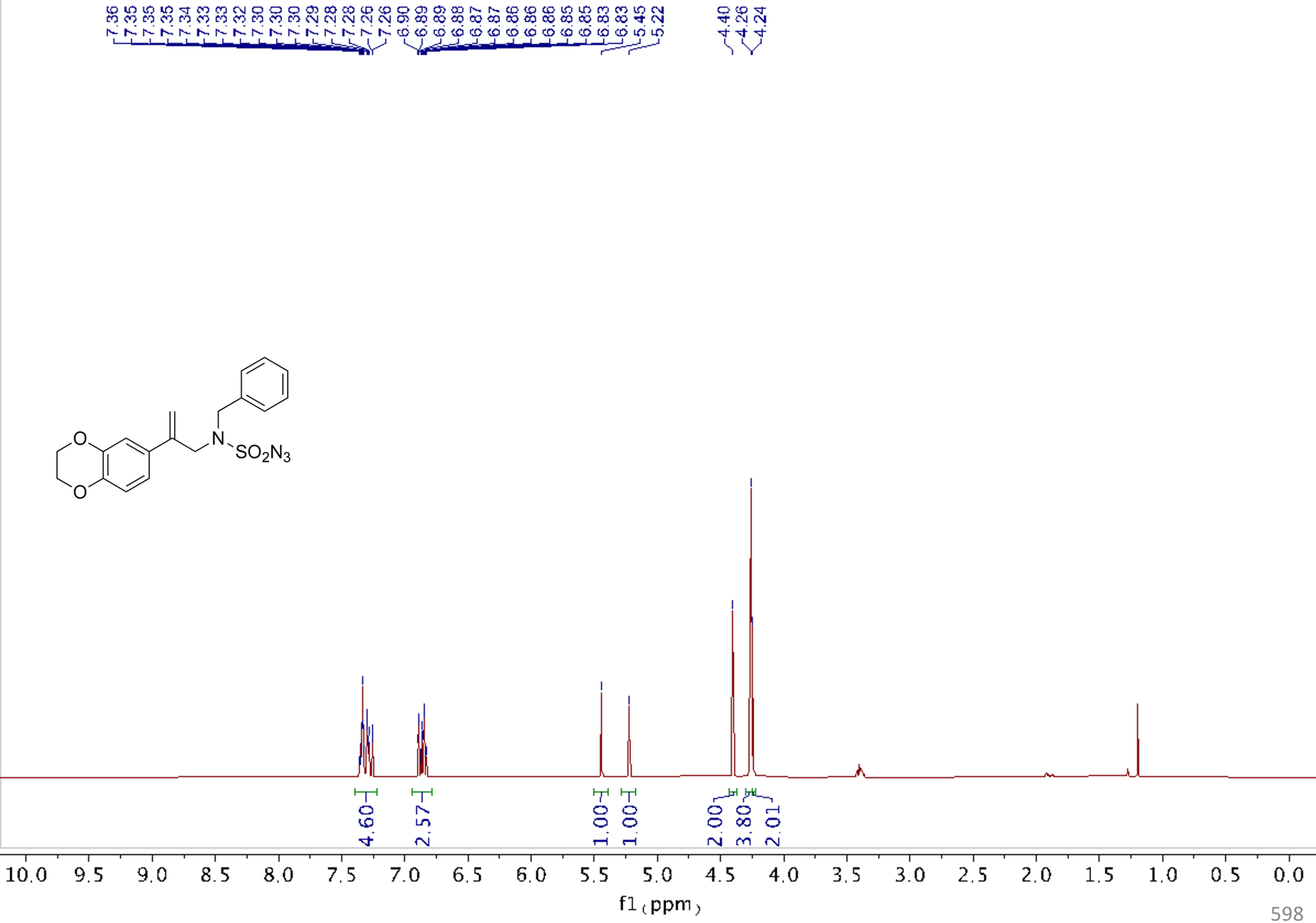
^{1}H NMR 5-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)benzo[*d*][1,3]dioxole 2.1o



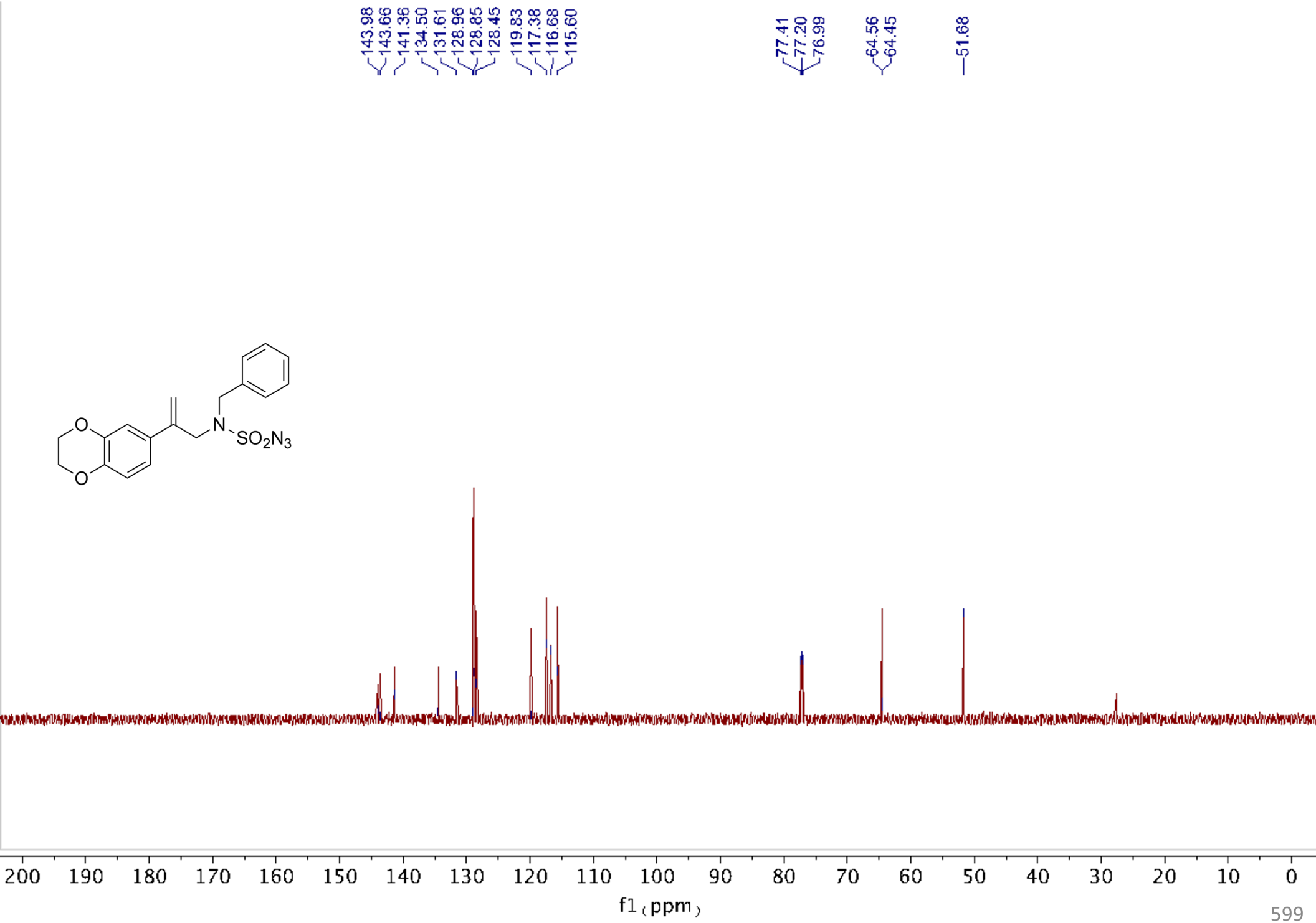
^{13}C NMR 5-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)benzo[*d*][1,3]dioxole 2.1o



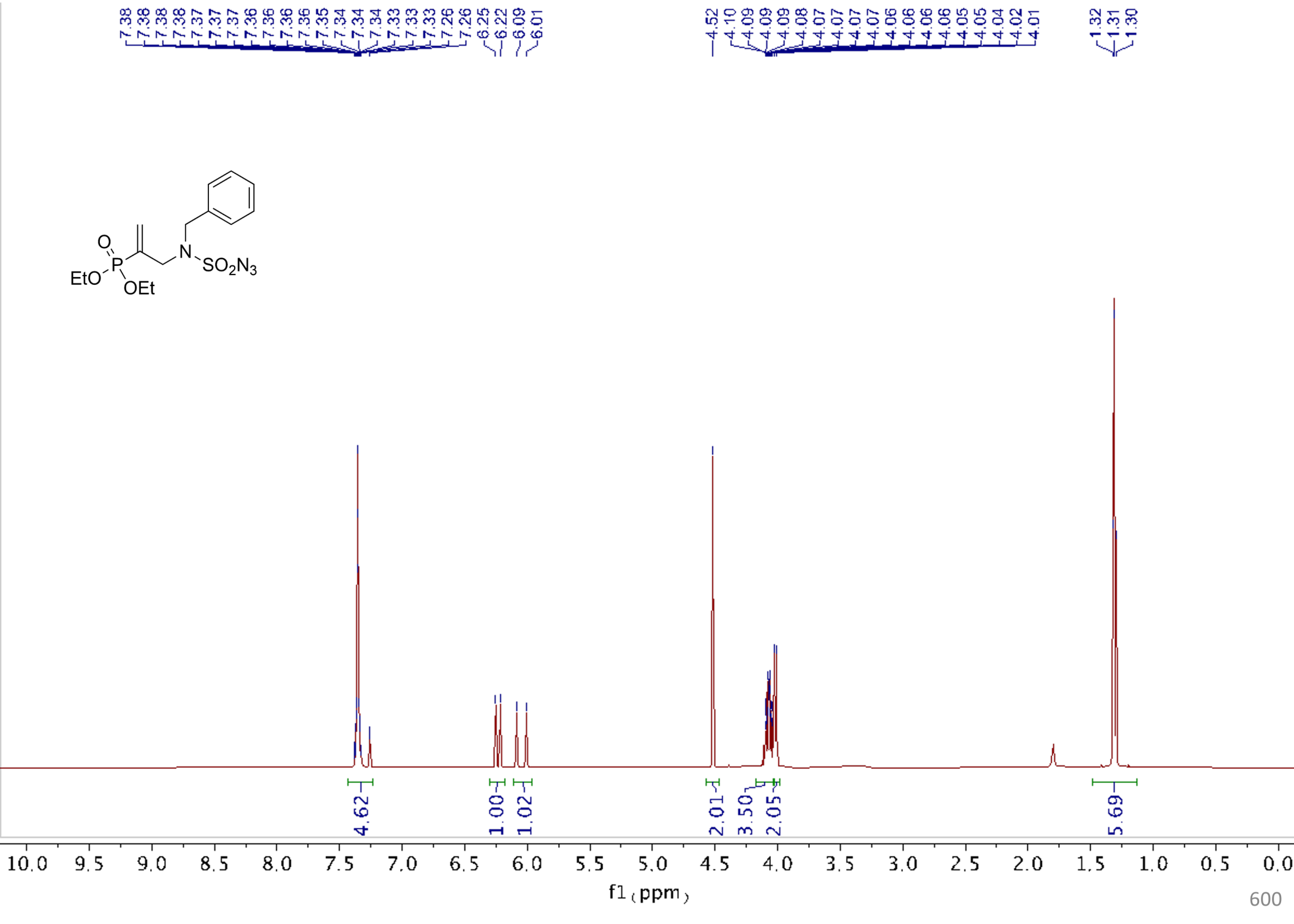
^{1}H NMR 6-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2,3-dihydrobenzo[*b*][1,4]dioxine 2.1p



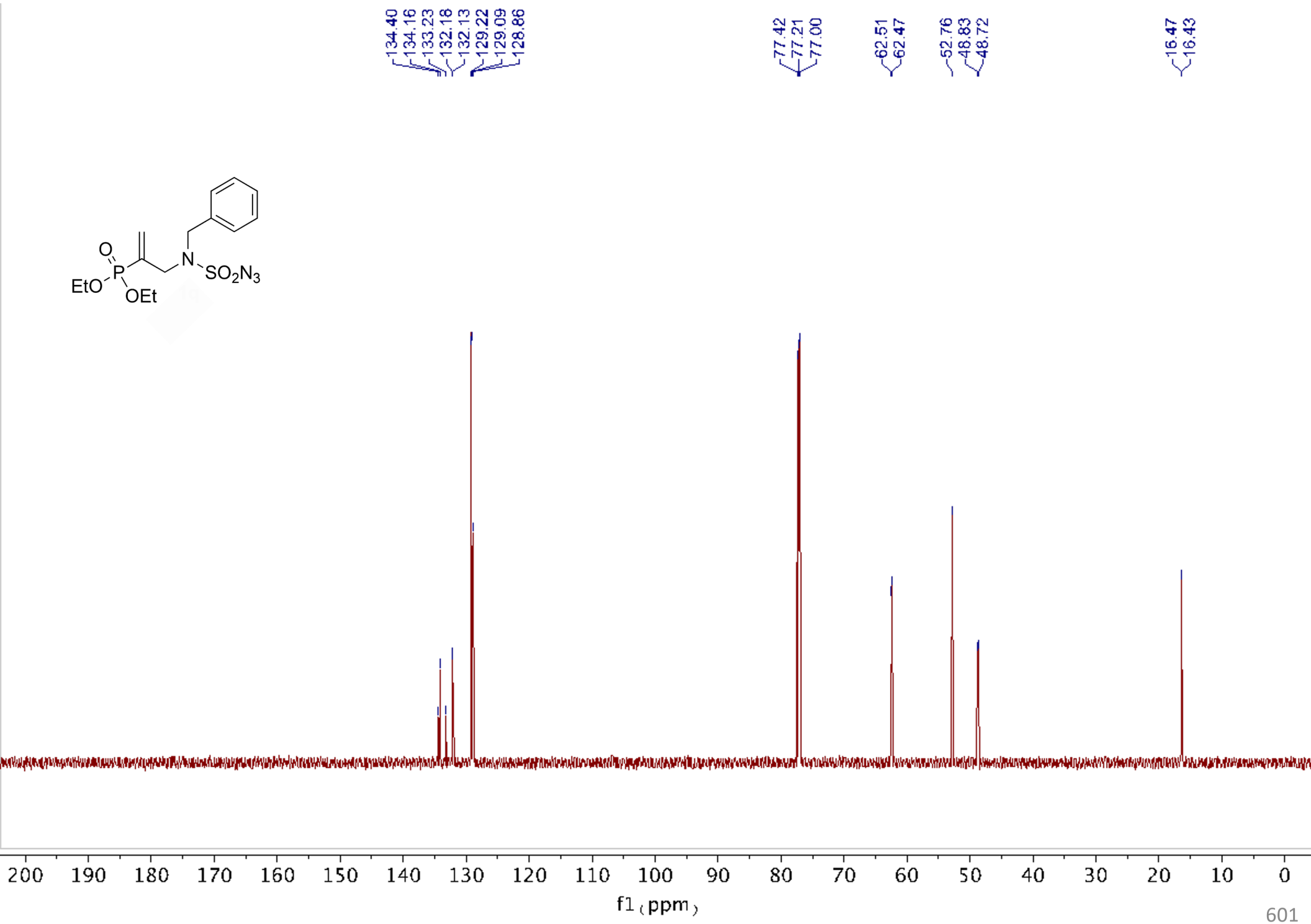
^{13}C NMR 6-(3-((Azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)-2,3-dihydrobenzo[*b*][1,4]dioxine 2.1p



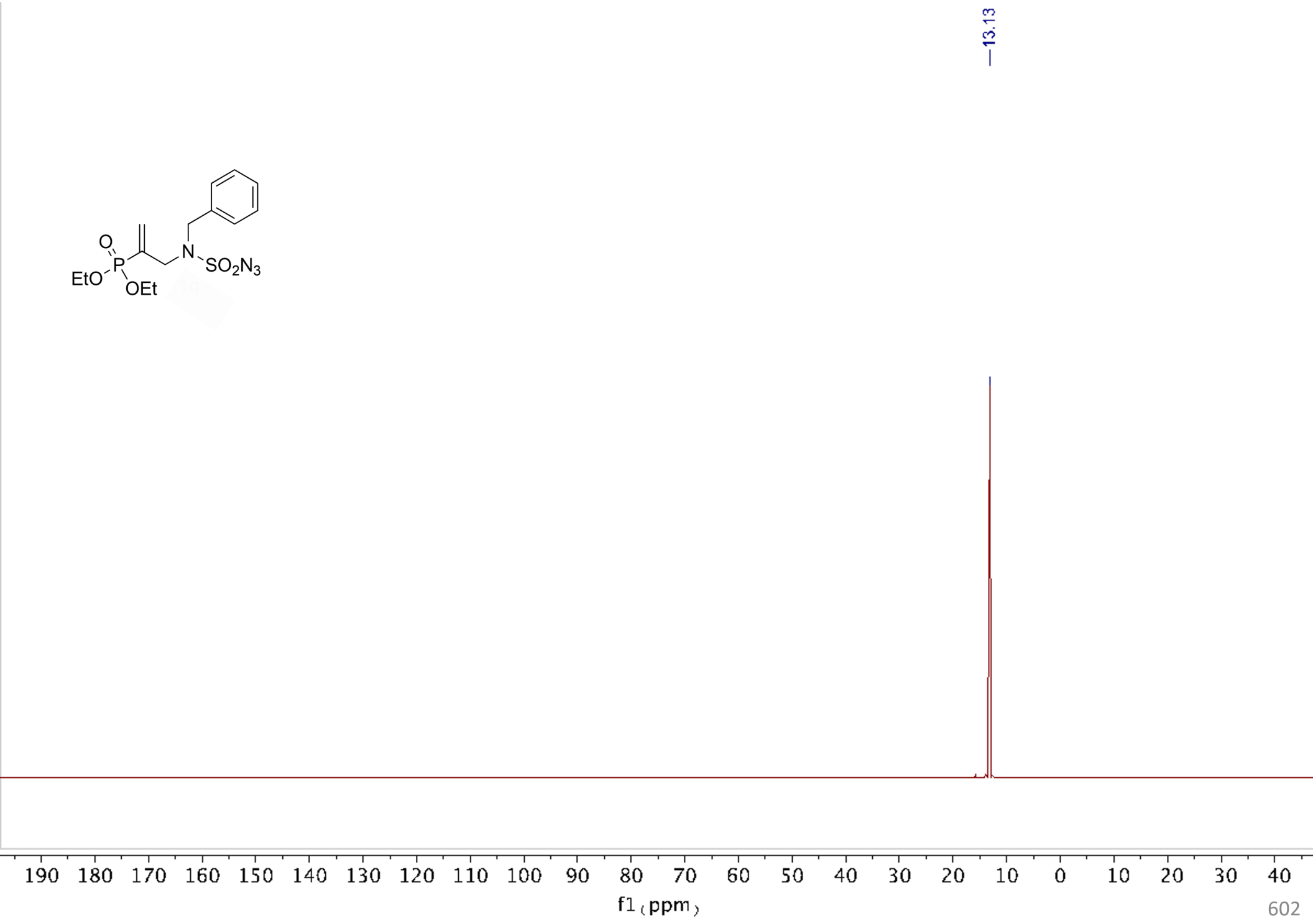
^{1}H NMR Diethyl (3-((azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)phosphonate 2.1q



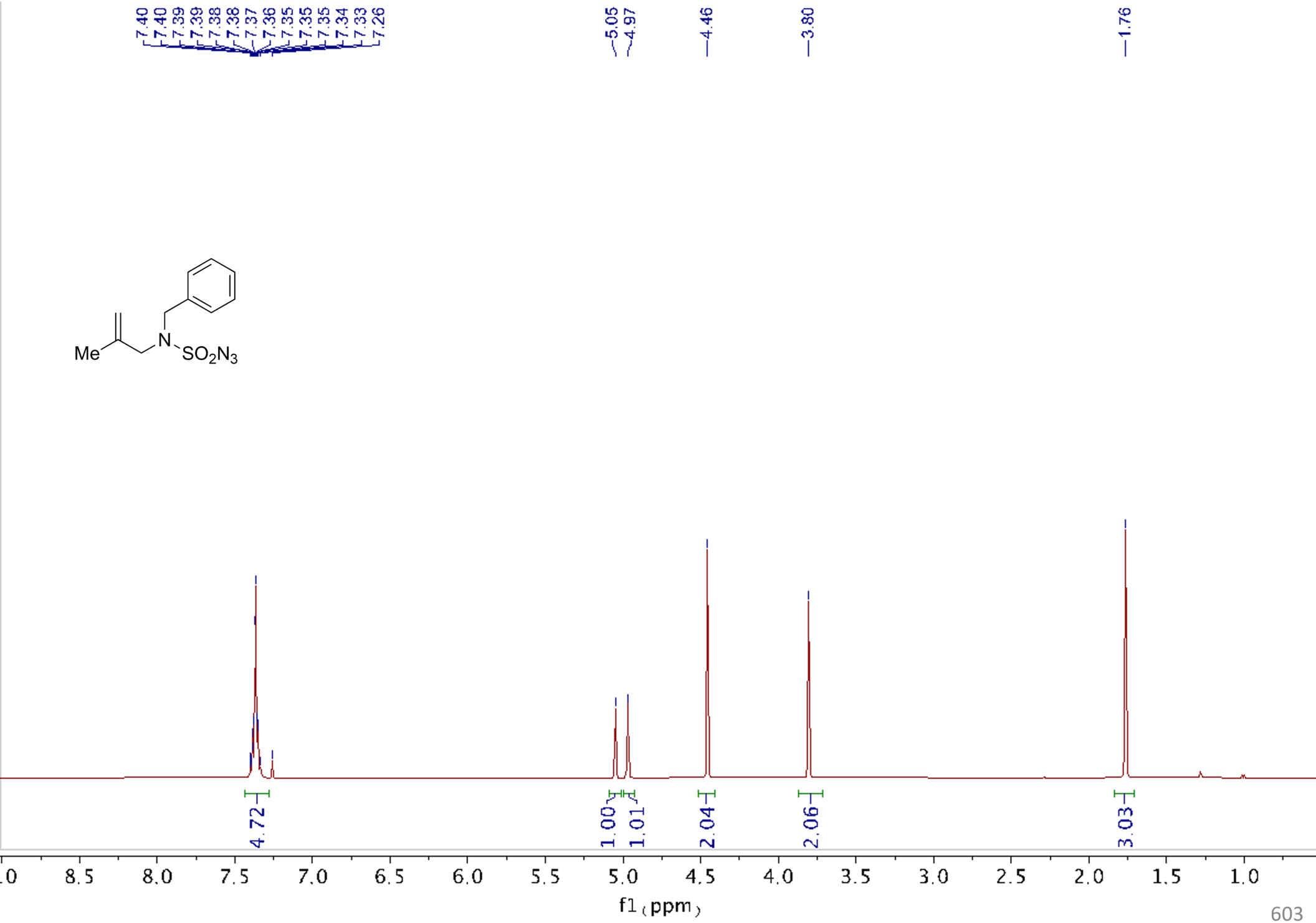
^{13}C NMR Diethyl (3-((azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)phosphonate 2.1q



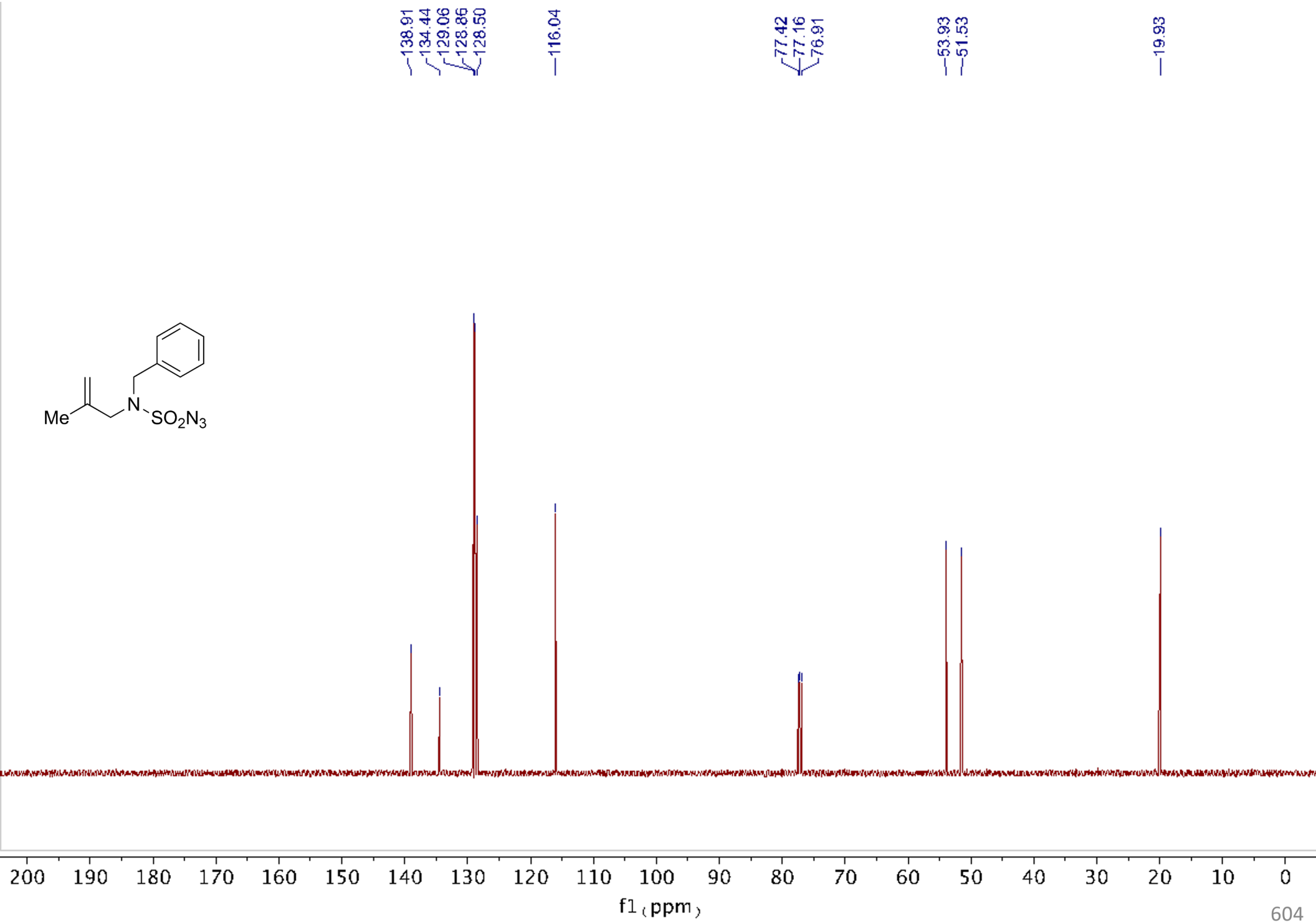
^{31}P NMR Diethyl (3-((azidosulfonyl)(benzyl)amino)prop-1-en-2-yl)phosphonate 2.1q



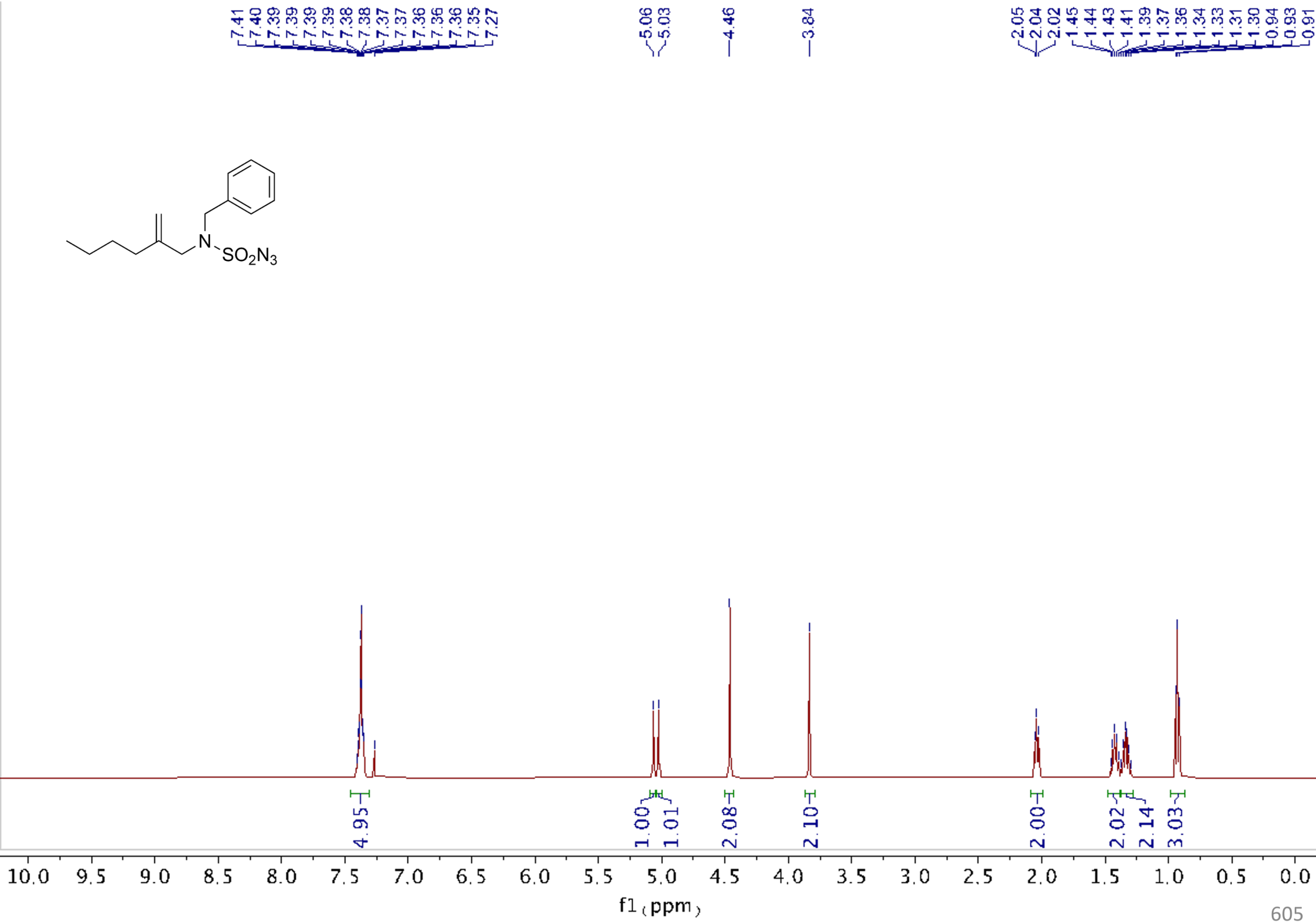
^{1}H NMR (((Azidosulfonyl)(2-methylallyl)amino)methyl)benzene 2.1t



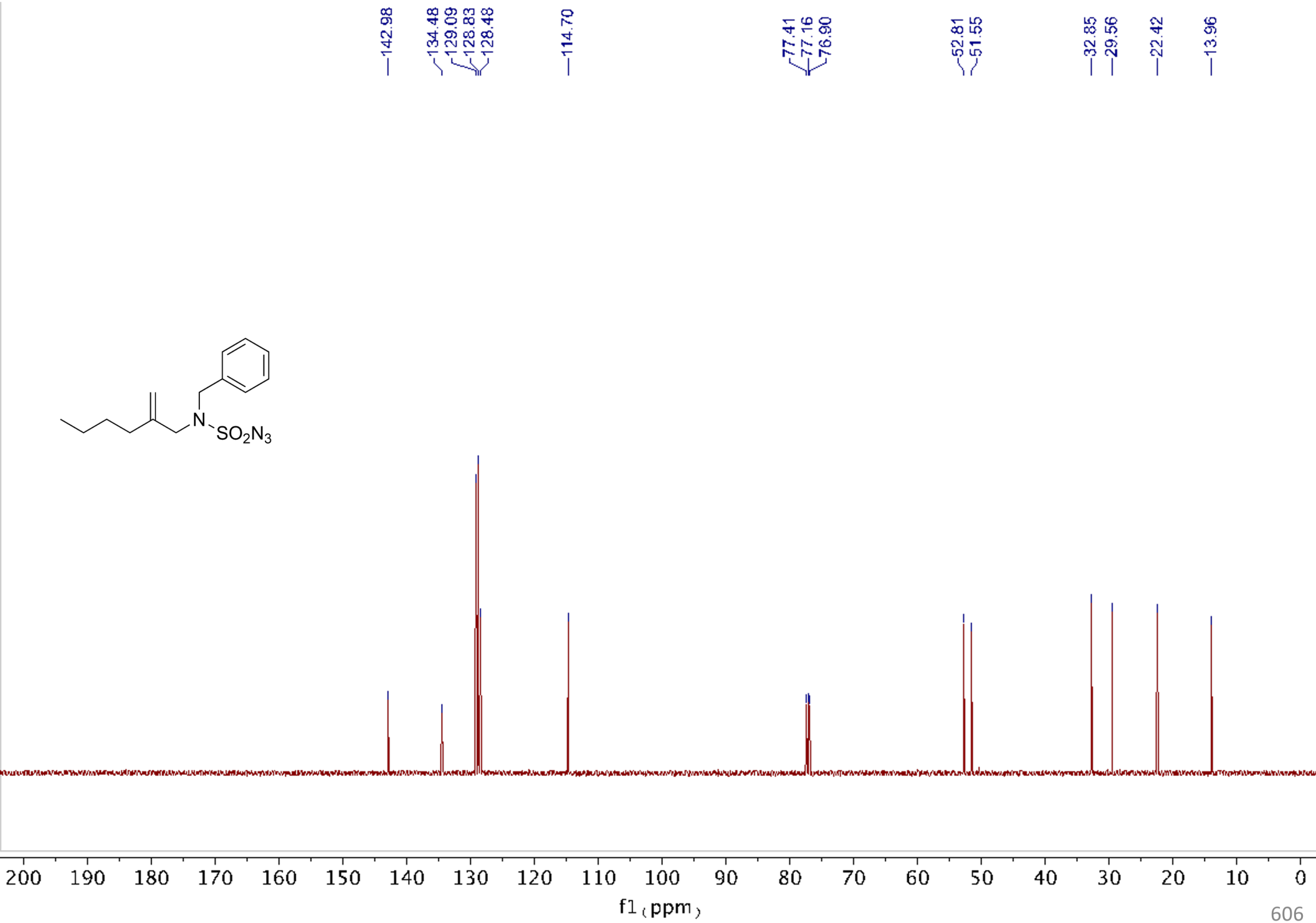
^{13}C NMR (((Azidosulfonyl)(2-methylallyl)amino)methyl)benzene 2.1t



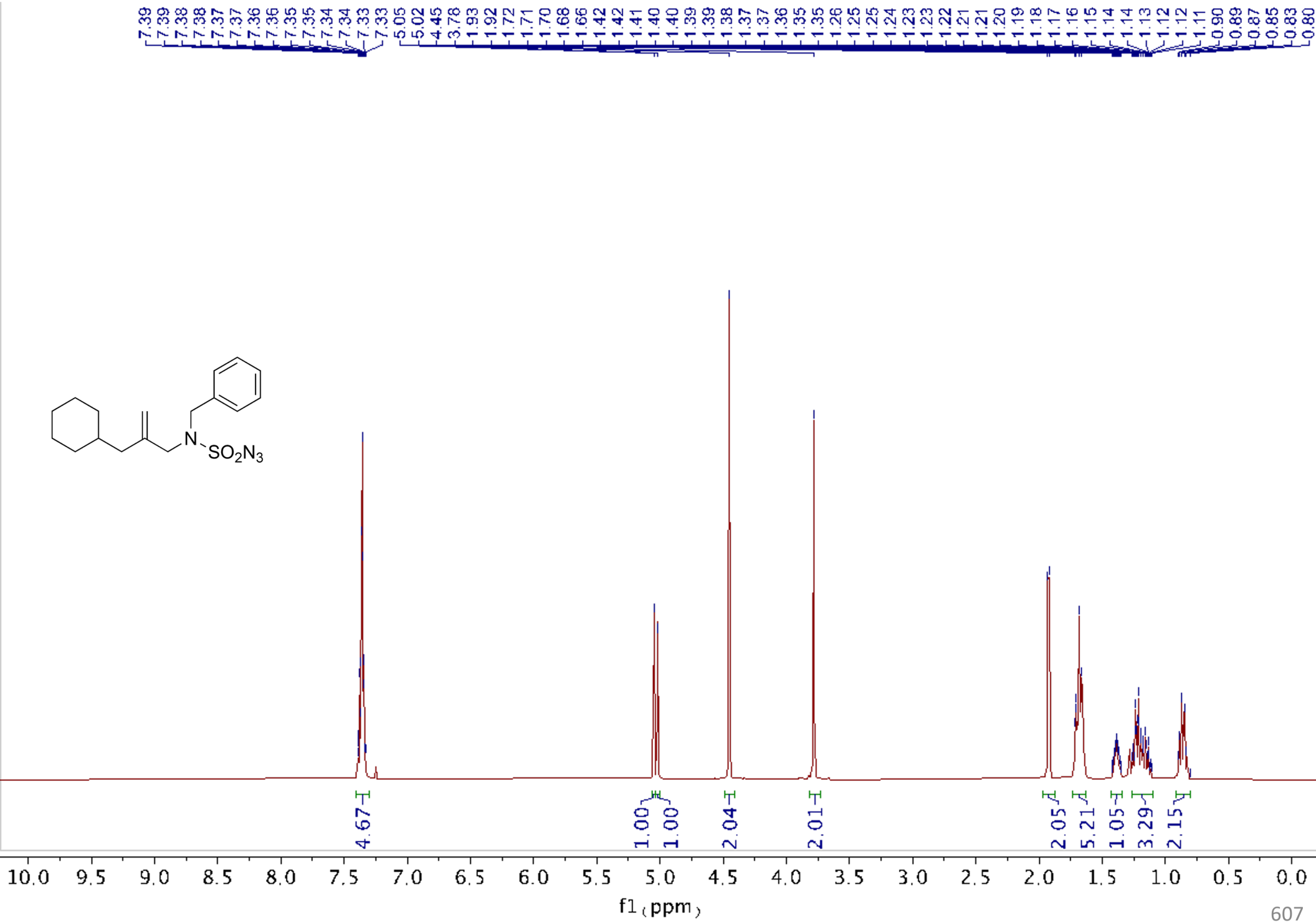
^{1}H NMR (((Azidosulfonyl)(2-methylenehexyl)amino)methyl)benzene 2.1u



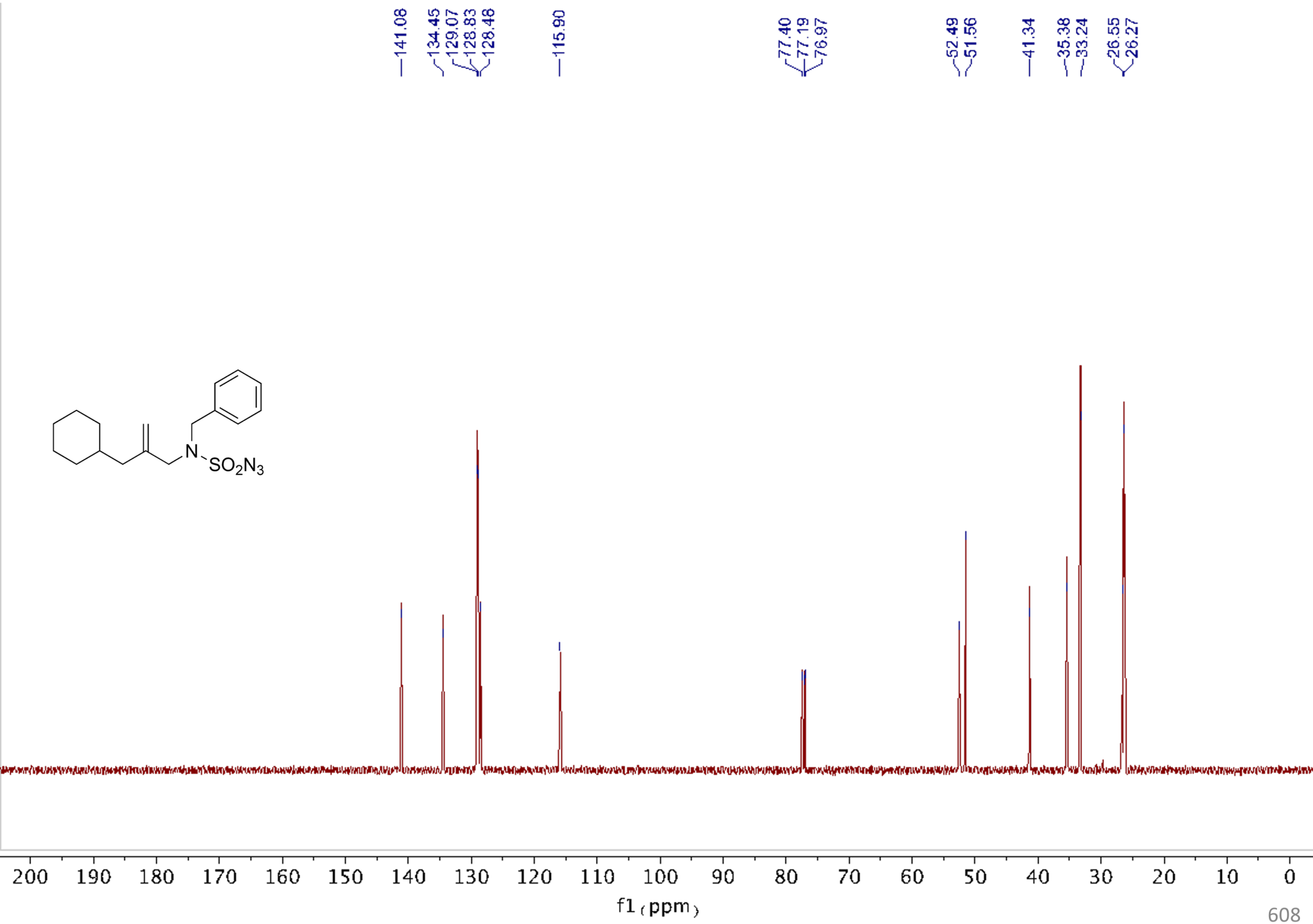
^{13}C NMR (((Azidosulfonyl)(2-methylenehexyl)amino)methyl)benzene 2.1u



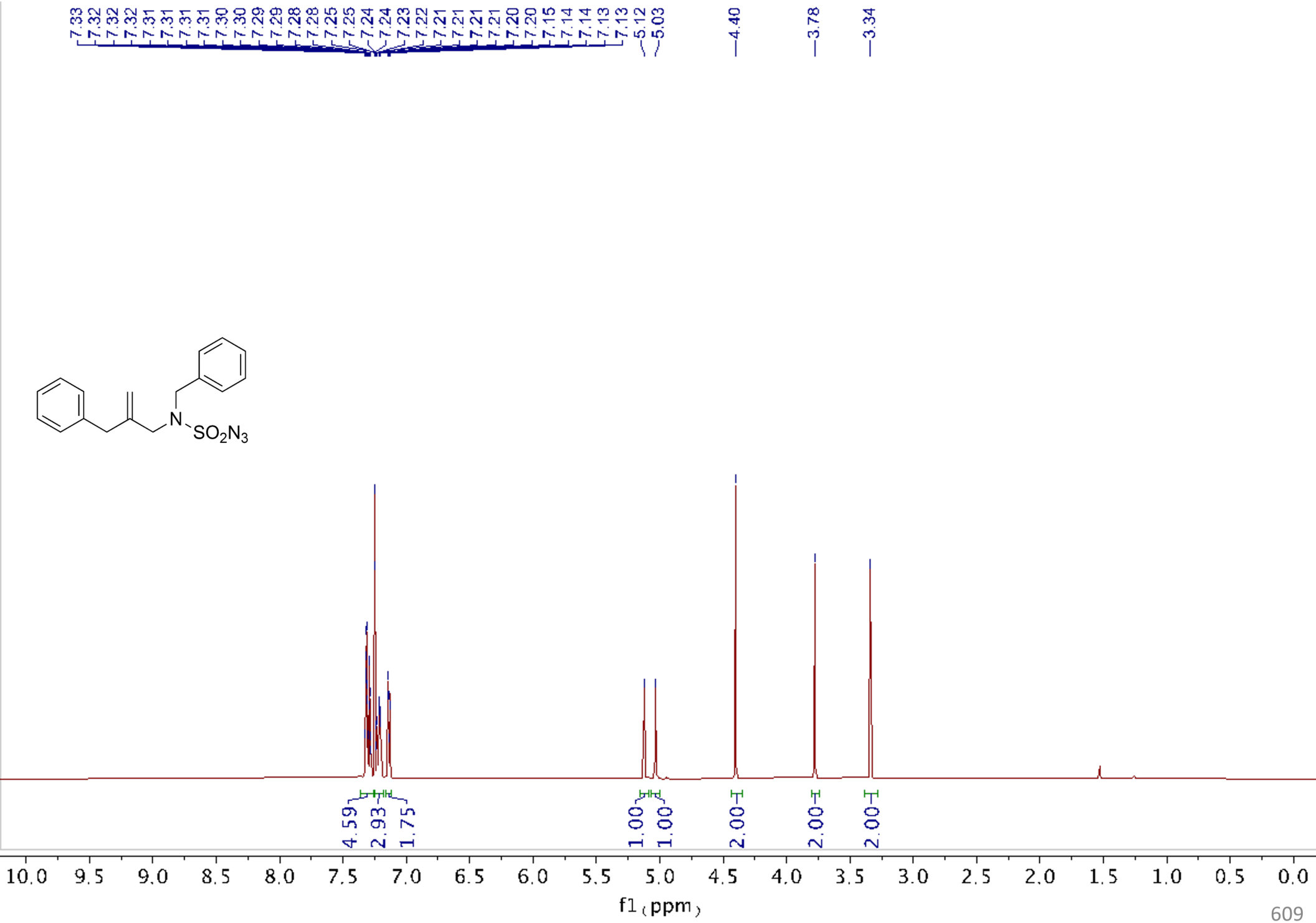
^{1}H NMR (((Azidosulfonyl)(2-(cyclohexylmethyl)allyl)amino)methyl)benzene 2.1v



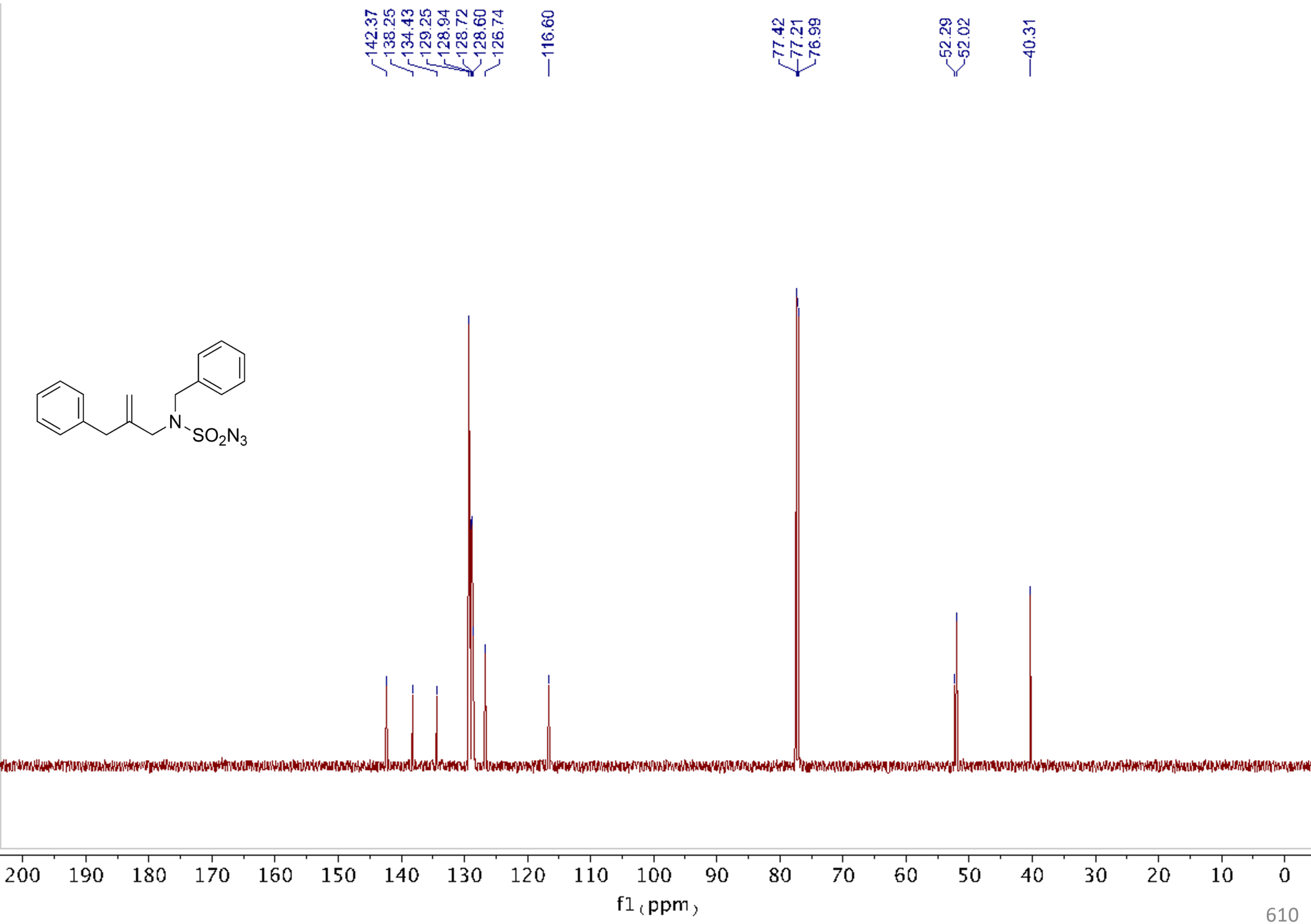
^{13}C NMR (((Azidosulfonyl)(2-(cyclohexylmethyl)allyl)amino)methyl)benzene 2.1v



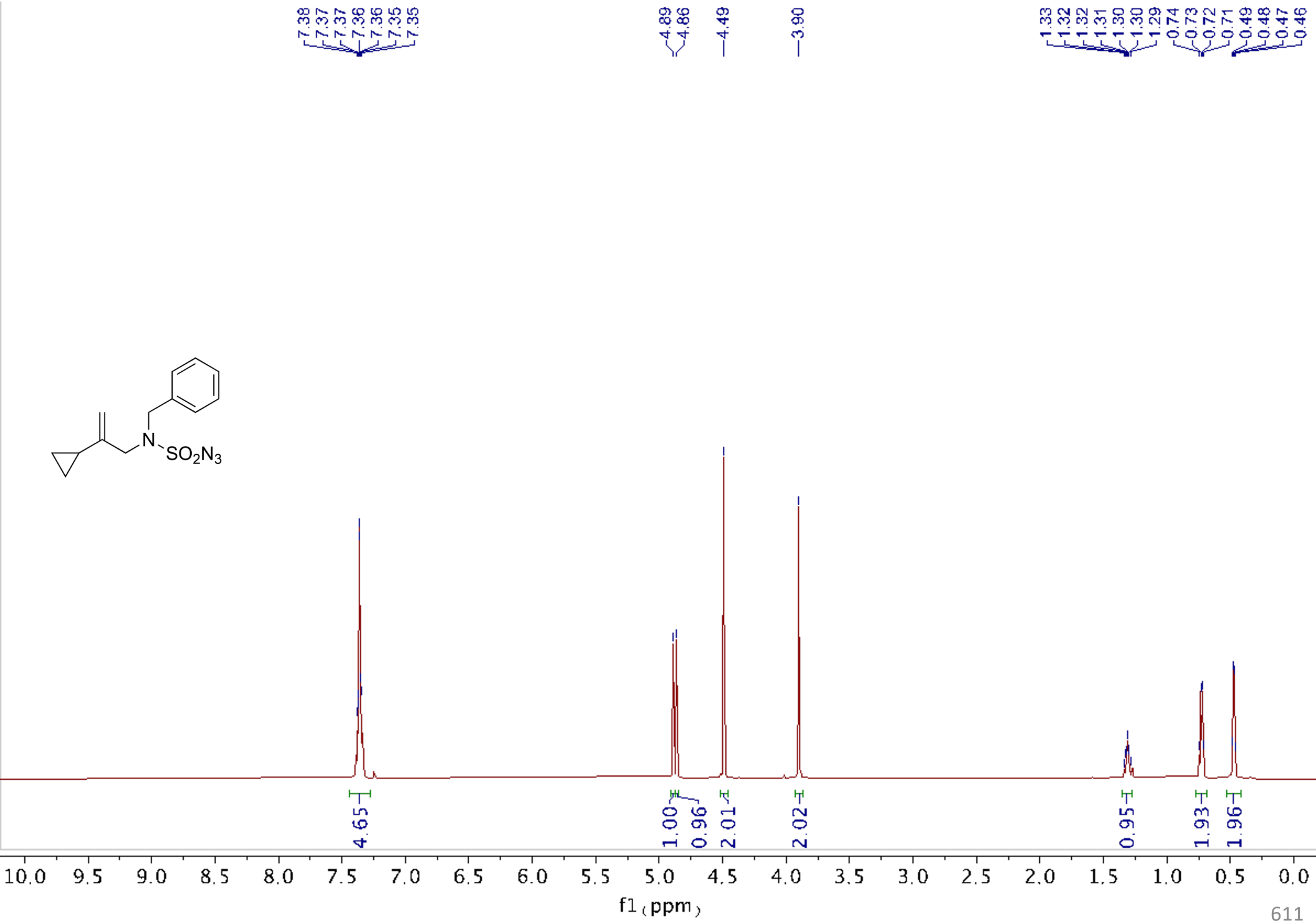
^{1}H NMR (((Azidosulfonyl)(2-benzylallyl)amino)methyl)benzene 2.1w



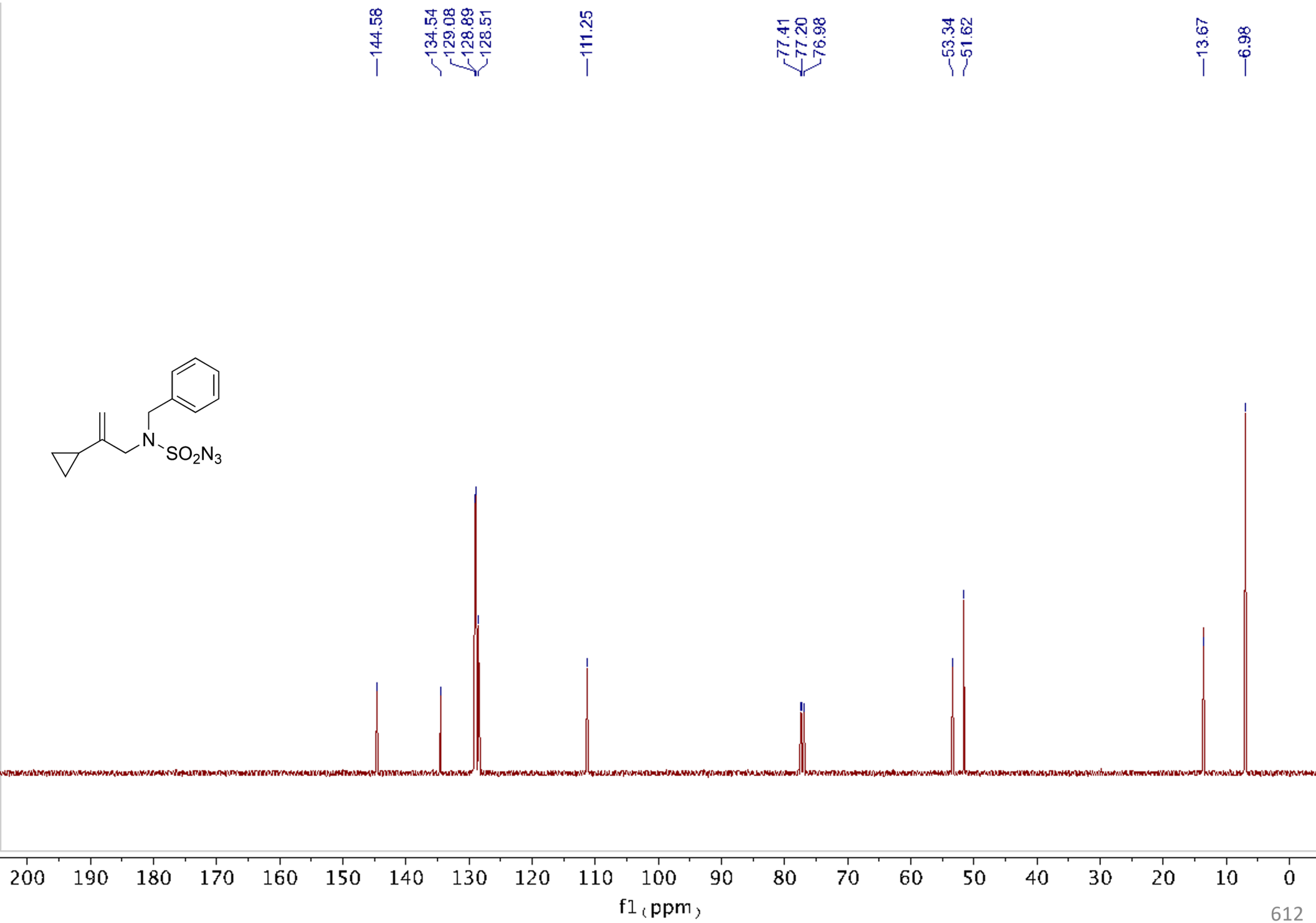
^{13}C NMR (((Azidosulfonyl)(2-benzylallyl)amino)methyl)benzene 2.1w



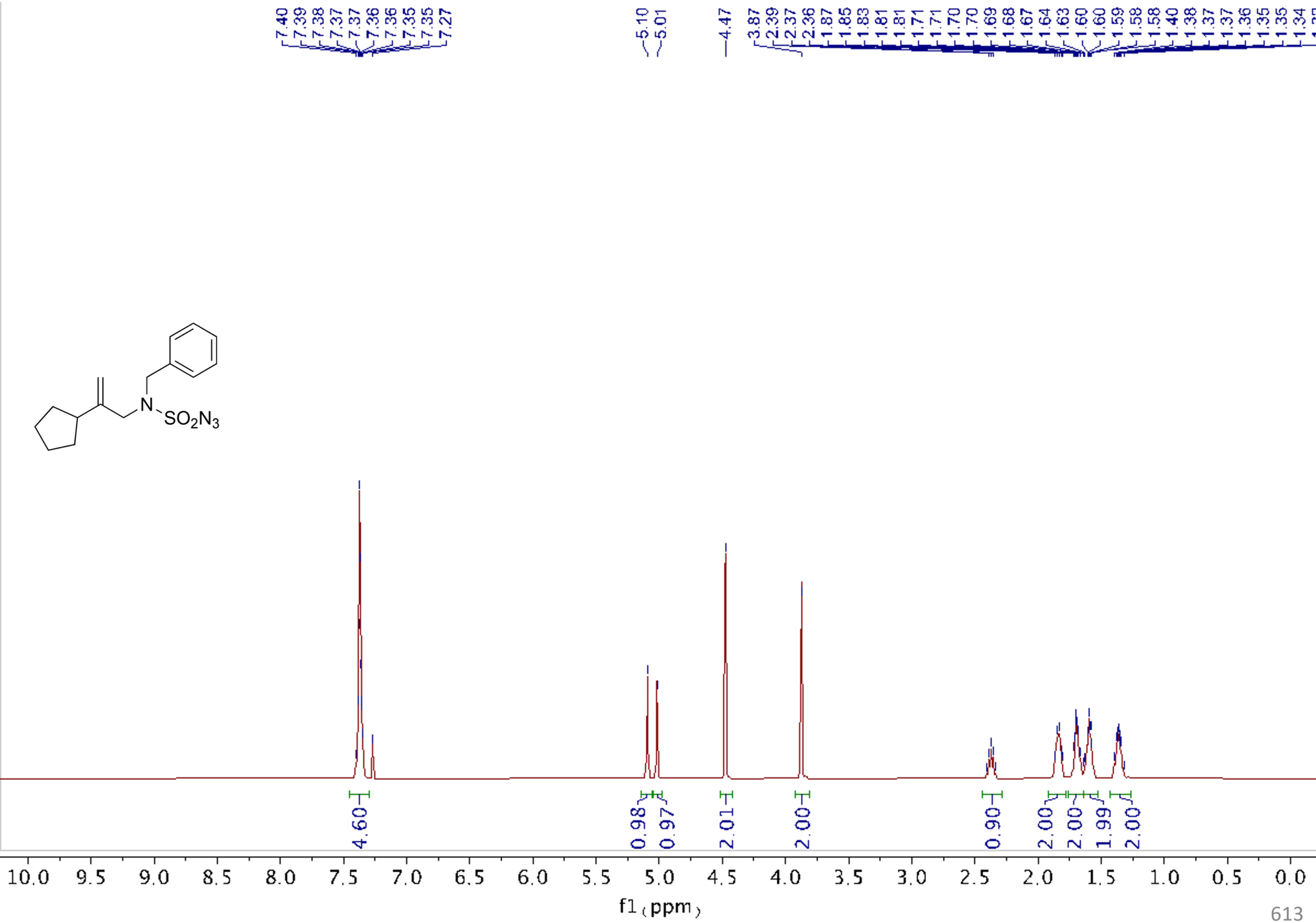
^{1}H NMR (((Azidosulfonyl)(2-cyclopropylallyl)amino)methyl)benzene 2.1x



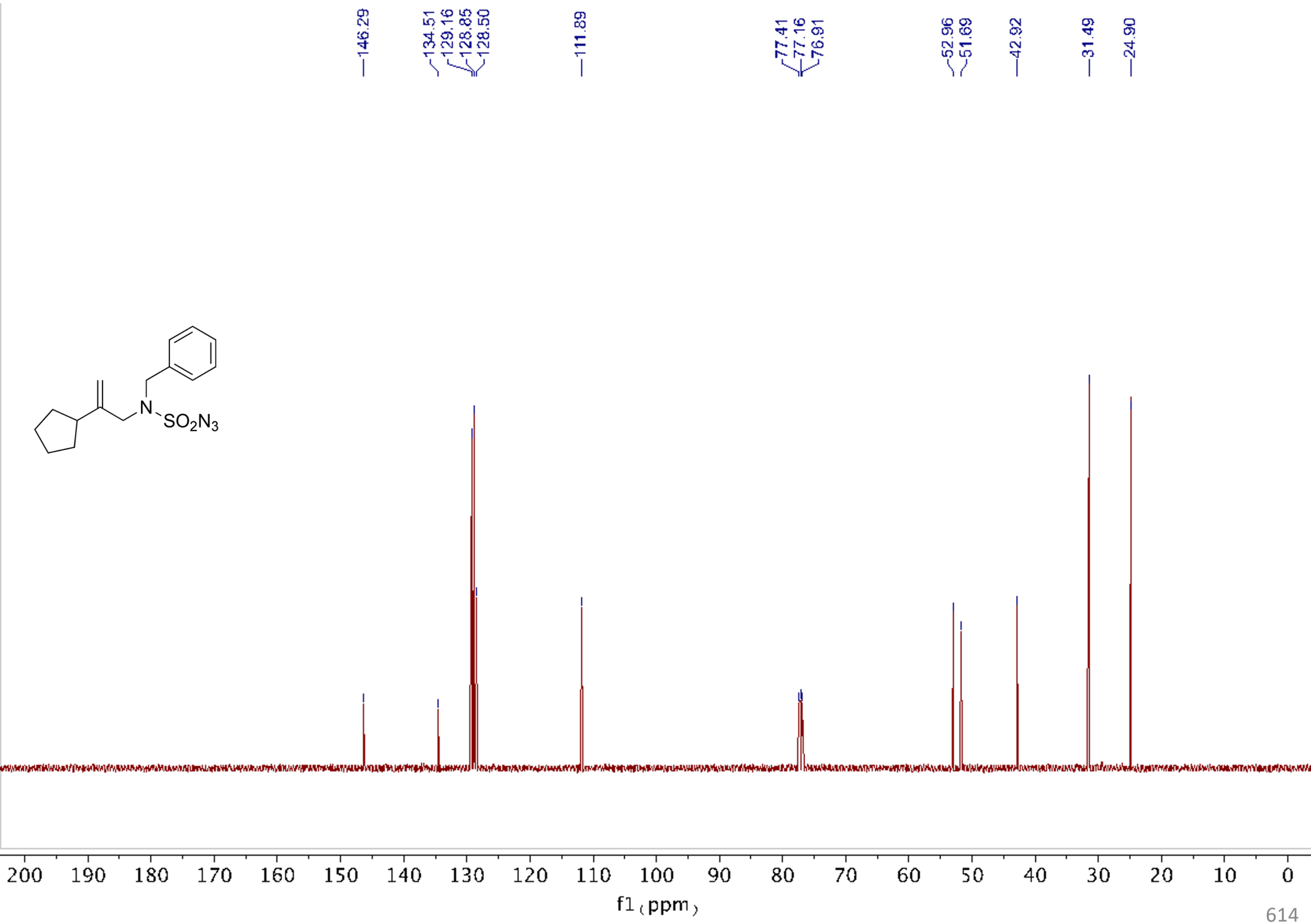
^{13}C NMR (((Azidosulfonyl)(2-cyclopropylallyl)amino)methyl)benzene 2.1x



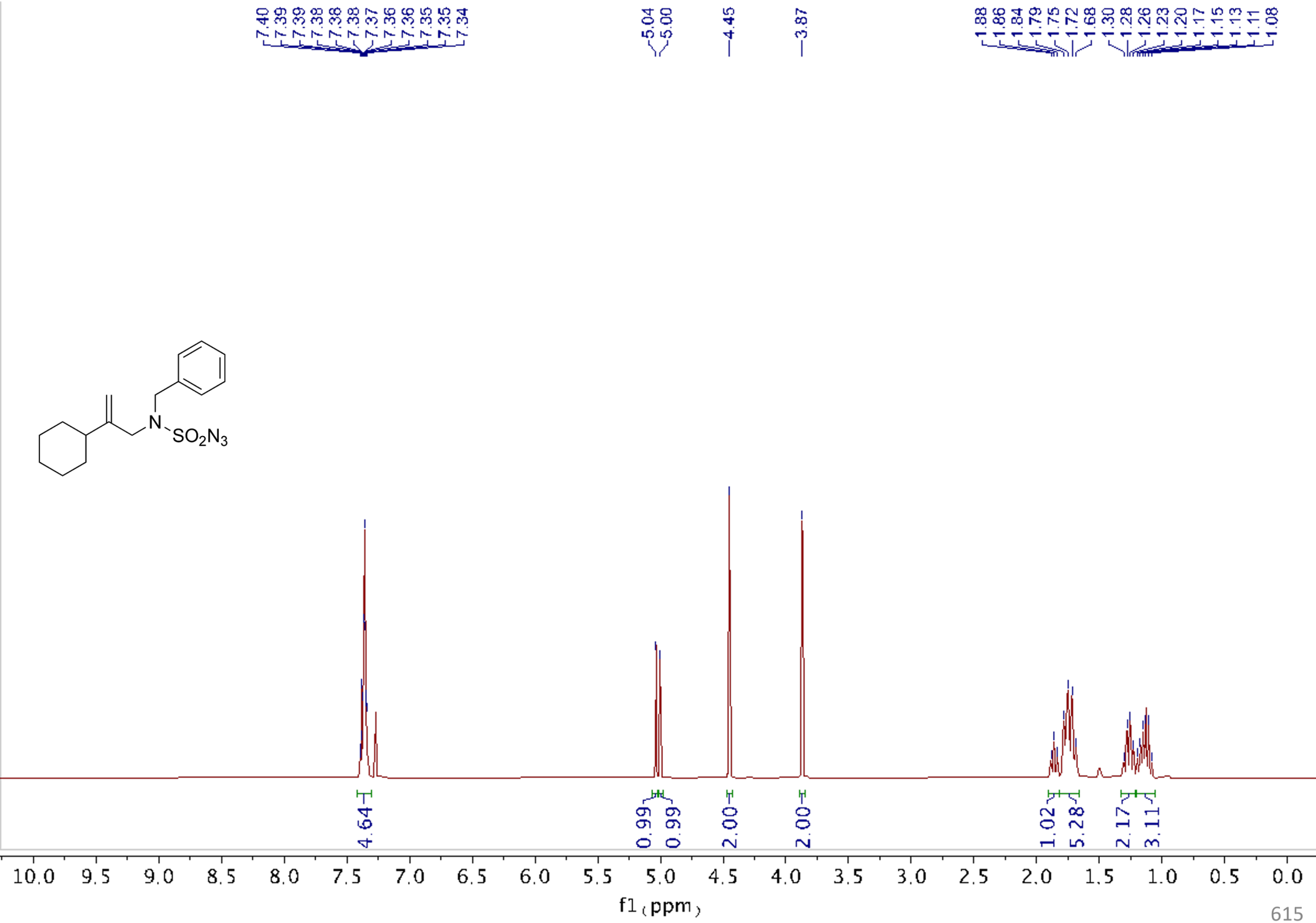
^{1}H NMR (((Azidosulfonyl)(2-cyclopentylallyl)amino)methyl)benzene 2.1y



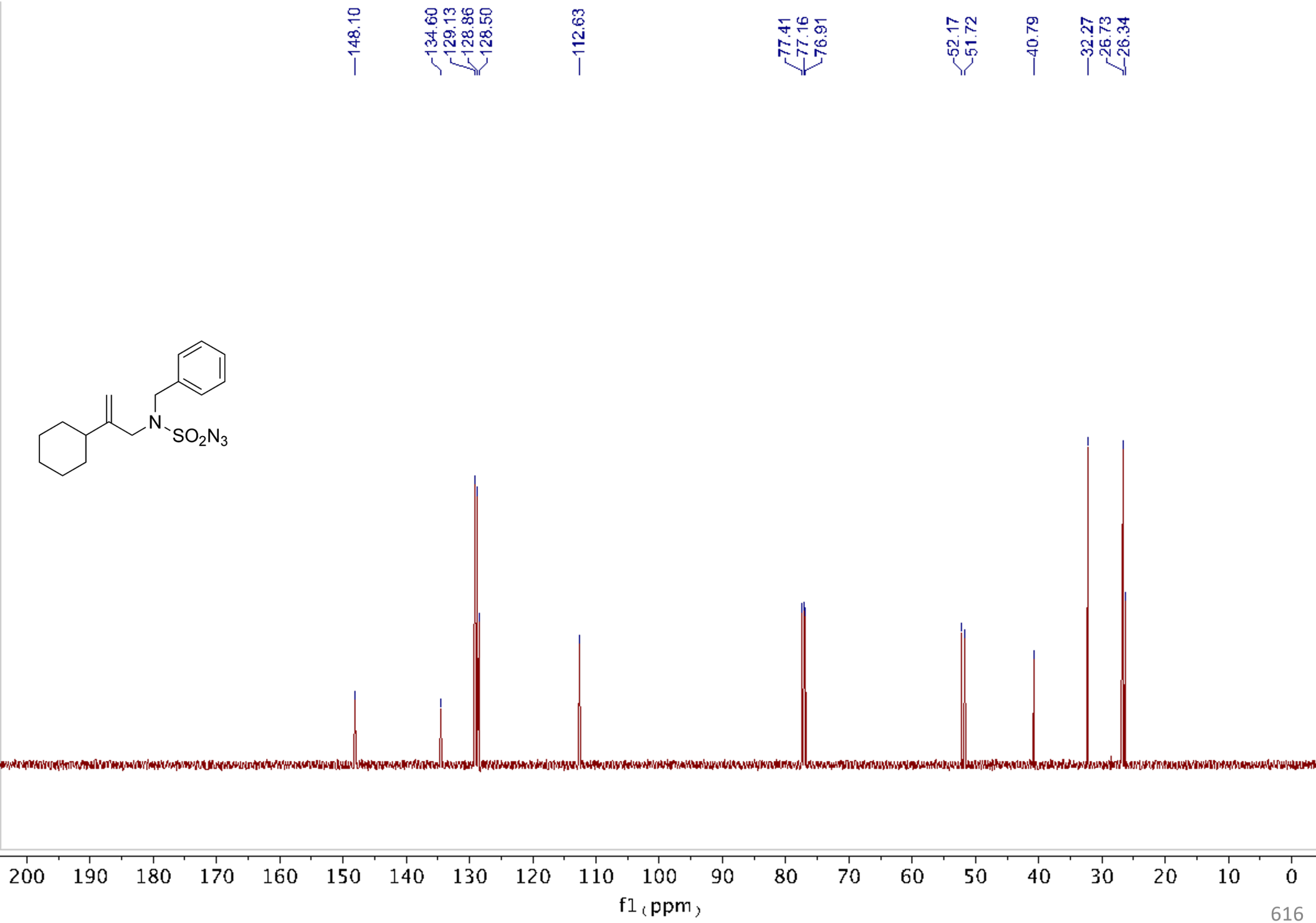
^{13}C NMR (((Azidosulfonyl)(2-cyclopentylallyl)amino)methyl)benzene 2.1y



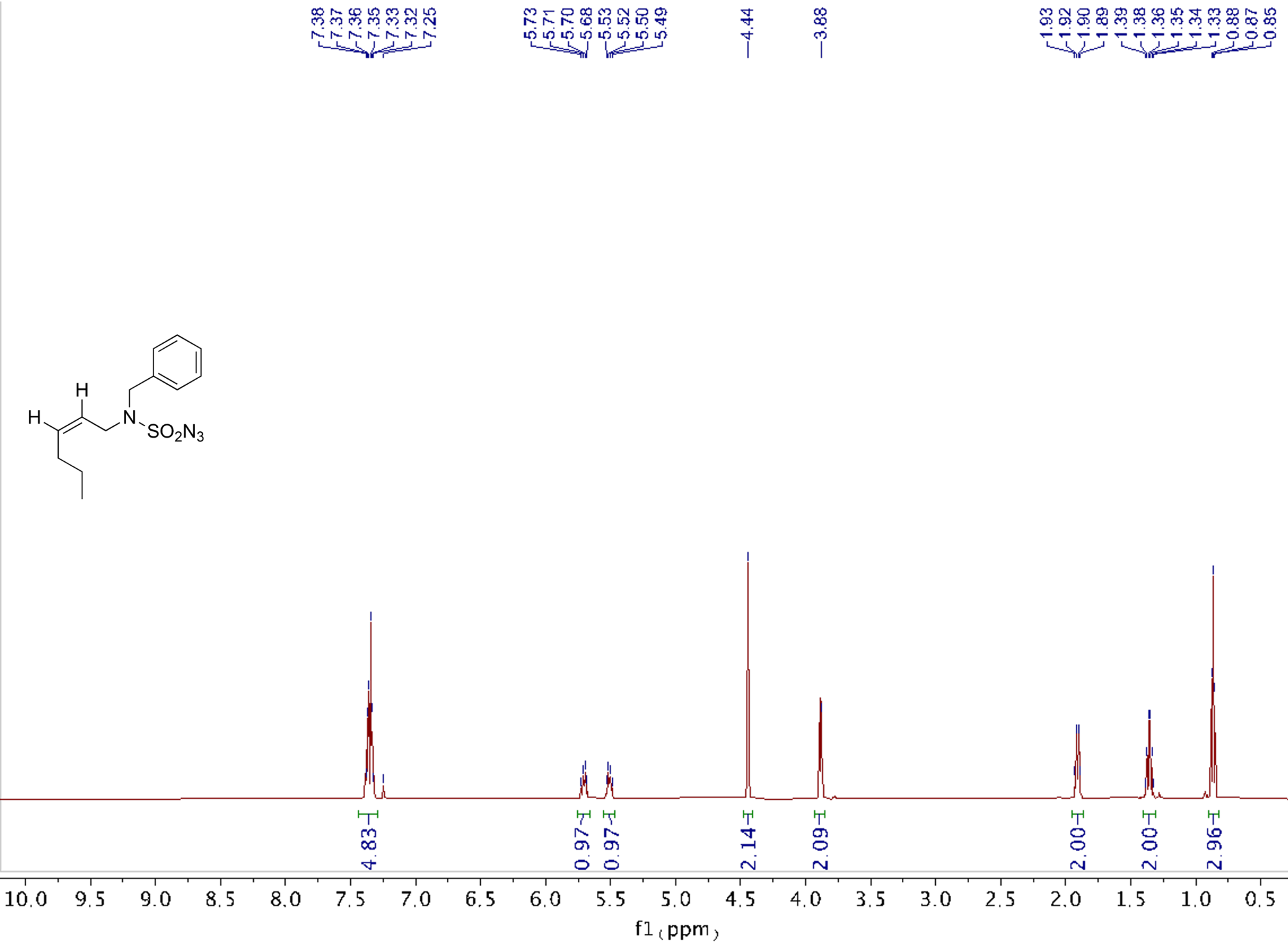
^{1}H NMR (((Azidosulfonyl)(2-cyclohexylallyl)amino)methyl)benzene 2.1z



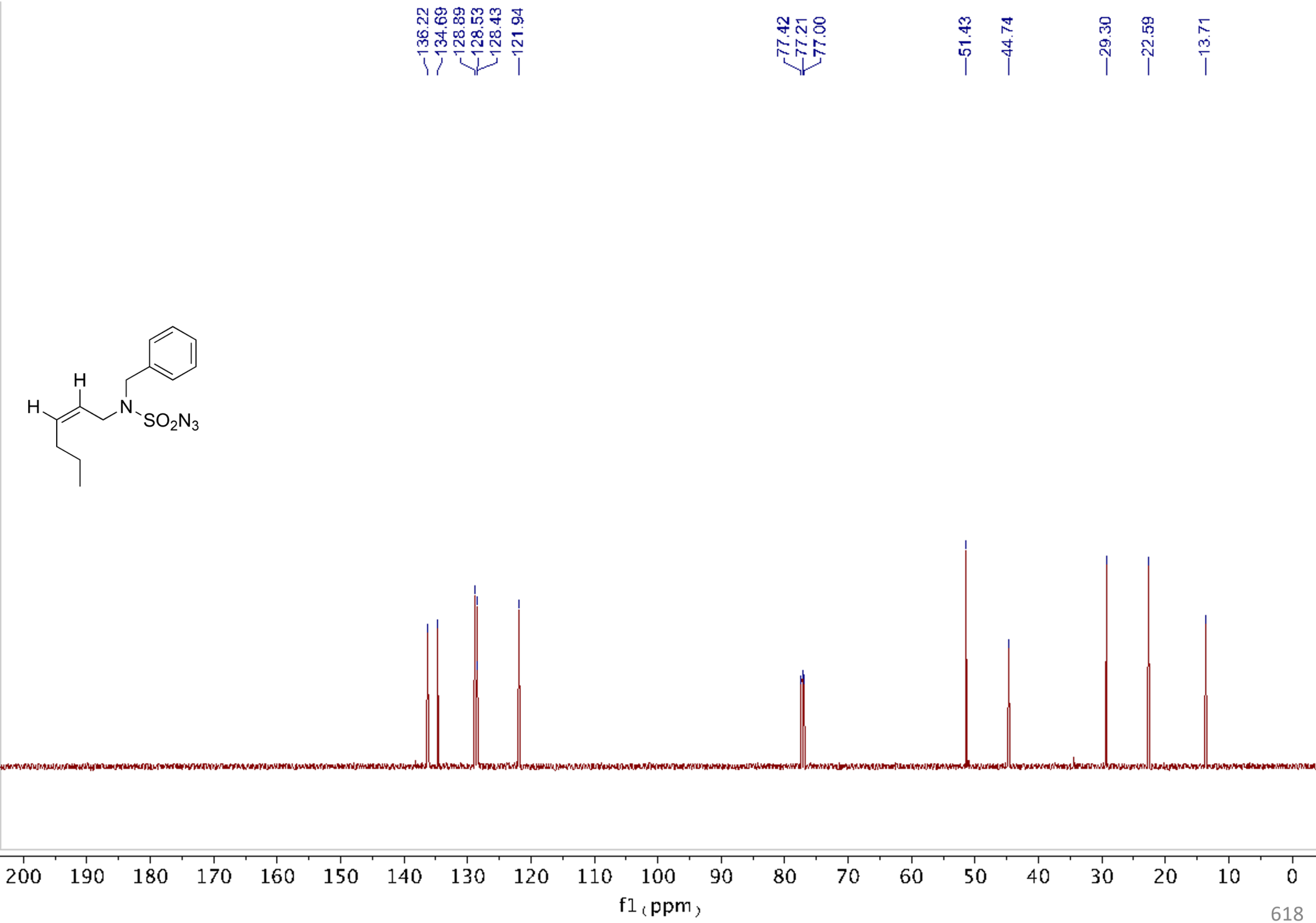
^{13}C NMR (((Azidosulfonyl)(2-cyclohexylallyl)amino)methyl)benzene 2.1z



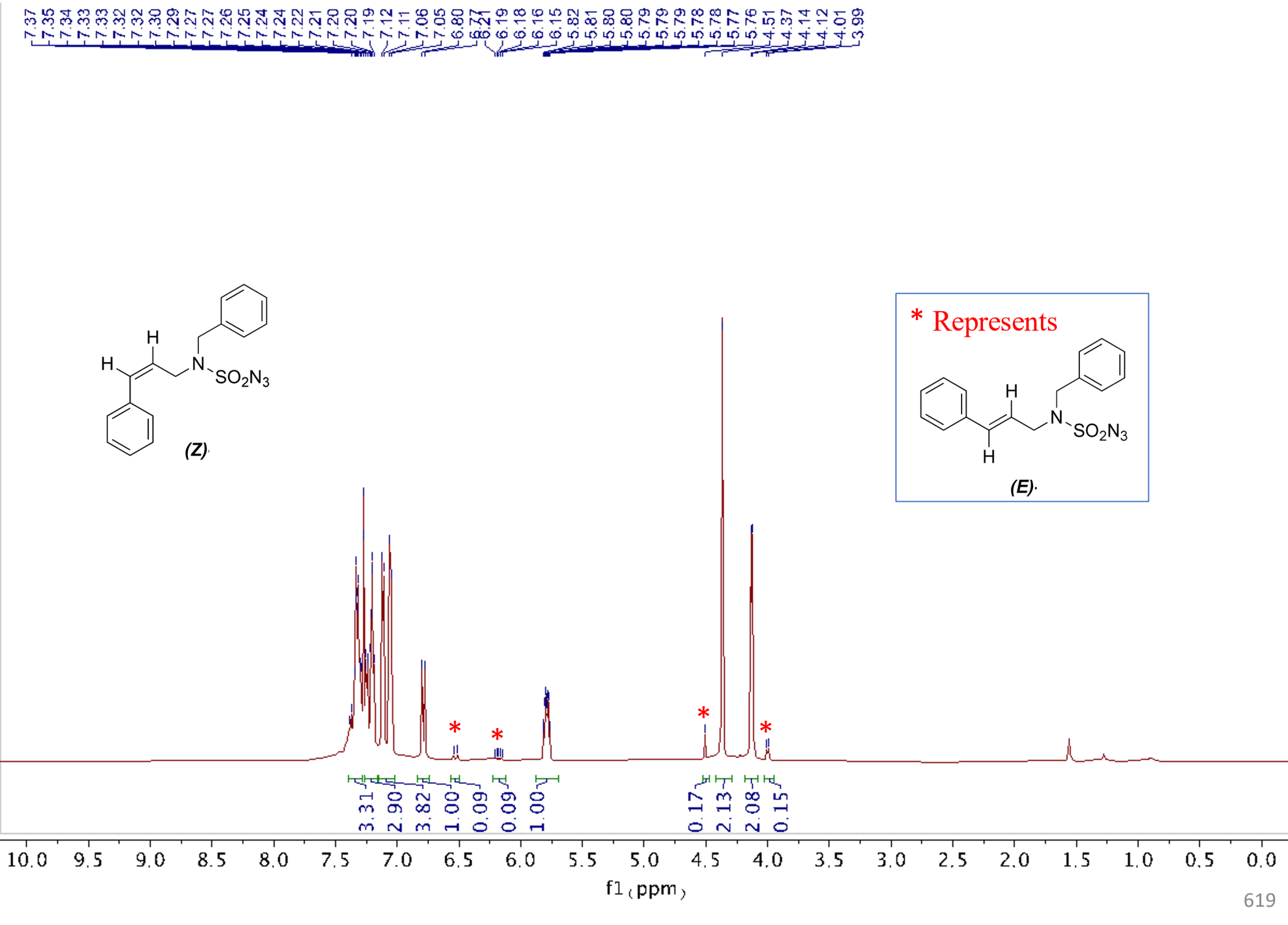
^{1}H NMR (*Z*)-(((Azidosulfonyl)(hex-2-en-1-yl)amino)methyl)benzene 2.1aa



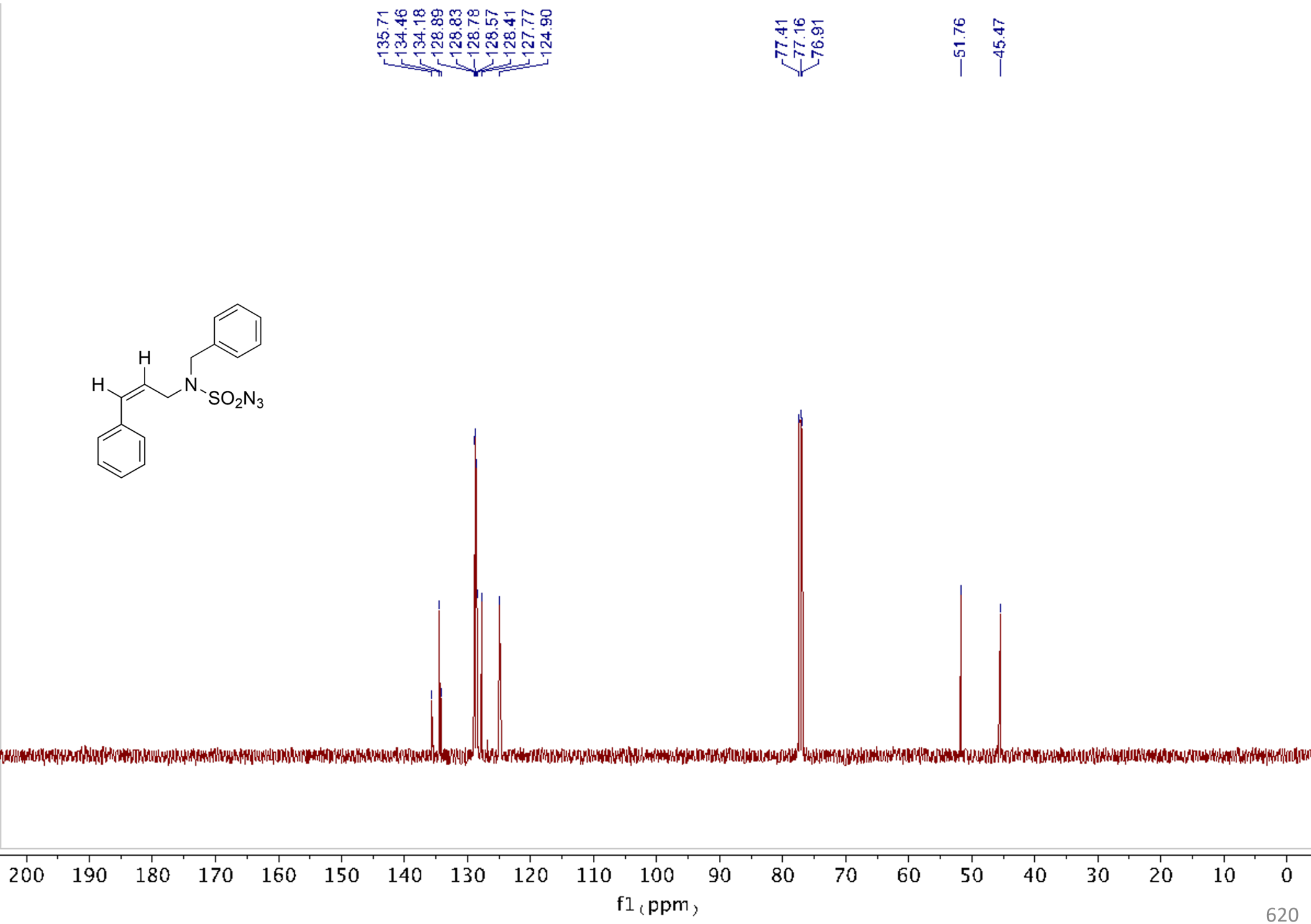
^{13}C NMR (*Z*)-(((Azidosulfonyl)(hex-2-en-1-yl)amino)methyl)benzene 2.1aa



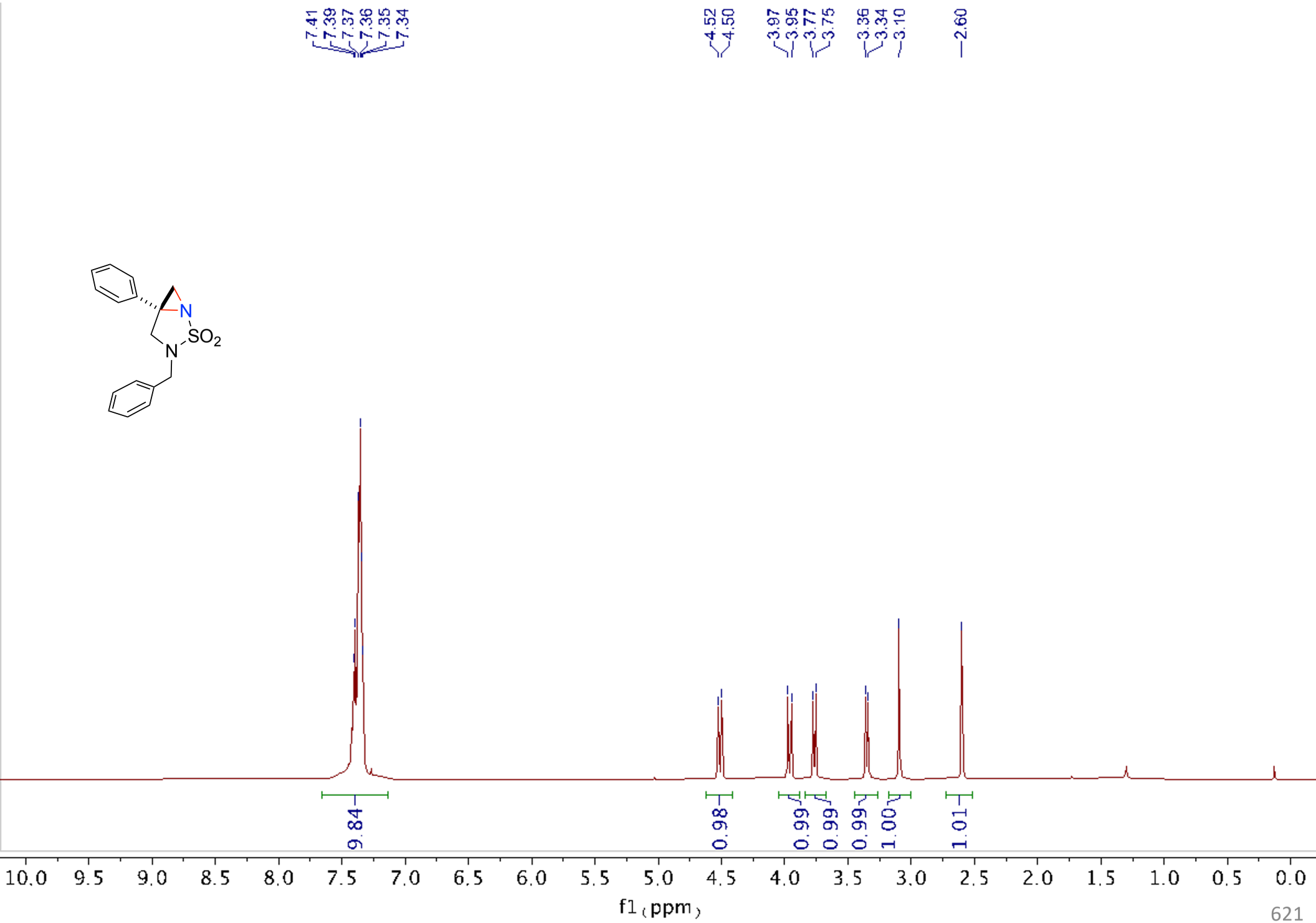
^{1}H NMR (*Z*)-(((Azidosulfonyl)(3-phenylallyl)amino)methyl)benzene 2.1ab



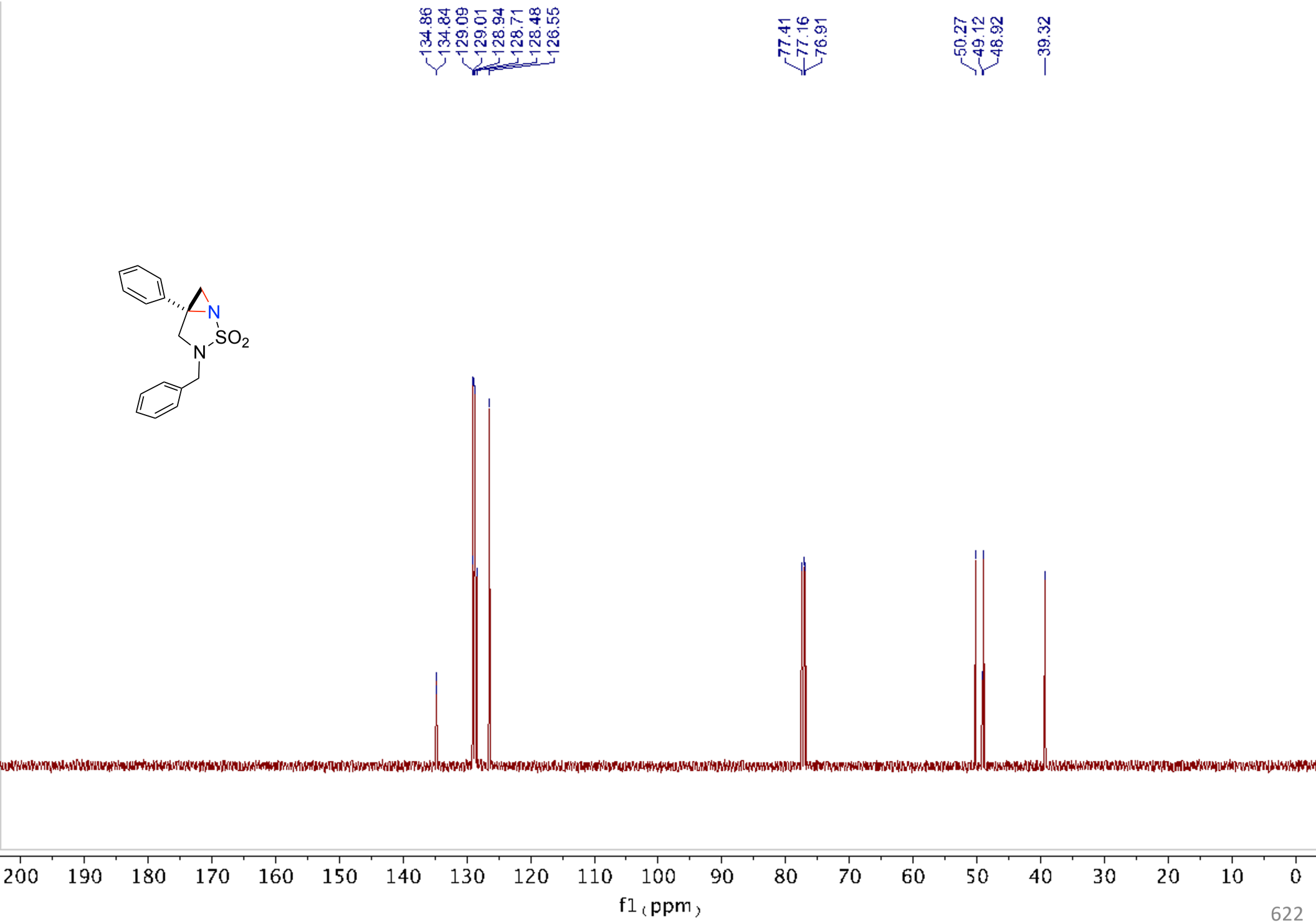
^{13}C NMR (*Z*)-(((Azidosulfonyl)(3-phenylallyl)amino)methyl)benzene 2.1ab



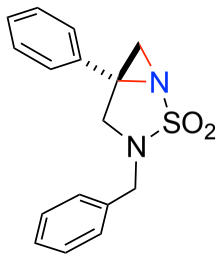
^{1}H NMR (*R*)-3-Benzyl-5-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2a



^{13}C NMR (*R*)-3-Benzyl-5-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2a



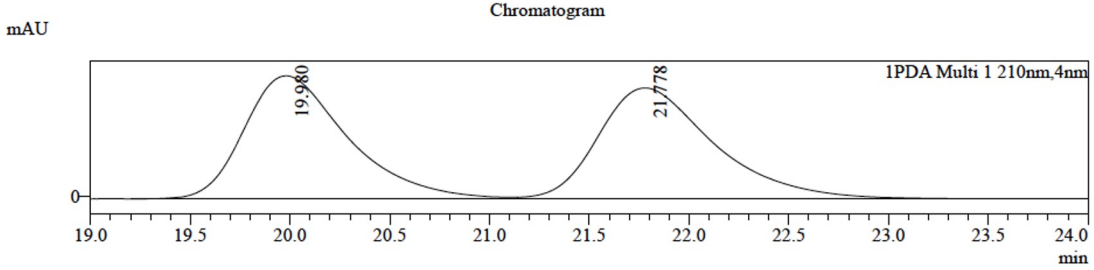
3-Benzyl-5-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2a



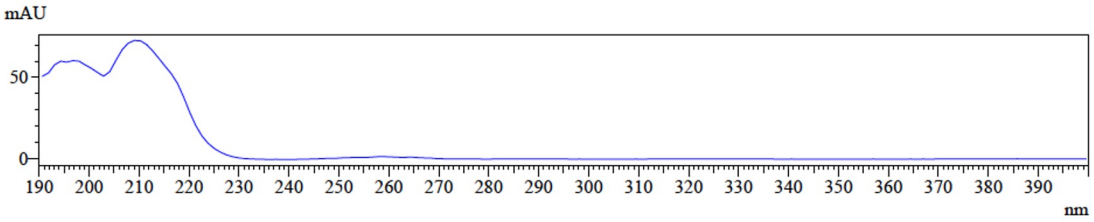
Sample Information

Data File	: H0X-0243_3-ODH-15%1.0mL.lcd
Sample Name	: H0X-0243_3-ODH-15%1.0mL
Sample ID	: H0X-0243_3-ODH-15%1.0mL
Method File	: H0X-15%-1.0ml-30MIN.lcm

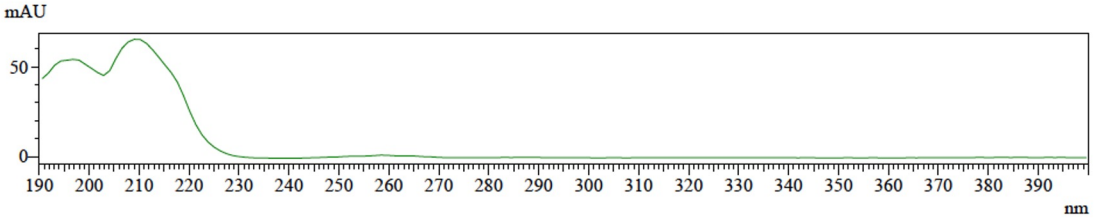
Chromatogram



UV Spectrum
Retention time = 19.980



UV Spectrum
Retention time = 21.778

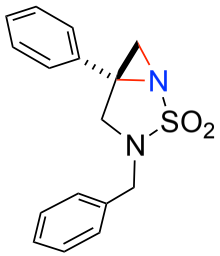


Peak Table

PDA Ch1 210nm

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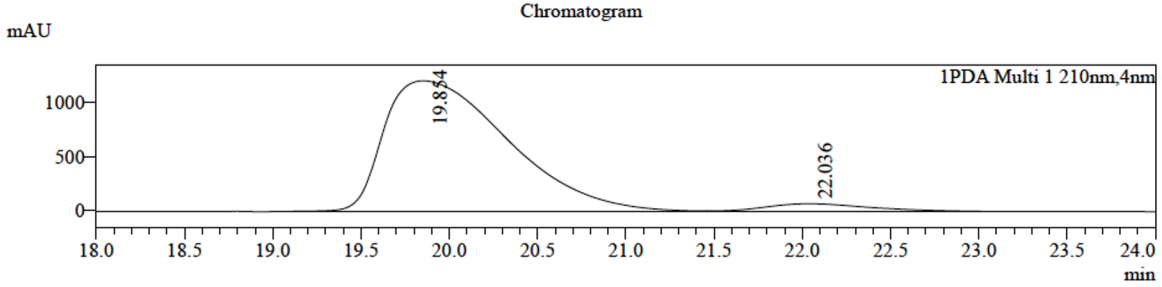
(*R*)-3-Benzyl-5-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2a



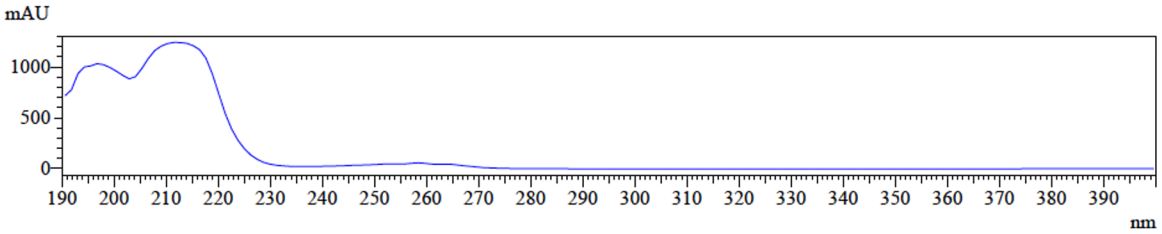
Sample Information

Data File	: H0X-0301-ODH-15%1.0mL.lcd
Sample Name	: H0X-0301-ODH-15%1.0mL
Sample ID	: H0X-0301-ODH-15%1.0mL
Method File	: H0X-15%-1.0ml-30MIN.lcm

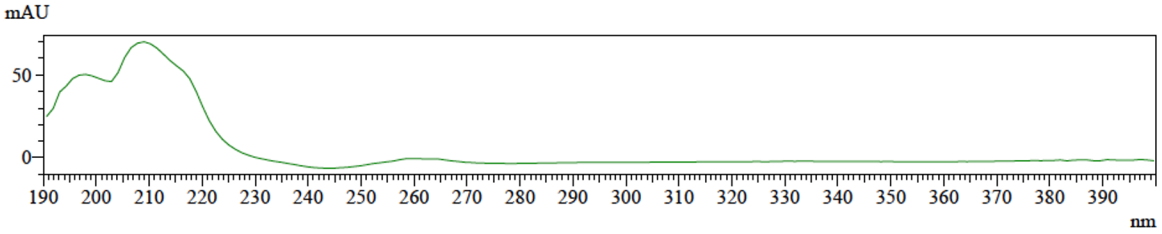
Chromatogram



UV Spectrum
Retention time = 19.854



UV Spectrum
Retention time = 22.036

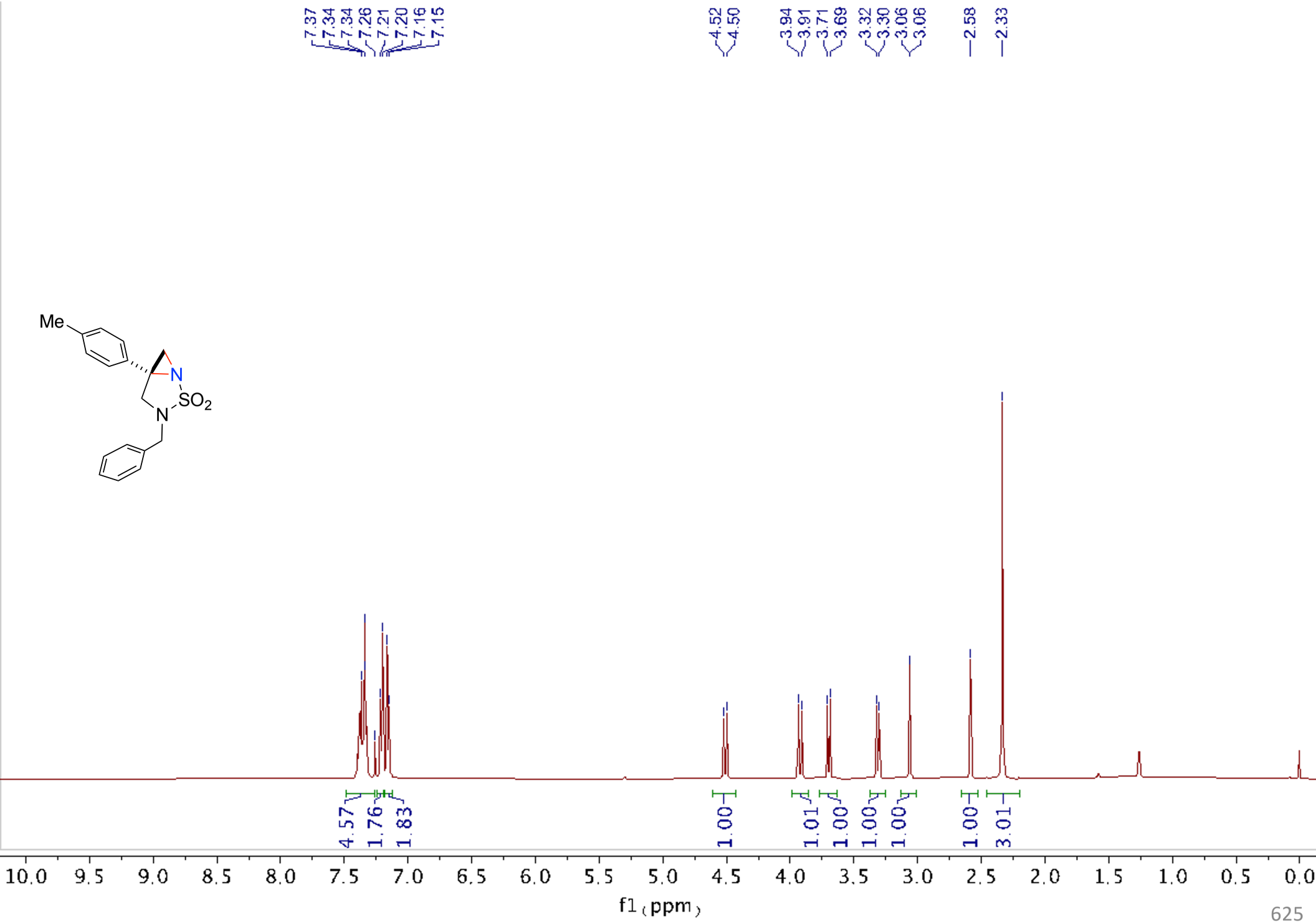


Peak Table

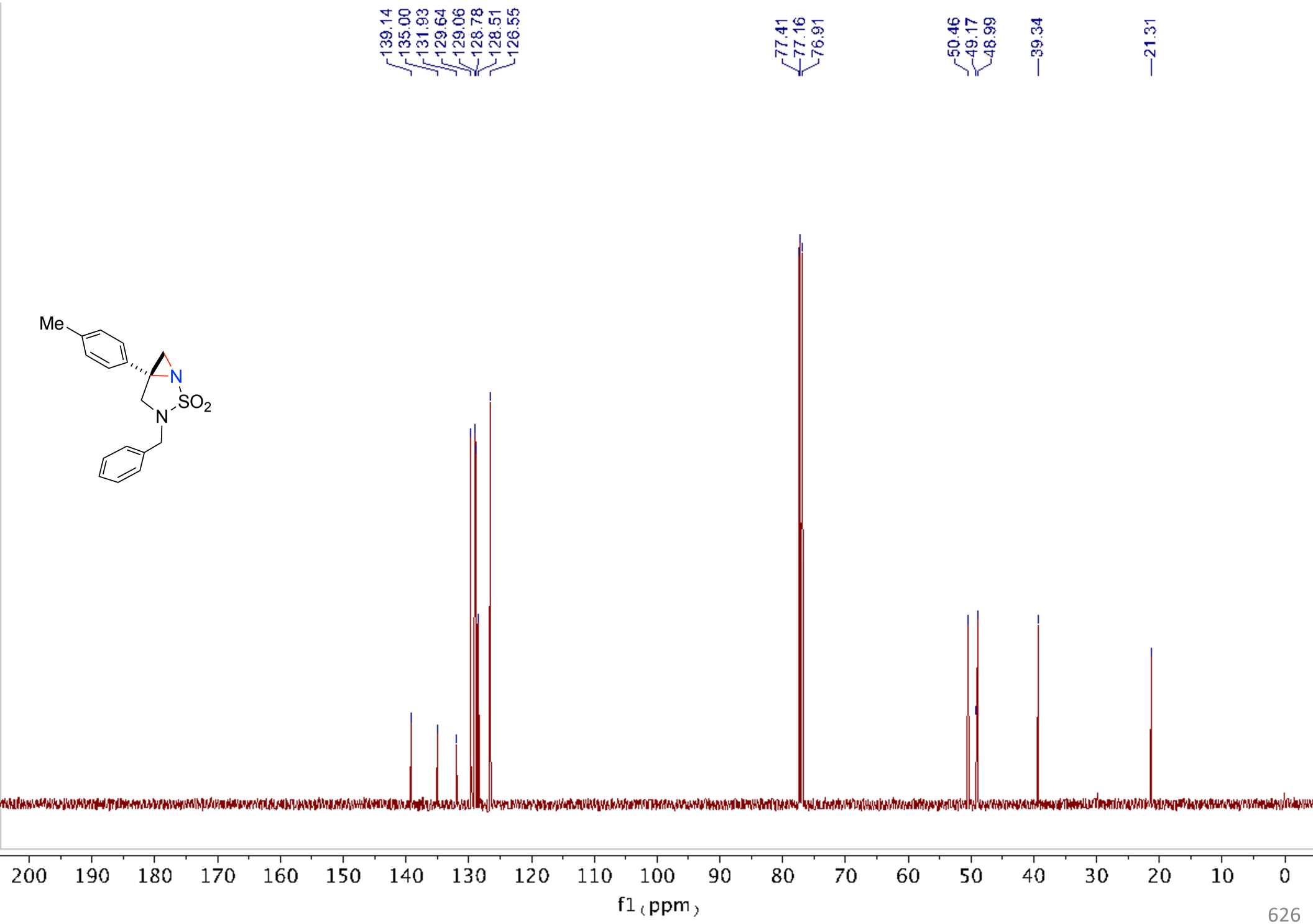
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	19.854	58780429	95.125
2	22.036	3012479	4.875
Total		61792908	100.000

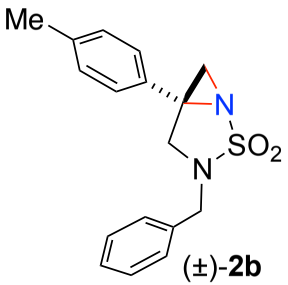
^{1}H NMR (*R*)-3-Benzyl-5-(*p*-tolyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2b



^{13}C NMR (*R*)-3-Benzyl-5-(*p*-tolyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2b



3-Benzyl-5-(*p*-tolyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2b

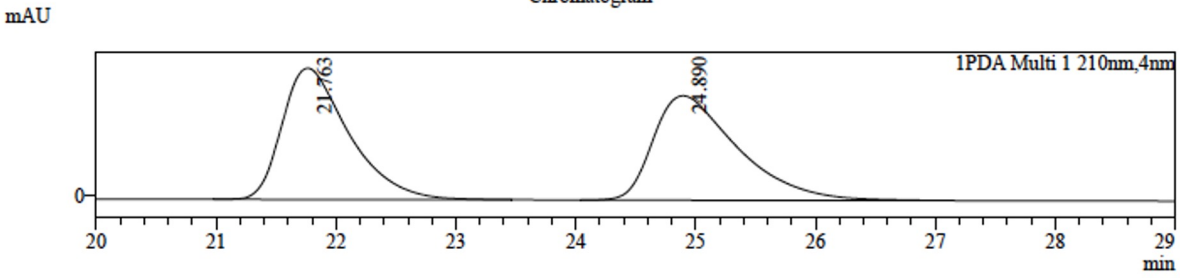


(±)-**2b**

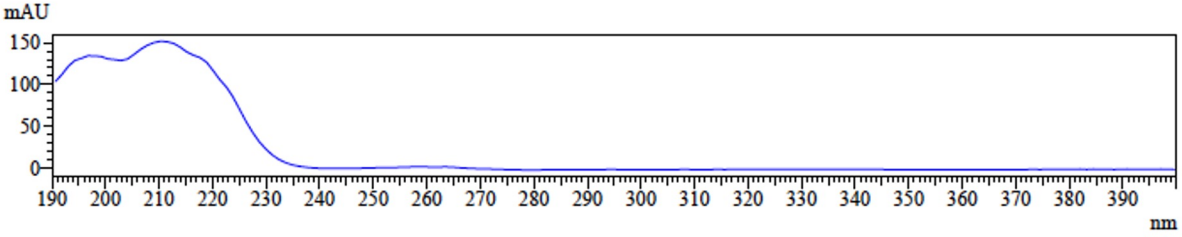
Sample Information

Data File	: H0X-0442_2nd-ODH-10%1.0mL.lcd
Sample Name	: H0X-0442_2nd-ODH-10%1.0mL
Sample ID	: H0X-0442_2nd-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-40MIN.lcm

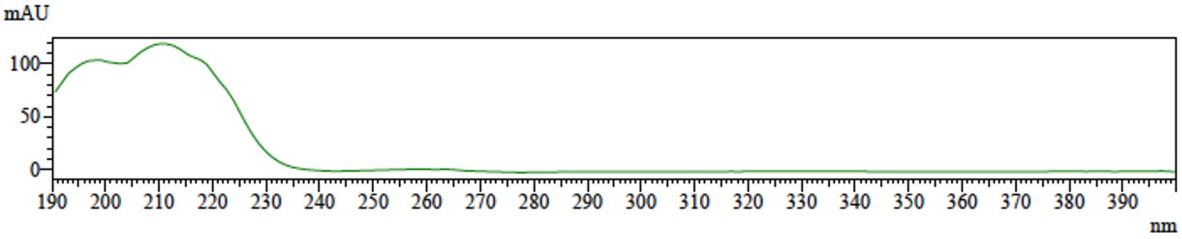
Chromatogram



UV Spectrum
Retention time = 21.763



UV Spectrum
Retention time = 24.890

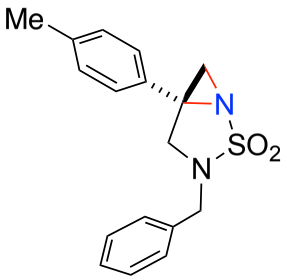


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
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2	24.890	5906934	50.072
Total		11796793	100.000

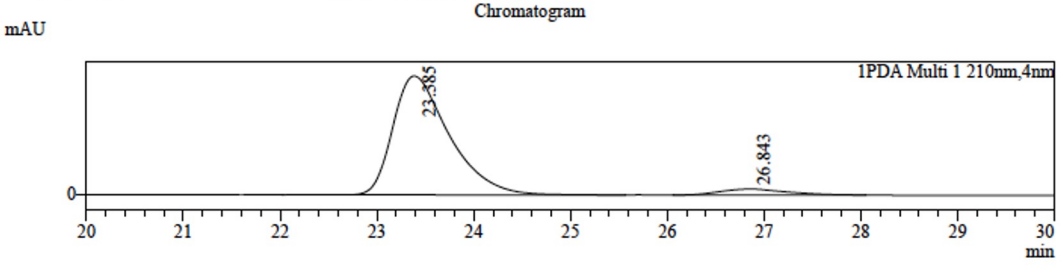
(*R*)-3-Benzyl-5-(*p*-tolyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2b



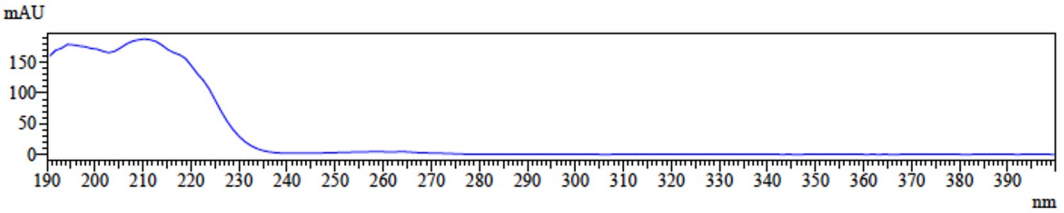
Sample Information

Data File	: H0X-0443-ODH-10%1.0mL.lcd
Sample Name	: H0X-0443-ODH-10%1.0mL
Sample ID	: H0X-0443-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-90MIN.lcm

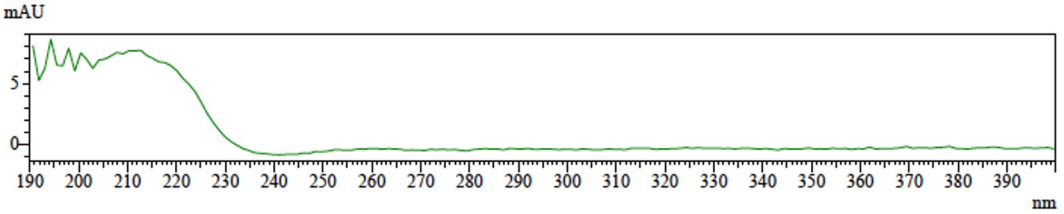
Chromatogram



UV Spectrum
Retention time = 23.385



UV Spectrum
Retention time = 26.843

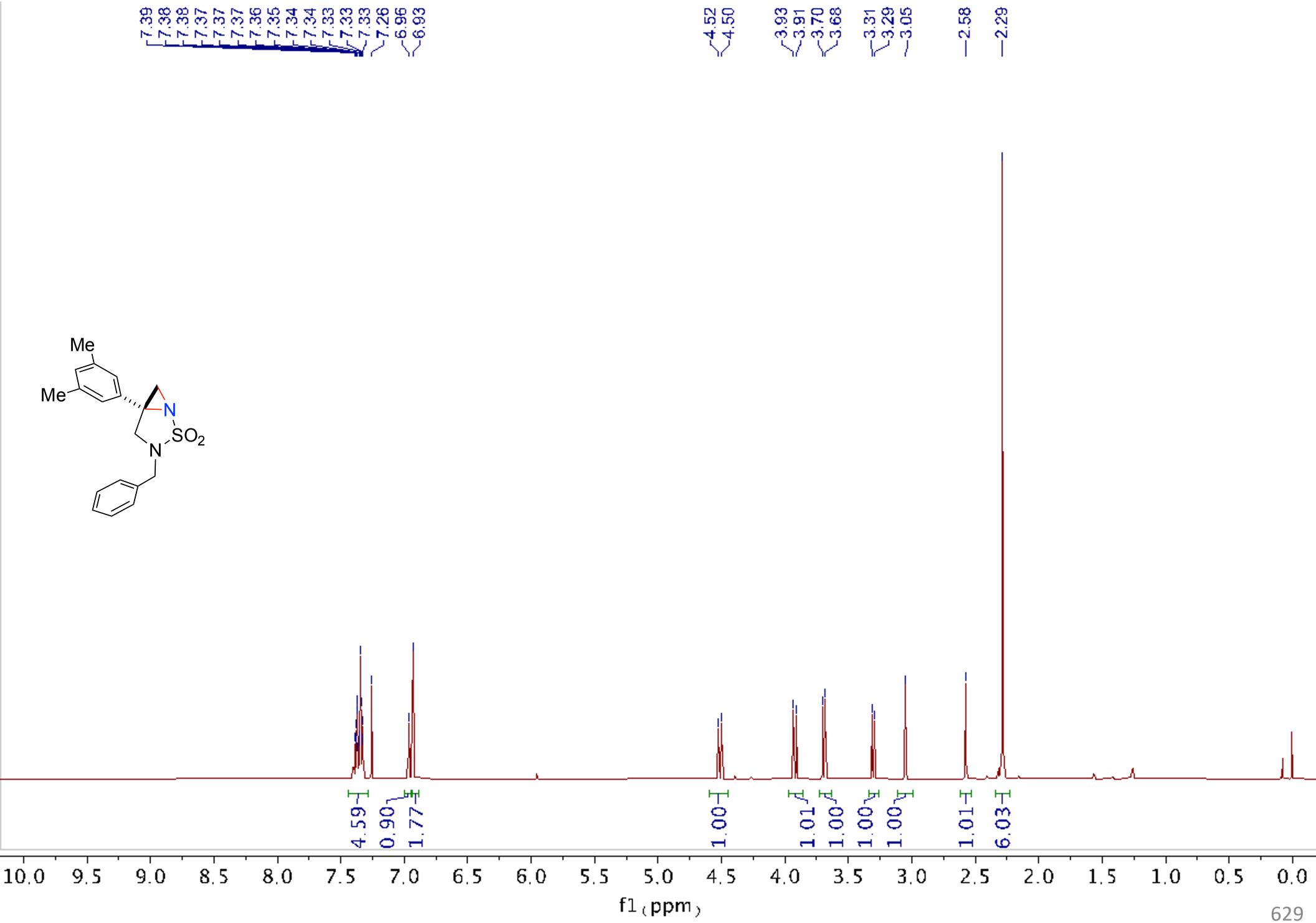


Peak Table

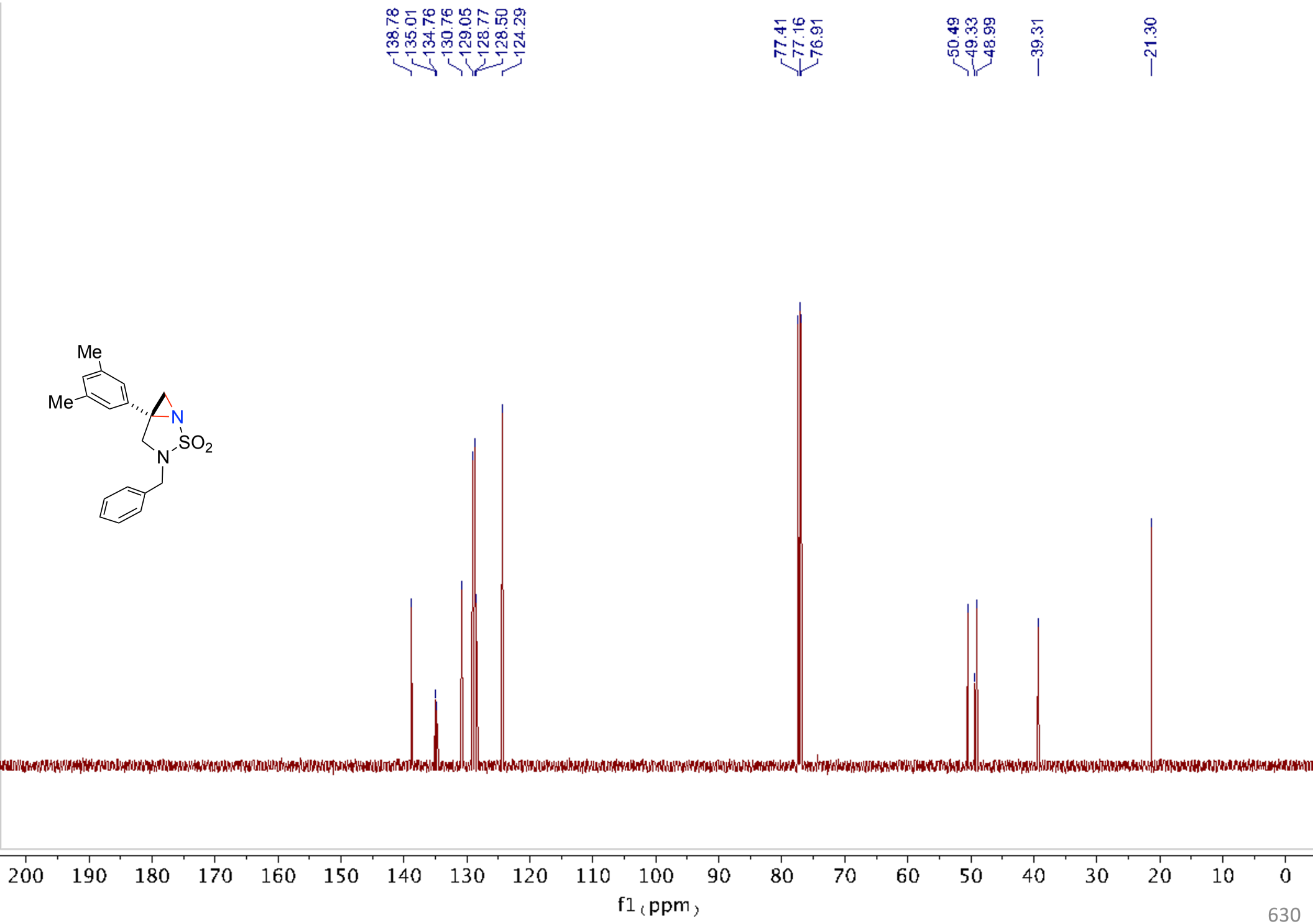
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	23.385	7494835	94.280
2	26.843	454733	5.720
Total		7949568	100.000

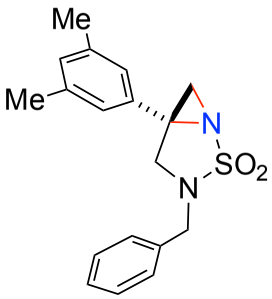
^{1}H NMR (*R*)-3-Benzyl-5-(3,5-dimethylphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2c



^{13}C NMR (*R*)-3-Benzyl-5-(3,5-dimethylphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2c



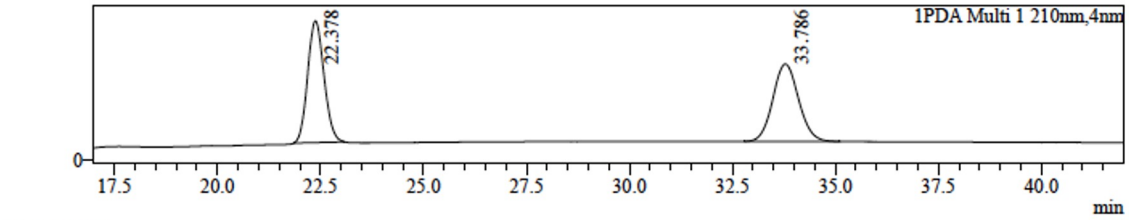
3-Benzyl-5-(3,5-dimethylphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2c



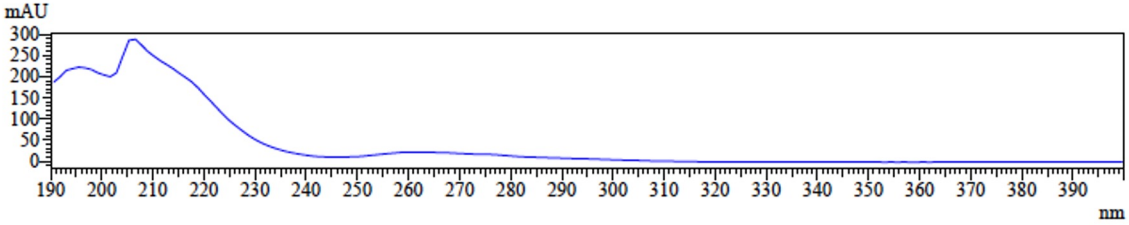
Sample Information

Data File	: H0X-0496-IC-20%1.0mL.lcd
Sample Name	: H0X-0496-IC-20%1.0mL
Sample ID	: H0X-0496-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

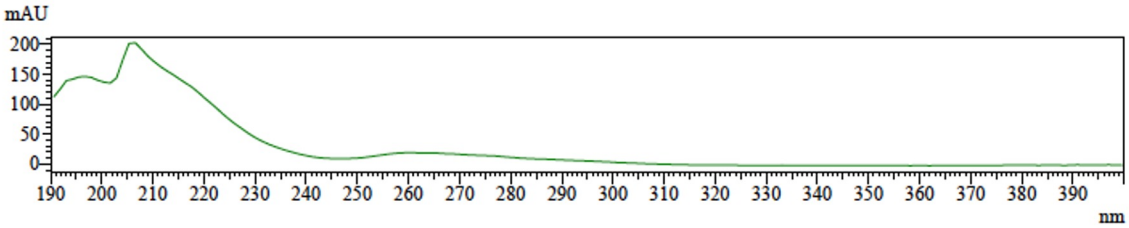
Chromatogram



UV Spectrum
Retention time = 22.378



UV Spectrum
Retention time = 33.786

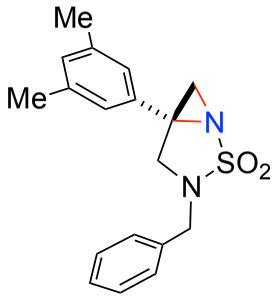


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	22.378	6013374	50.002
2	33.786	6012865	49.998
Total		12026238	100.000

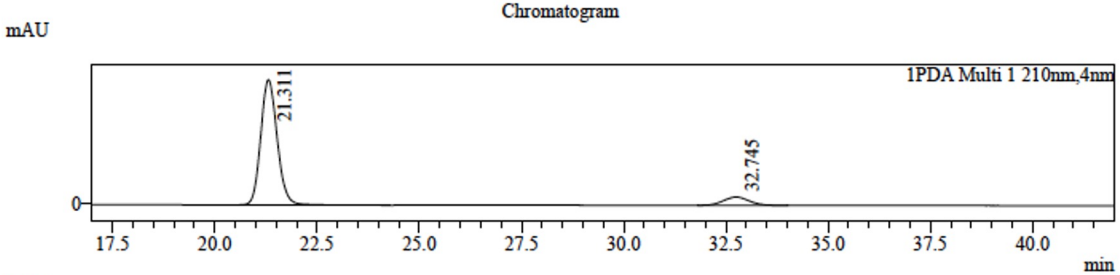
(*R*)-3-Benzyl-5-(3,5-dimethylphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2c



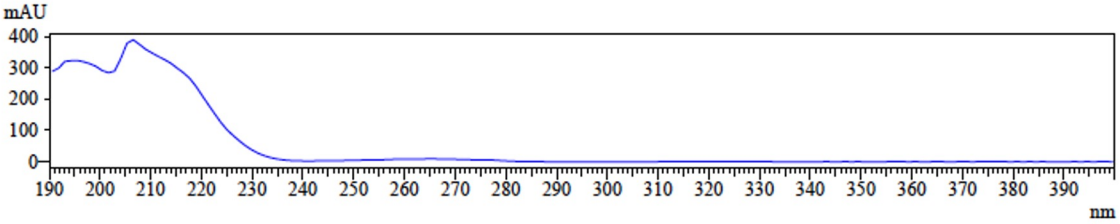
Sample Information

Data File	: H0X-0497-IC-20%1.0mL.lcd
Sample Name	: H0X-0497-IC-20%1.0mL
Sample ID	: H0X-0497-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

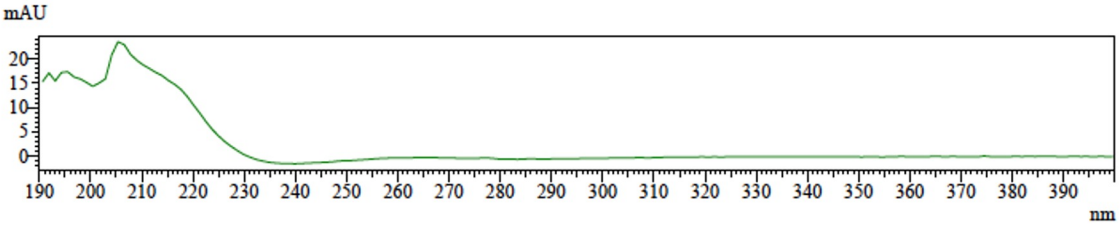
Chromatogram



UV Spectrum
Retention time = 21.311



UV Spectrum
Retention time = 32.745

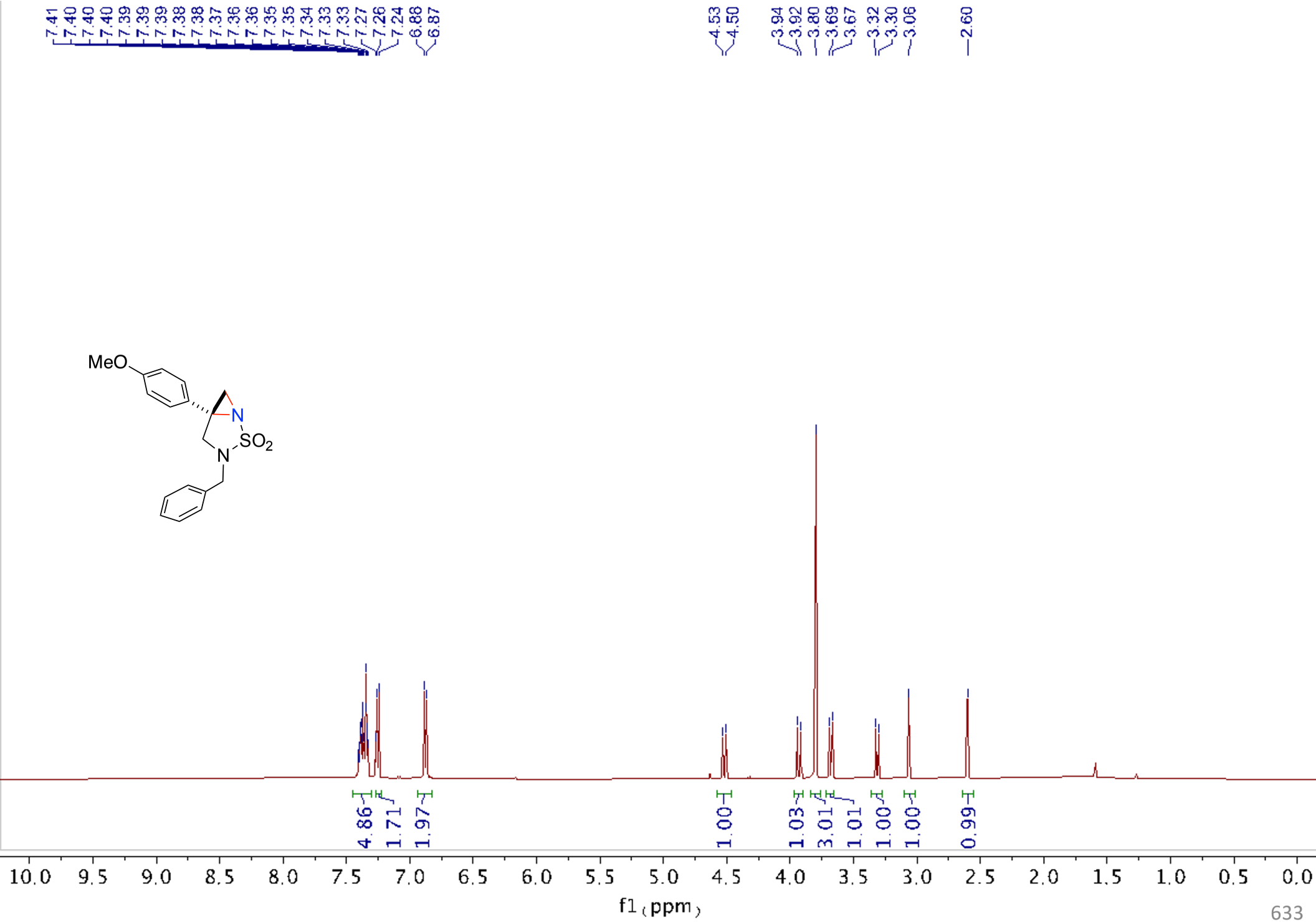


Peak Table

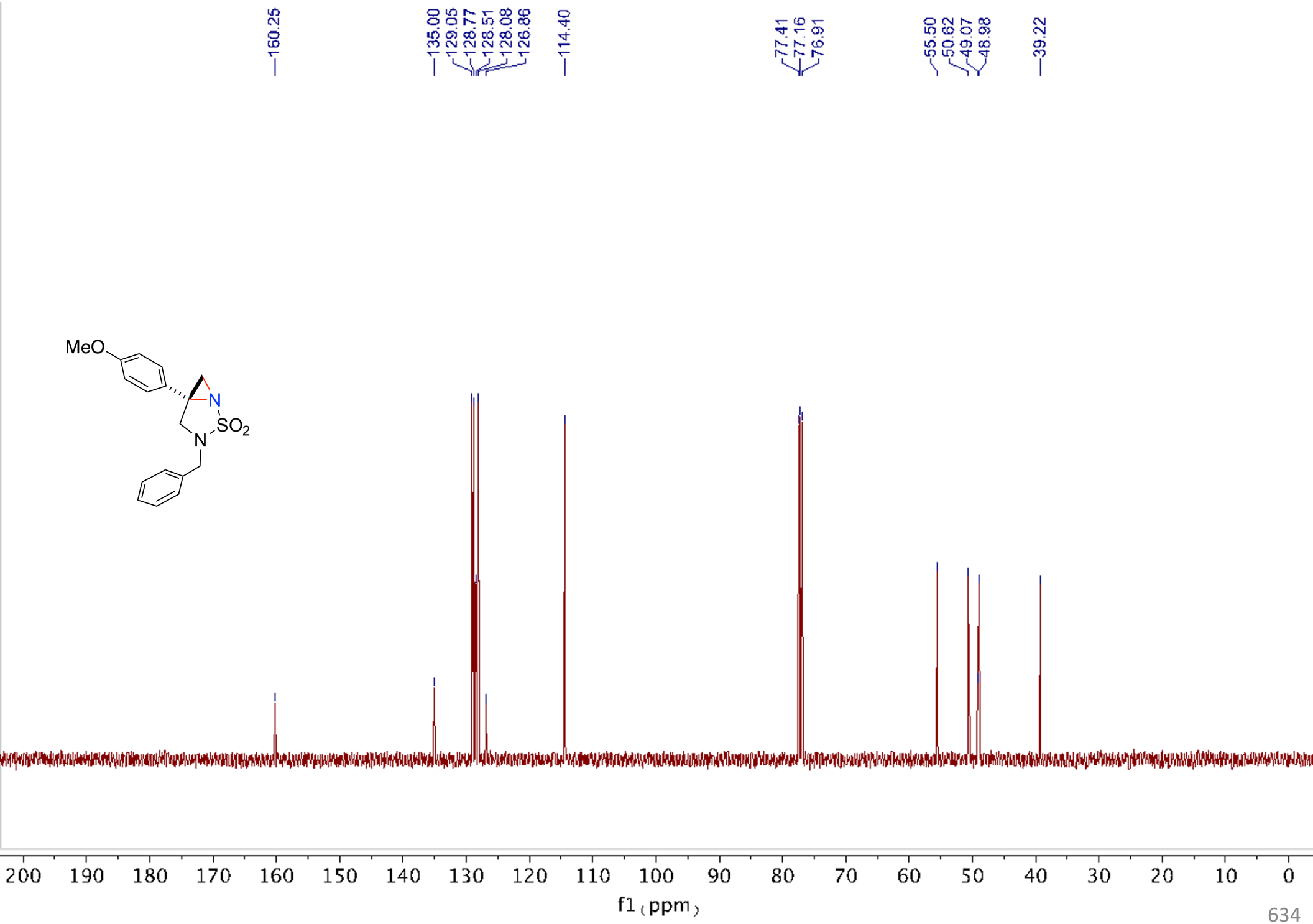
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	21.311	9816052	90.703
2	32.745	1006080	9.297
Total		10822132	100.000

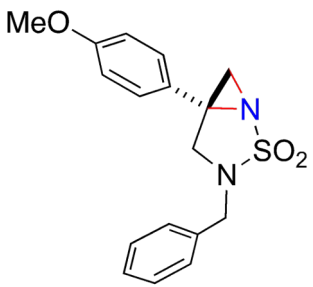
^{1}H NMR (*R*)-3-Benzyl-5-(4-methoxyphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2d



^{13}C NMR (*R*)-3-Benzyl-5-(4-methoxyphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2d



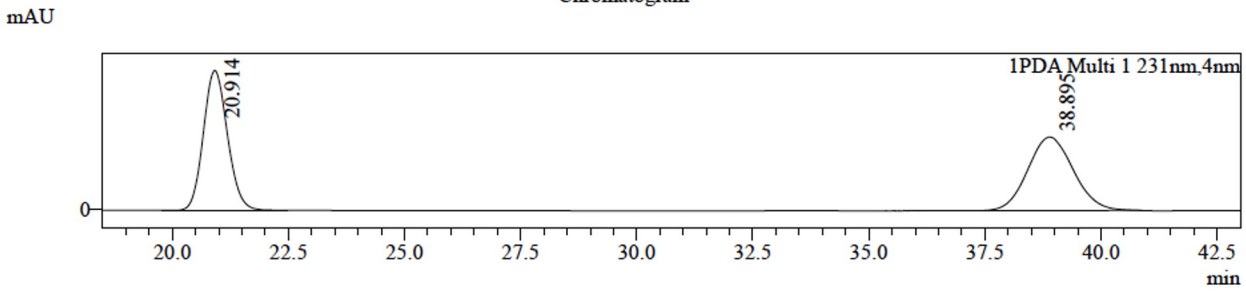
3-Benzyl-5-(4-methoxyphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2d



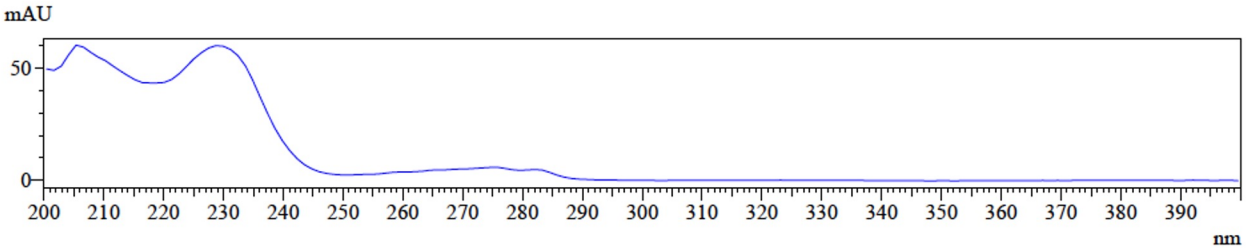
Sample Information

Data File	: H0X-0871-IC-30%1.0mL.lcd
Sample Name	: H0X-0871-IC-30%1.0mL
Sample ID	: H0X-0871-IC-30%1.0mL
Method File	: H0X-30%-1.0ml--60MIN.lcm

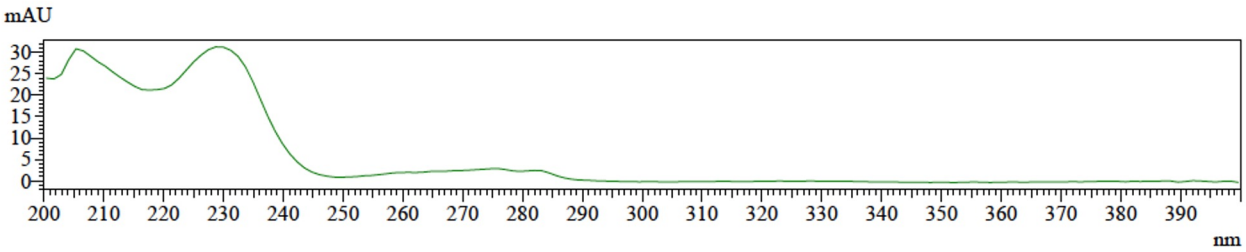
Chromatogram



UV Spectrum
Retention time = 20.914



UV Spectrum
Retention time = 38.895

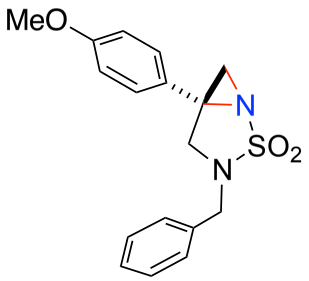


Peak Table

PDA Ch1 231nm

Peak#	Ret. Time	Area	Area%
1	20.914	2004743	50.074
2	38.895	1998813	49.926
Total		4003556	100.000

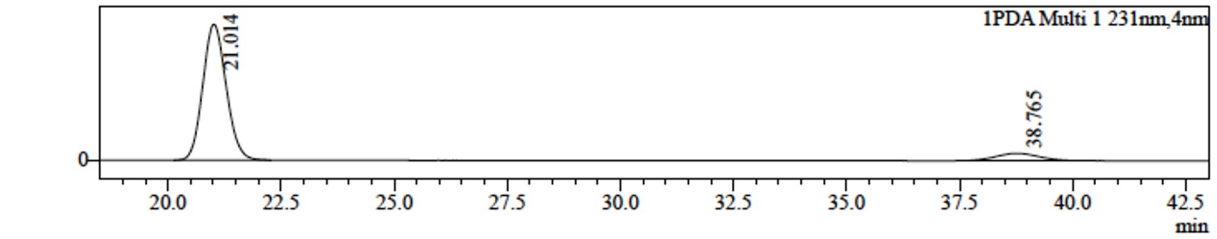
(*R*)-3-Benzyl-5-(4-methoxyphenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2d



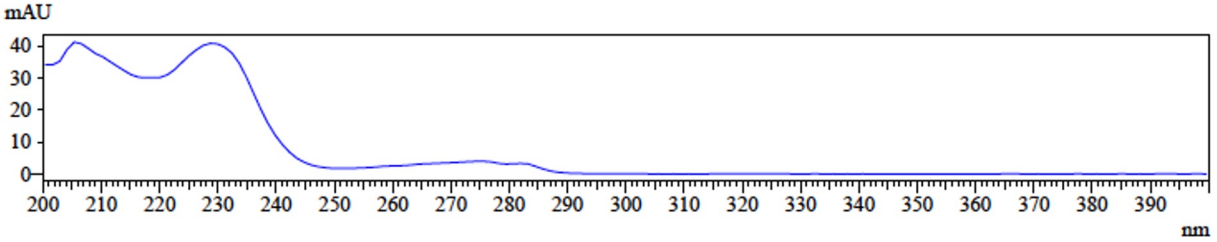
Sample Information

Data File	: H0X-0872_2-IC-30%1.0mL.lcd
Sample Name	: H0X-0872_2-IC-30%1.0mL
Sample ID	: H0X-0872_2-IC-30%1.0mL
Method File	: H0X-30%-1.0ml--60MIN.lcm

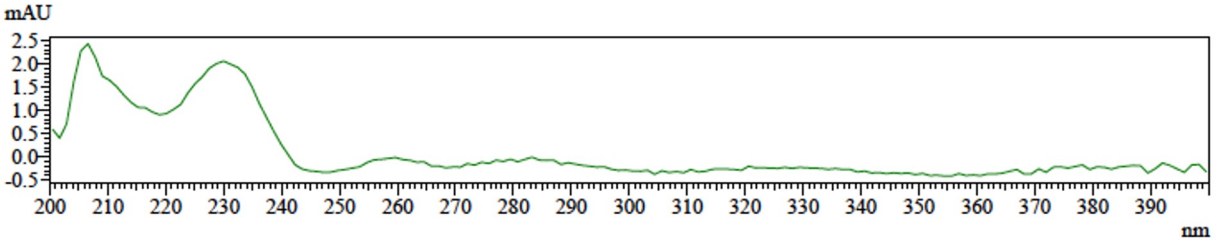
Chromatogram



UV Spectrum
Retention time = 21.014



UV Spectrum
Retention time = 38.765

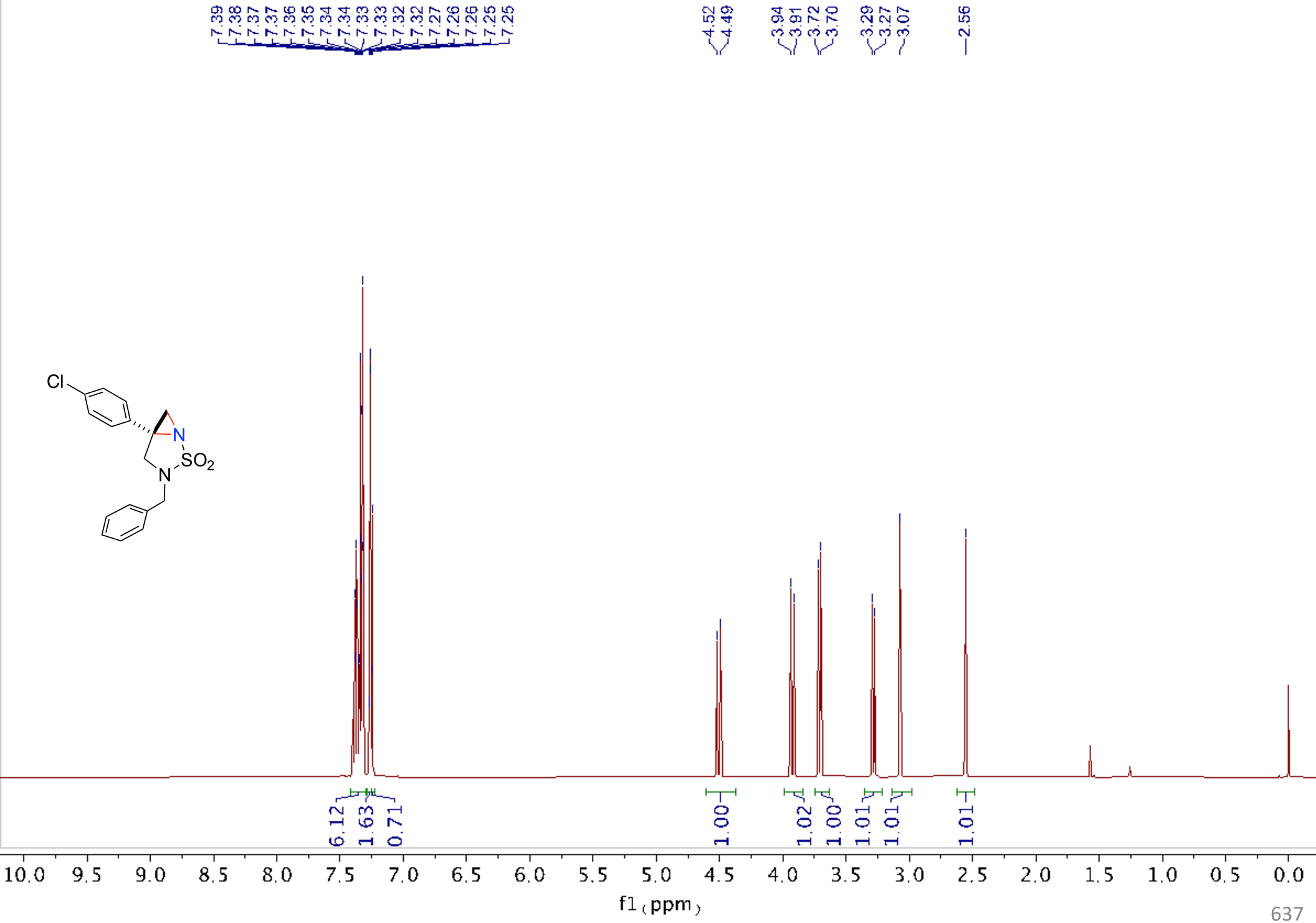


Peak Table

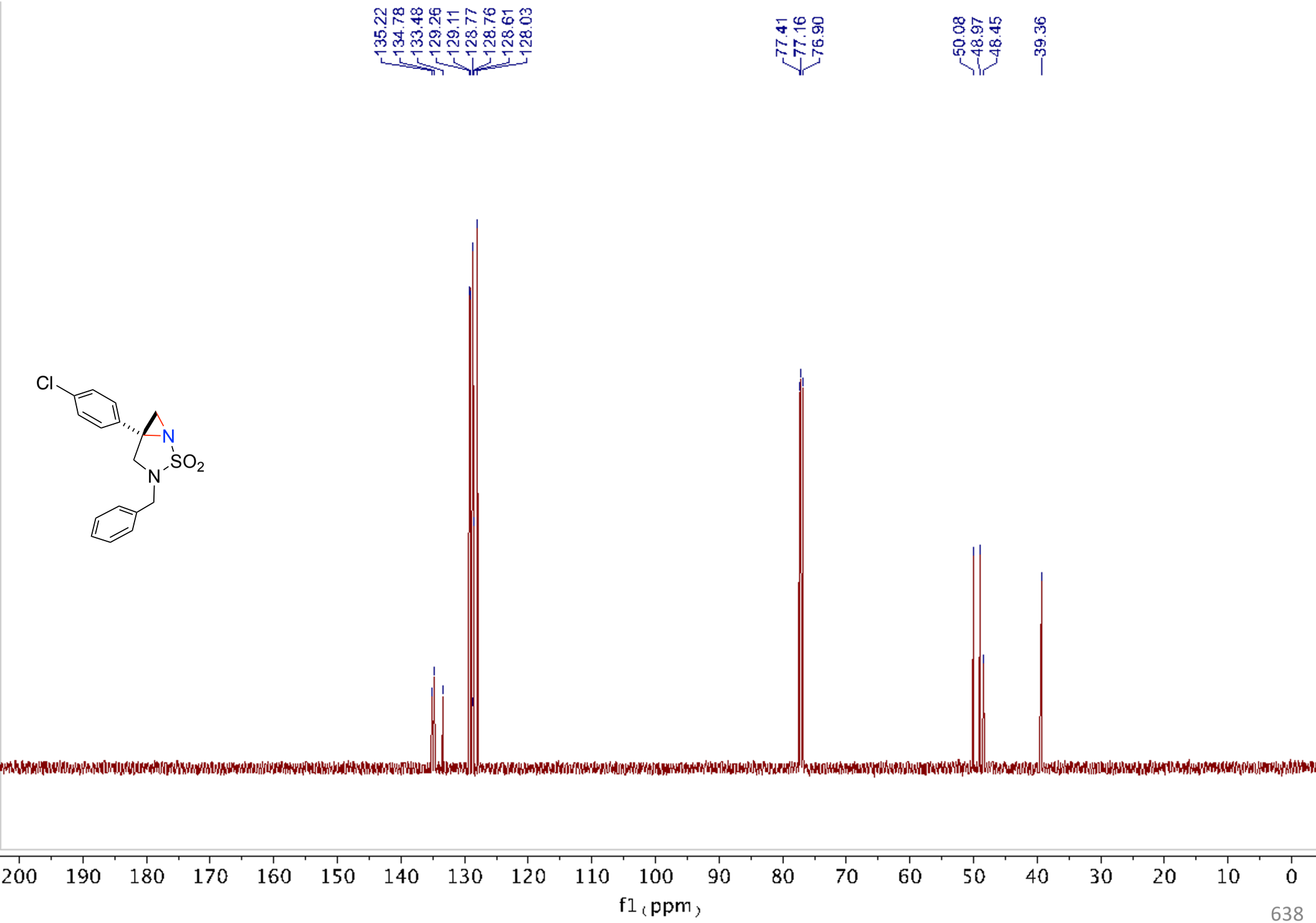
PDA Ch1 231nm

Peak#	Ret. Time	Area	Area%
1	21.014	1357130	91.410
2	38.765	127528	8.590
Total		1484658	100.000

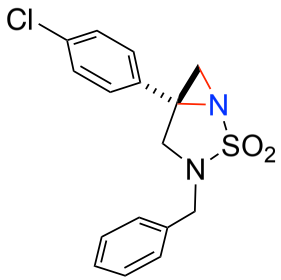
^{1}H NMR (*R*)-3-Benzyl-5-(4-chlorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2e



^{13}C NMR (*R*)-3-Benzyl-5-(4-chlorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2e



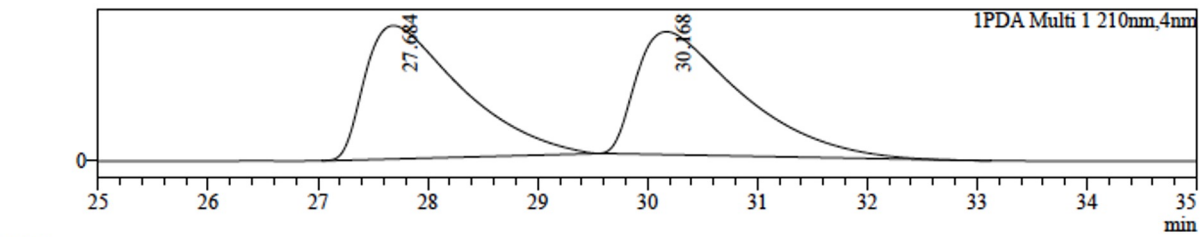
3-Benzyl-5-(4-chlorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2e



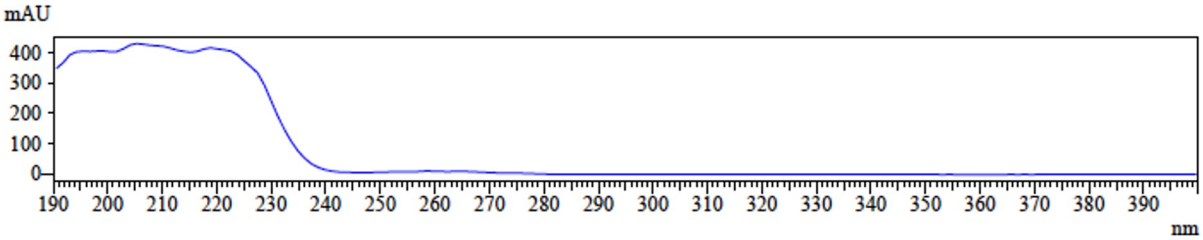
Sample Information

Data File	: H0X-0401-ODH-10%1.0mL.lcd
Sample Name	: H0X-0401-ODH-10%1.0mL
Sample ID	: H0X-0401-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-90MIN.lcm

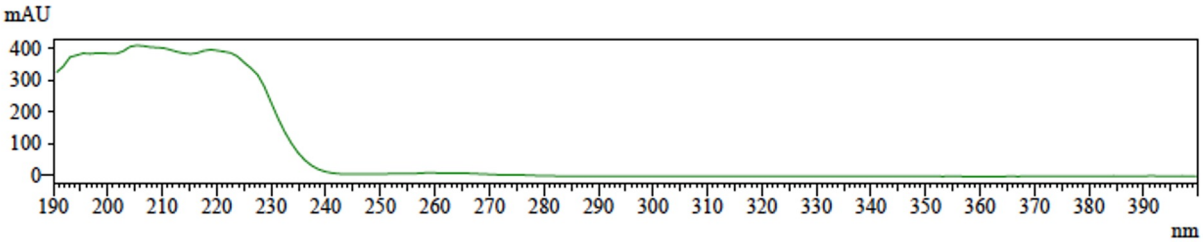
Chromatogram



UV Spectrum
Retention time = 27.684



UV Spectrum
Retention time = 30.168

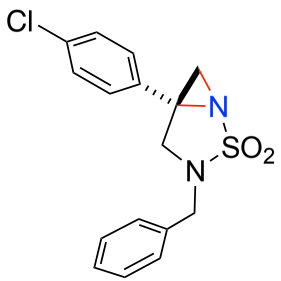


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	27.684	25124272	49.960
2	30.168	25164990	50.040
Total		50289262	100.000

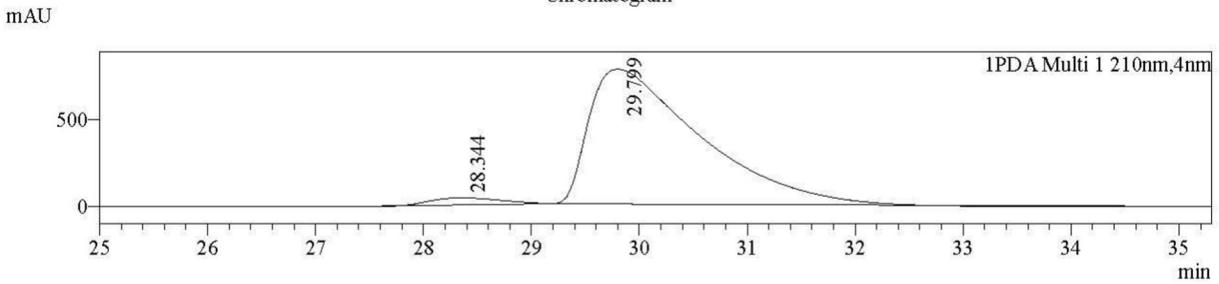
(*R*)-3-Benzyl-5-(4-chlorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2e



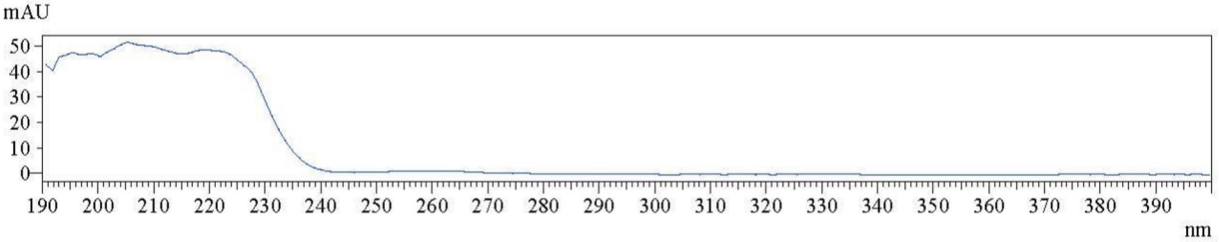
Sample Information

Data File	: H0X-0402-ODH-10%1.0mL.lcd
Sample Name	: H0X-0402-ODH-10%1.0mL001
Sample ID	: H0X-0402-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-90MIN.lcm

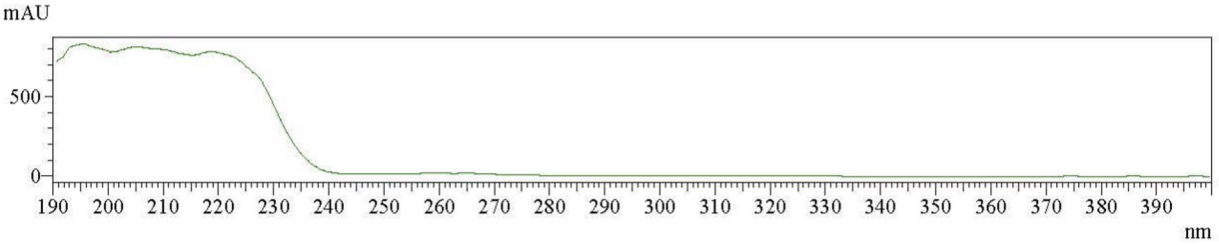
Chromatogram



UV Spectrum
Retention time = 28.344



UV Spectrum
Retention time = 29.799

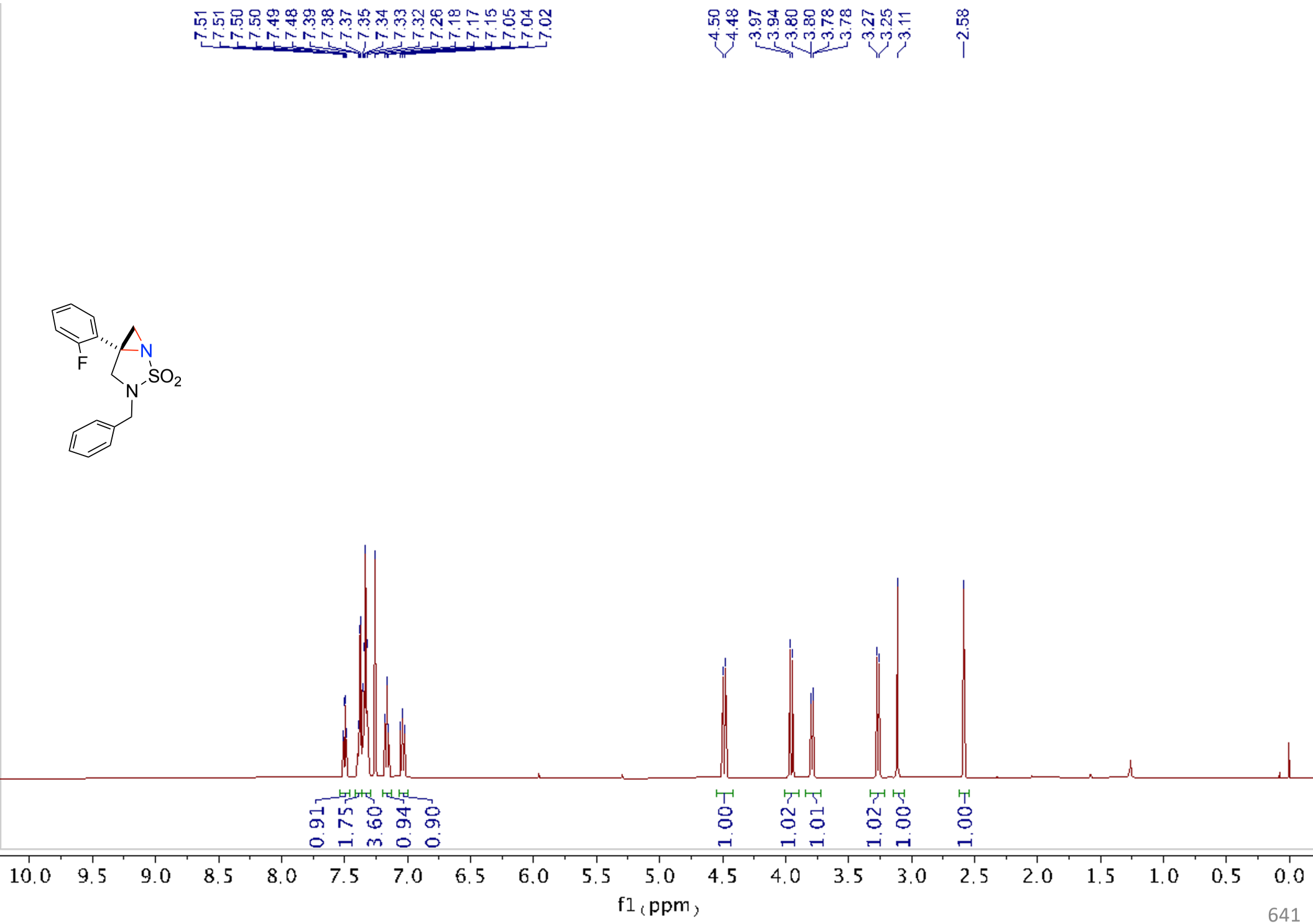


Peak Table

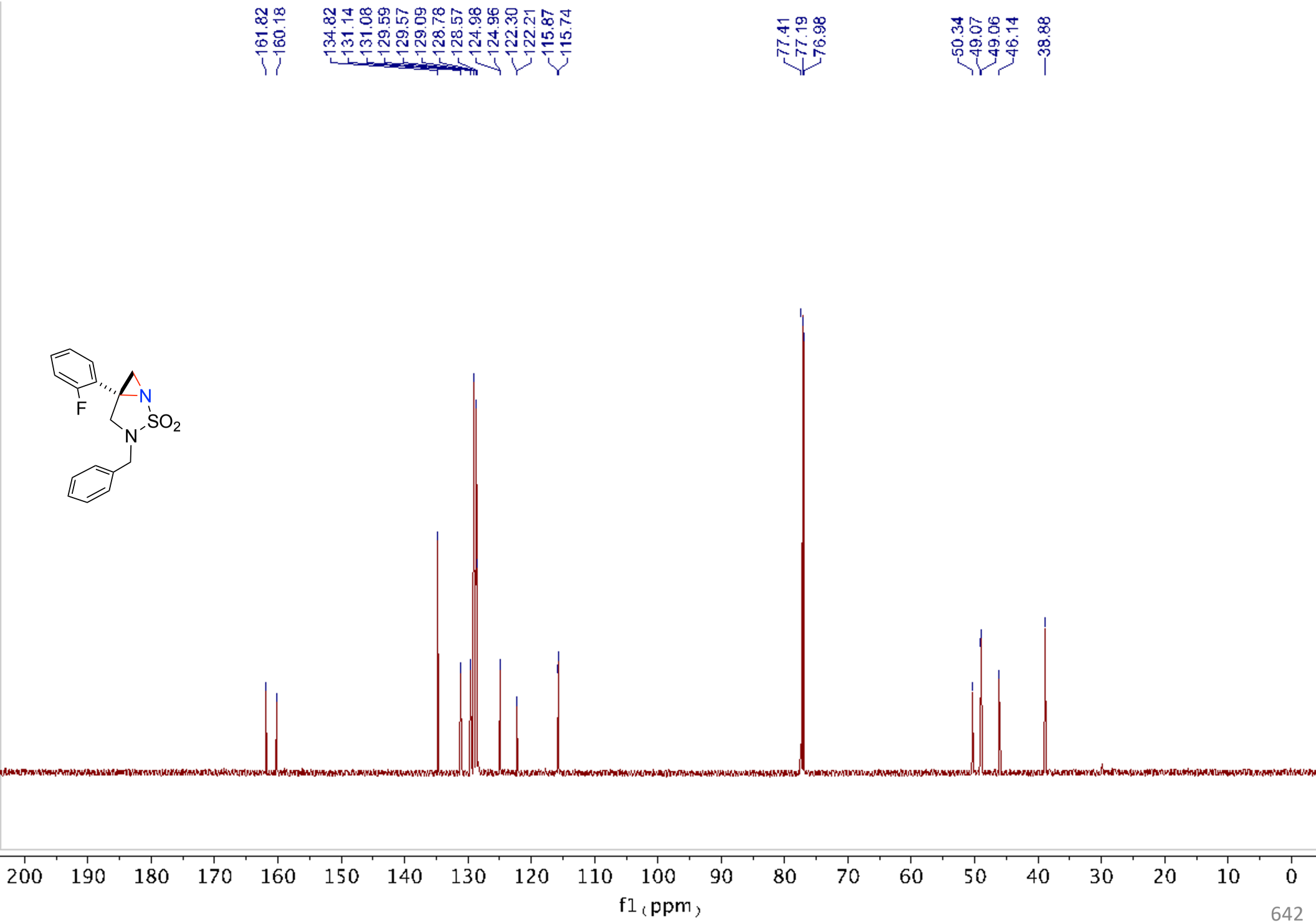
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	28.344	1795353	3.174
2	29.799	54776993	96.826
Total		56572346	100.000

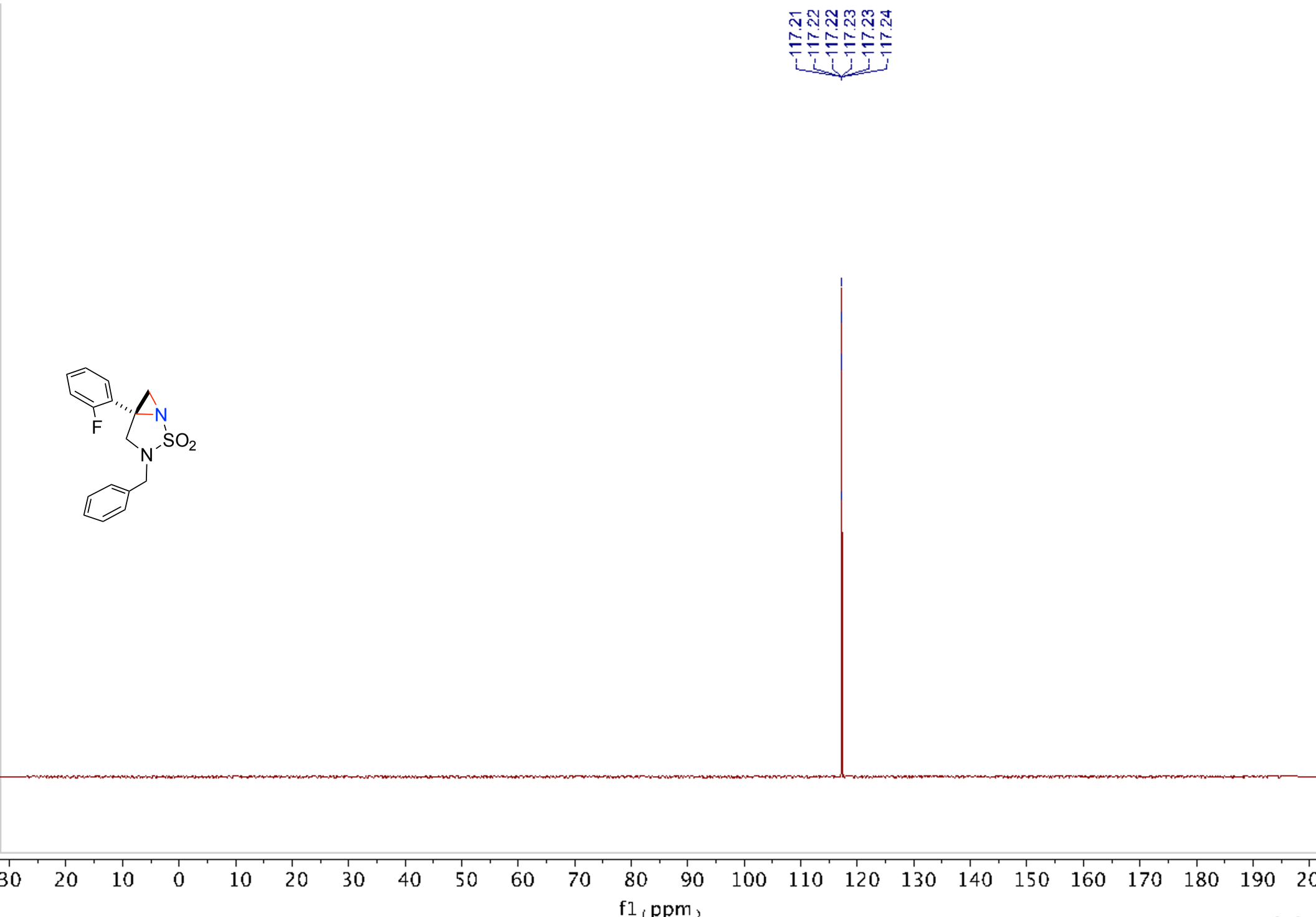
^{1}H NMR (*R*)-3-Benzyl-5-(2-fluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2f



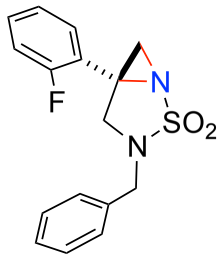
^{13}C NMR (*R*)-3-Benzyl-5-(2-fluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2f



^{19}F NMR (*R*)-3-Benzyl-5-(2-fluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2f



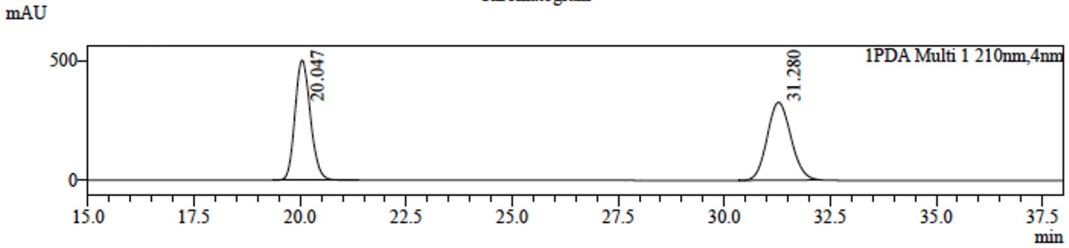
3-Benzyl-5-(2-fluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2f



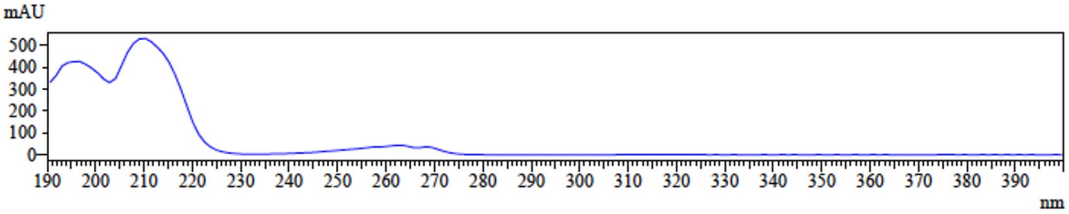
Sample Information

Data File	: H0X-0487_2nd-IC-20%1.0mL.lcd
Sample Name	: H0X-0487_2nd-IC-20%1.0mL
Sample ID	: H0X-0487_2nd-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

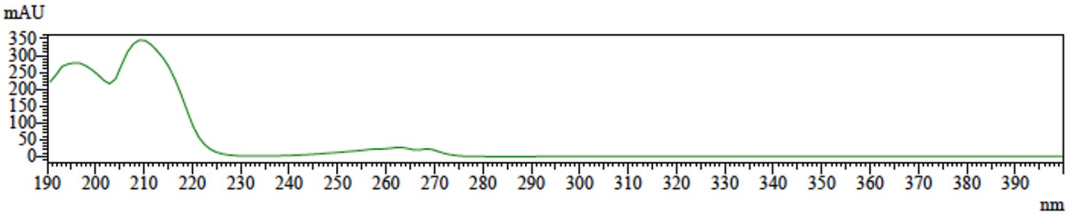
Chromatogram



UV Spectrum
Retention time = 20.047



UV Spectrum
Retention time = 31.280

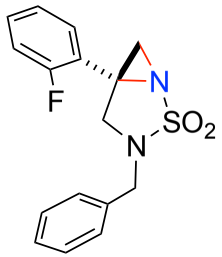


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	20.047	12732551	49.978
2	31.280	12743643	50.022
Total		25476193	100.000

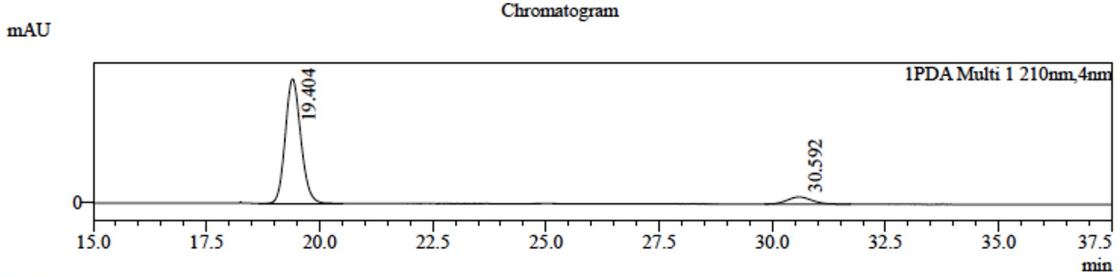
(*R*)-3-Benzyl-5-(2-fluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2f



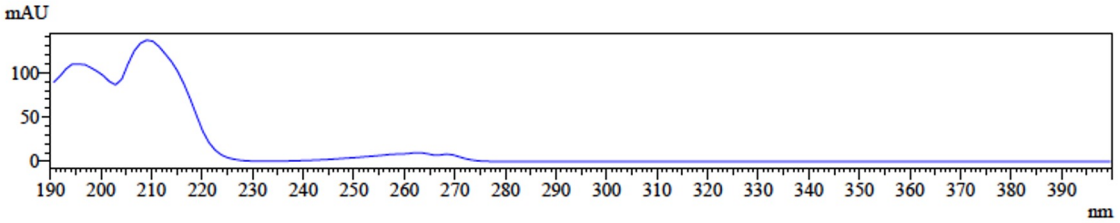
Sample Information

Data File	: H0X-0488_2nd-IC-20%1.0mL.lcd
Sample Name	: H0X-0488_2nd-IC-20%1.0mL
Sample ID	: H0X-0488_2nd-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

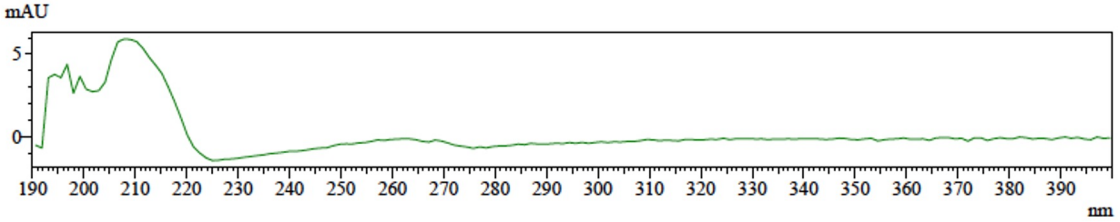
Chromatogram



UV Spectrum
Retention time = 19.404



UV Spectrum
Retention time = 30.592

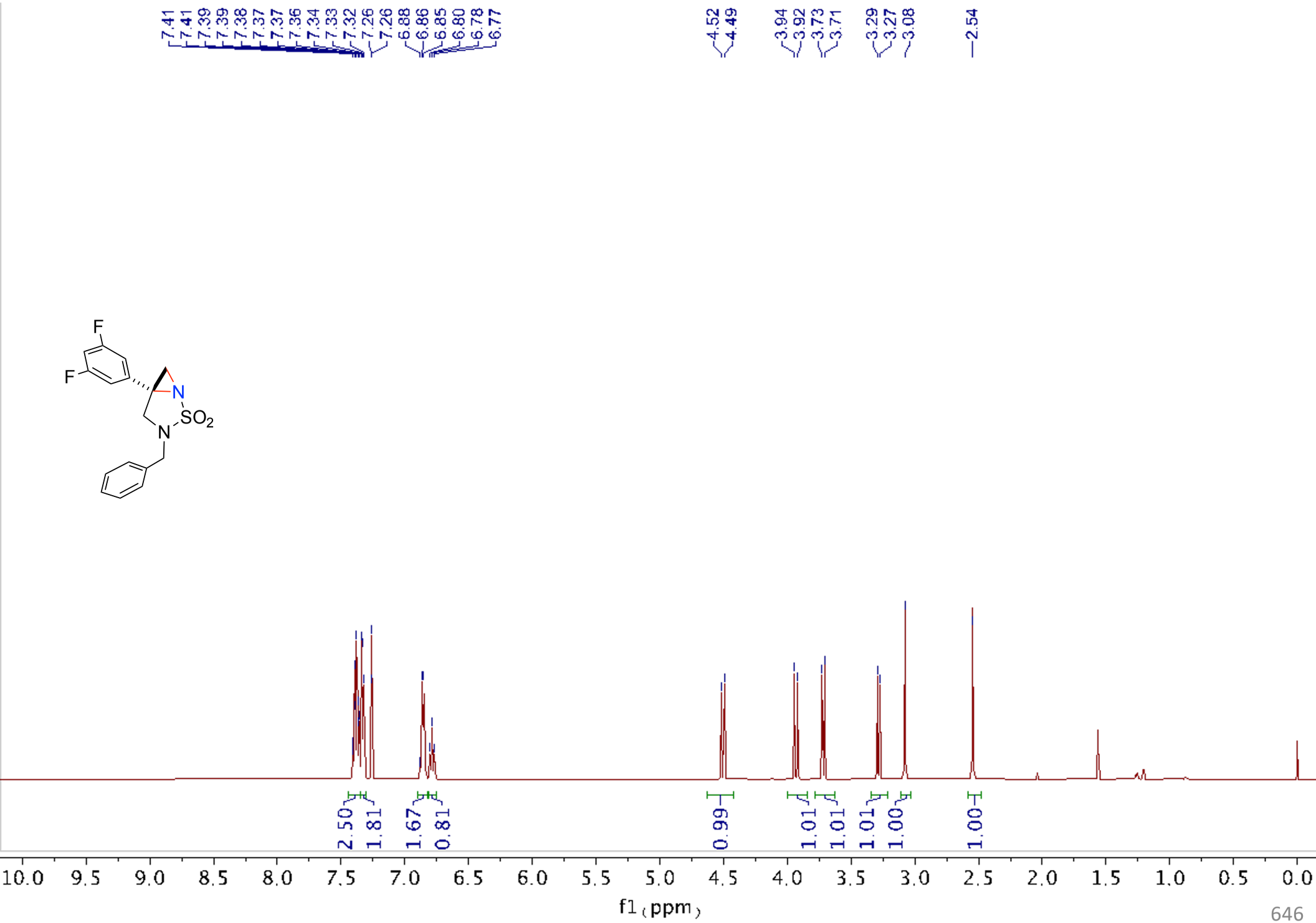


Peak Table

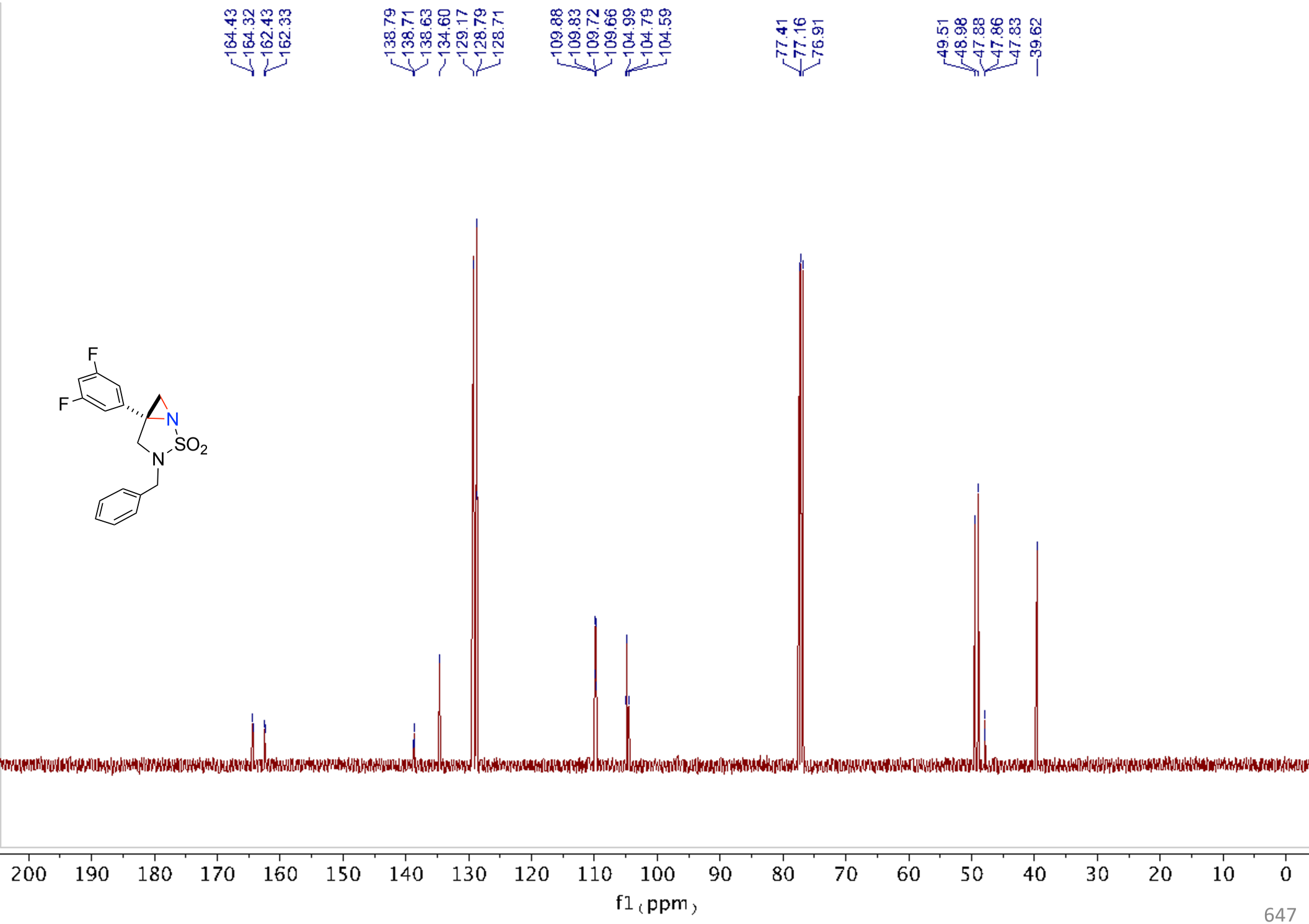
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	19.404	3069113	91.641
2	30.592	279930	8.359
Total		3349043	100.000

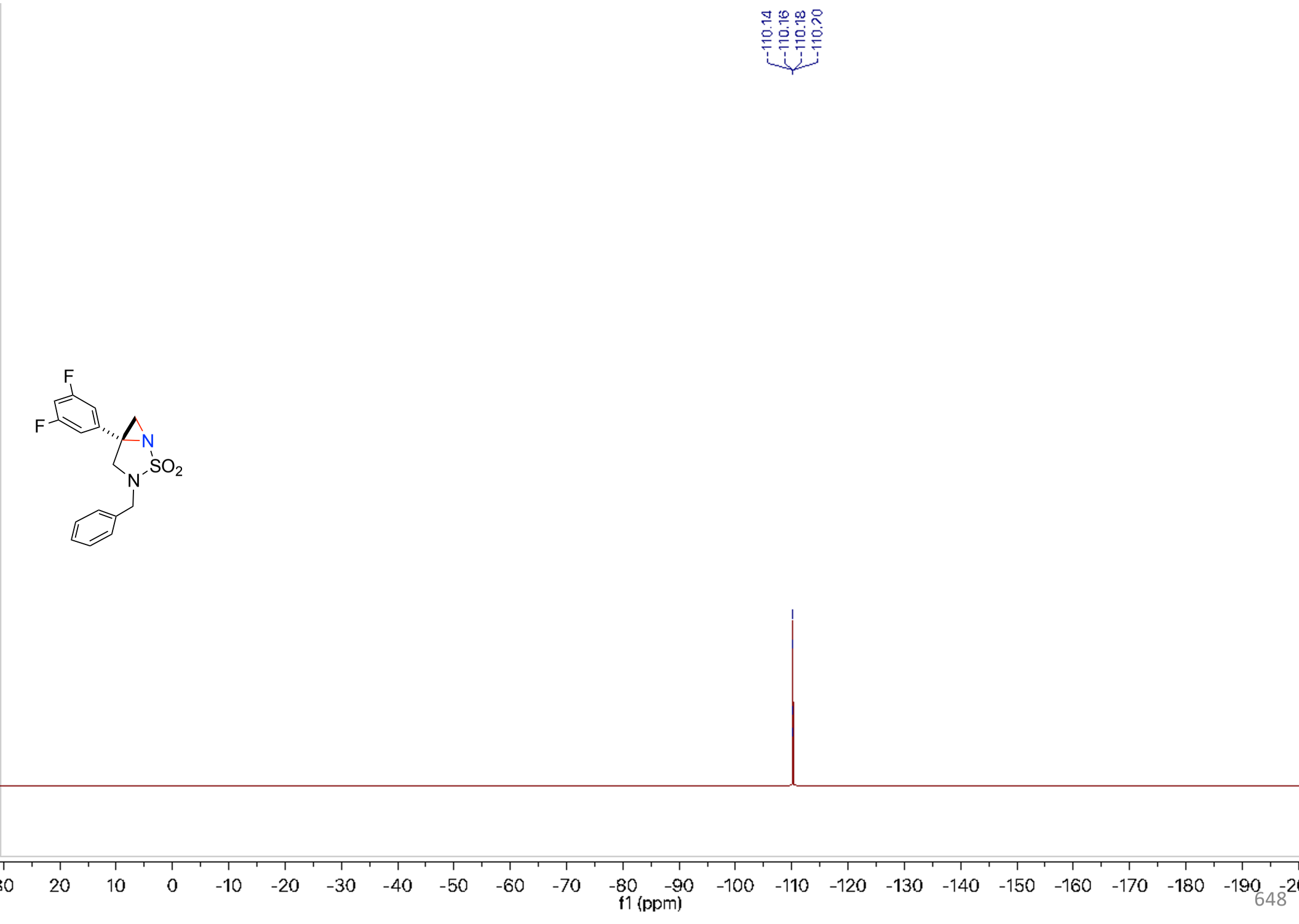
^{1}H NMR (*R*)-3-Benzyl-5-(3,5-difluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2g



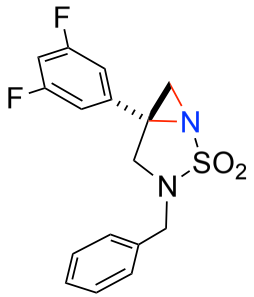
^{13}C NMR (*R*)-3-Benzyl-5-(3,5-difluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2g



^{19}F NMR (*R*)-3-Benzyl-5-(3,5-difluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2g



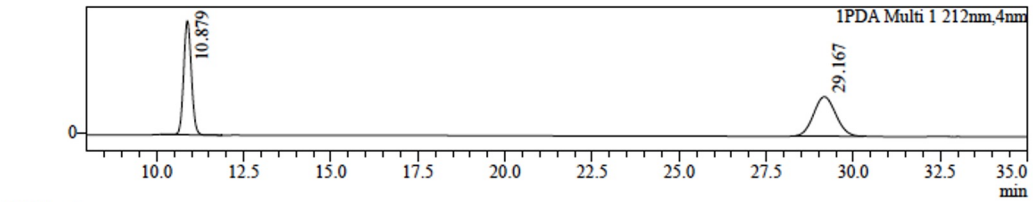
3-Benzyl-5-(3,5-difluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2g



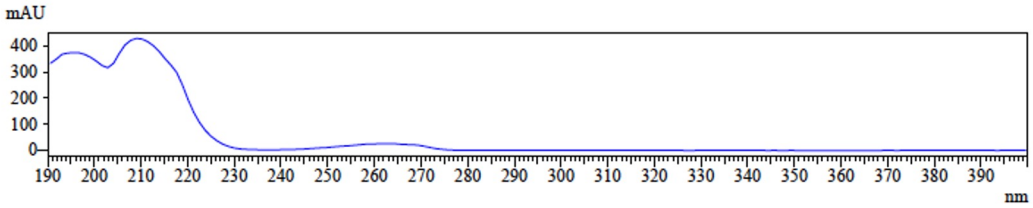
Sample Information

Data File	: H0X-0535-IC-20%1.0mL.lcd
Sample Name	: H0X-0535-IC-20%1.0mL
Sample ID	: H0X-0535-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

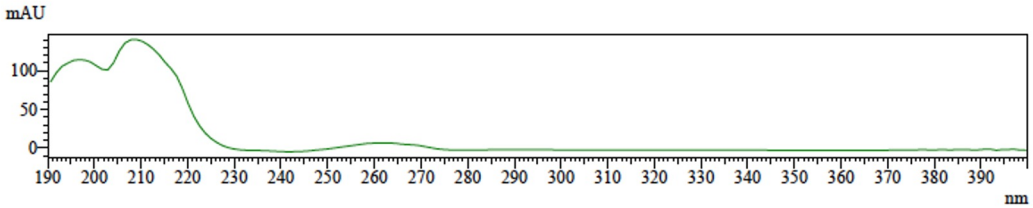
Chromatogram



UV Spectrum
Retention time = 10.879



UV Spectrum
Retention time = 29.167

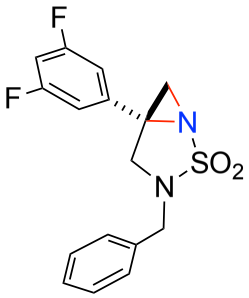


Peak Table

PDA Ch1 212nm

Peak#	Ret. Time	Area	Area%
1	10.879	6267498	49.909
2	29.167	6290257	50.091
Total		12557755	100.000

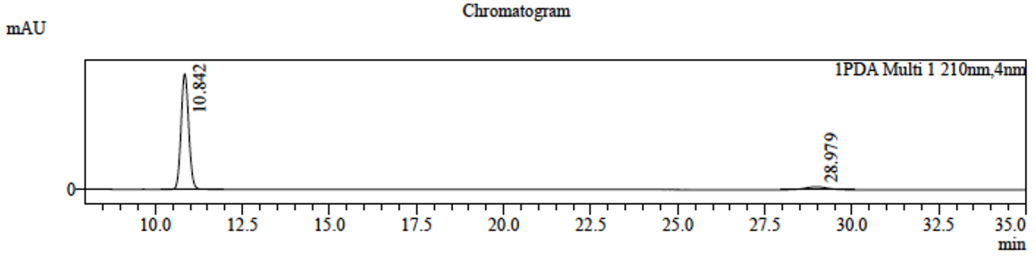
(*R*)-3-Benzyl-5-(3,5-difluorophenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2g



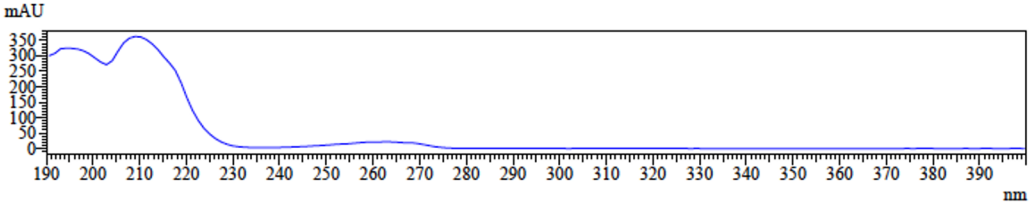
Sample Information

Data File : H0X-0536-IC-20%1.0mL.lcd
Sample Name : H0X-0536-IC-20%1.0mL
Sample ID : H0X-0536-IC-20%1.0mL
Method File : H0X-20%-1.0ml-60MIN.lcm

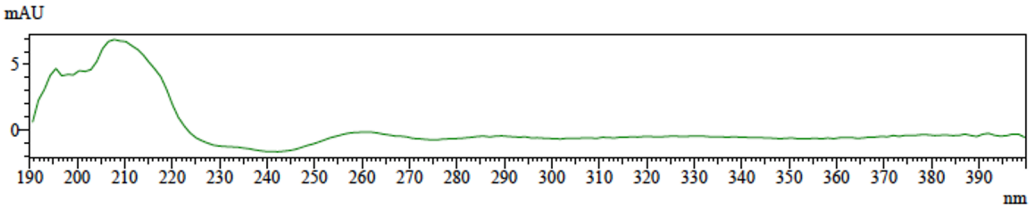
Chromatogram



UV Spectrum
Retention time = 10.842



UV Spectrum
Retention time = 28.979

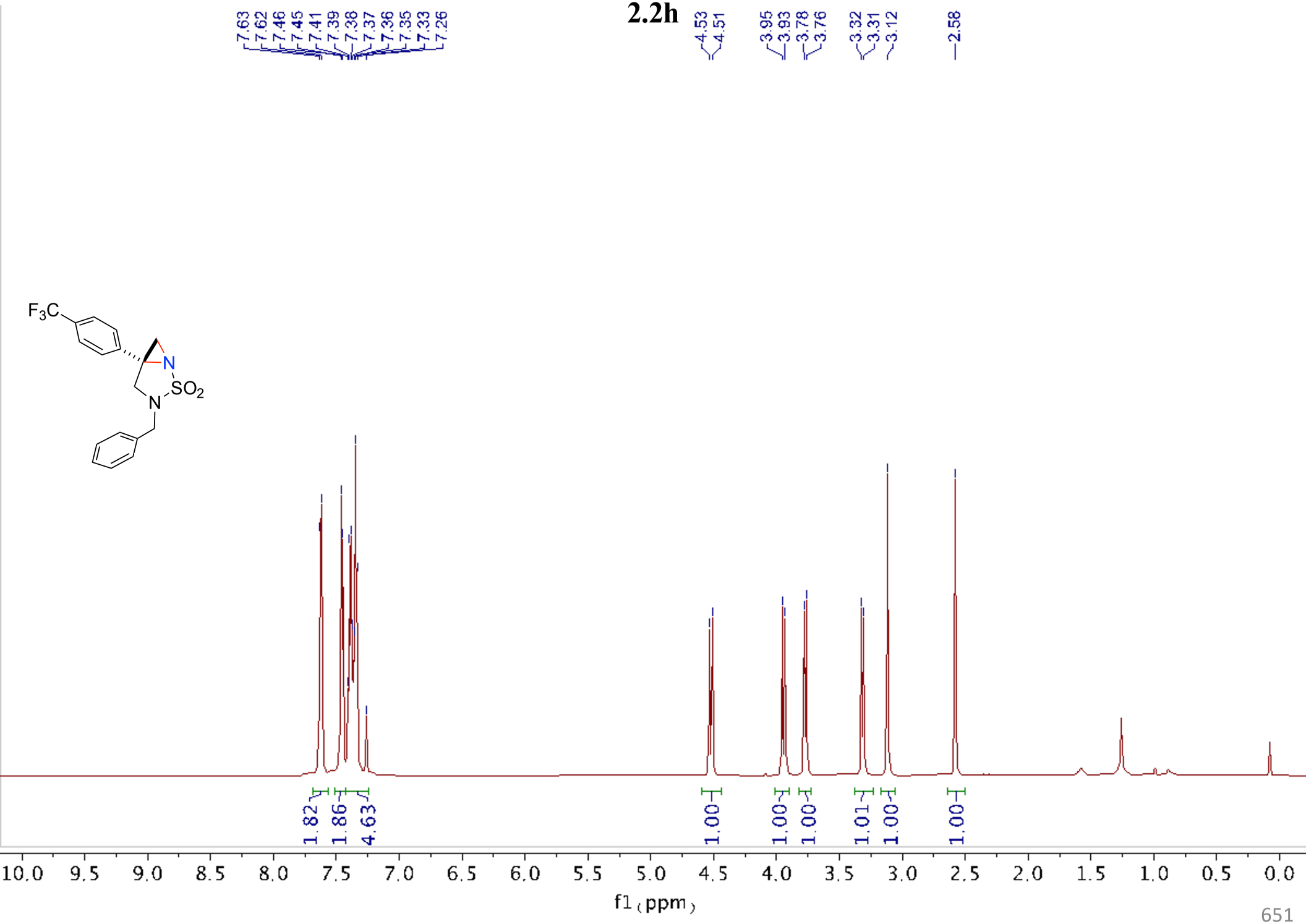


Peak Table

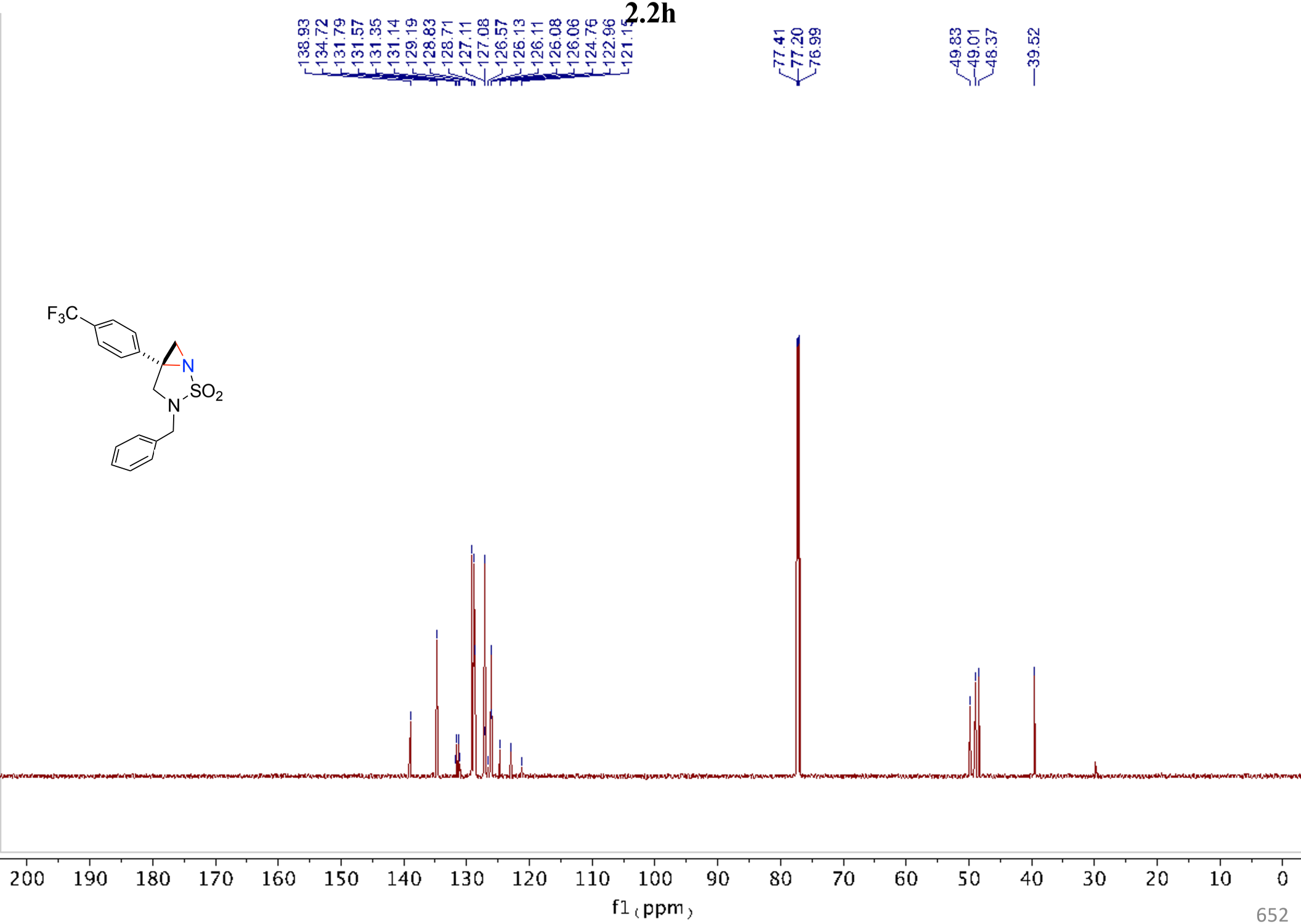
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	10.842	5315237	93.280
2	28.979	382920	6.720
Total		5698158	100.000

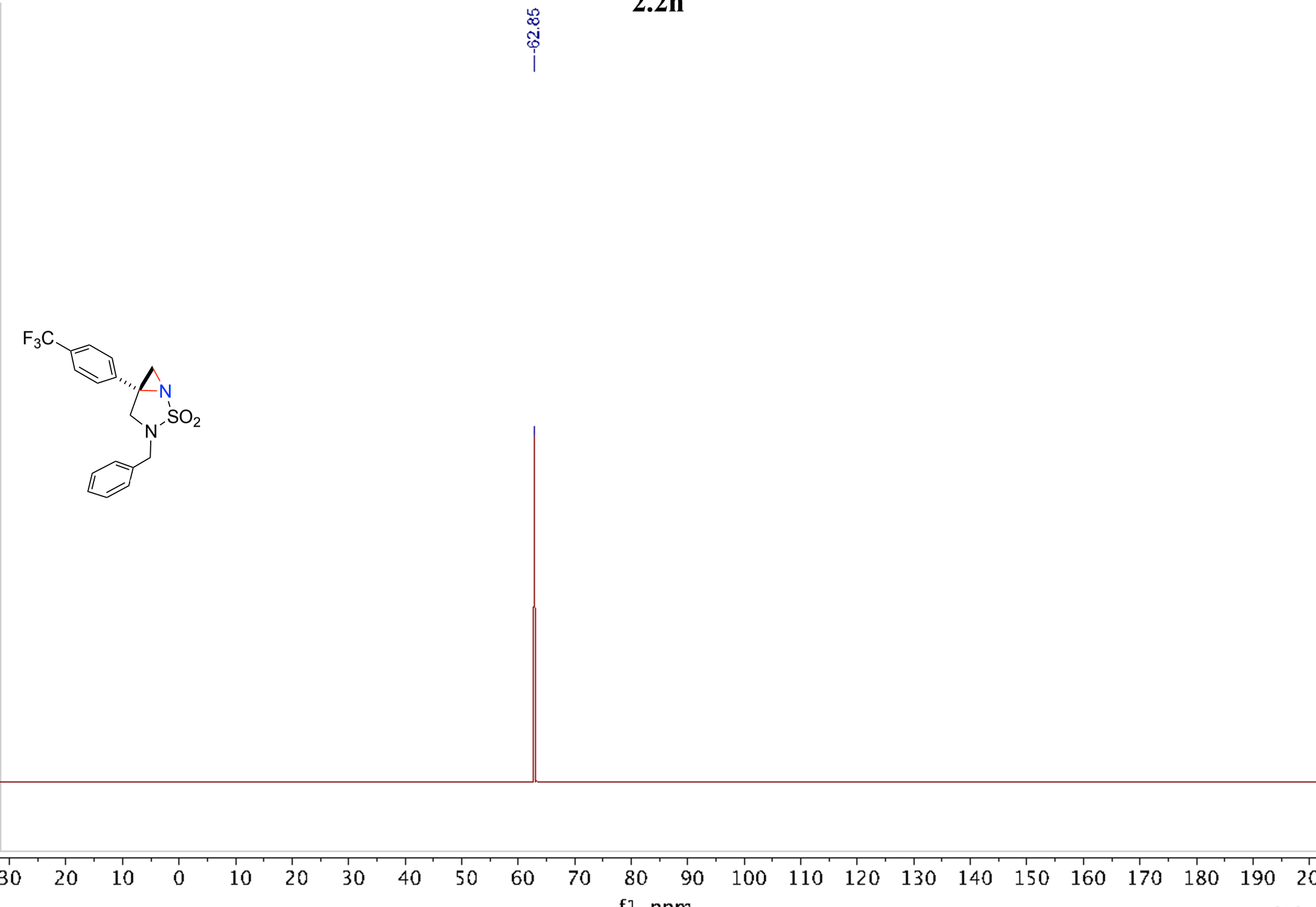
^{1}H NMR (*R*)-3-Benzyl-5-(4-(trifluoromethyl)phenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2h



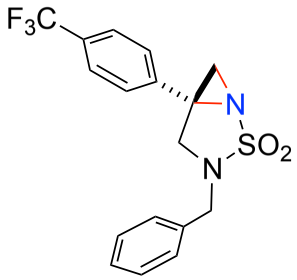
^{13}C NMR (*R*)-3-Benzyl-5-(4-(trifluoromethyl)phenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2h



^{19}F NMR (*R*)-3-Benzyl-5-(4-(trifluoromethyl)phenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2h



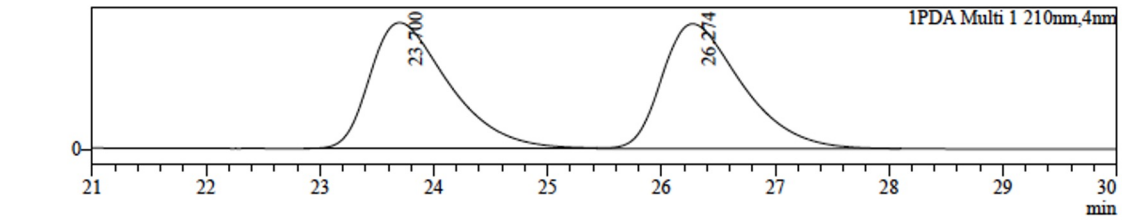
3-Benzyl-5-(4-(trifluoromethyl)phenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2h



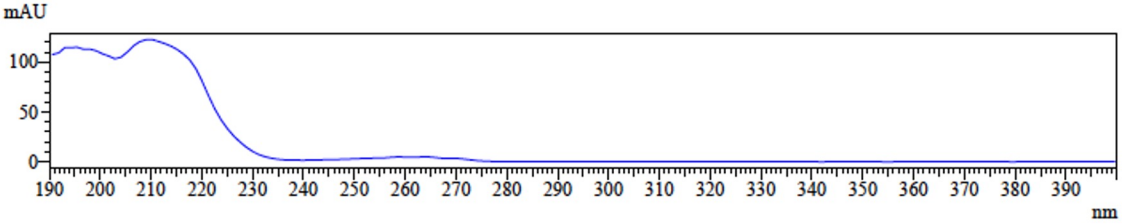
Sample Information

Data File	: H0X-0447_3rd-ODH-10%1.0mL.lcd
Sample Name	: H0X-0447_3rd-ODH-10%1.0mL
Sample ID	: H0X-0447_3rd-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-40MIN.lcm

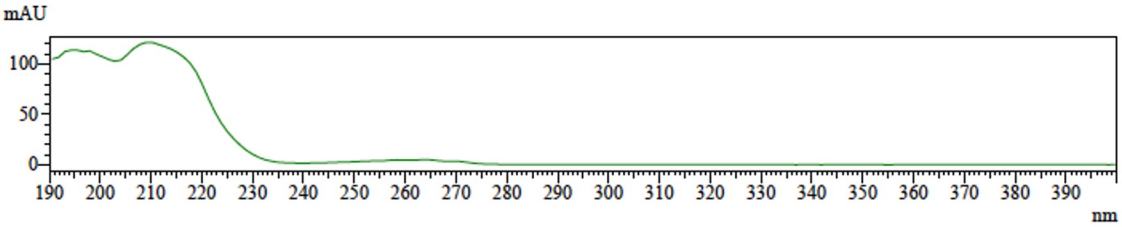
Chromatogram



UV Spectrum
Retention time = 23.700



UV Spectrum
Retention time = 26.274

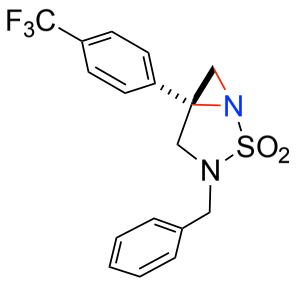


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	23.700	5755889	49.980
2	26.274	5760568	50.020
Total		11516457	100.000

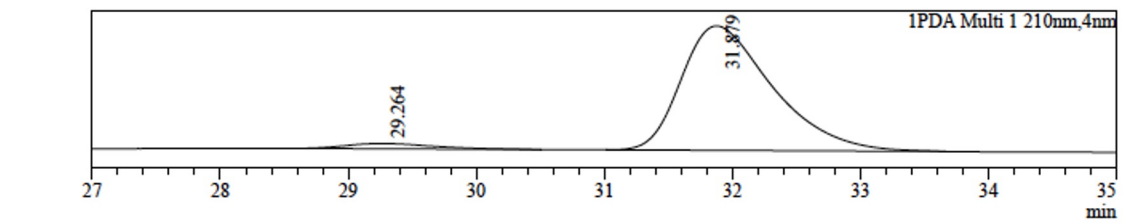
(*R*)-3-Benzyl-5-(4-(trifluoromethyl)phenyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2h



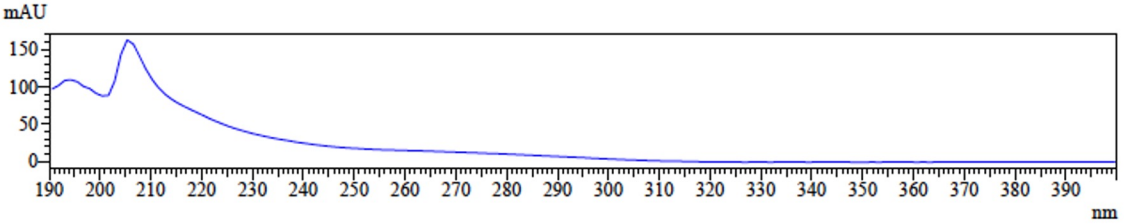
Sample Information

Data File	: H0X-0446-ODH-10%1.0mL.lcd
Sample Name	: H0X-0446-ODH-10%1.0mL
Sample ID	: H0X-0446-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-90MIN.lcm

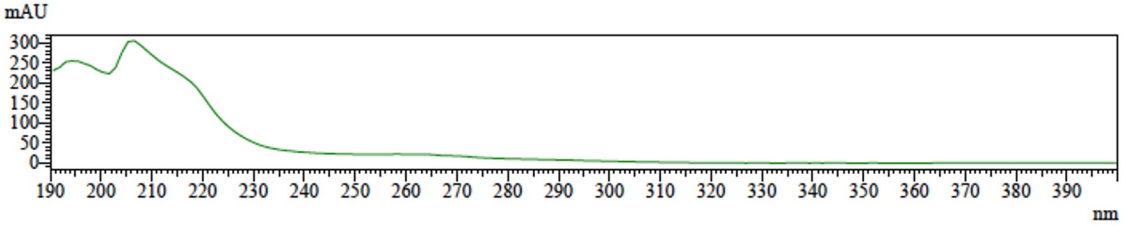
Chromatogram



UV Spectrum
Retention time = 29.264



UV Spectrum
Retention time = 31.879

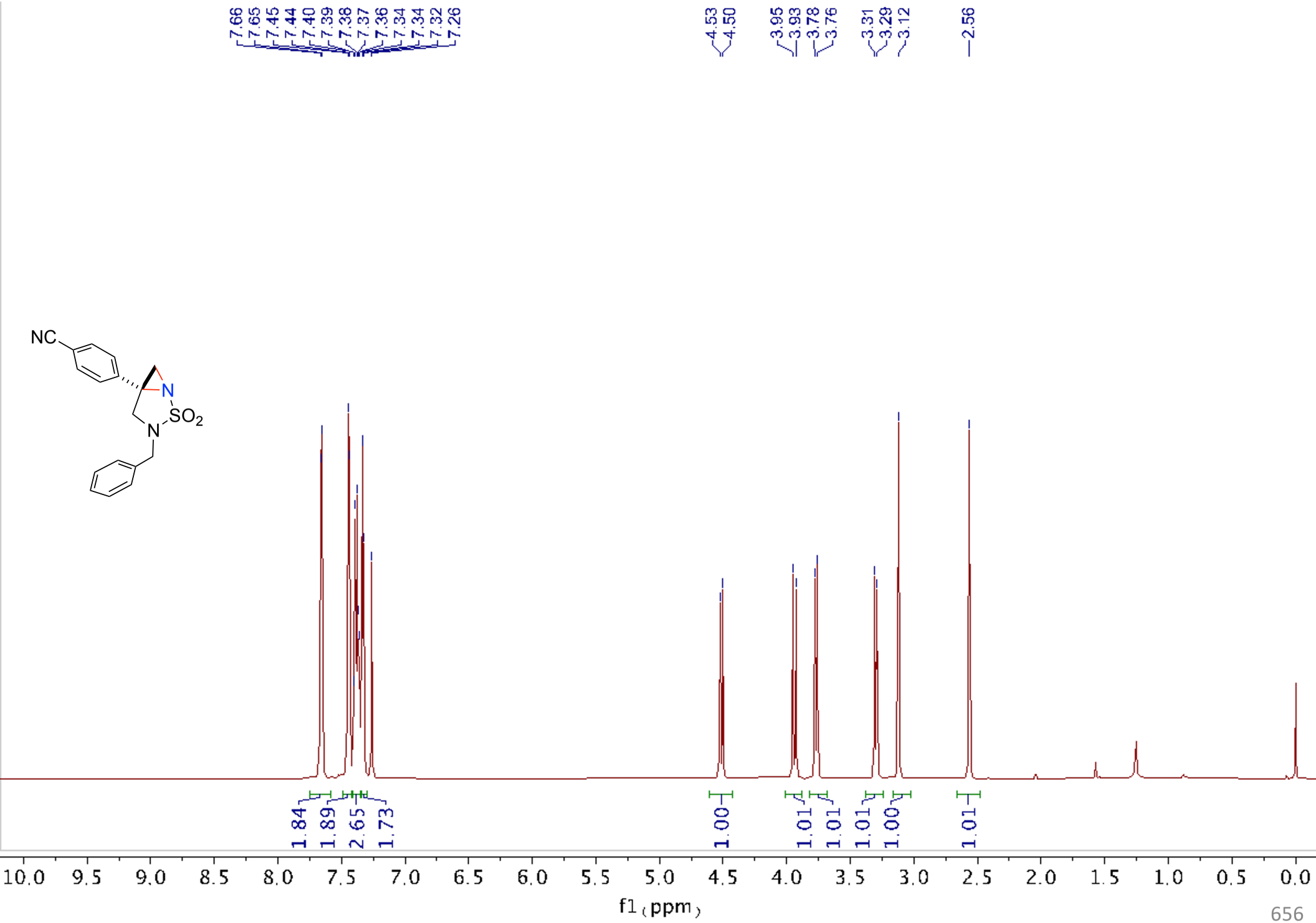


Peak Table

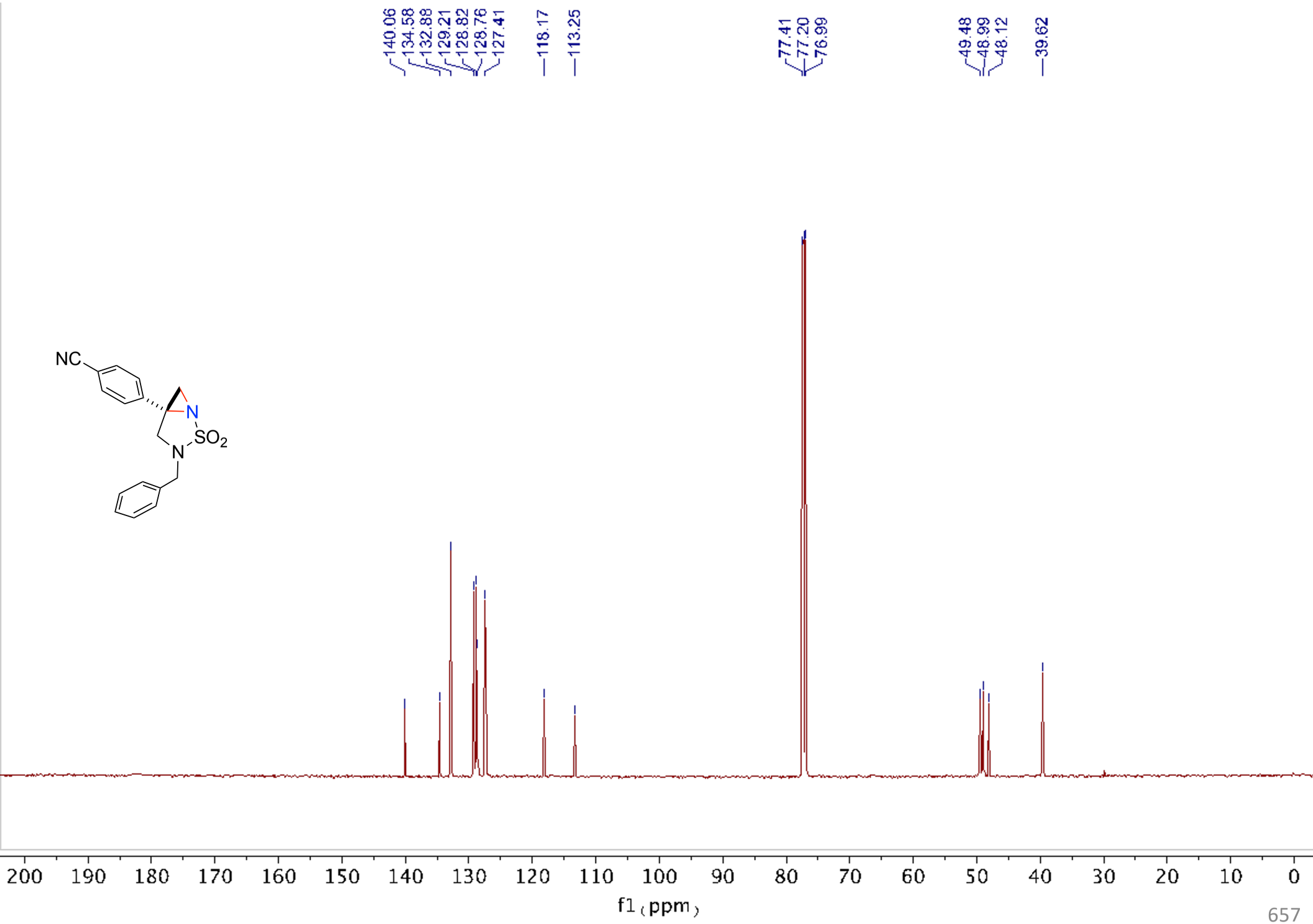
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	29.264	329408	3.921
2	31.879	8071938	96.079
Total		8401346	100.000

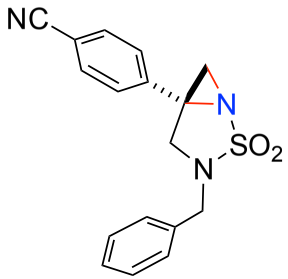
^{1}H NMR (*R*)-4-(3-Benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)benzonitrile 2.2i



^{13}C NMR (*R*)-4-(3-Benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)benzonitrile 2.2i



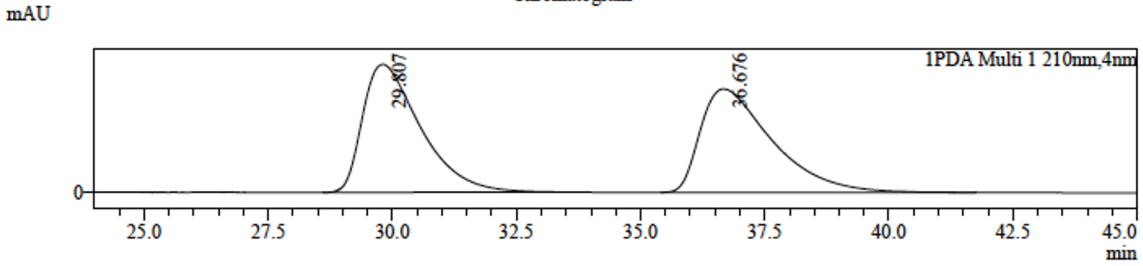
4-(3-Benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)benzonitrile 2.2i



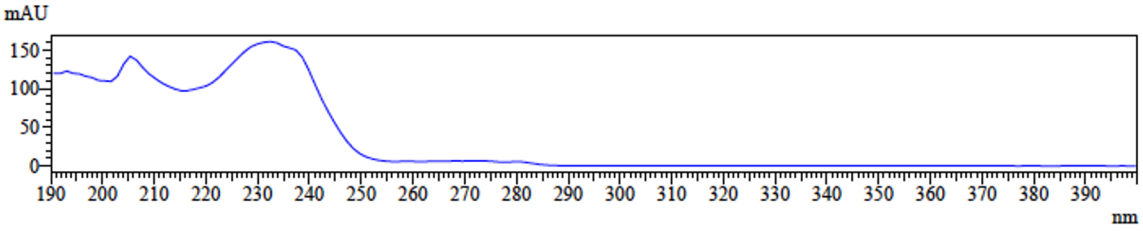
Sample Information

Data File	: H0X-0452-ODH-20%1.0mL.lcd
Sample Name	: H0X-0452-ODH-20%1.0mL
Sample ID	: H0X-0452-ODH-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

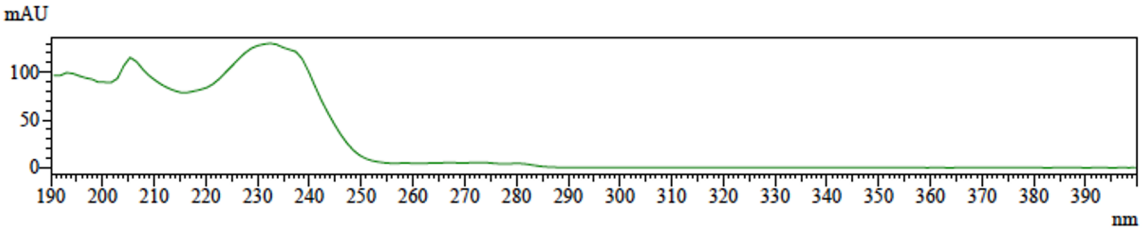
Chromatogram



UV Spectrum
Retention time = 29.807



UV Spectrum
Retention time = 36.676

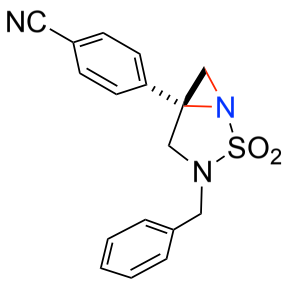


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	29.807	9388573	50.064
2	36.676	9364531	49.936
Total		18753104	100.000

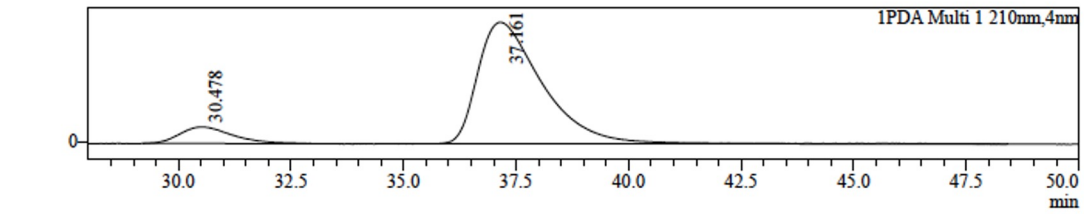
(*R*)-4-(3-Benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)benzonitrile 2.2i



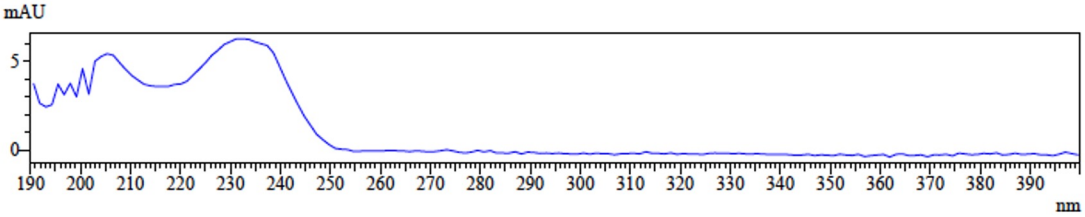
Sample Information

Data File	: H0X-0453-ODH-20%1.0mL.lcd
Sample Name	: H0X-0453-ODH-20%1.0mL
Sample ID	: H0X-0453-ODH-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

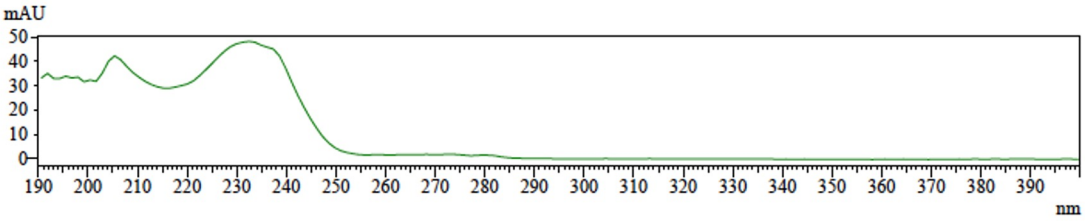
Chromatogram



UV Spectrum
Retention time = 30.478



UV Spectrum
Retention time = 37.161

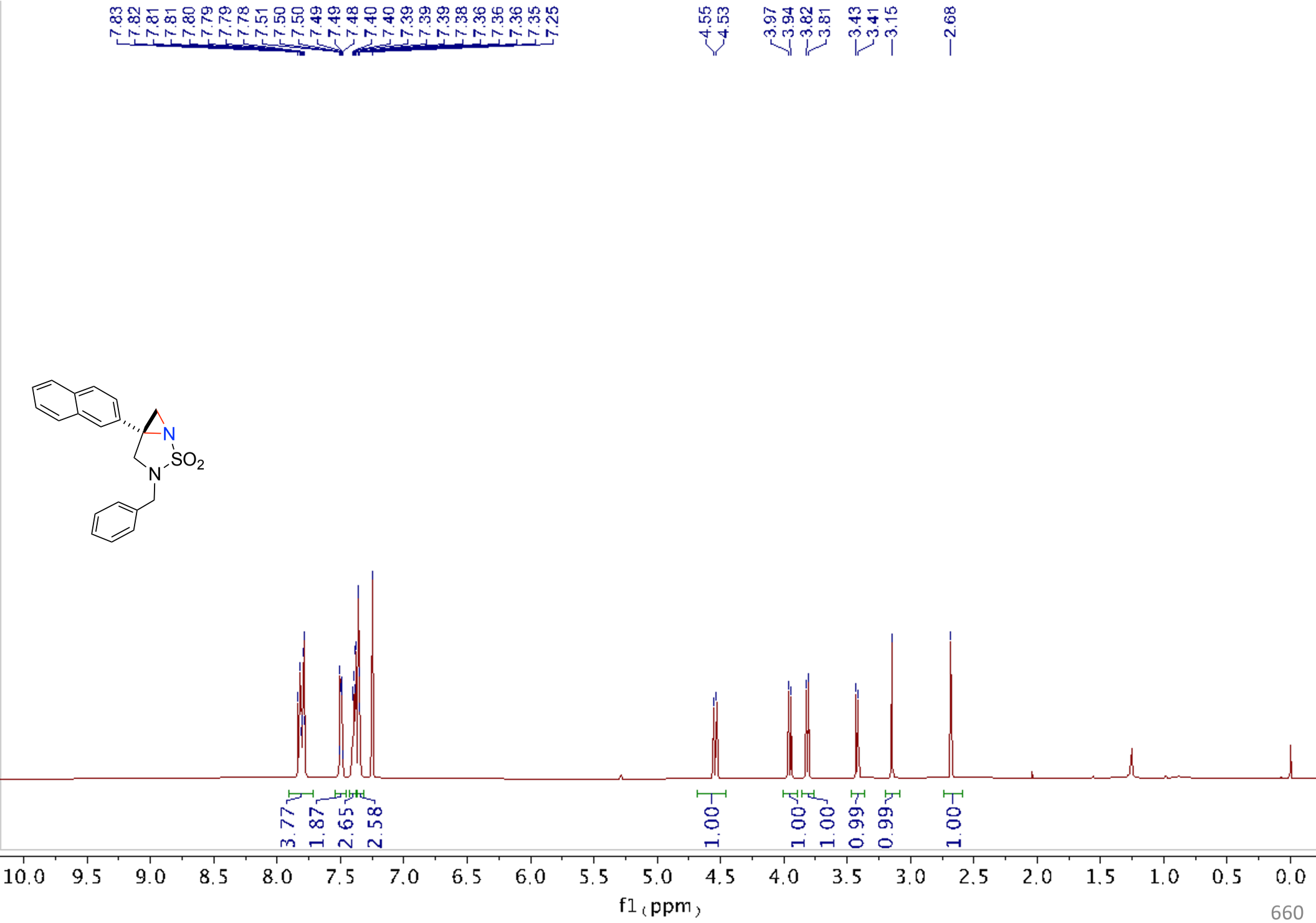


Peak Table

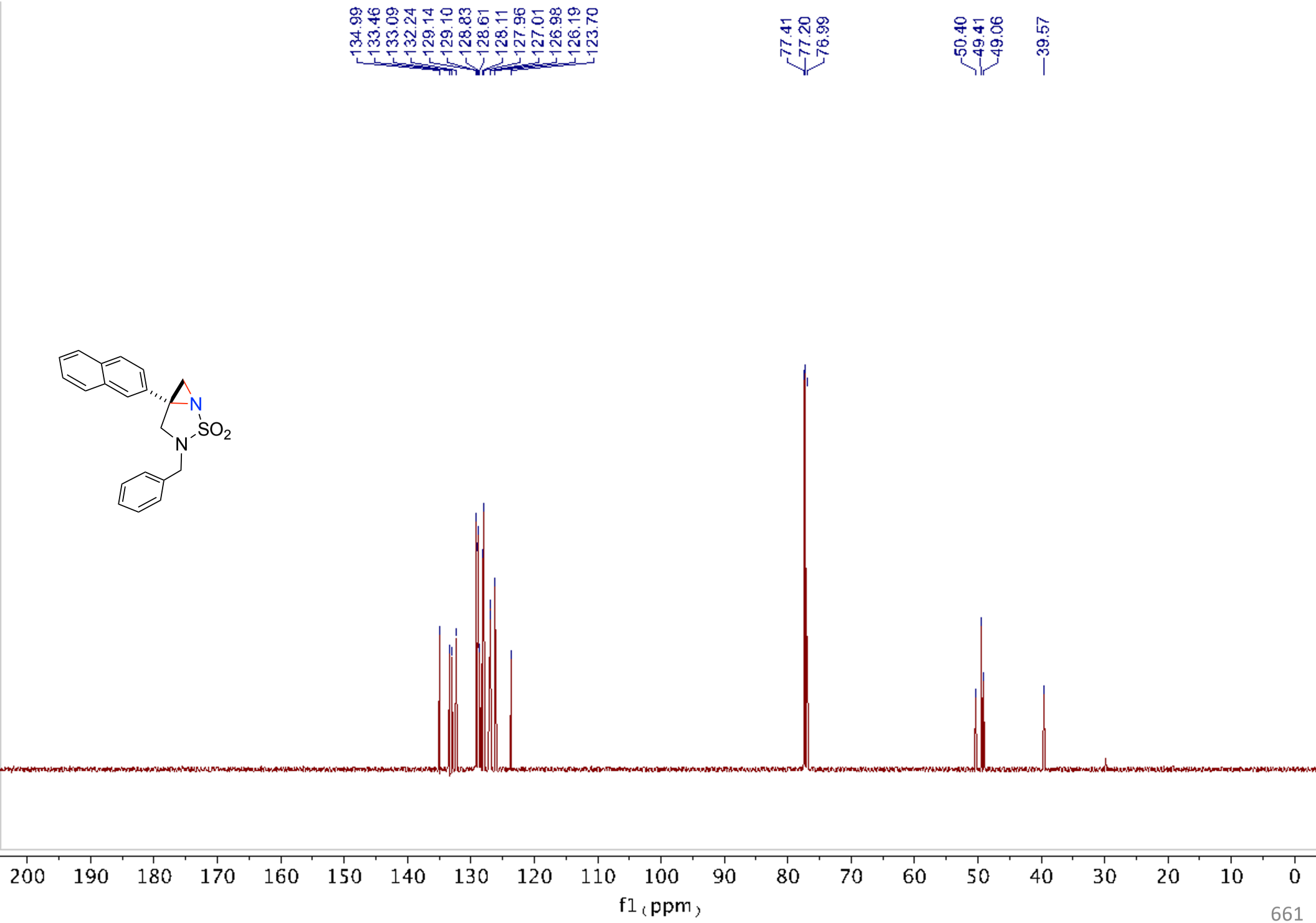
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	30.478	382085	9.867
2	37.161	3490149	90.133
Total		3872234	100.000

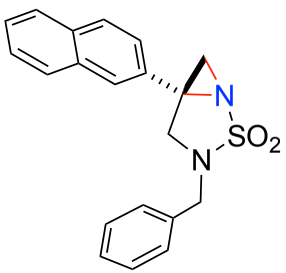
^{1}H NMR (*R*)-3-Benzyl-5-(naphthalen-2-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2j



^{13}C NMR (*R*)-3-Benzyl-5-(naphthalen-2-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2j



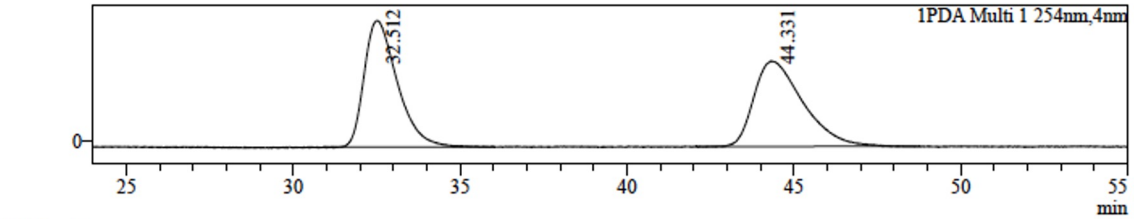
3-Benzyl-5-(naphthalen-2-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2j



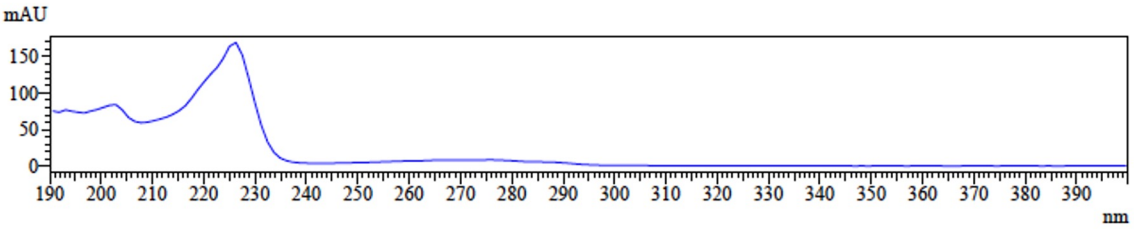
Sample Information

Data File	: H0X-0461-ODH-10%1.0mL.lcd
Sample Name	: H0X-0461-ODH-10%1.0mL
Sample ID	: H0X-0461-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-40MIN.lcm

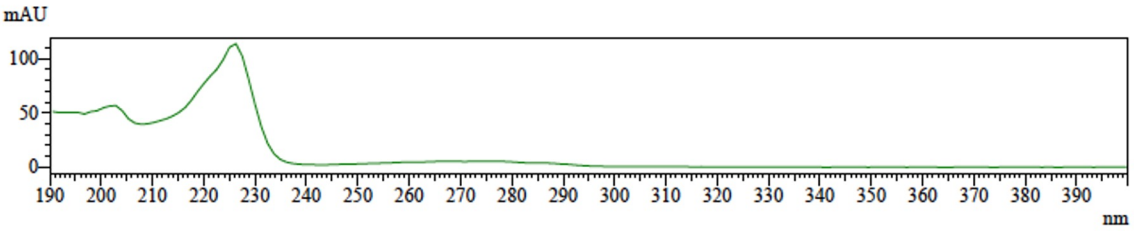
Chromatogram



UV Spectrum
Retention time = 32.512



UV Spectrum
Retention time = 44.331

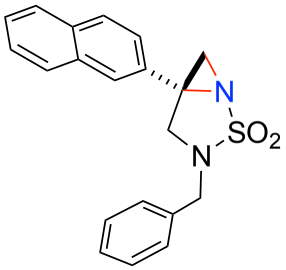


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	32.512	392774	50.032
2	44.331	392264	49.968
Total		785037	100.000

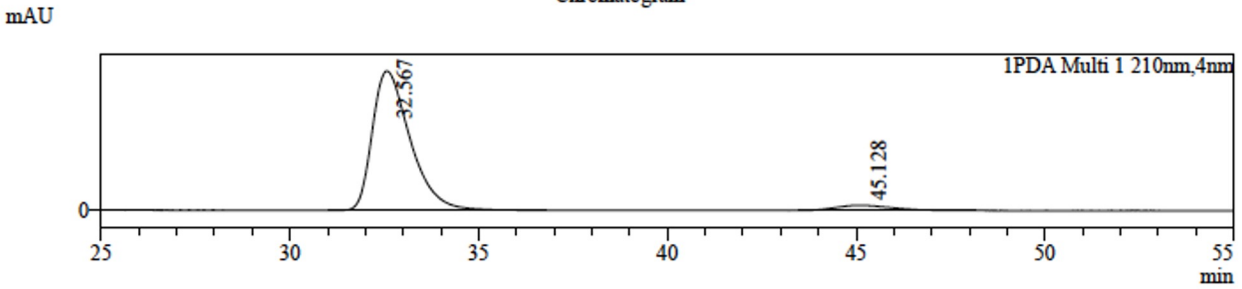
(*R*)-3-Benzyl-5-(naphthalen-2-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2j



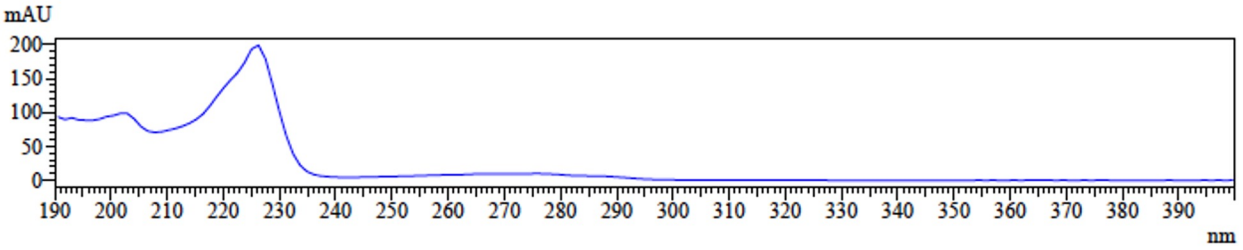
Sample Information

Data File	: H0X-0462-ODH-10%1.0mL.lcd
Sample Name	: H0X-0462-ODH-10%1.0mL
Sample ID	: H0X-0462-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-40MIN.lcm

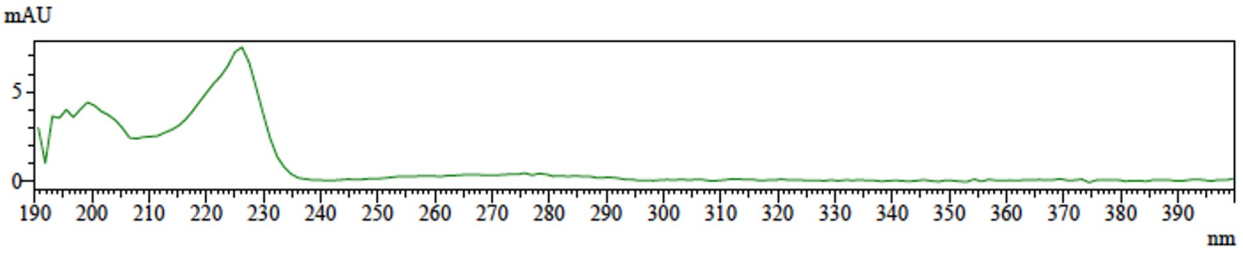
Chromatogram



UV Spectrum
Retention time = 32.567



UV Spectrum
Retention time = 45.128

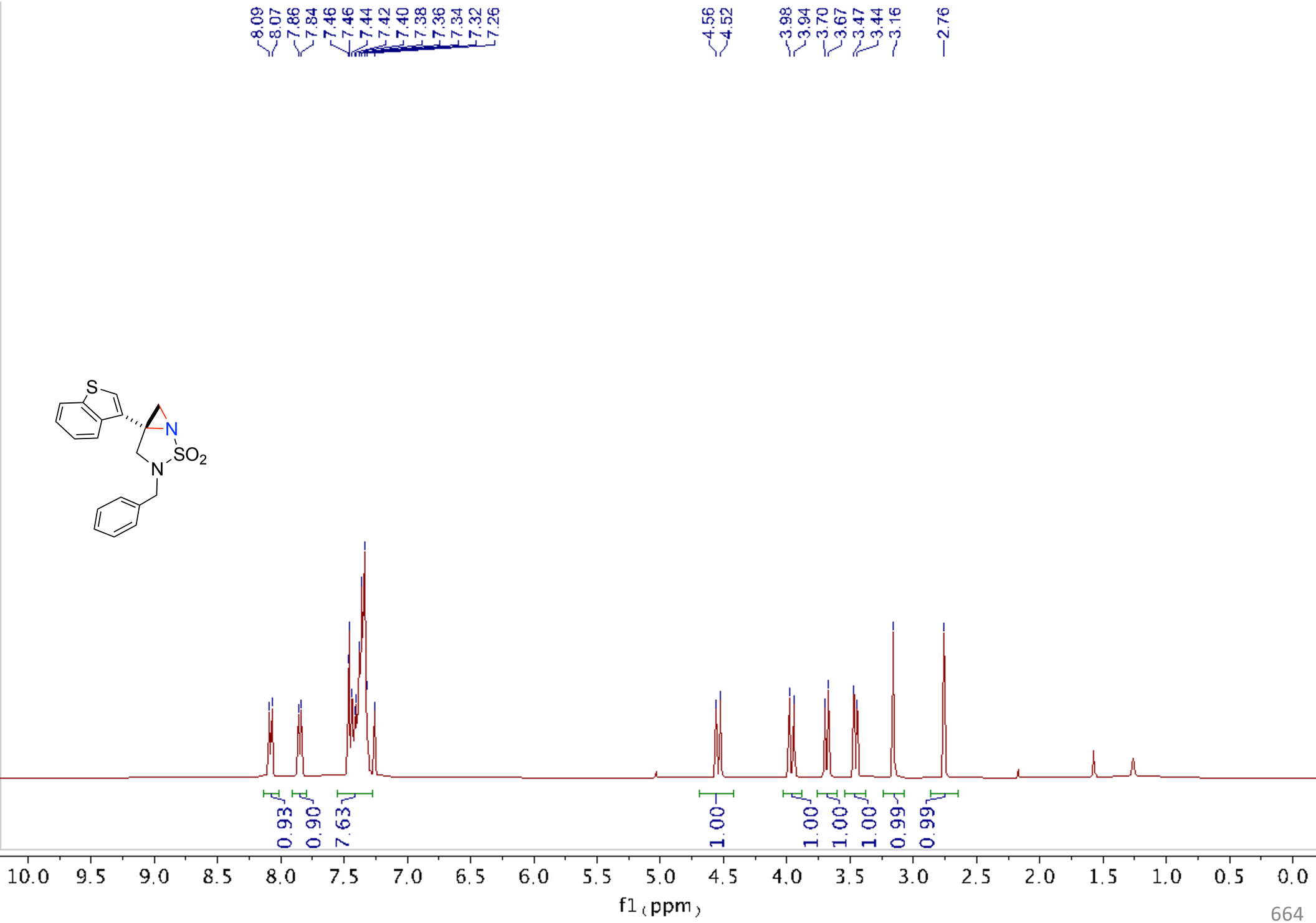


Peak Table

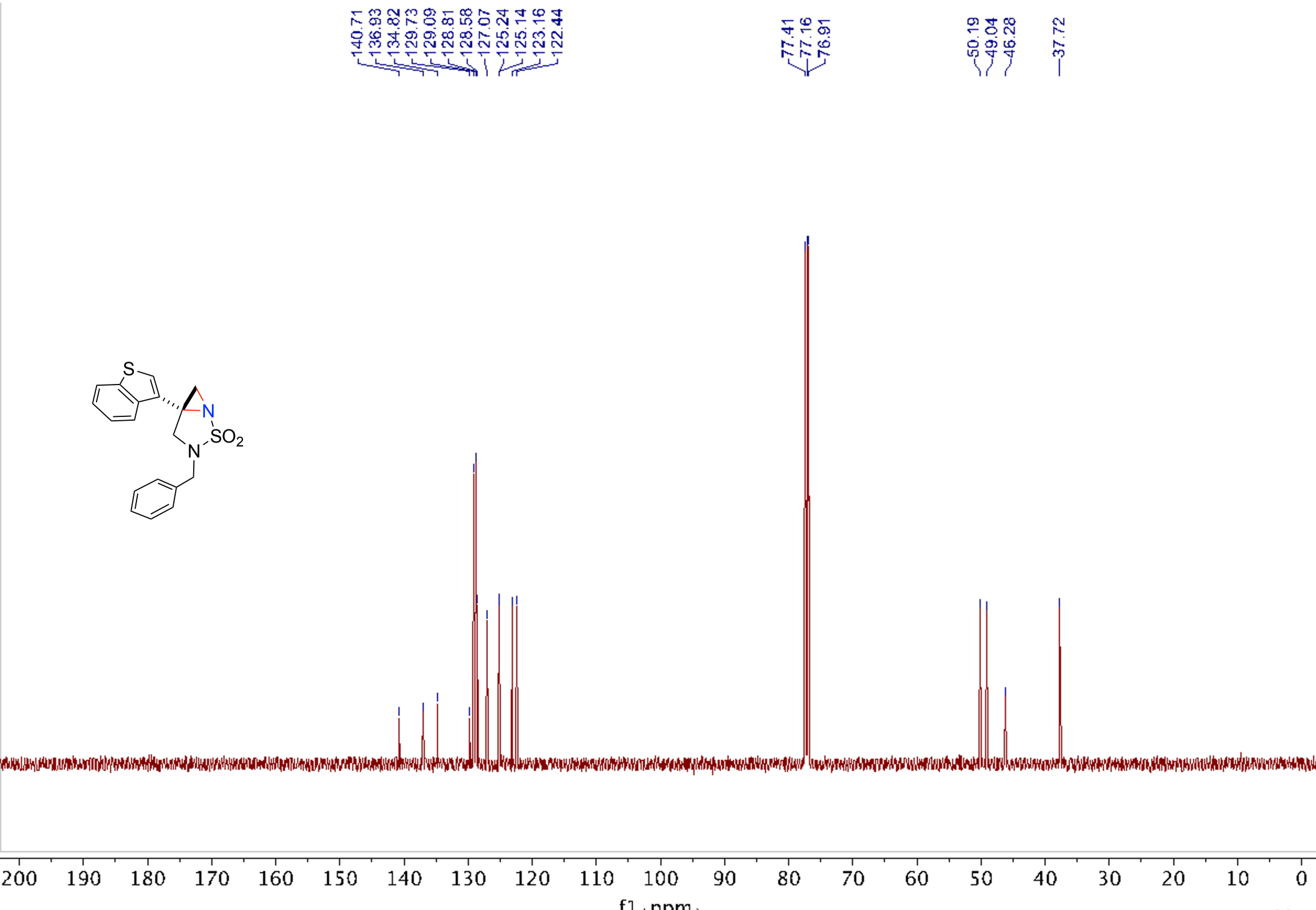
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	32.567	5286704	94.885
2	45.128	284987	5.115
Total		5571691	100.000

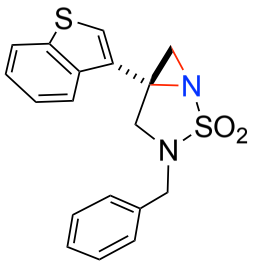
^{1}H NMR (*R*)-5-(Benzo[*b*]thiophen-3-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2k



^{13}C NMR (*R*)-5-(Benzo[*b*]thiophen-3-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2k



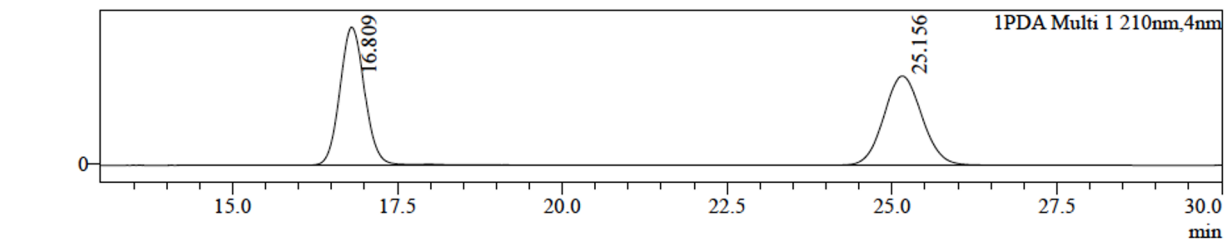
5-(Benzo[*b*]thiophen-3-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2k



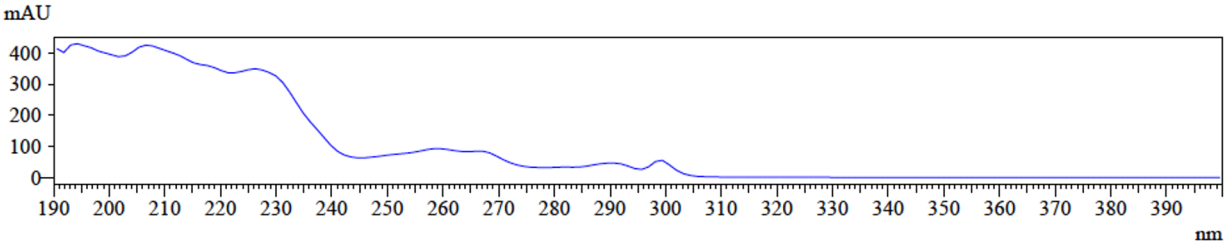
Sample Information

Data File	: H0X-0753--IC-20%1.0mL.lcd
Sample Name	: H0X-0753--IC-20%1.0mL
Sample ID	: H0X-0753--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

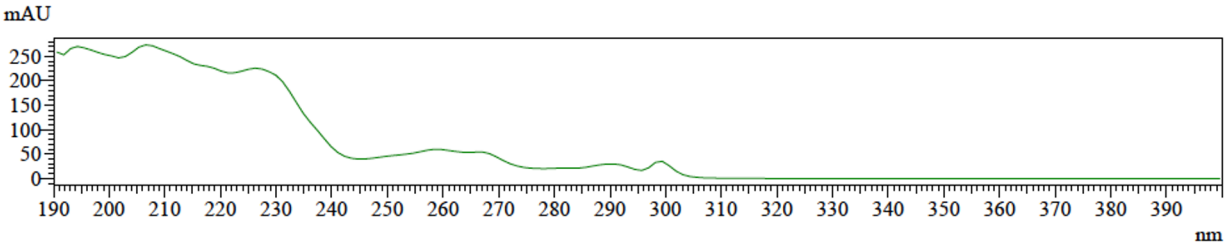
Chromatogram



UV Spectrum
Retention time = 16.809



UV Spectrum
Retention time = 25.156

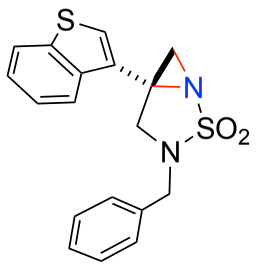


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	16.809	10750733	50.259
2	25.156	10640129	49.741
Total		21390862	100.000

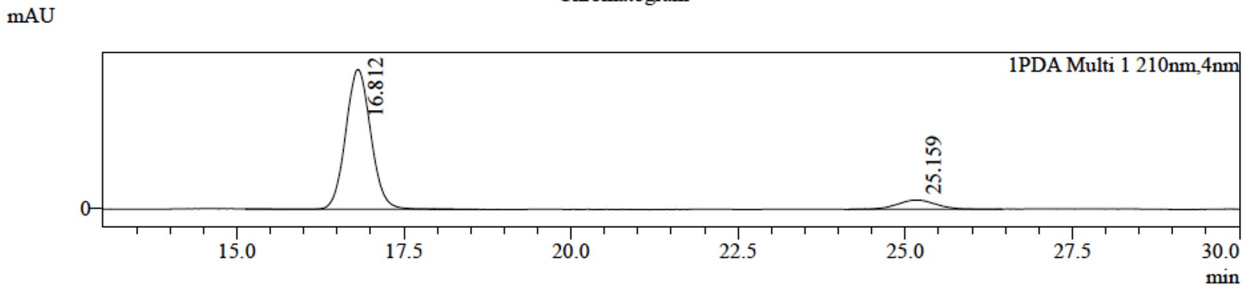
(*R*)-5-(Benzo[*b*]thiophen-3-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2k



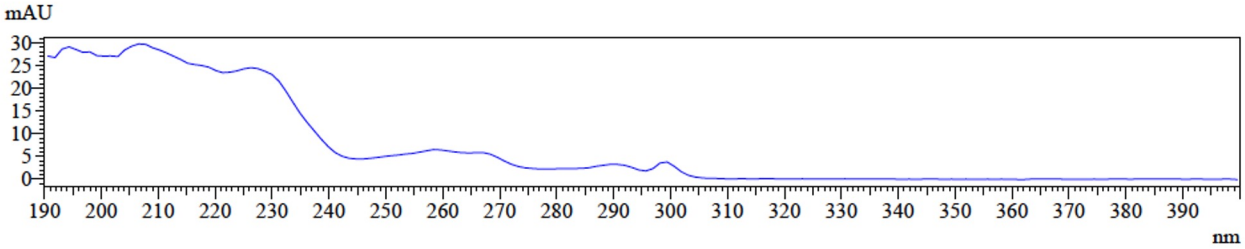
Sample Information

Data File	: H0X-0754--IC-20%1.0mL.lcd
Sample Name	: H0X-0754--IC-20%1.0mL
Sample ID	: H0X-0754--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

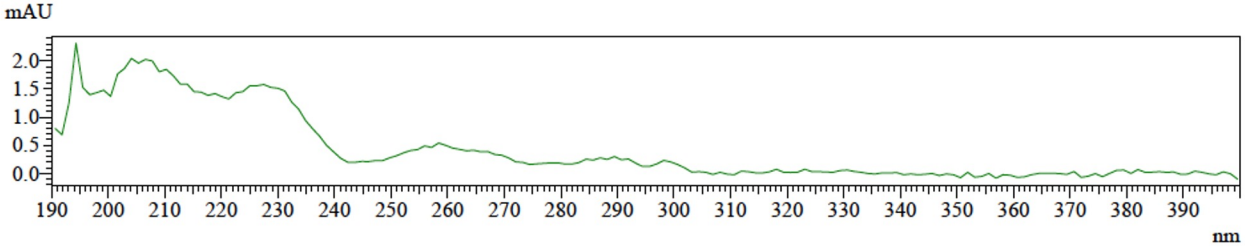
Chromatogram



UV Spectrum
Retention time = 16.812



UV Spectrum
Retention time = 25.159

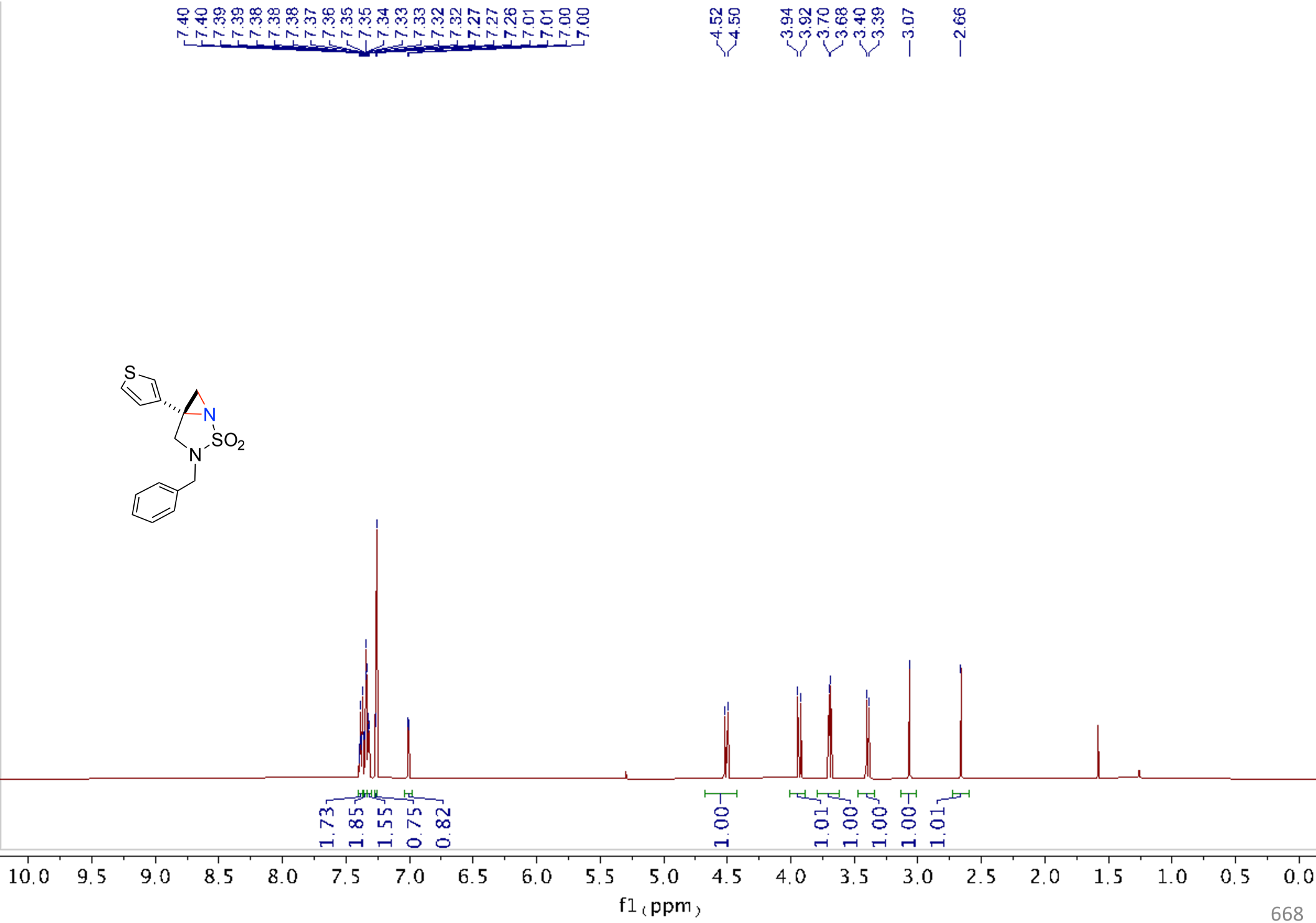


Peak Table

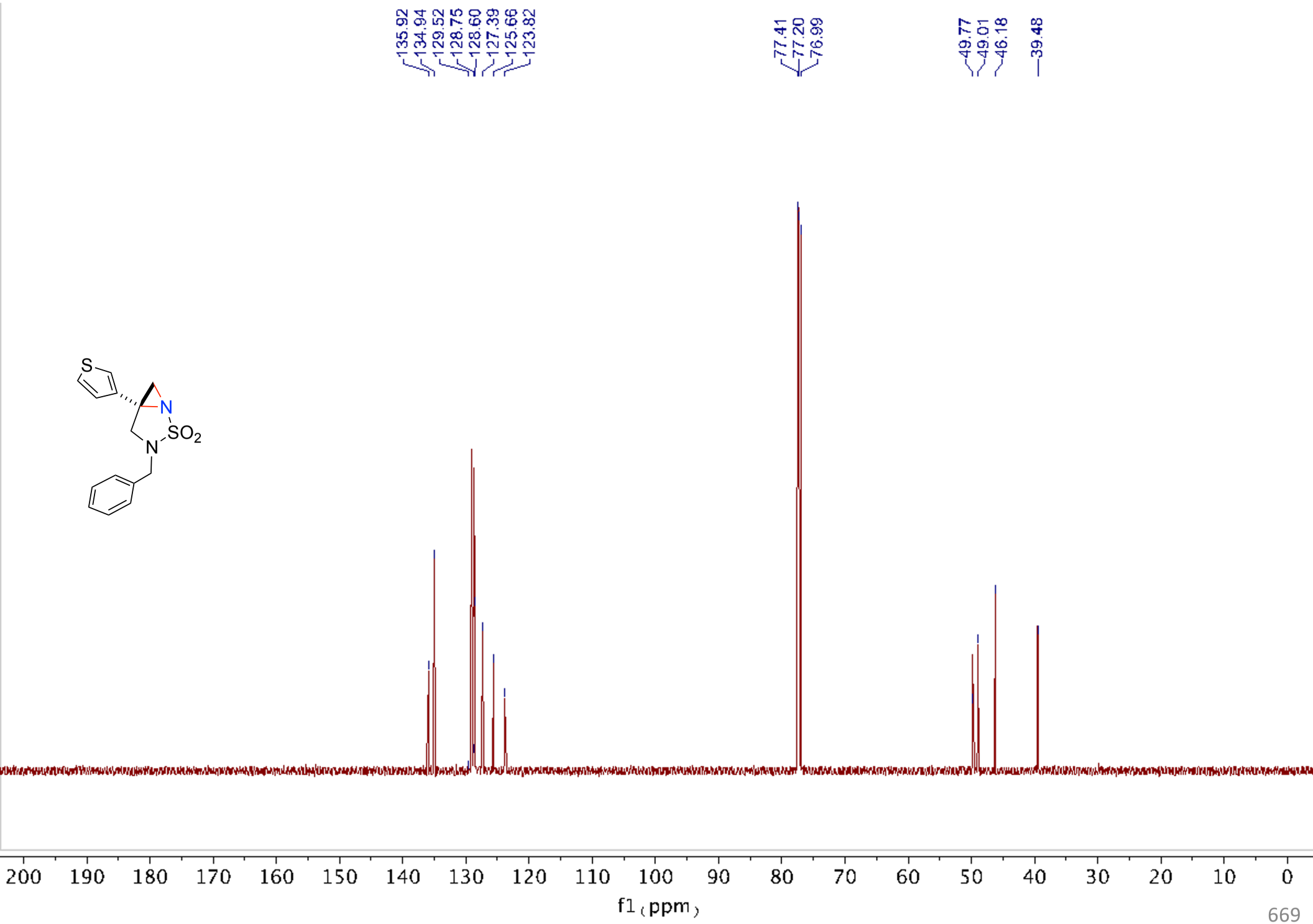
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	16.812	742020	90.814
2	25.159	75053	9.186
Total		817073	100.000

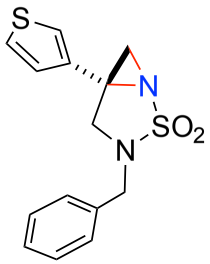
^{1}H NMR (*R*)-3-Benzyl-5-(thiophen-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2l



^{13}C NMR (*R*)-3-Benzyl-5-(thiophen-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2l



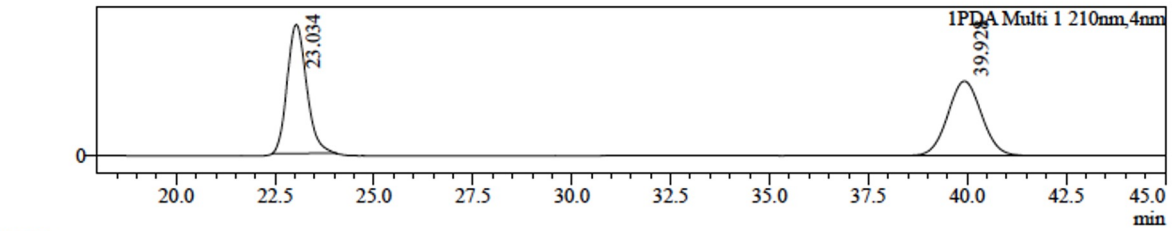
3-Benzyl-5-(thiophen-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2l



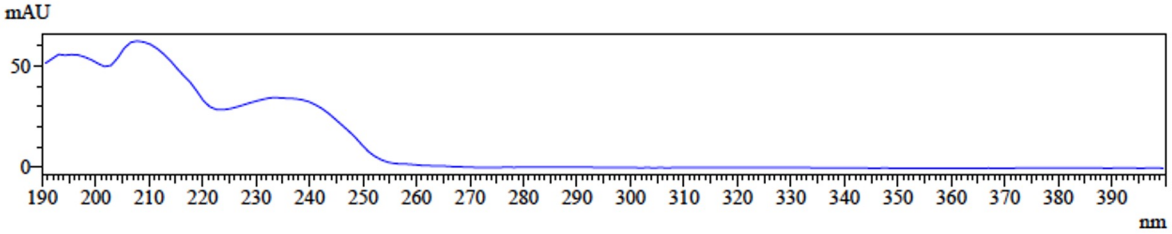
Sample Information

Data File	: H0X-0609-IC-20%1.0mL.lcd
Sample Name	: H0X-0609-IC-20%1.0mL
Sample ID	: H0X-0609-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

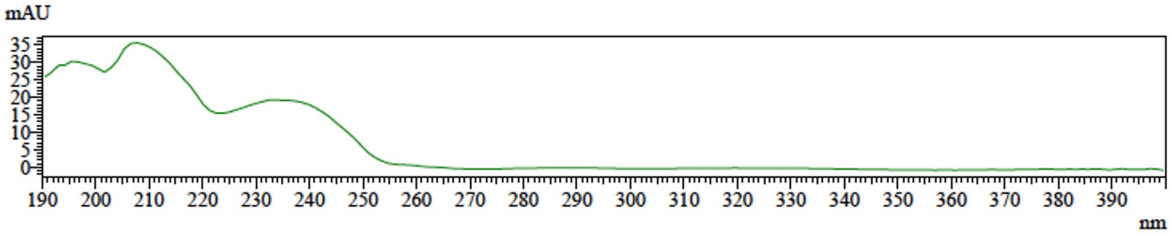
Chromatogram



UV Spectrum
Retention time = 23.034



UV Spectrum
Retention time = 39.928

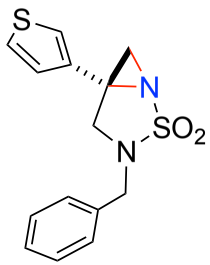


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	23.034	1974100	49.955
2	39.928	1977695	50.045
Total		3951795	100.000

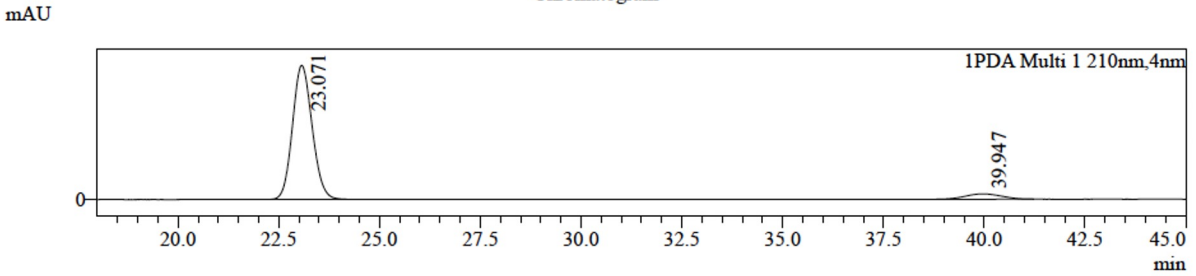
(*R*)-3-Benzyl-5-(thiophen-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2l



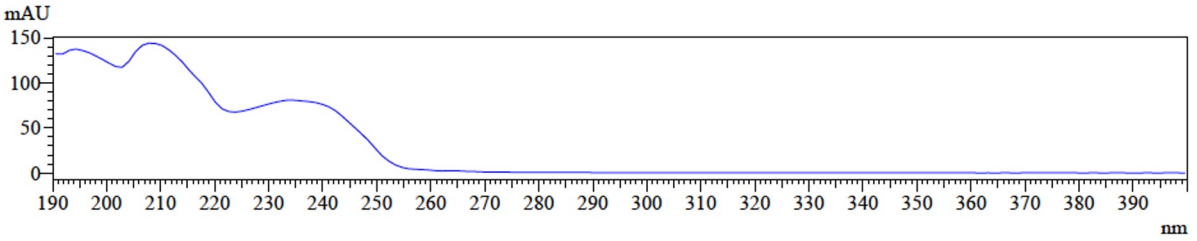
Sample Information

Data File	: H0X-0610-IC-20%1.0mL.lcd
Sample Name	: H0X-0610-IC-20%1.0mL
Sample ID	: H0X-0610-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

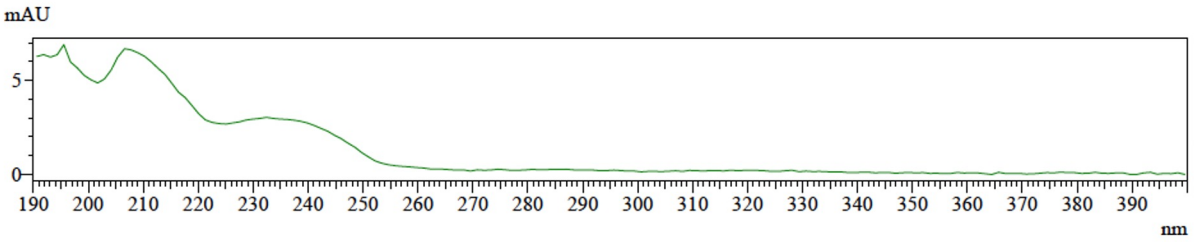
Chromatogram



UV Spectrum
Retention time = 23.071



UV Spectrum
Retention time = 39.947

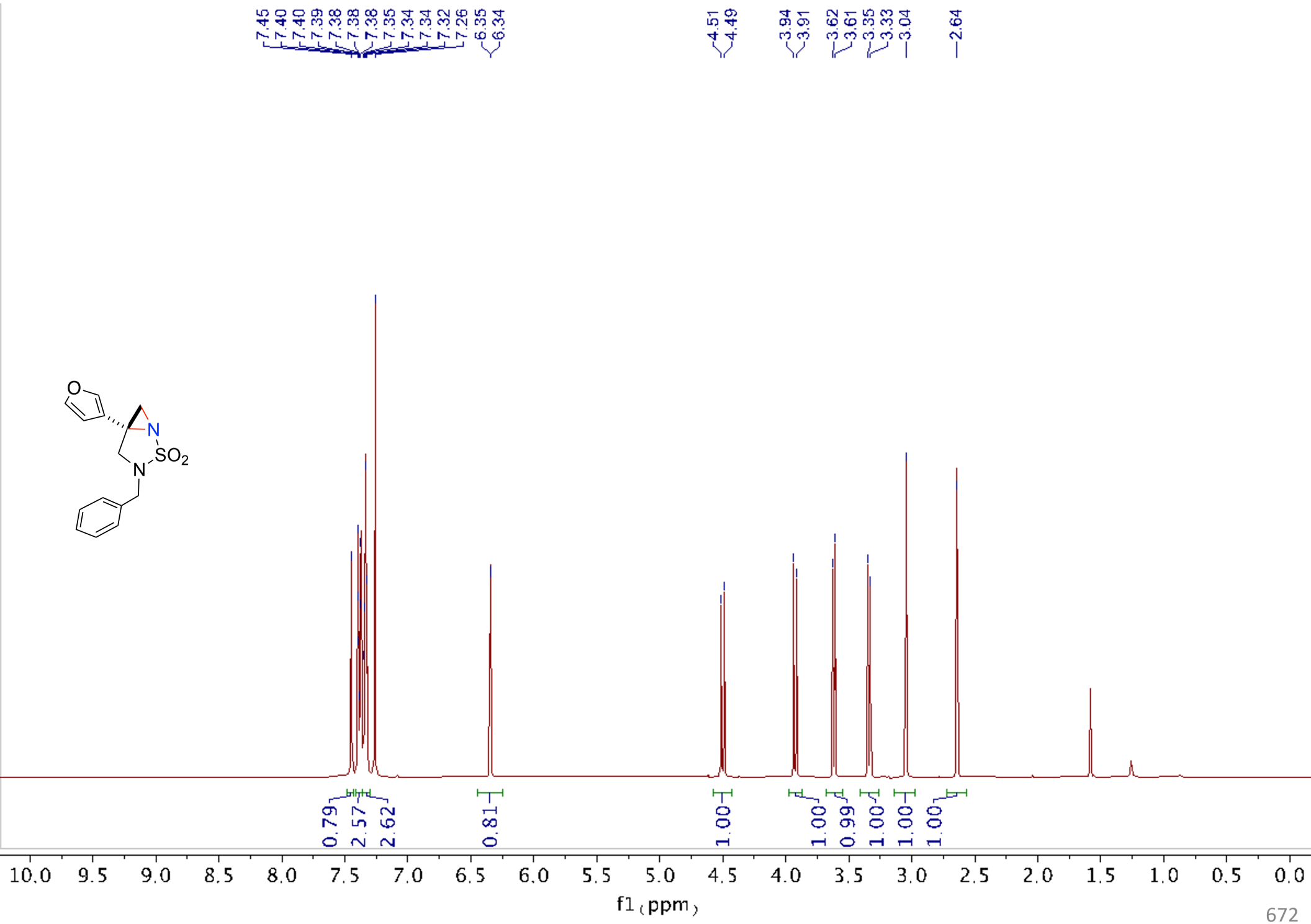


Peak Table

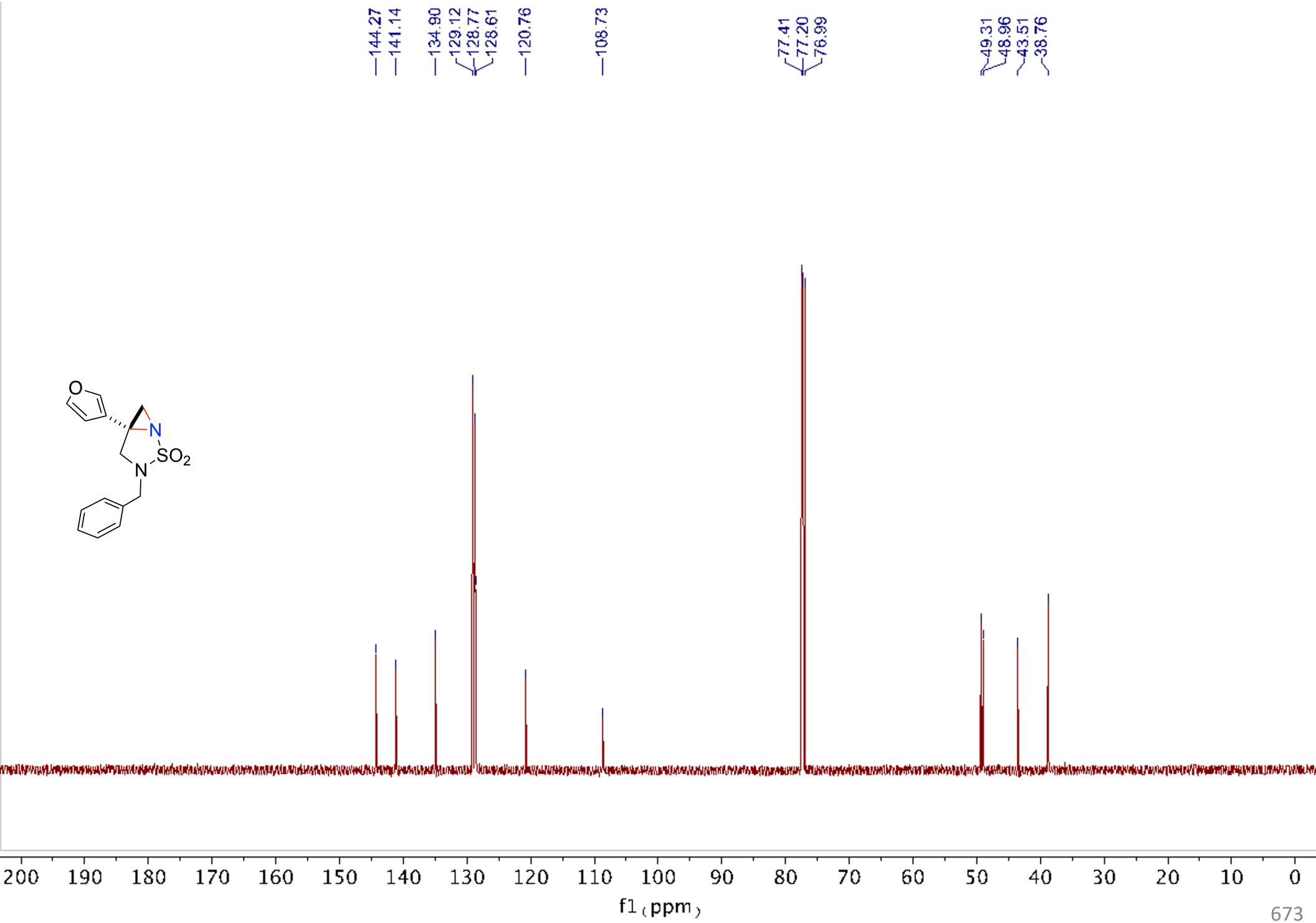
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	23.071	4650451	93.175
2	39.947	340642	6.825
Total		4991093	100.000

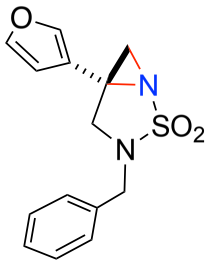
^{1}H NMR (*R*)-3-Benzyl-5-(furan-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2m



^{13}C NMR (*R*)-3-Benzyl-5-(furan-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2m



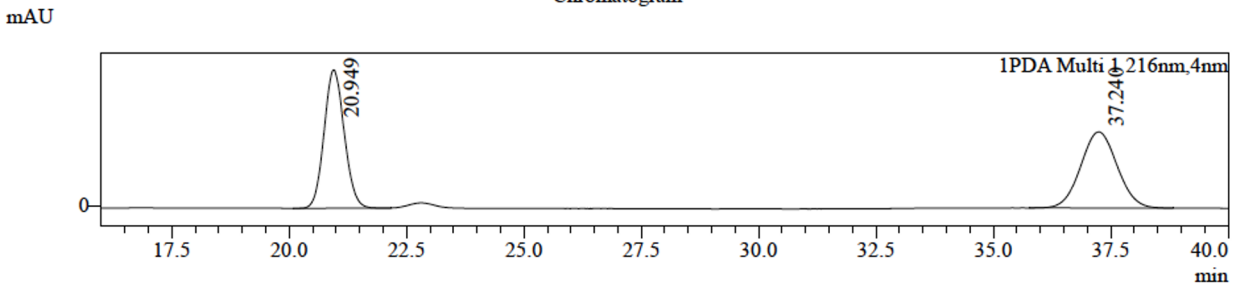
3-Benzyl-5-(furan-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2m



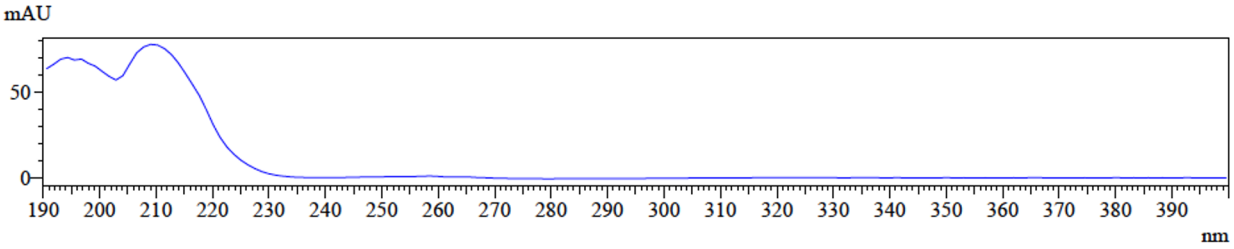
Sample Information

Data File	: H0X-0601-IC-20%1.0mL.lcd
Sample Name	: H0X-0601-IC-20%1.0mL
Sample ID	: H0X-0601-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

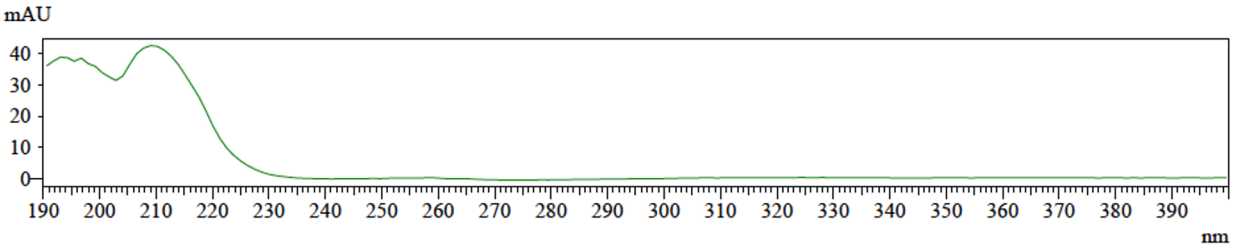
Chromatogram



UV Spectrum
Retention time = 20.949



UV Spectrum
Retention time = 37.240

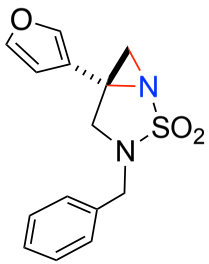


Peak Table

PDA Ch1 216nm

Peak#	Ret. Time	Area	Area%
1	20.949	1745327	50.153
2	37.240	1734674	49.847
Total		3480002	100.000

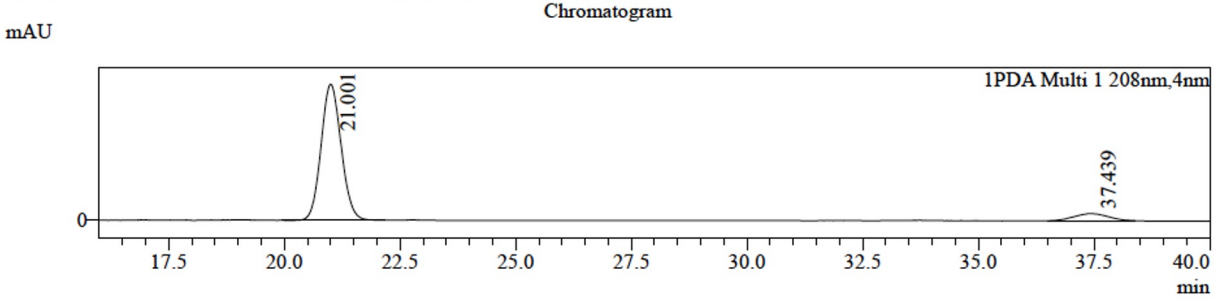
(*R*)-3-Benzyl-5-(furan-3-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2m



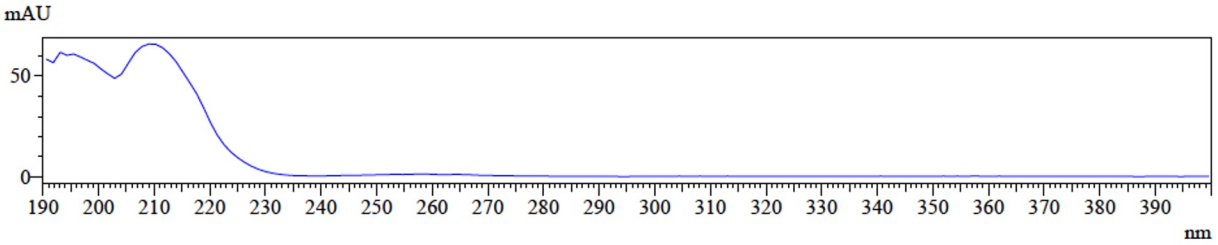
Sample Information

Data File : H0X-0602-IC-20%1.0mL.lcd
Sample Name : H0X-0602-IC-20%1.0mL
Sample ID : H0X-0602-IC-20%1.0mL
Method File : H0X-20%-1.0ml-60MIN.lcm

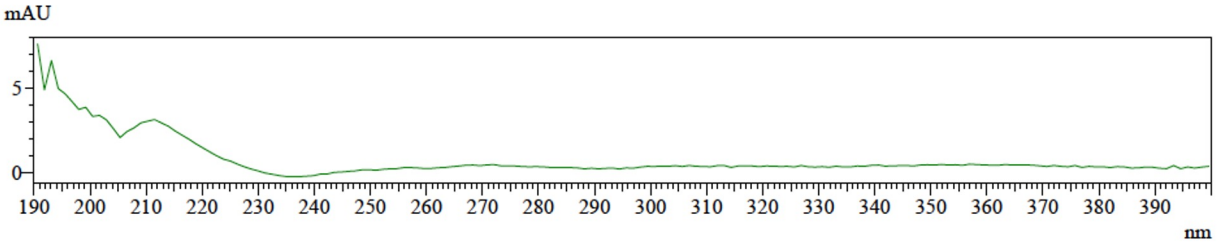
Chromatogram



UV Spectrum
Retention time = 21.001



UV Spectrum
Retention time = 37.439

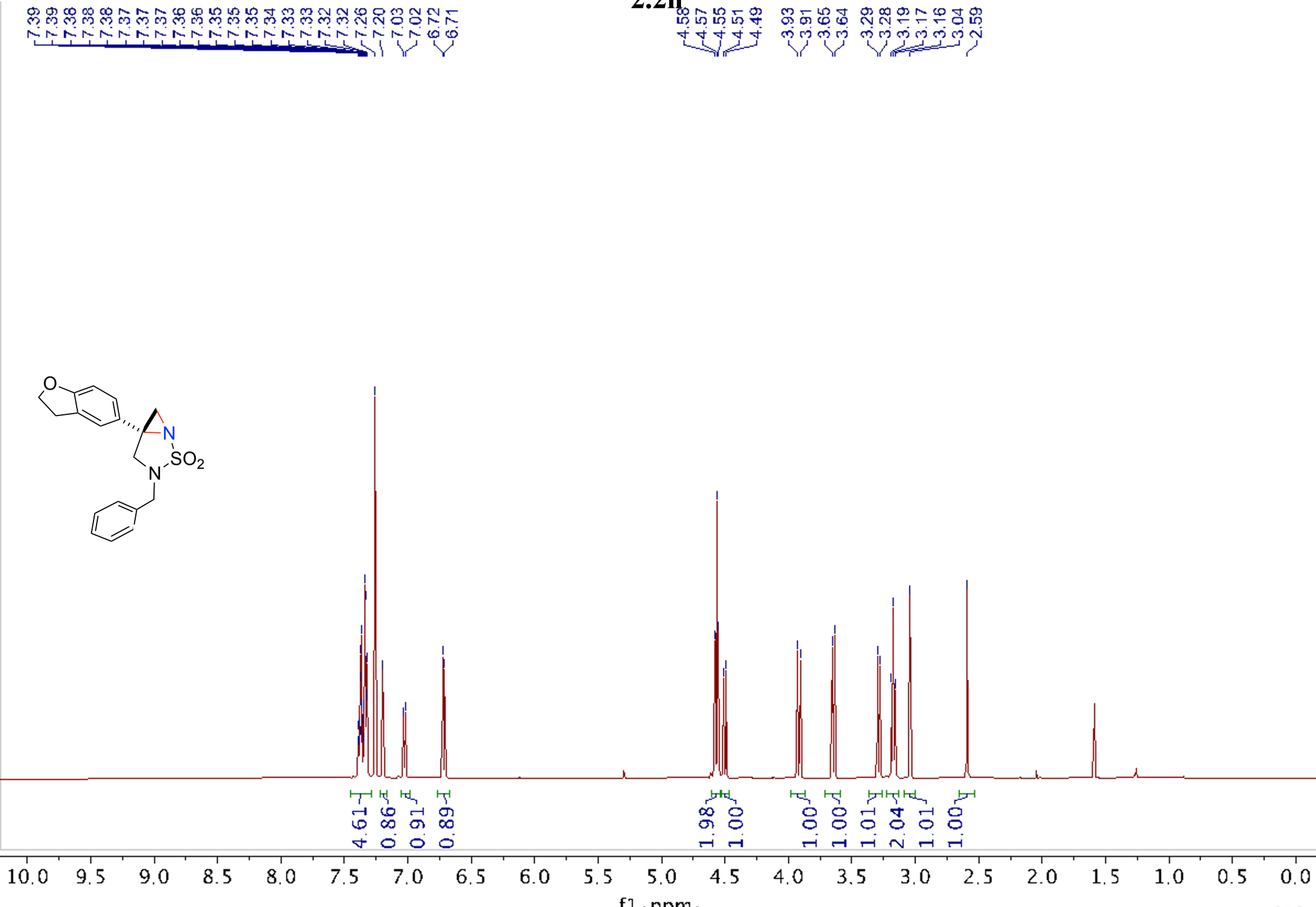


Peak Table

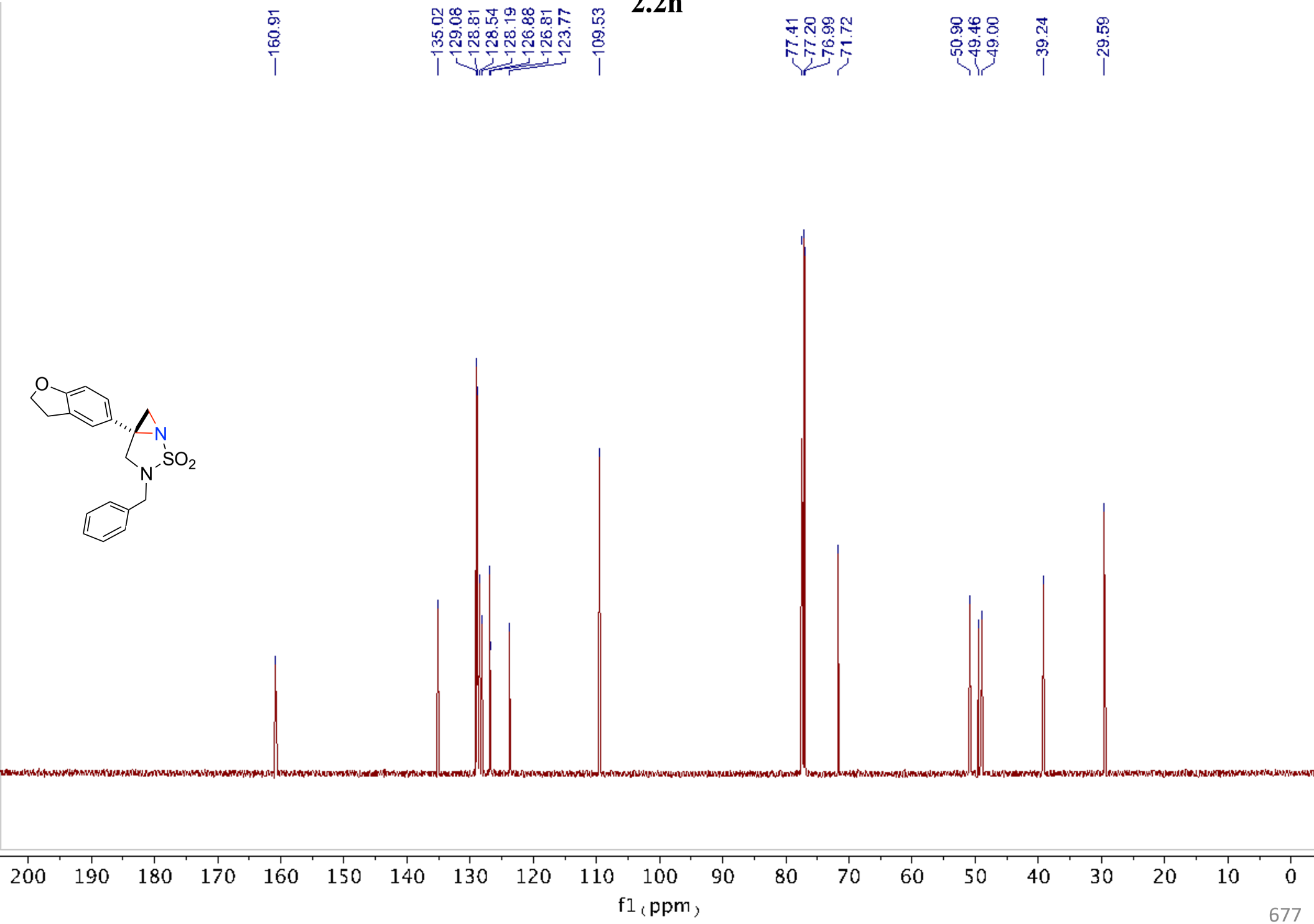
PDA Ch1 208nm

Peak#	Ret. Time	Area	Area%
1	21.001	1862259	91.811
2	37.439	166111	8.189
Total		2028370	100.000

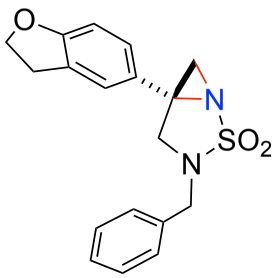
^{1}H NMR (*R*)-3-Benzyl-5-(2,3-dihydrobenzofuran-5-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2n



^{13}C NMR (*R*)-3-Benzyl-5-(2,3-dihydrobenzofuran-5-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2n



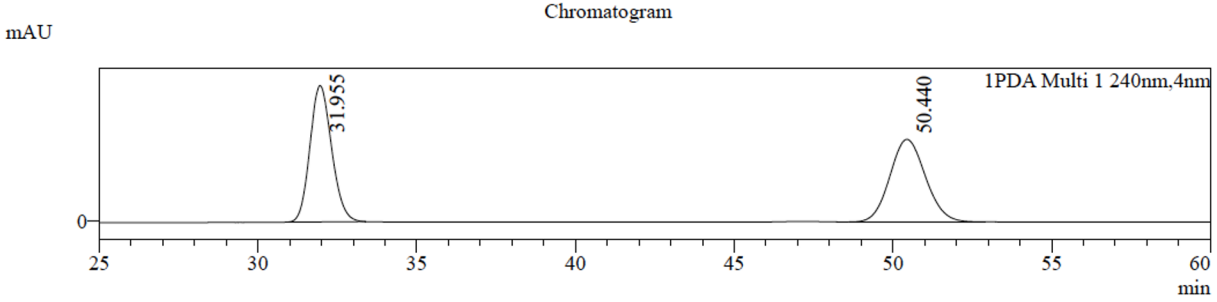
3-Benzyl-5-(2,3-dihydrobenzofuran-5-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2n



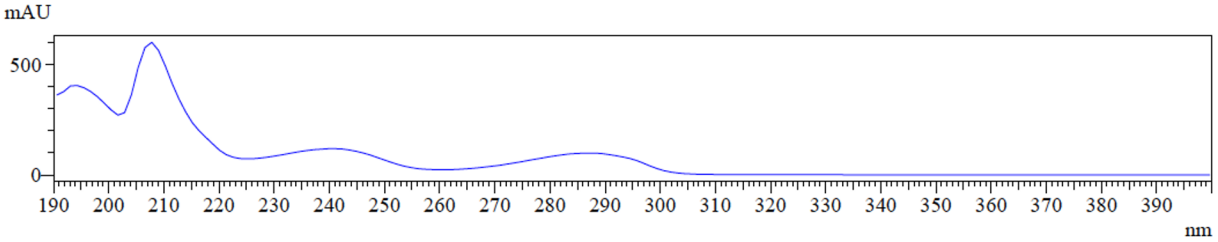
Sample Information

Data File	: H0X-060X-RAC-IC-30%1.0mL001.lcd
Sample Name	: H0X-060X-RAC-IC-30%1.0mL
Sample ID	: H0X-060X-RAC-IC-30%1.0mL
Method File	: H0X-30%-1.0ml--60MIN.lcm

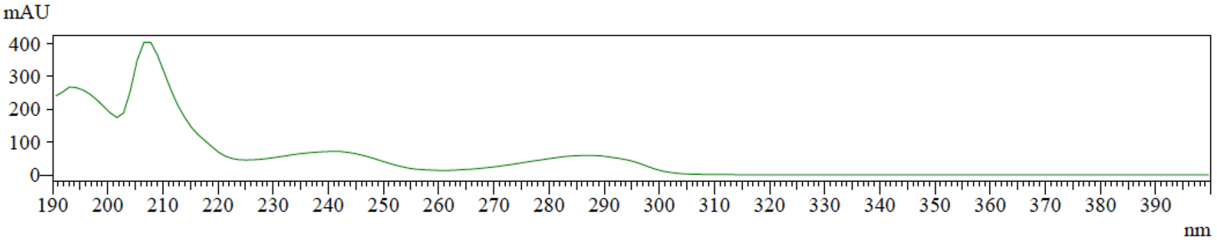
Chromatogram



UV Spectrum
Retention time = 31.955



UV Spectrum
Retention time = 50.440

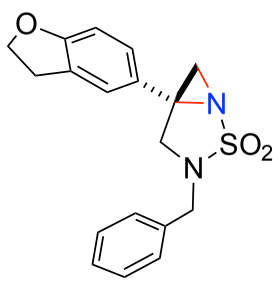


Peak Table

PDA Ch1 240nm

Peak#	Ret. Time	Area	Area%
1	31.955	5540845	50.172
2	50.440	5502782	49.828
Total		11043627	100.000

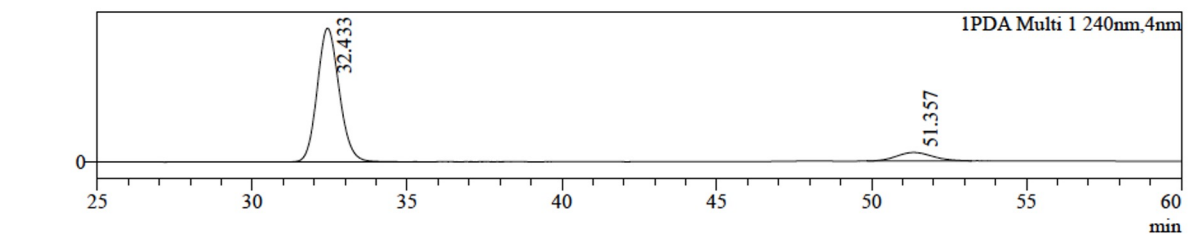
(*R*)-3-Benzyl-5-(2,3-dihydrobenzofuran-5-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2n



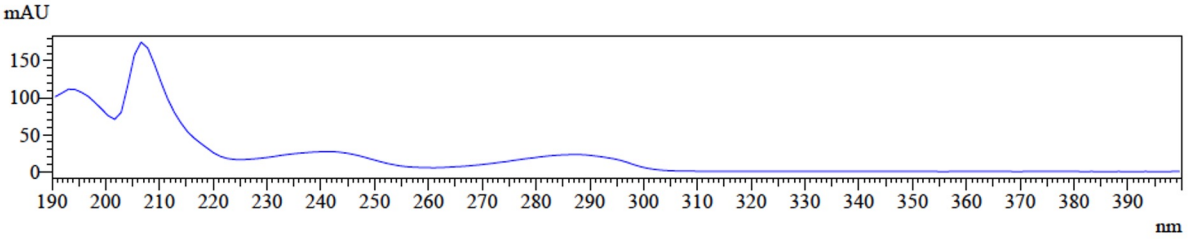
Sample Information

Data File	: H0X-060X-CHIRAL-IC-30%1.0mL.lcd
Sample Name	: H0X-060X-CHIRAL-IC-30%1.0mL
Sample ID	: H0X-060X-CHIRAL-IC-30%1.0mL
Method File	: H0X-30%-1.0ml--60MIN.lcm

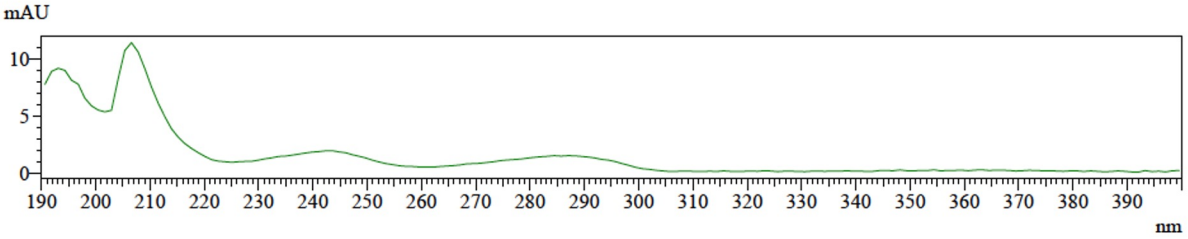
Chromatogram



UV Spectrum
Retention time = 32.433



UV Spectrum
Retention time = 51.357

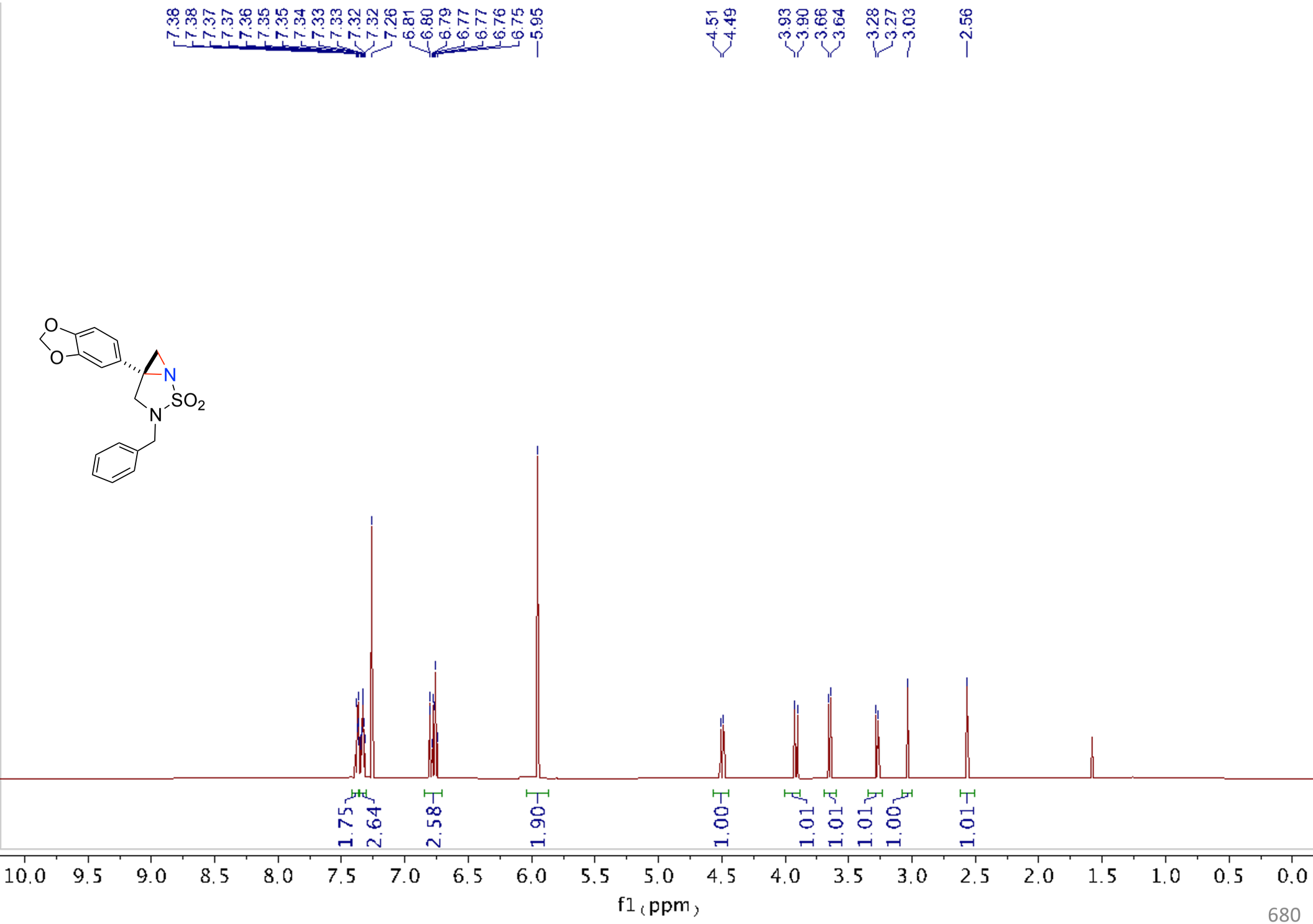


Peak Table

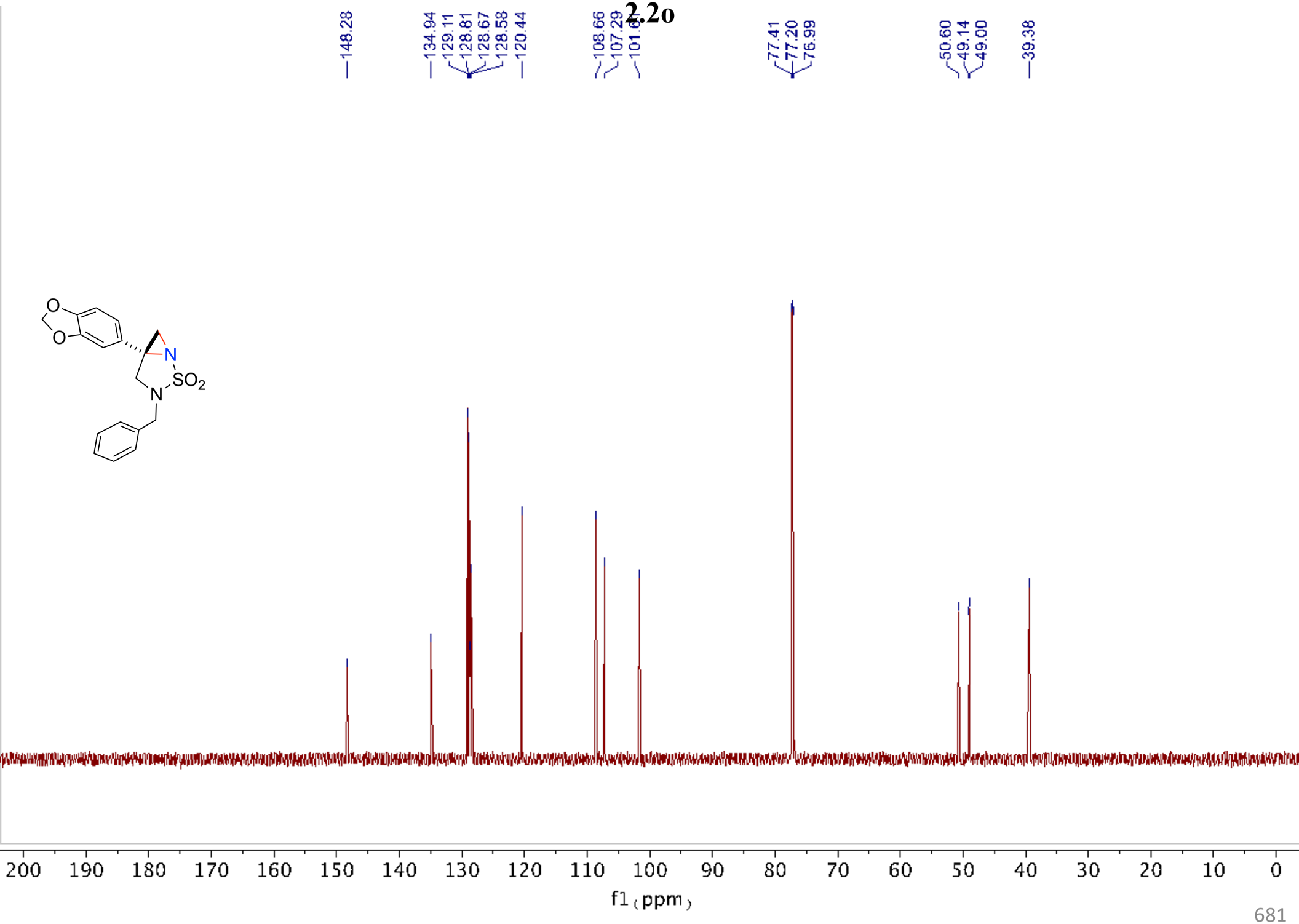
PDA Ch1 240nm

Peak#	Ret. Time	Area	Area%
1	32.433	1302579	90.631
2	51.357	134653	9.369
Total		1437232	100.000

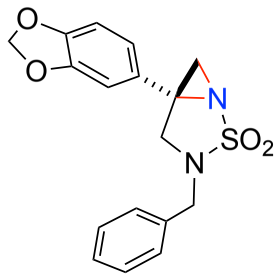
^{1}H NMR (*R*)-5-(Benzo[*d*][1,3]dioxol-5-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2o



^{13}C NMR (*R*)-5-(Benzo[*d*][1,3]dioxol-5-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2o



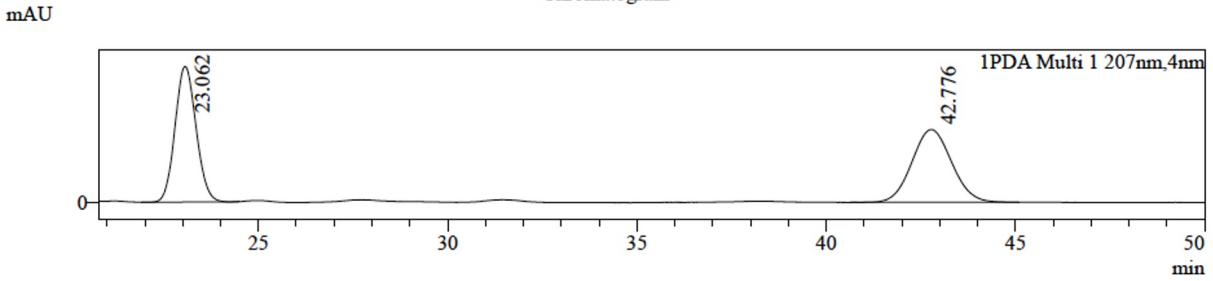
5-(Benzo[*d*][1,3]dioxol-5-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2o



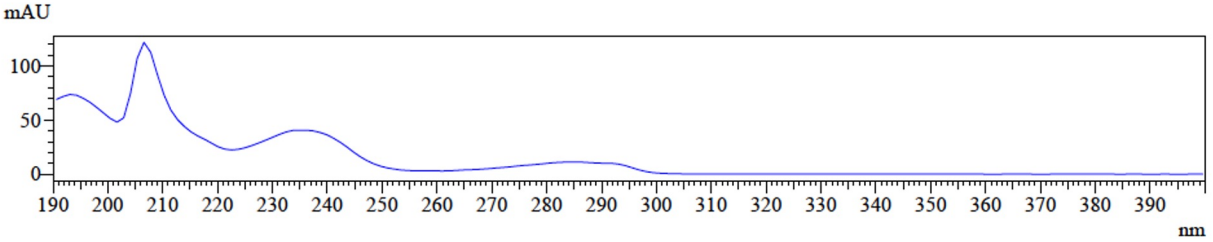
Sample Information

Data File	: H0X-0599_3rd-IC-30%1.0mL.lcd
Sample Name	: H0X-0599_3rd-IC-30%1.0mL
Sample ID	: H0X-0599_3rd-IC-30%1.0mL
Method File	: H0X-30%-1.0ml-90MIN.lcm

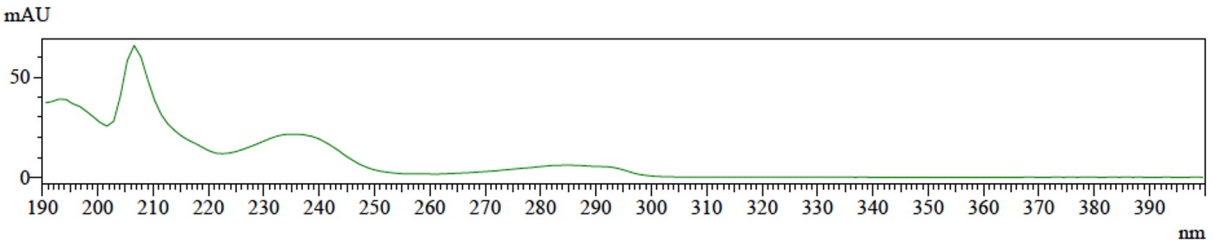
Chromatogram



UV Spectrum
Retention time = 23.062



UV Spectrum
Retention time = 42.776

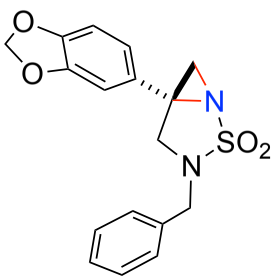


Peak Table

PDA Ch1 207nm

Peak#	Ret. Time	Area	Area%
1	23.062	3722931	49.642
2	42.776	3776681	50.358
Total		7499611	100.000

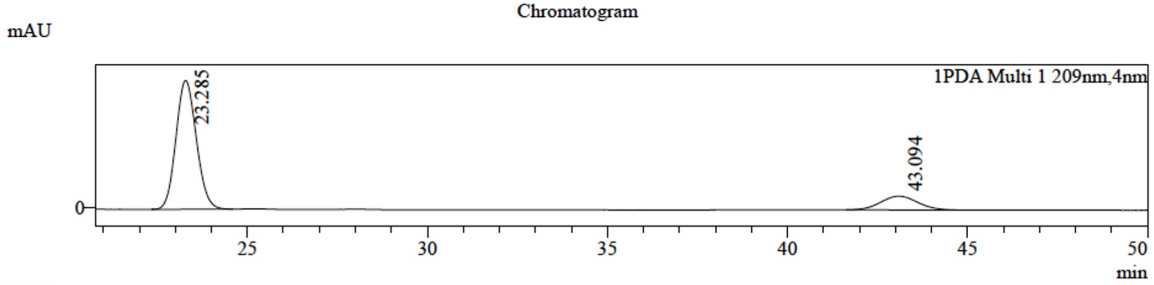
(*R*)-5-(Benzo[*d*][1,3]dioxol-5-yl)-3-benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2o



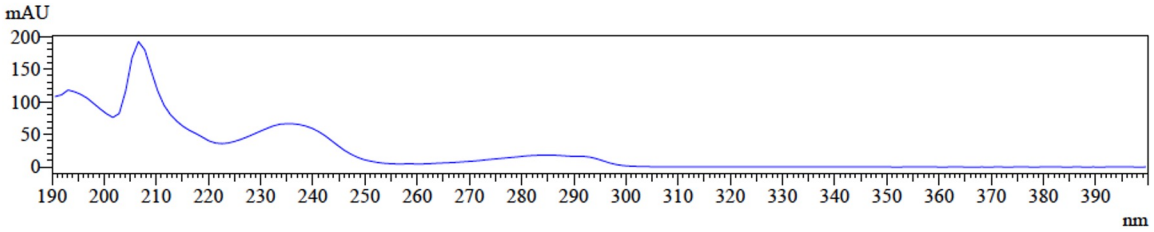
Sample Information

Data File : H0X-0600-IC-30%1.0mL.lcd
Sample Name : H0X-0600-IC-30%1.0mL
Sample ID : H0X-0600-IC-30%1.0mL
Method File : H0X-30%-1.0ml-90MIN.lcm

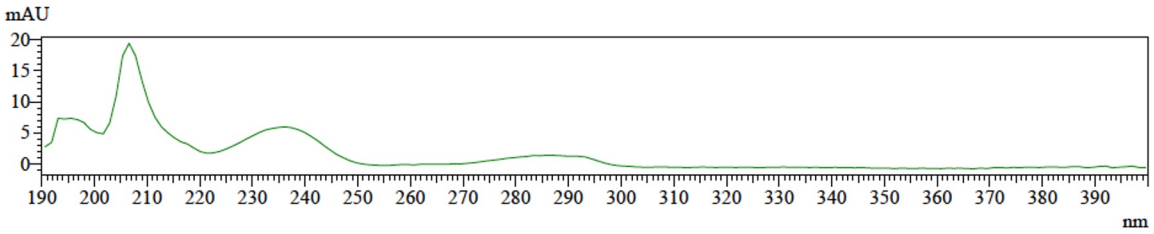
Chromatogram



UV Spectrum
Retention time = 23.285



UV Spectrum
Retention time = 43.094

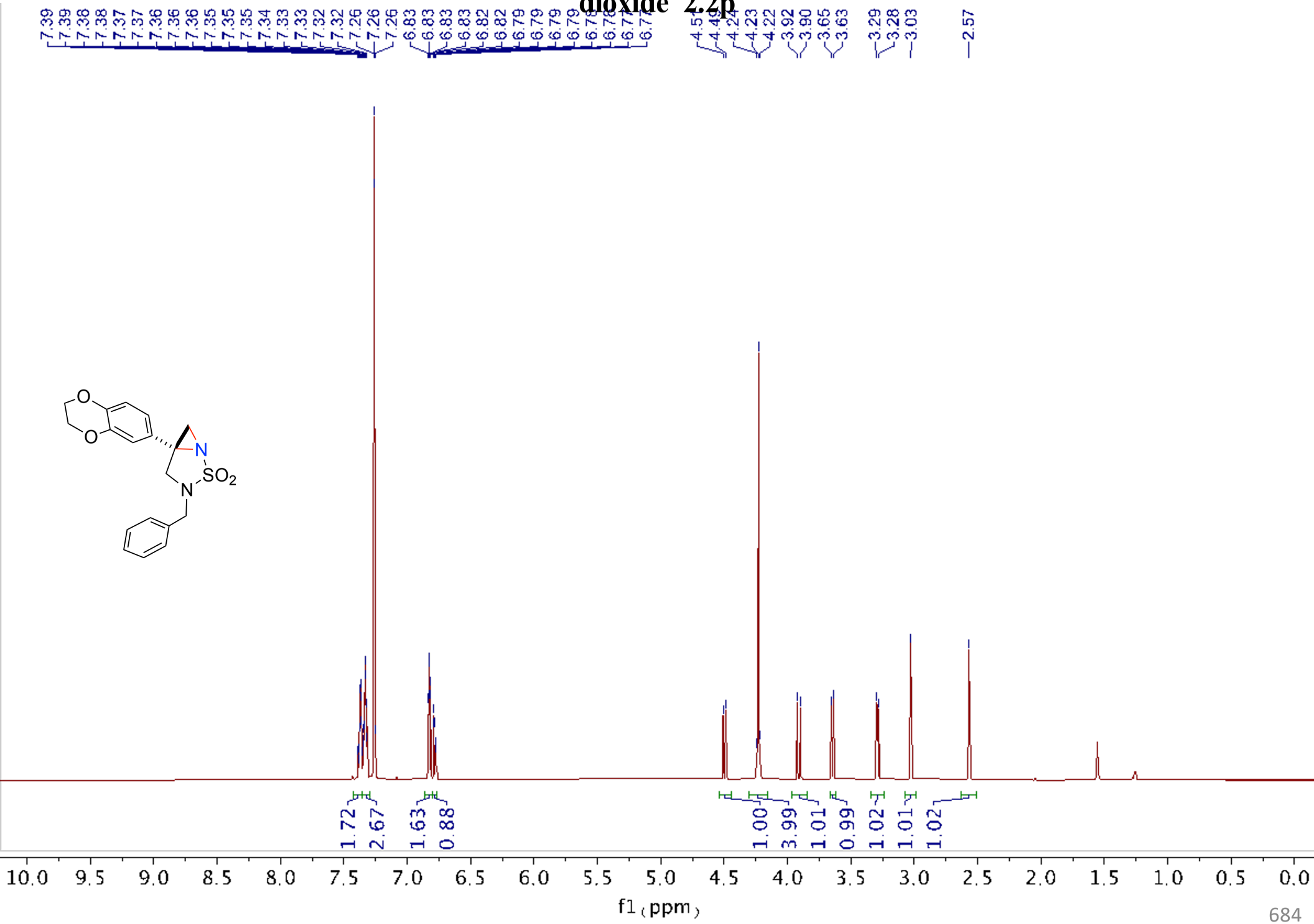


Peak Table

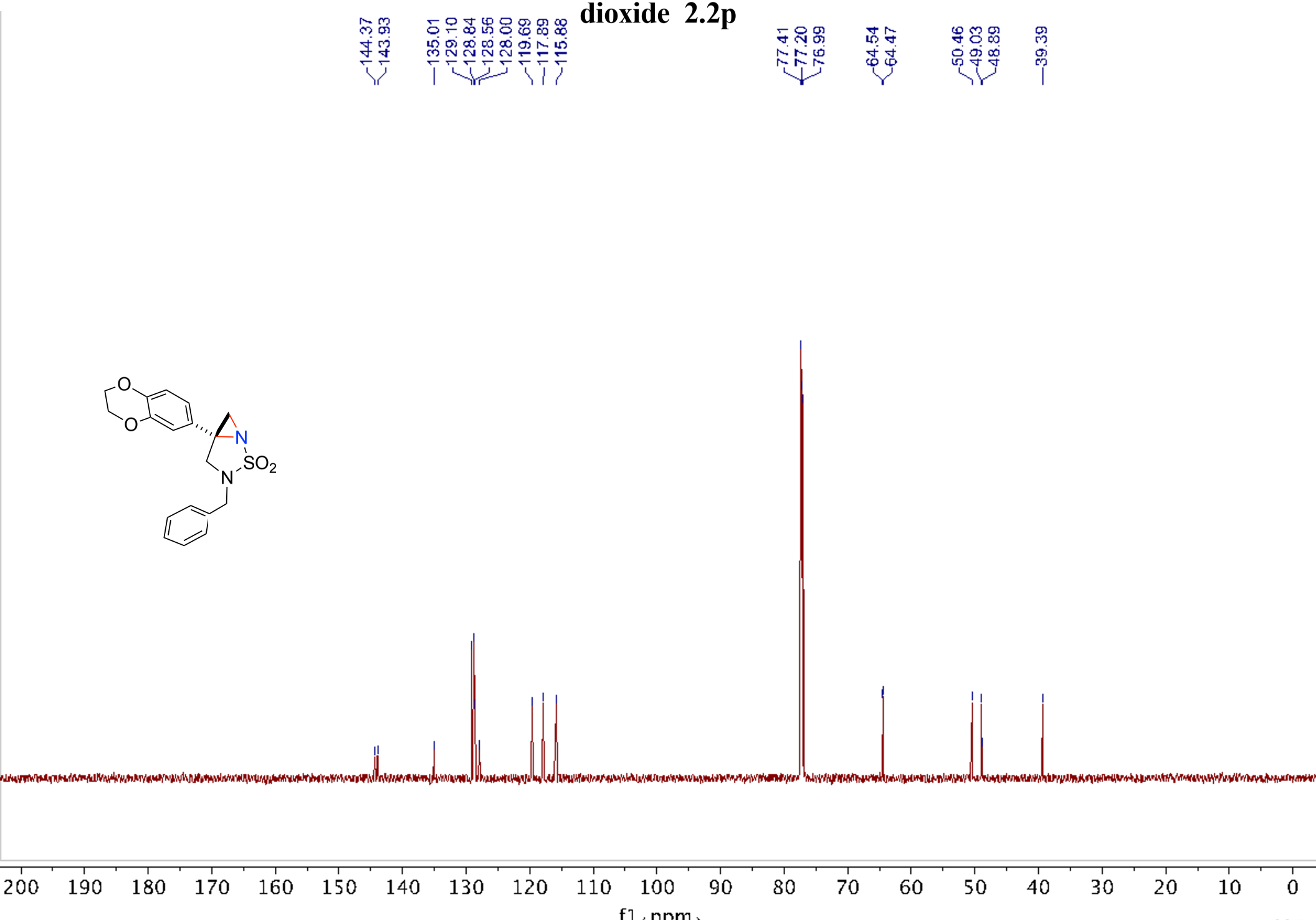
PDA Ch1 209nm

Peak#	Ret. Time	Area	Area%
1	23.285	5558979	83.824
2	43.094	1072740	16.176
Total		6631719	100.000

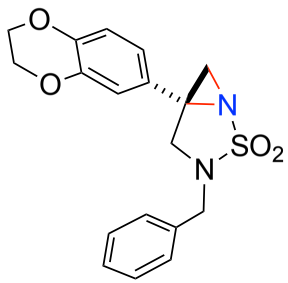
^{1}H NMR (*R*)-3-Benzyl-5-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2p



^{13}C NMR (*R*)-3-Benzyl-5-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2p



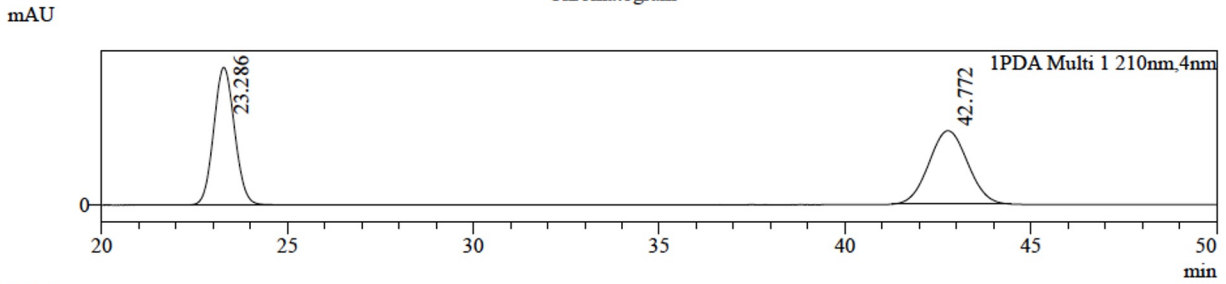
3-Benzyl-5-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2p



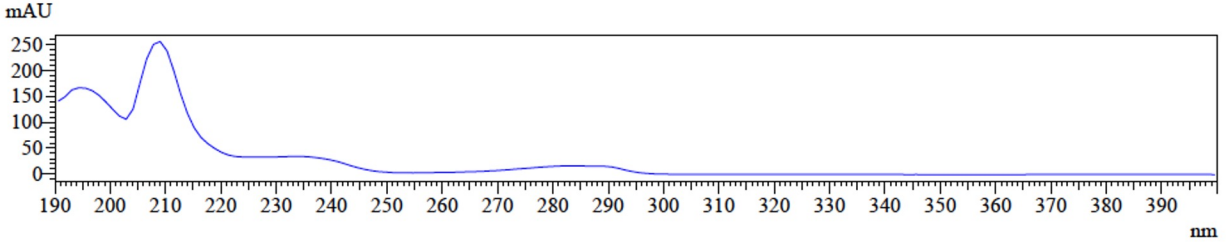
Sample Information

Data File	: H0X-0918-IC-30%1.0mL001.lcd
Sample Name	: H0X-0918-IC-30%1.0mL001
Sample ID	: H0X-0918-IC-30%1.0mL001
Method File	: H0X-30%-1.0ml-60MIN.lcm

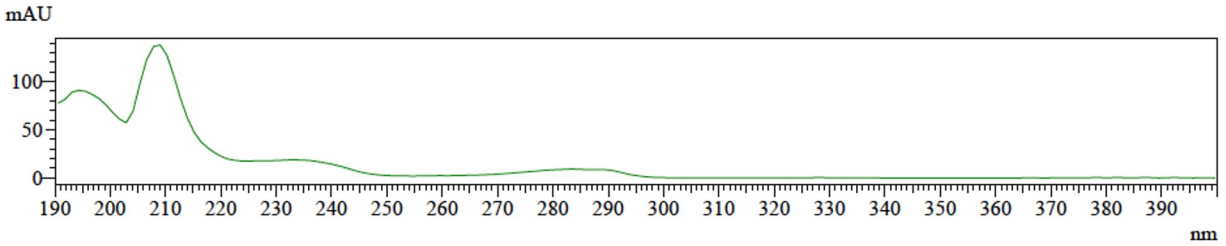
Chromatogram



UV Spectrum
Retention time = 23.286



UV Spectrum
Retention time = 42.772

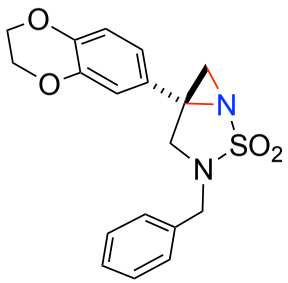


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	23.286	7978535	50.080
2	42.772	7953109	49.920
Total		15931644	100.000

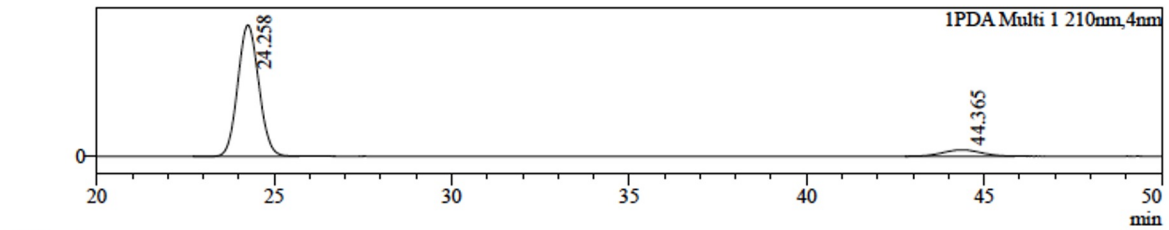
(*R*)-3-Benzyl-5-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2p



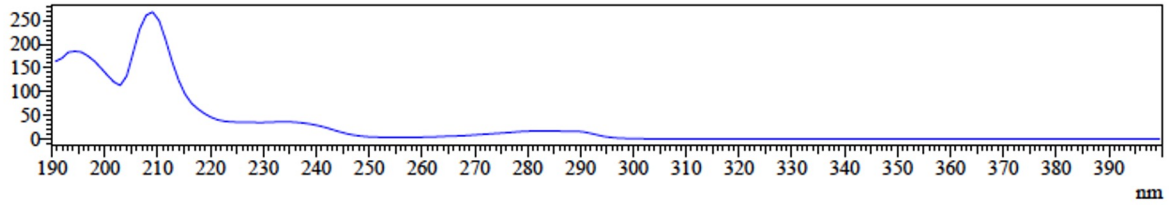
Sample Information

Data File	: H0X-0919-IC-30%1.0mL001.lcd
Sample Name	: H0X-0919-IC-30%1.0mL001
Sample ID	: H0X-0919-IC-30%1.0mL001
Method File	: H0X-30%-1.0ml-60MIN.lcm

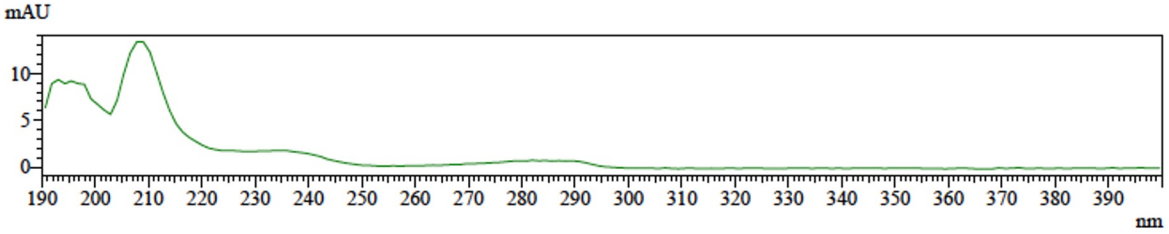
Chromatogram



UV Spectrum
Retention time = 24.258



UV Spectrum
Retention time = 44.365

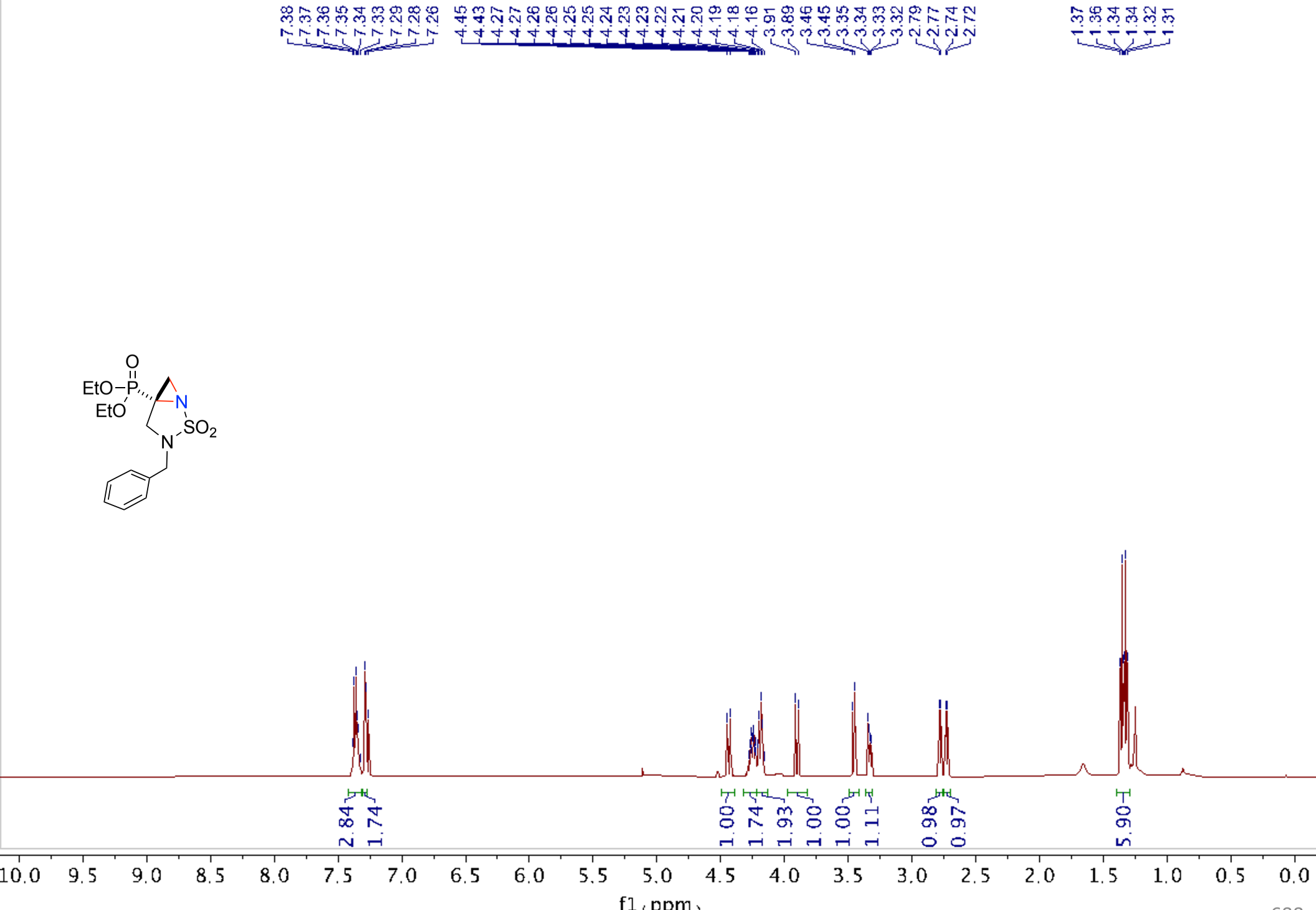


Peak Table

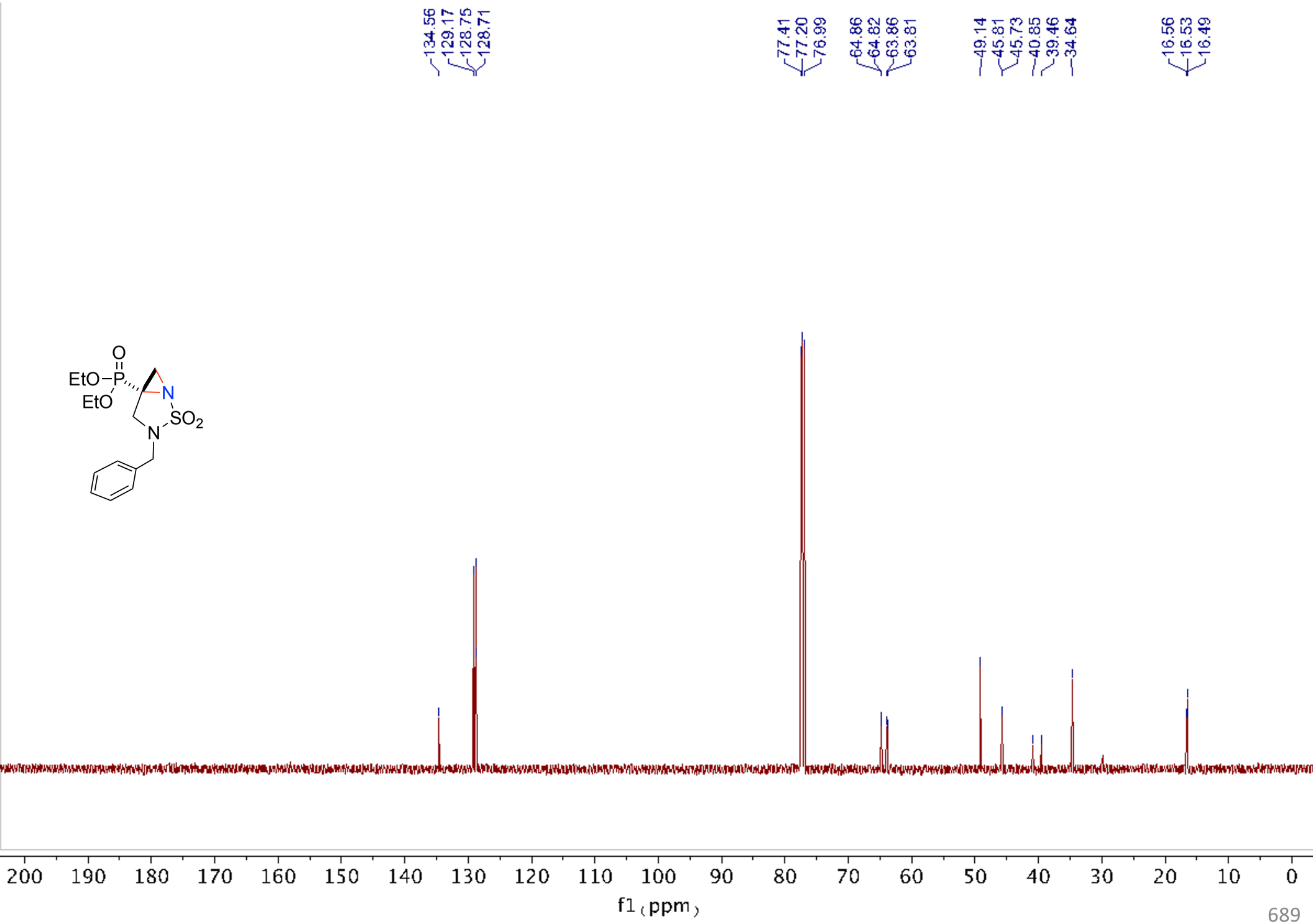
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	24.258	8895289	91.784
2	44.365	796219	8.216
Total		9691508	100.000

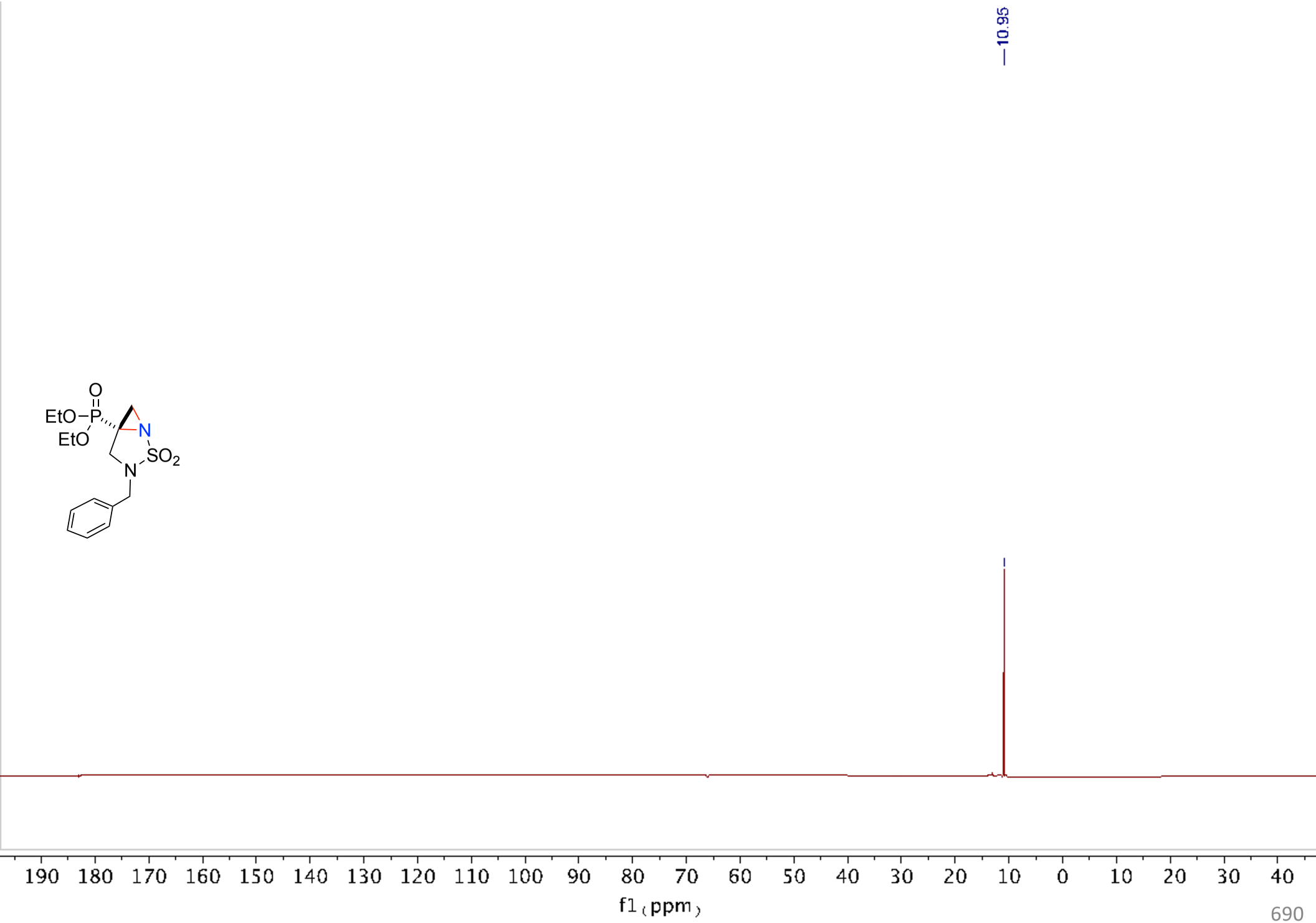
^{1}H NMR Diethyl (*S*)-(3-benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)phosphonate 2.2q



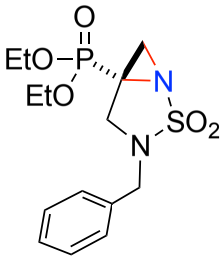
^{13}C NMR Diethyl (*S*)-(3-benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)phosphonate 2.2q



^{31}P NMR Diethyl (*S*)-(3-benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)phosphonate 2.2q



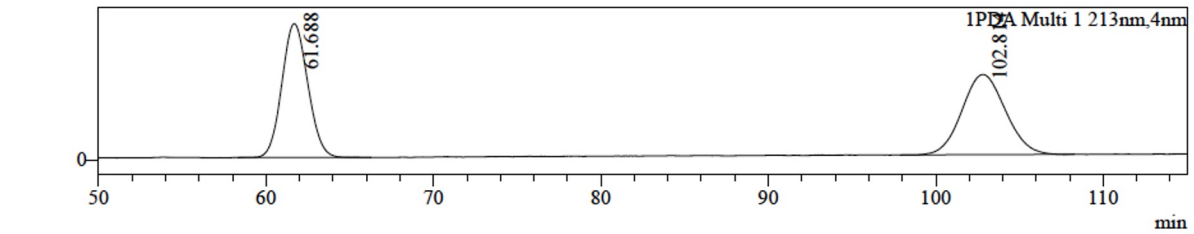
Diethyl (3-benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)phosphonate 2.2q



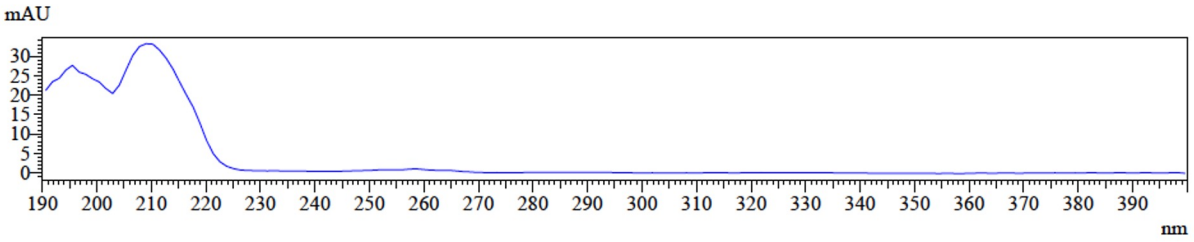
Sample Information

Data File	: H0X-0755-RAC-IC-20%1.0mL004.lcd
Sample Name	: H0X-0755-RAC-IC-20%1.0mL003
Sample ID	: H0X-0755-RAC-IC-20%1.0mL003
Method File	: H0X-20%-1.0ml-90MIN.lcm

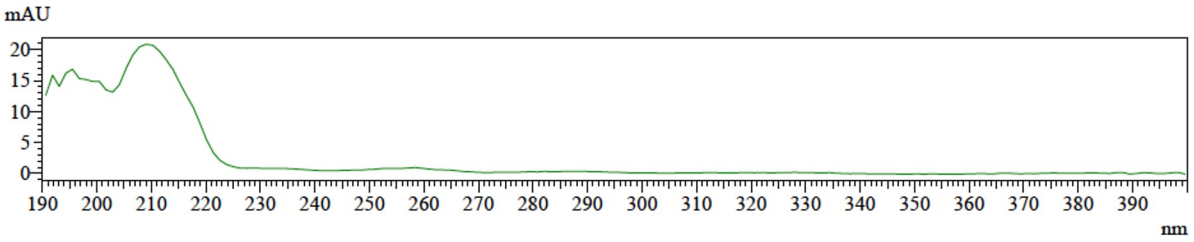
Chromatogram



UV Spectrum
Retention time = 61.688



UV Spectrum
Retention time = 102.814

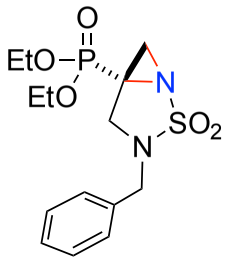


Peak Table

PDA Ch1 213nm

Peak#	Ret. Time	Area	Area%
1	61.688	2996426	49.922
2	102.814	3005832	50.078
Total		6002258	100.000

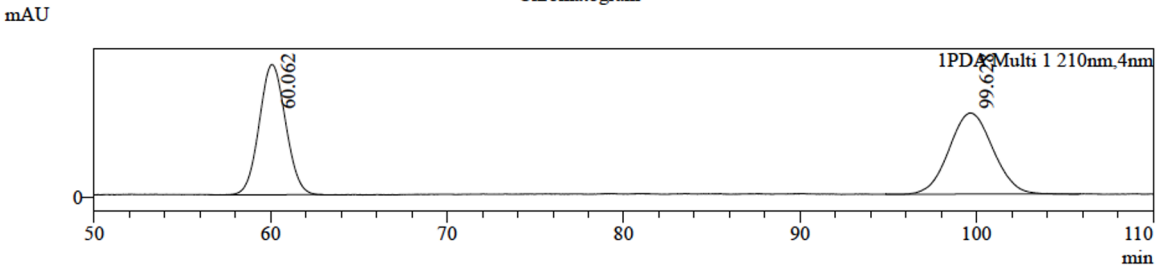
Diethyl (*S*)-(3-benzyl-2,2-dioxido-2-thia-1,3-diazabicyclo[3.1.0]hexan-5-yl)phosphonate 2.2q



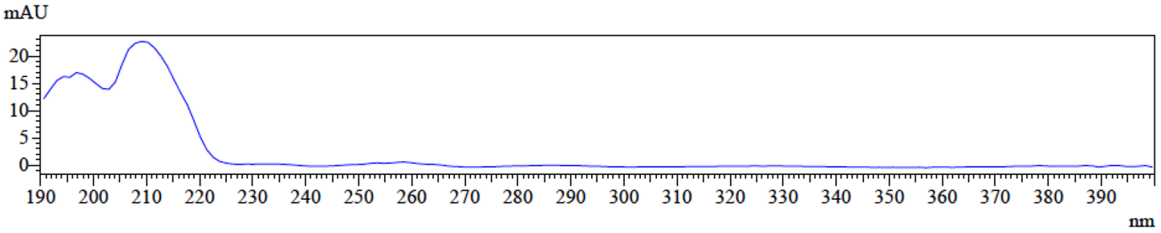
Sample Information

Data File	: H0X-756_F4-IC-20%-1.0 mL.lc.lcd
Sample Name	: H0X-756_F4-IC-20%-1.0 mL.lc
Sample ID	: H0X-756_F4-IC-20%-1.0 mL.lc
Method File	: H0X-20%-1.0ml-120MIN.lcm

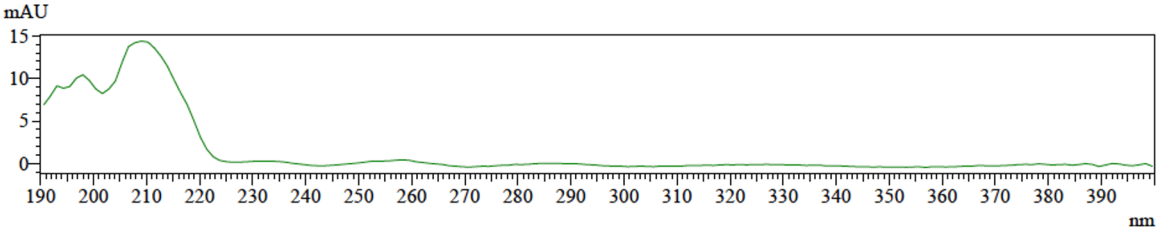
Chromatogram



UV Spectrum
Retention time = 60.062



UV Spectrum
Retention time = 99.628

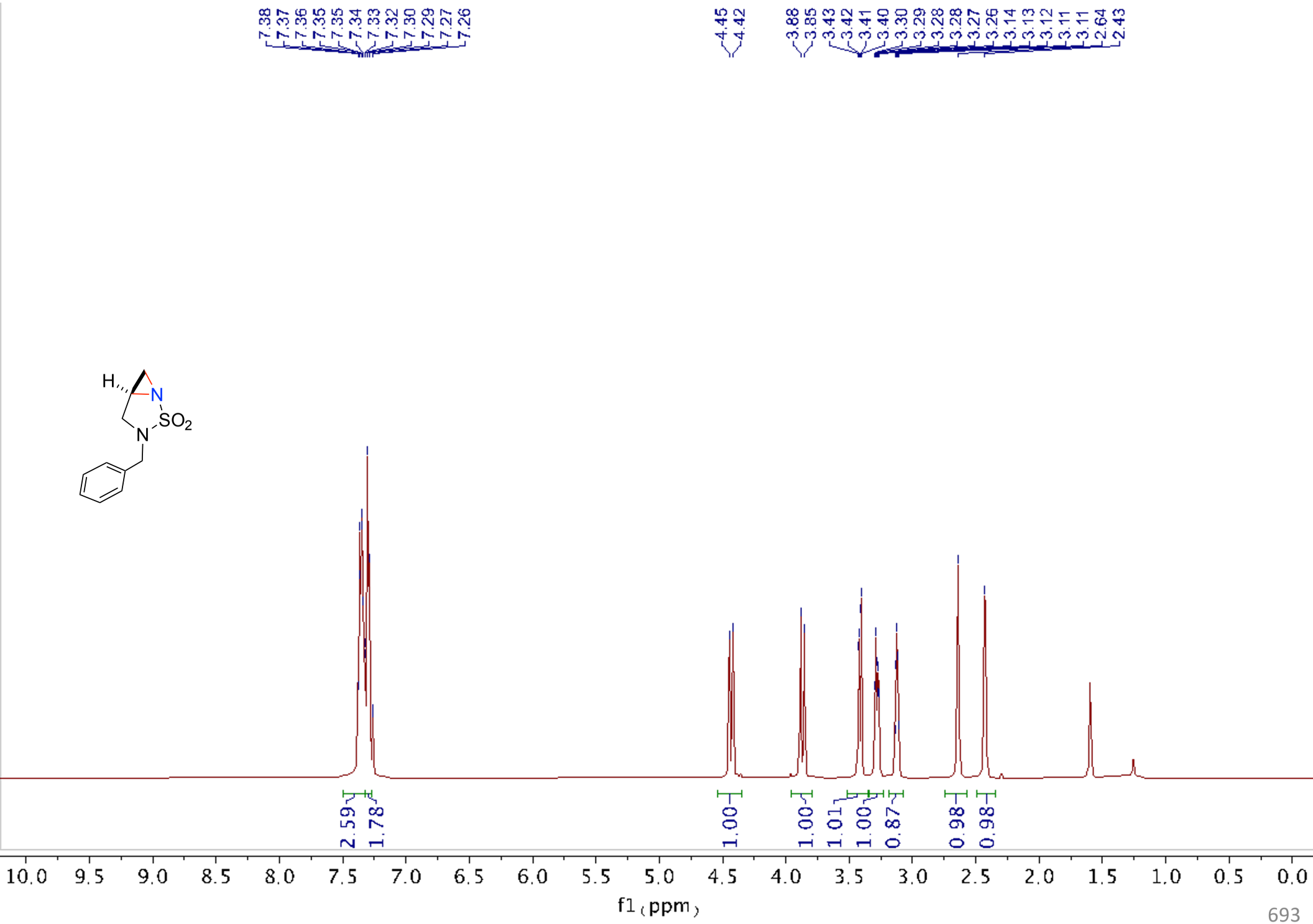


Peak Table

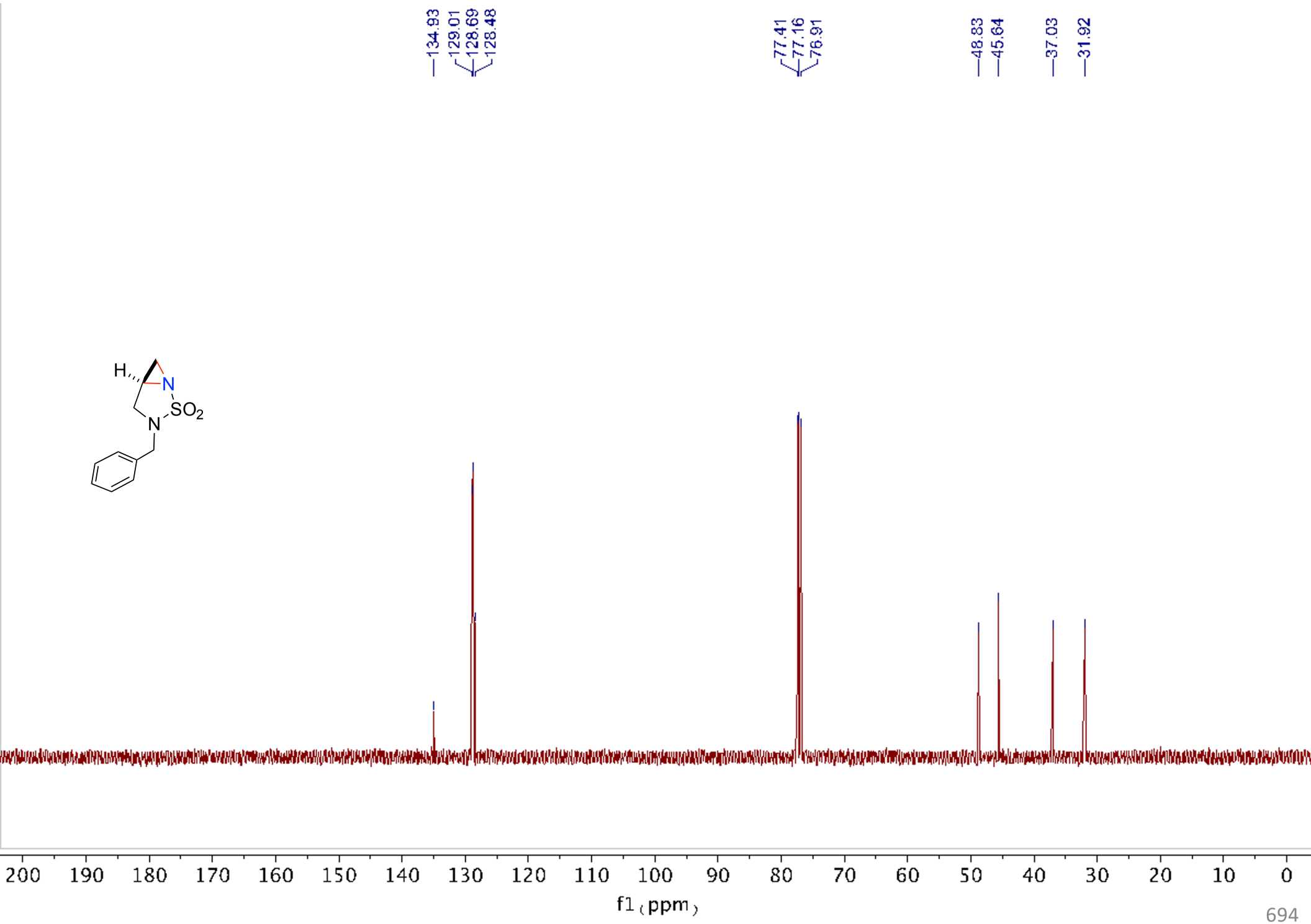
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	60.062	2156989	49.159
2	99.628	2230789	50.841
Total		4387778	100.000

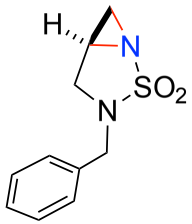
^{1}H NMR (*R*)-3-Benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2r



^{13}C NMR (*R*)-3-Benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2r



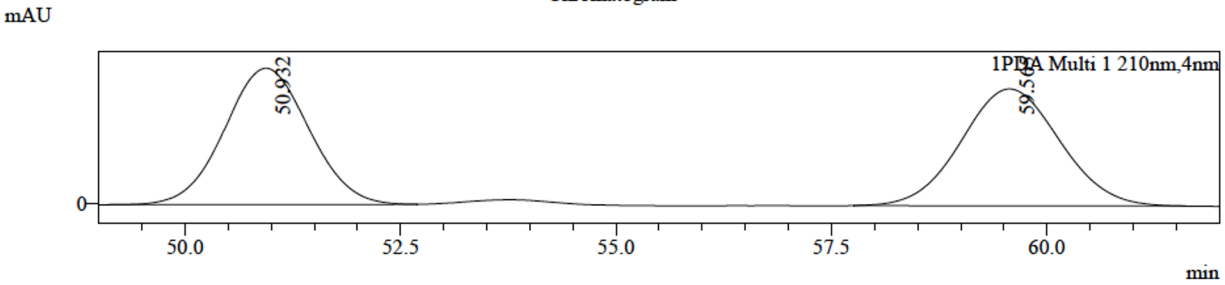
3-Benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2r



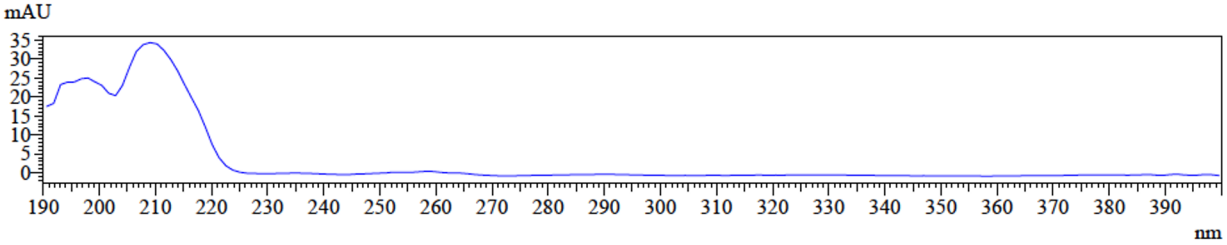
Sample Information

Data File	: H0X-0873_2-IC-20%-1.0 mL.lc.lcd
Sample Name	: H0X-0873_2-IC-20%-1.0 mL.lc
Sample ID	: H0X-0873_2-IC-20%-1.0 mL.lc
Method File	: H0X-20%-1.0ml-90MIN.lcm

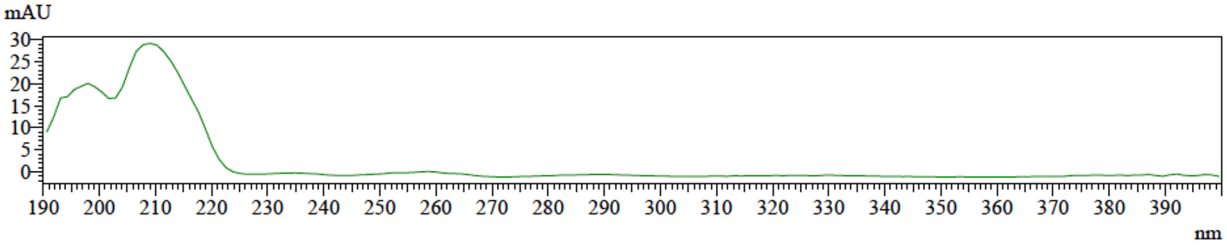
Chromatogram



UV Spectrum
Retention time = 50.932



UV Spectrum
Retention time = 59.565

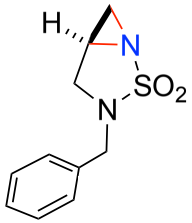


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	50.932	2184525	49.999
2	59.565	2184638	50.001
Total		4369163	100.000

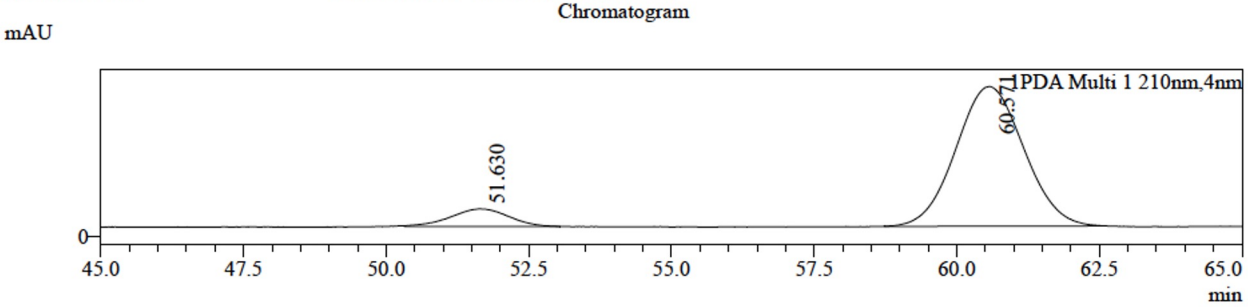
(*R*)-3-Benzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2r



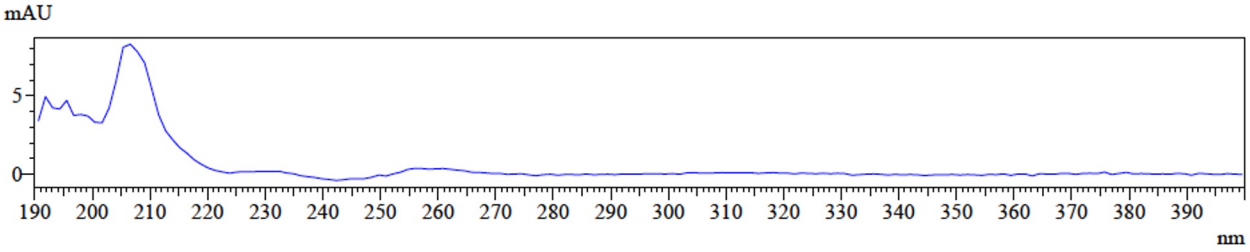
Sample Information

Data File	: H0X-0874_3-IC-20%-1.0 mL.lcd
Sample Name	: H0X-0874_3-IC-20%-1.0 mL
Sample ID	: H0X-0874_3-IC-20%-1.0 mL
Method File	: H0X-20%-1.0ml-90MIN.lcm

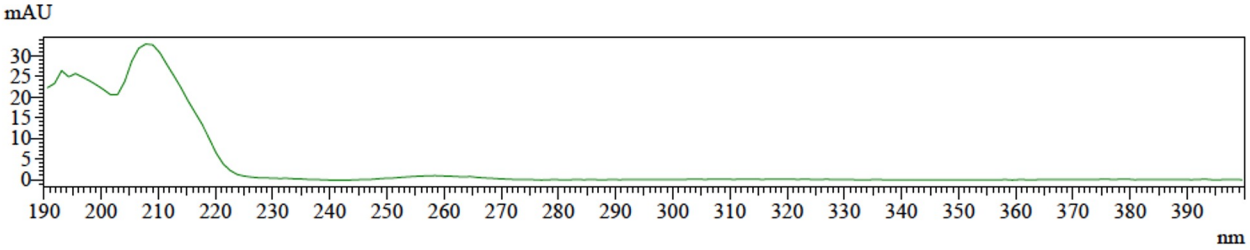
Chromatogram



UV Spectrum
Retention time = 51.630



UV Spectrum
Retention time = 60.571

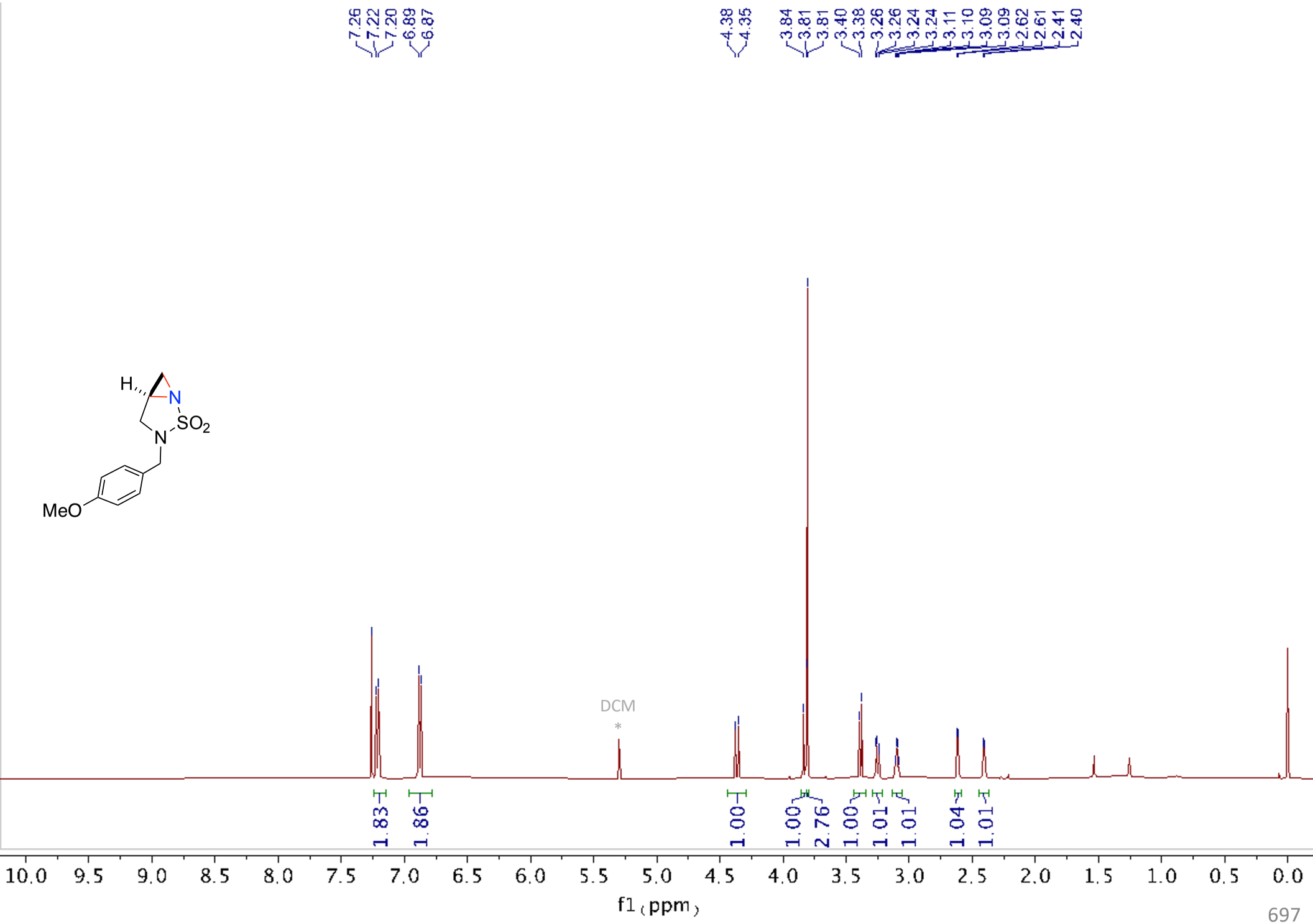


Peak Table

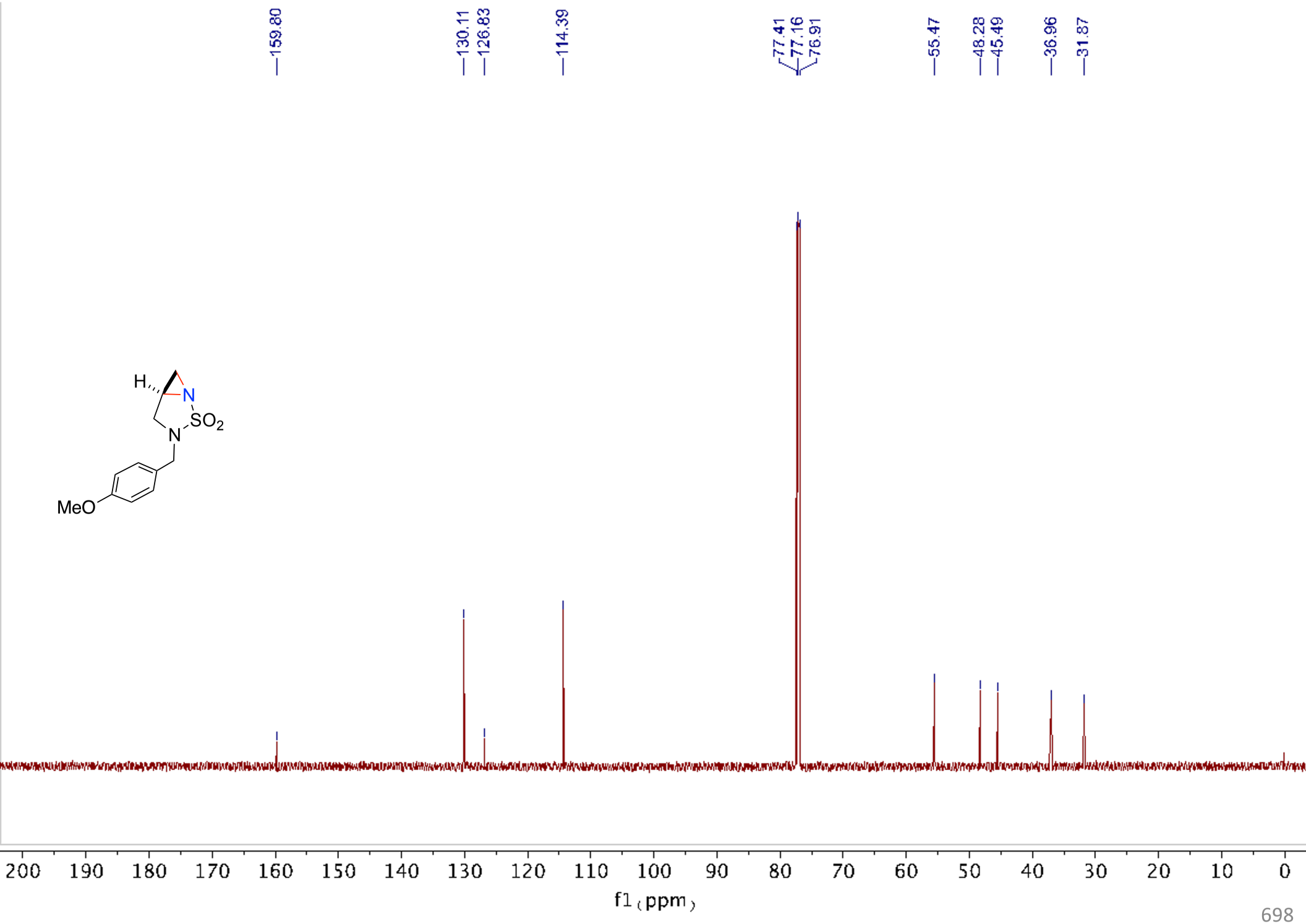
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	51.630	241711	9.718
2	60.571	2245469	90.282
Total		2487180	100.000

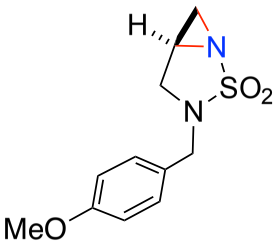
^{1}H NMR (*R*)-3-(4-Methoxybenzyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2s



^{13}C NMR (*R*)-3-(4-Methoxybenzyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2s



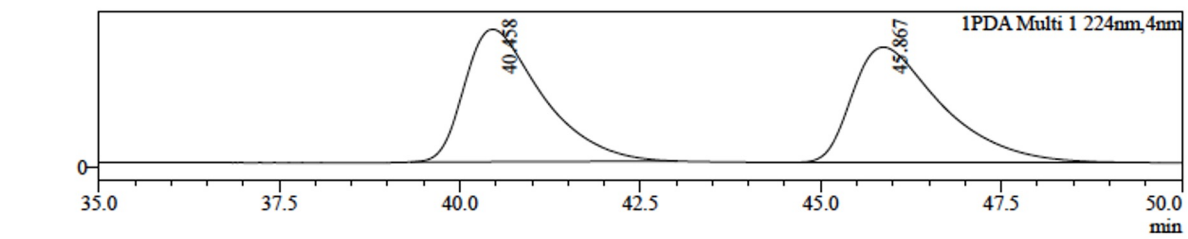
3-(4-Methoxybenzyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2s



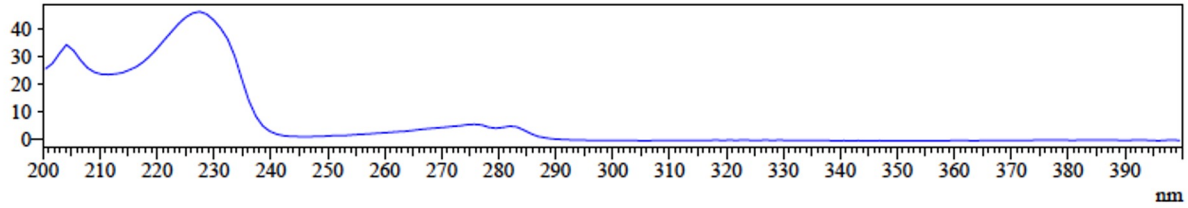
Sample Information

Data File	: H0X-0413_2nd-ODH-10%1.0mL.lcd
Sample Name	: H0X-0413_2nd-ODH-10%1.0mL
Sample ID	: H0X-0413_2nd-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-90MIN.lcm

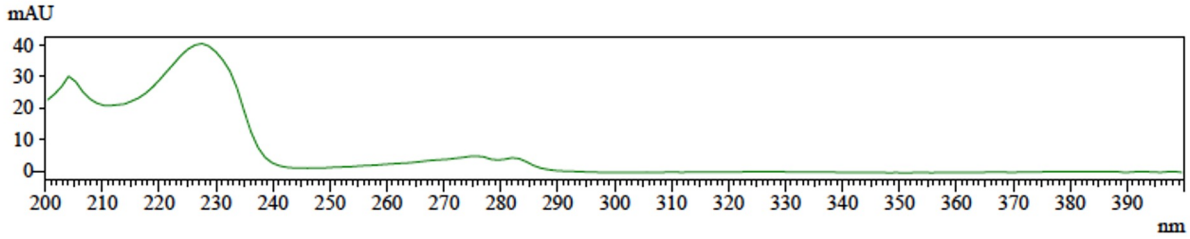
Chromatogram



UV Spectrum
Retention time = 40.458



UV Spectrum
Retention time = 45.867

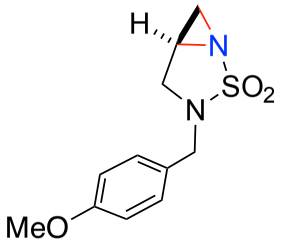


Peak Table

PDA Ch1 224nm

Peak#	Ret. Time	Area	Area%
1	40.458	2941871	49.882
2	45.867	2955823	50.118
Total		5897694	100.000

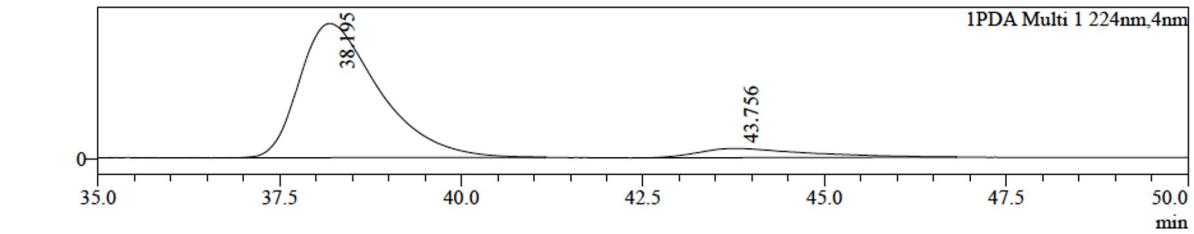
(*R*)-3-(4-Methoxybenzyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2s



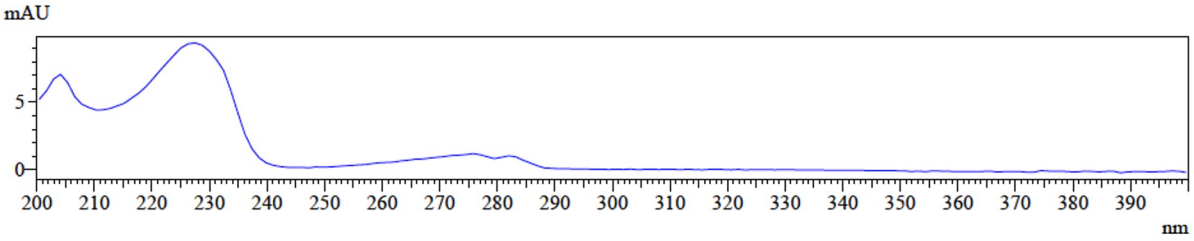
Sample Information

Data File	: H0X-0412_4th-ODH-10%1.0mL.lcd
Sample Name	: H0X-0412_4th-ODH-10%1.0mL
Sample ID	: H0X-0412_4th-ODH-10%1.0mL
Method File	: H0X-10%-1.0ml-60MIN.lcm

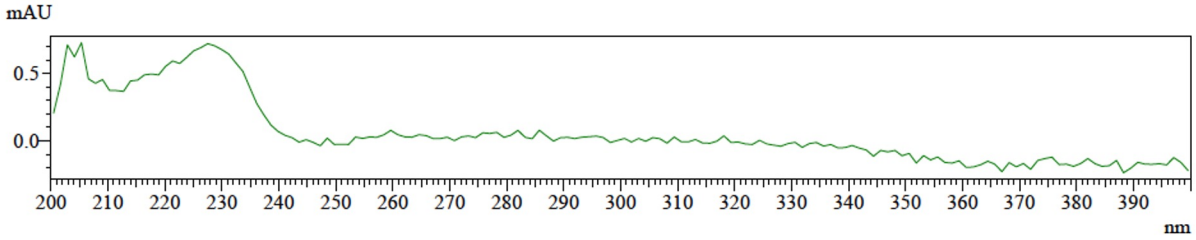
Chromatogram



UV Spectrum
Retention time = 38.195



UV Spectrum
Retention time = 43.756

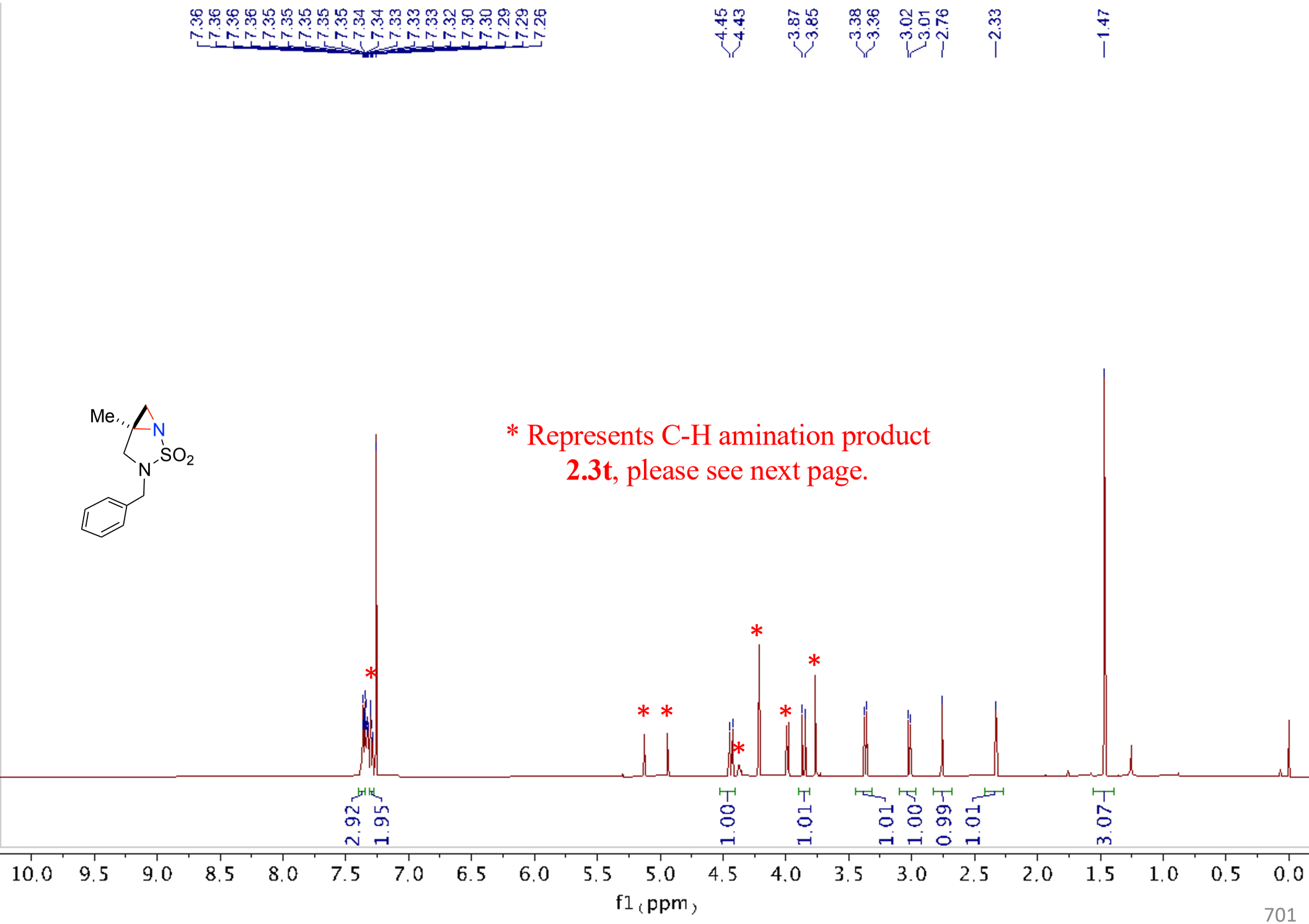


Peak Table

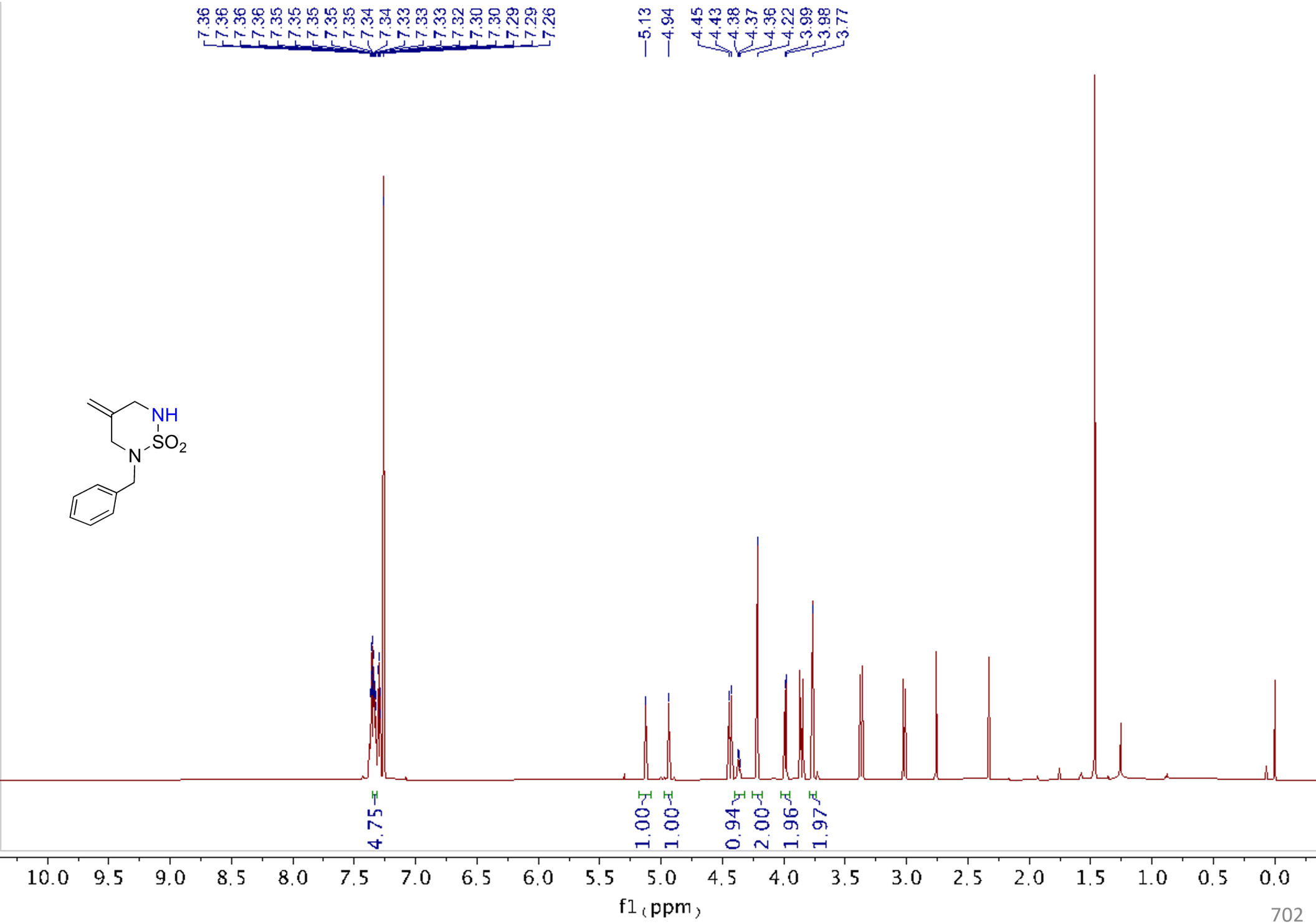
PDA Ch1 224nm

Peak#	Ret. Time	Area	Area%
1	38.195	631931	91.454
2	43.756	59054	8.546
Total		690985	100.000

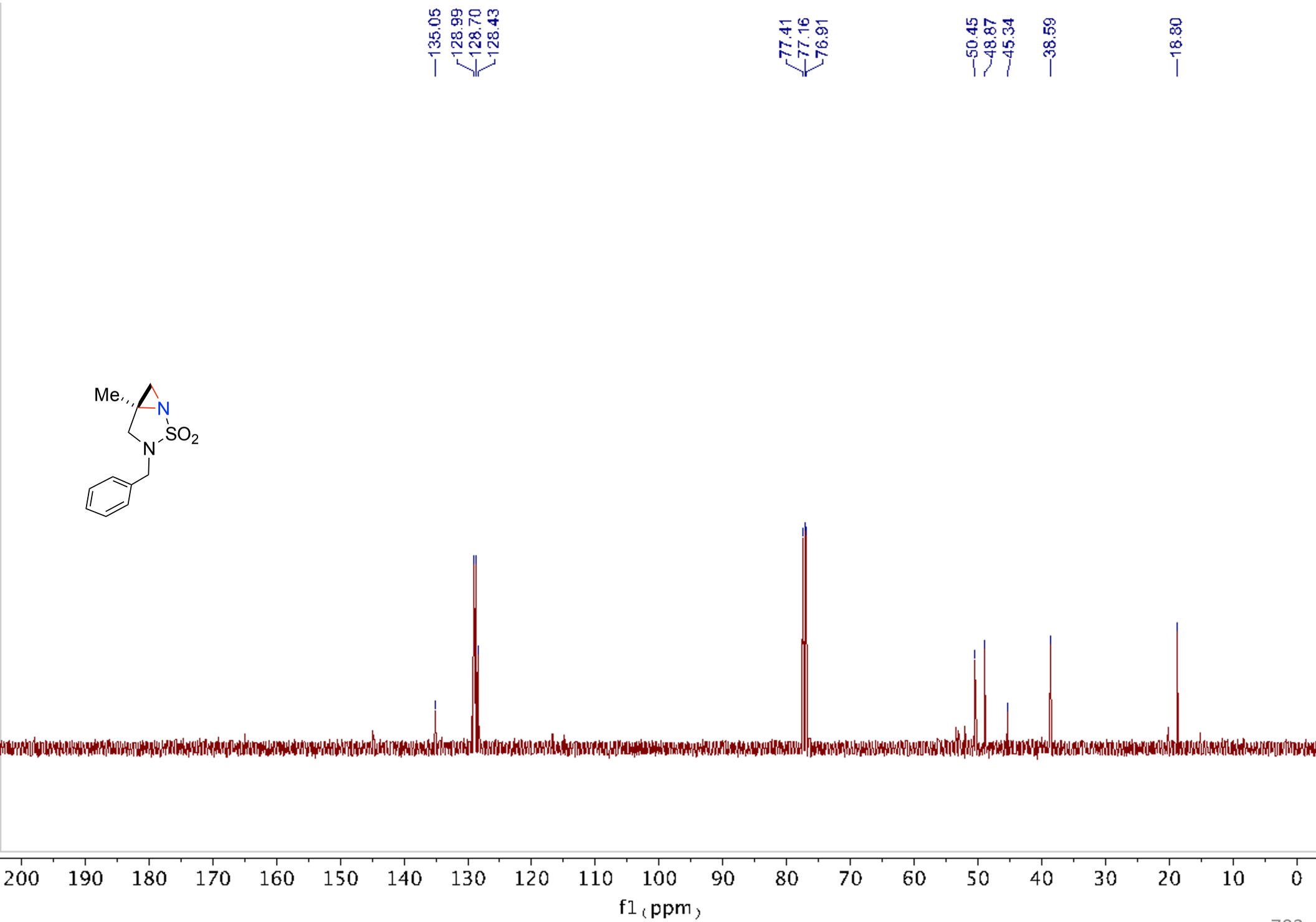
^{1}H NMR (*R*)-3-Benzyl-5-methyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2t



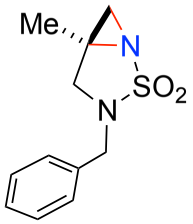
^{1}H NMR 2-benzyl-4-methylene-1,2,6-thiadiazinane 1,1-dioxide 2.3t



^{13}C NMR (*R*)-3-Benzyl-5-methyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2t



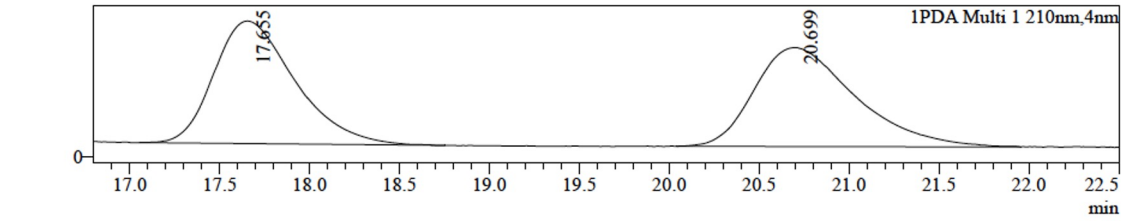
3-Benzyl-5-methyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2t



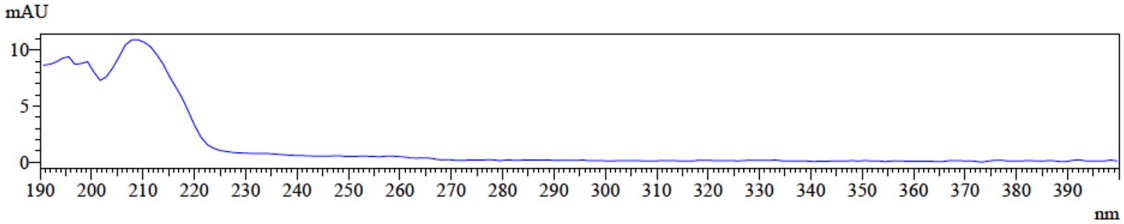
Sample Information

Data File	: H0X-0469_3-ODH-10%-1.0mL.lcd
Sample Name	: H0X-0469_3-ODH-10%-1.0mL
Sample ID	: H0X-0469_3-ODH-10%-1.0mL
Method File	: H0X-10%-1.0ml-60MIN.lcm

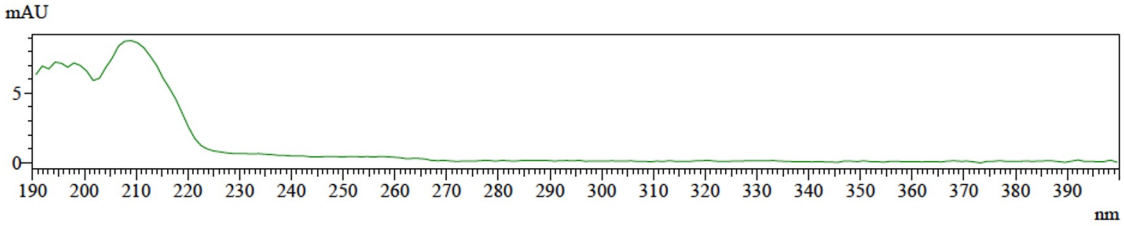
Chromatogram



UV Spectrum
Retention time = 17.655



UV Spectrum
Retention time = 20.699

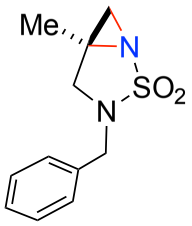


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	17.655	290178	49.870
2	20.699	291687	50.130
Total		581865	100.000

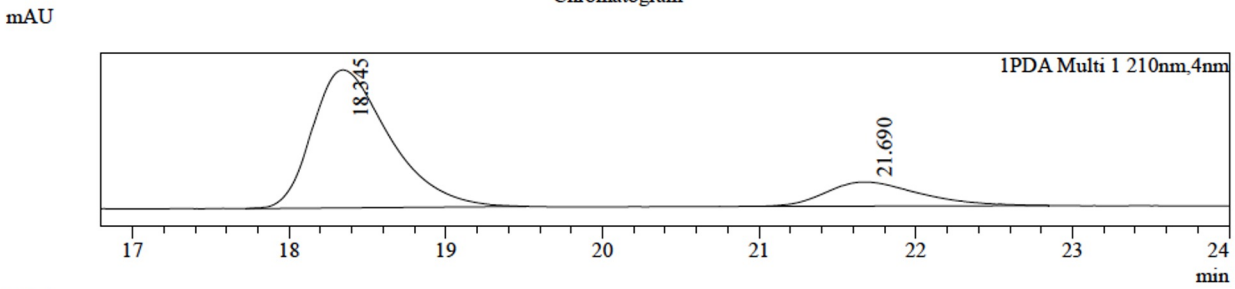
(*R*)-3-Benzyl-5-methyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2t



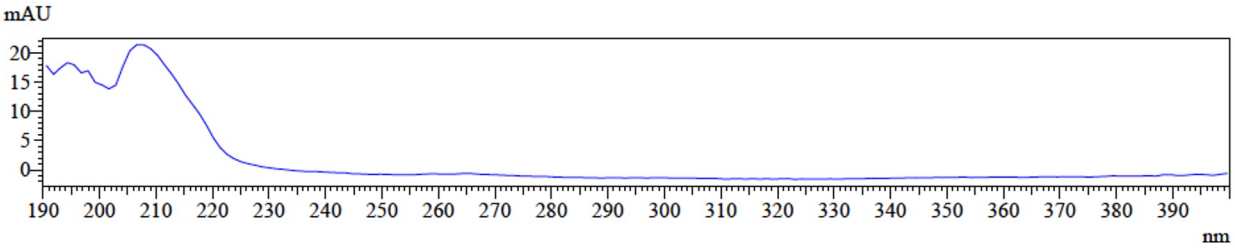
Sample Information

Data File	: H0X-0470_6-ODH-10%-1.0ml.lcd
Sample Name	: H0X-0470_6-ODH-10%-1.0ml
Sample ID	: H0X-0470_6-ODH-10%-1.0ml
Method File	: H0X-10%-1.0ml-30MIN.lcm

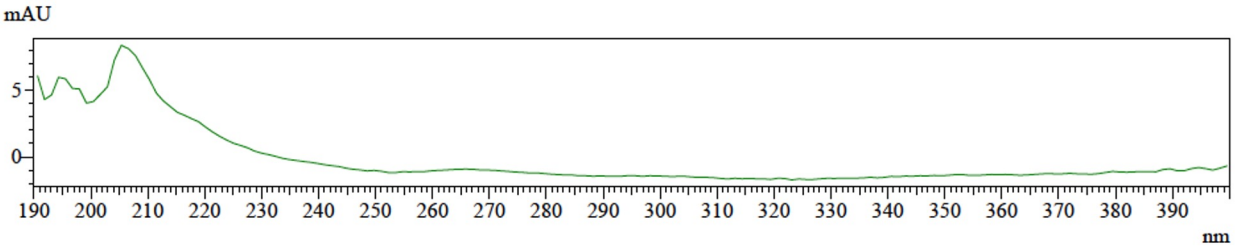
Chromatogram



UV Spectrum
Retention time = 18.345



UV Spectrum
Retention time = 21.690

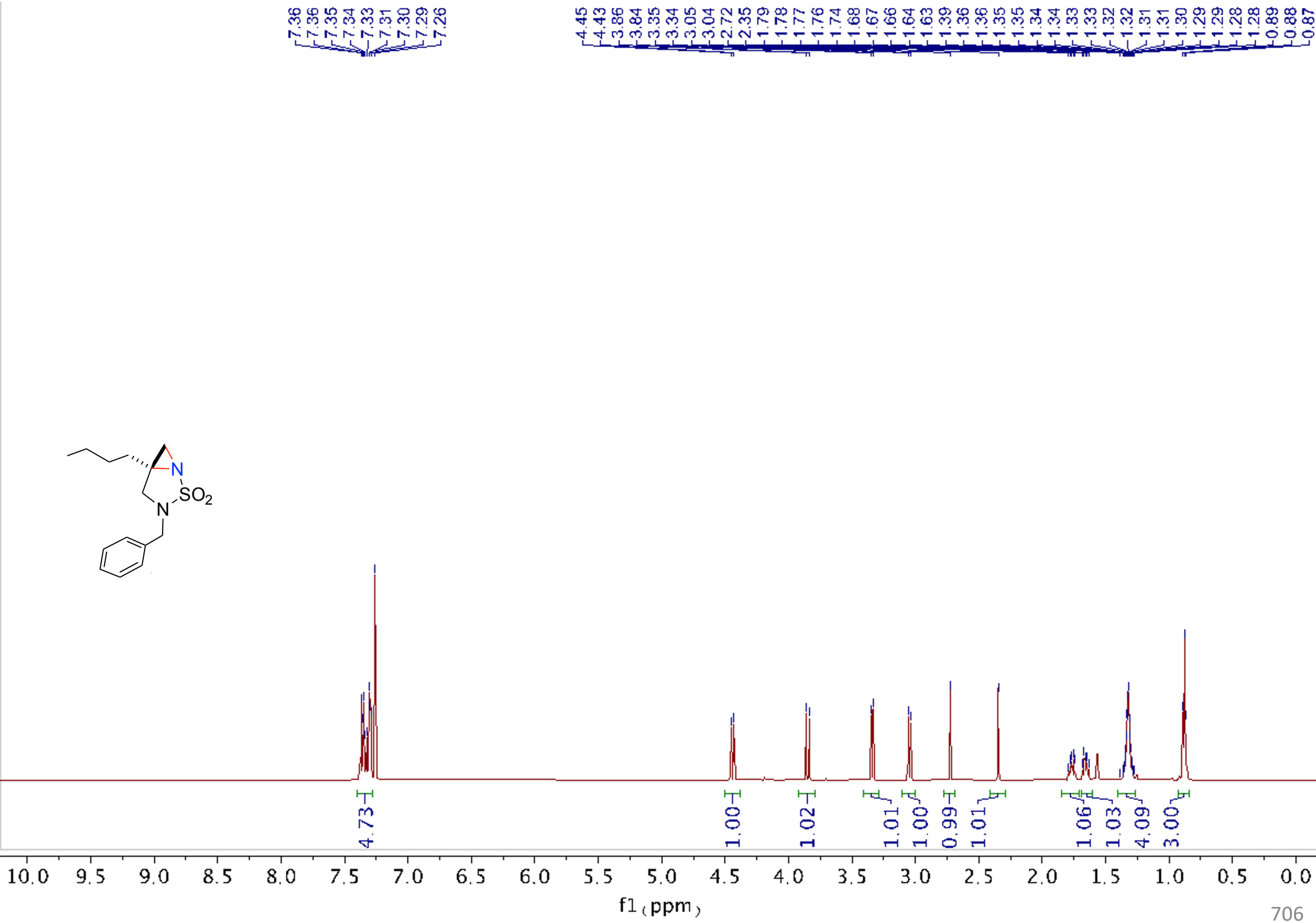


Peak Table

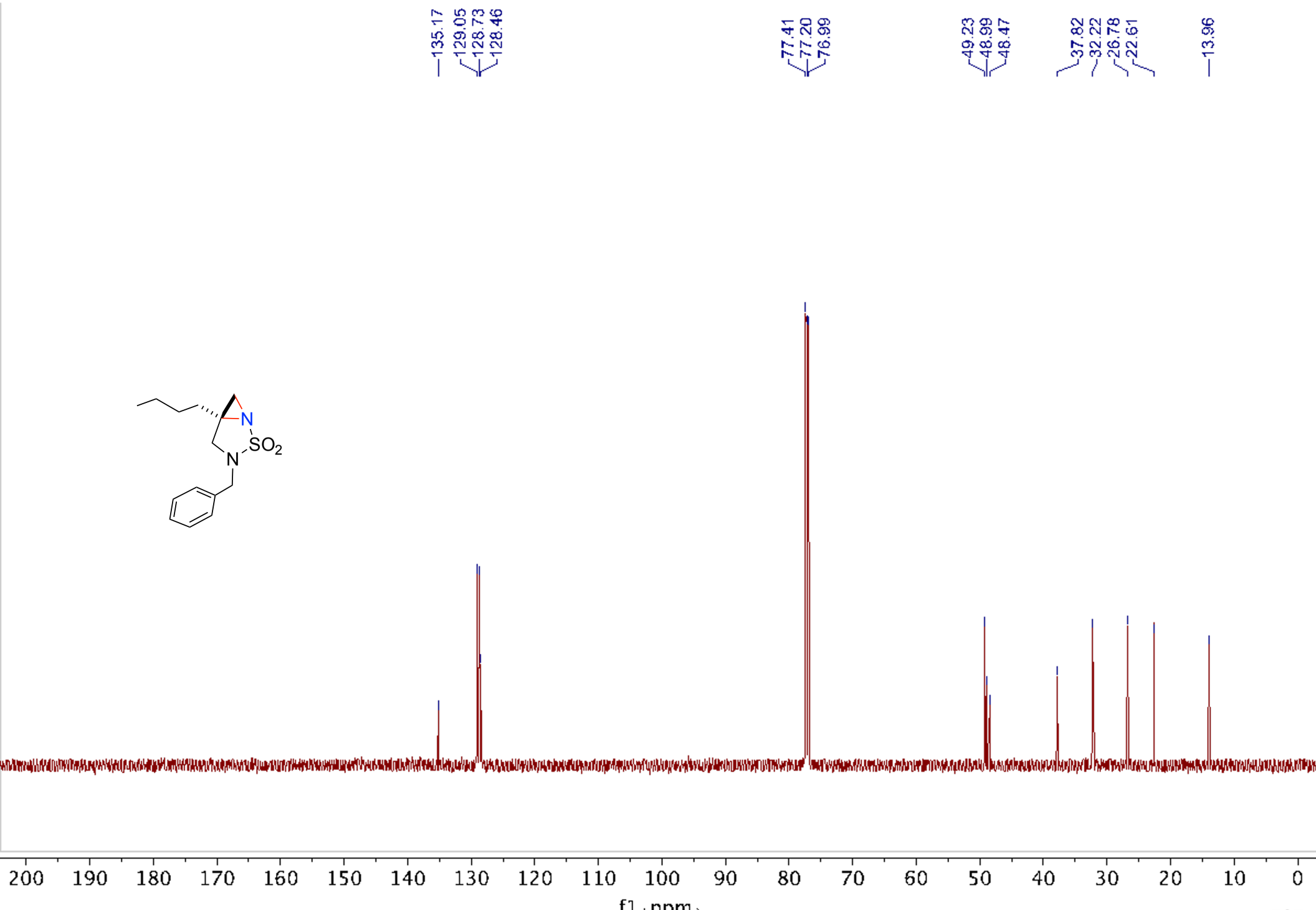
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	18.345	547631	82.467
2	21.690	116431	17.533
Total		664062	100.000

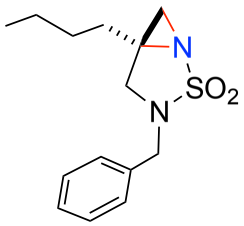
^{1}H NMR (*R*)-3-Benzyl-5-butyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2u



^{13}C NMR (*R*)-3-Benzyl-5-butyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2u



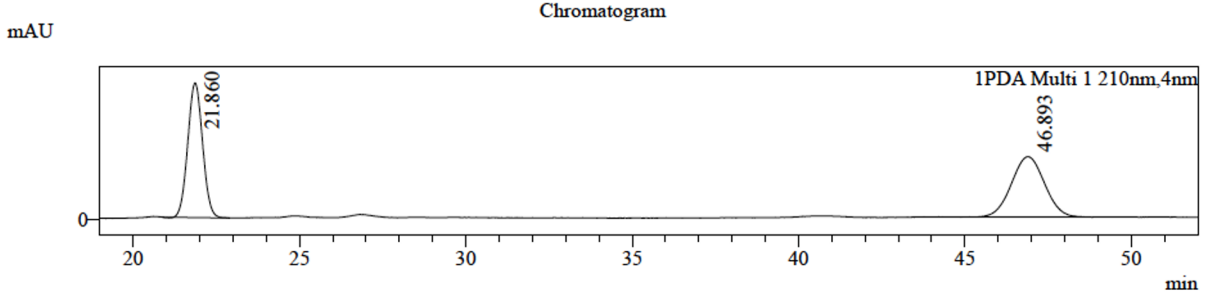
^{13}C NMR (*R*)-3-Benzyl-5-butyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2u



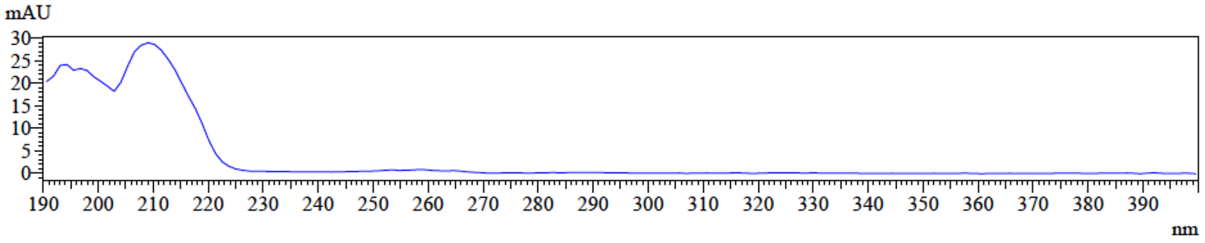
Sample Information

Data File	: H0X-880-16-IC-20%-1.0 mL.lcd
Sample Name	: H0X-880-16-IC-20%-1.0 mL
Sample ID	: H0X-880-16-IC-20%-1.0 mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

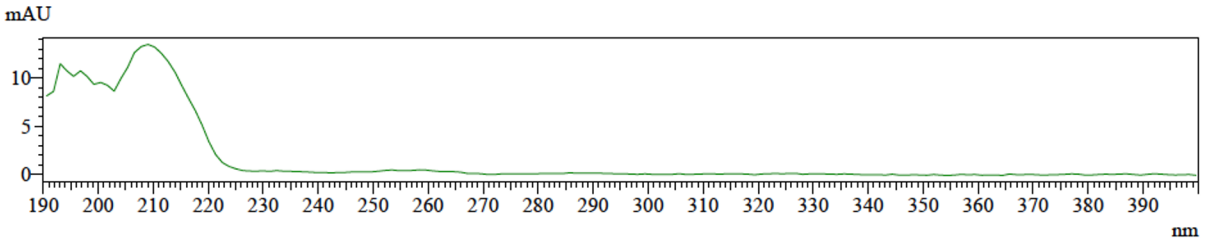
Chromatogram



UV Spectrum
Retention time = 21.860



UV Spectrum
Retention time = 46.893

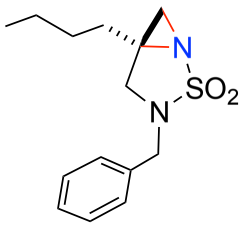


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	21.860	819356	49.939
2	46.893	821373	50.061
Total		1640729	100.000

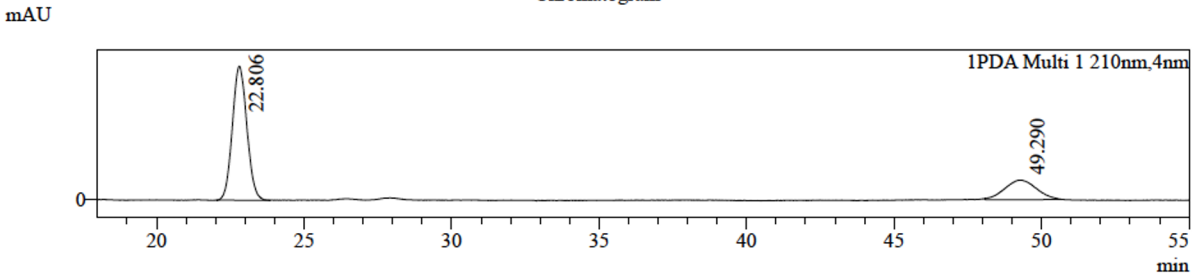
^{13}C NMR (*R*)-3-Benzyl-5-butyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2u



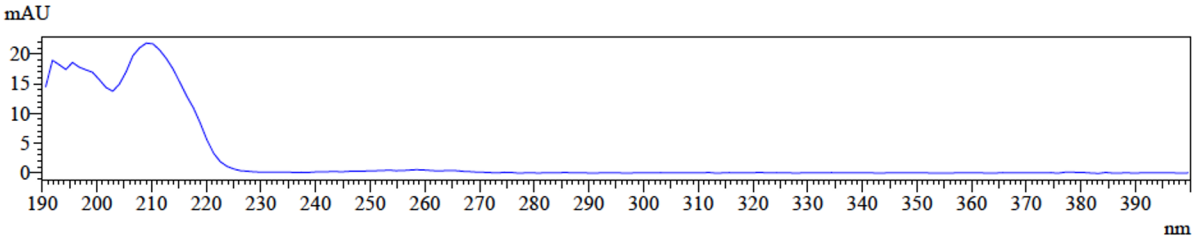
Sample Information

Data File	: H0X-838_F-IC-20%-1.0 mL.lc.lcd
Sample Name	: H0X-838_F-IC-20%-1.0 mL.lc
Sample ID	: H0X-838_F-IC-20%-1.0 mL.lc
Method File	: H0X-20%-1.0ml-60MIN.lcm

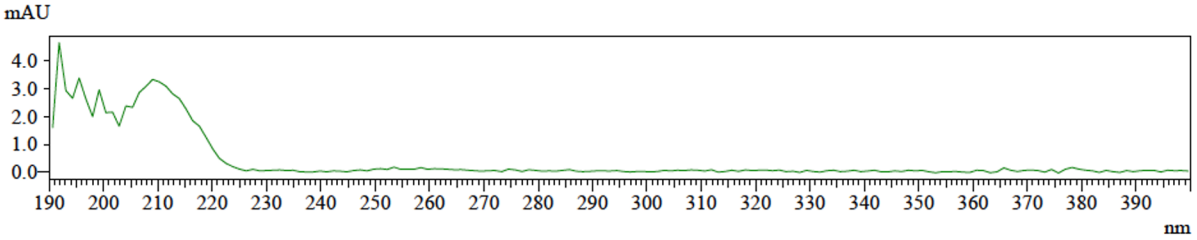
Chromatogram



UV Spectrum
Retention time = 22.806



UV Spectrum
Retention time = 49.290

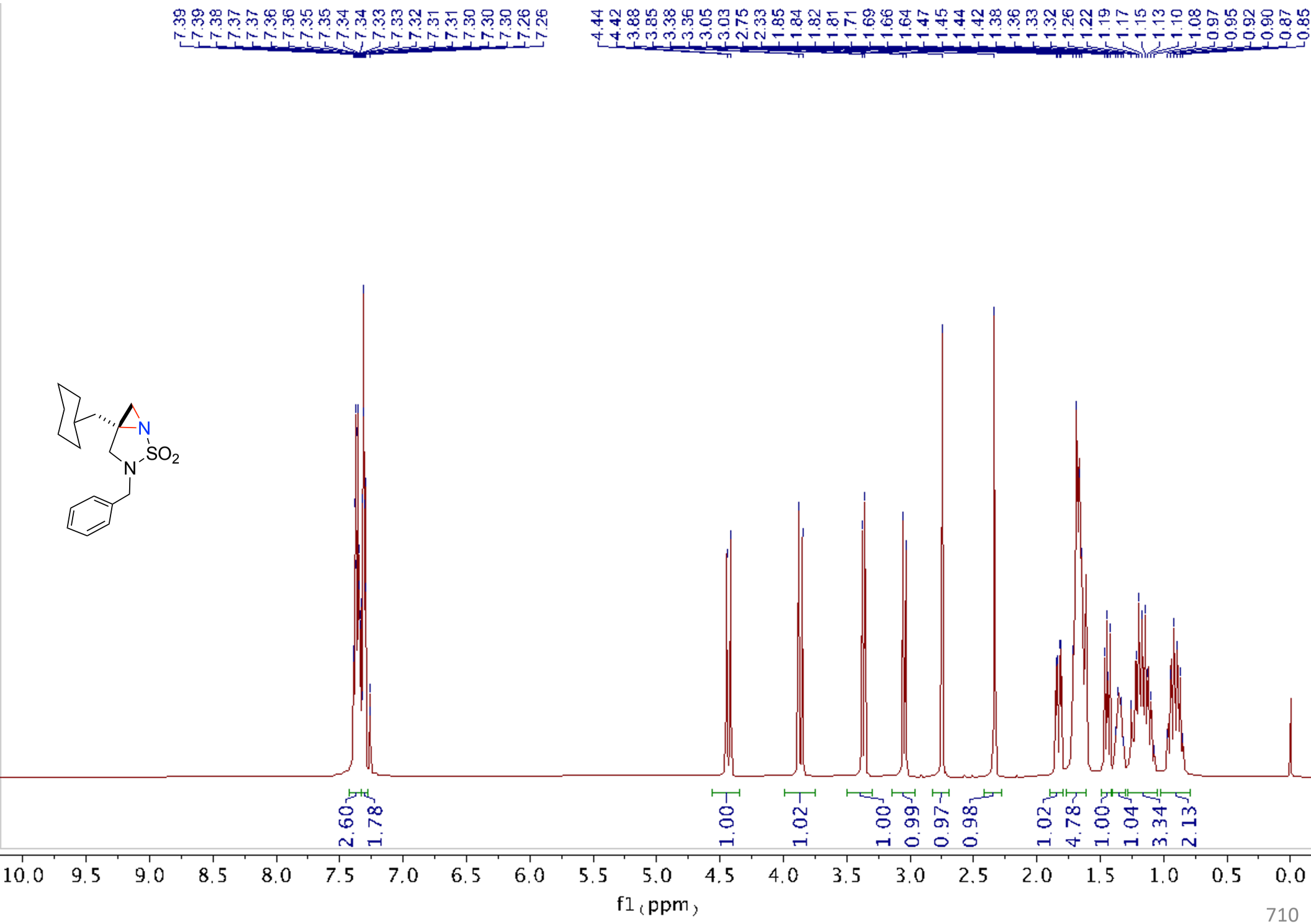


Peak Table

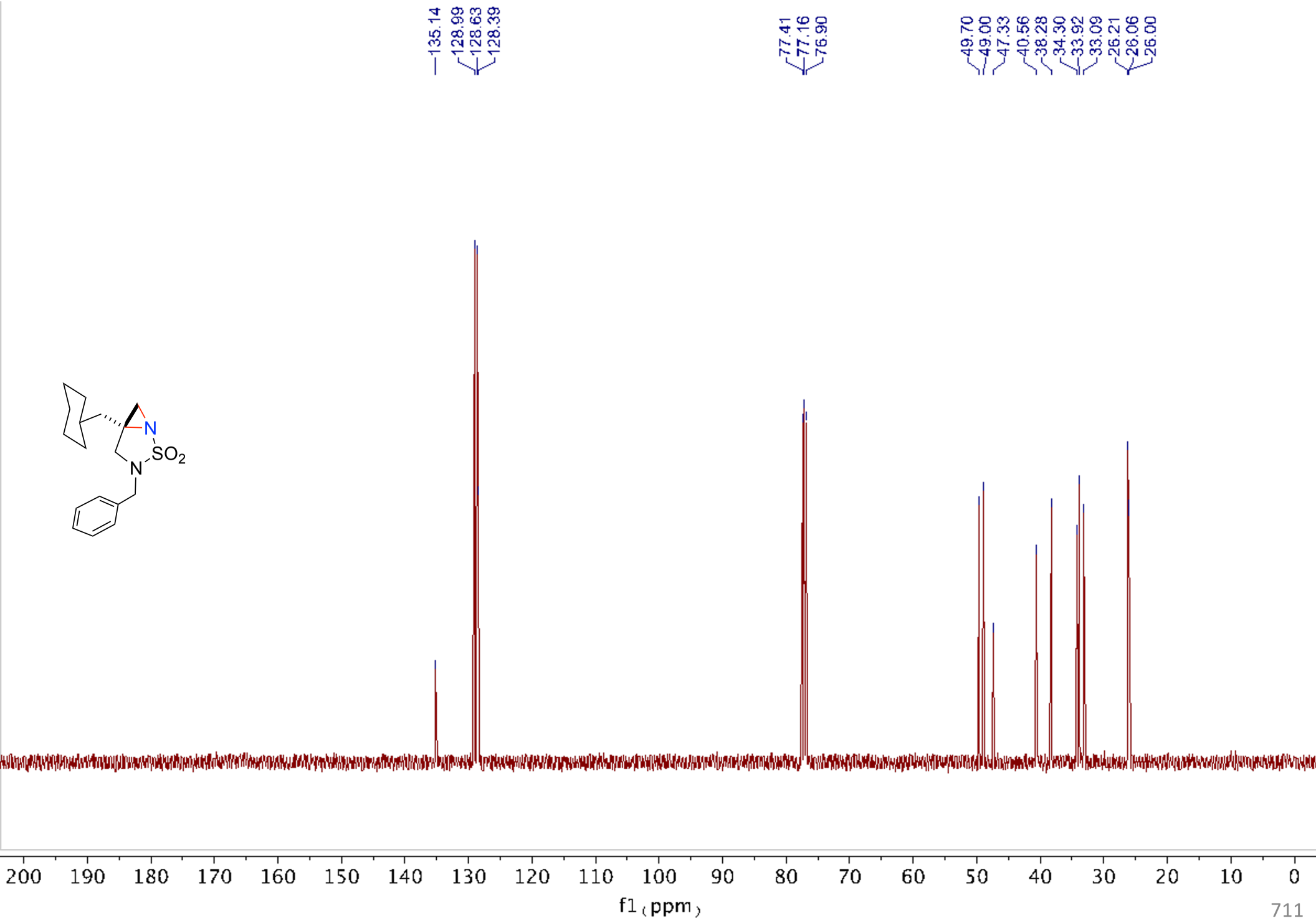
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	22.806	695423	76.012
2	49.290	219469	23.988
Total		914892	100.000

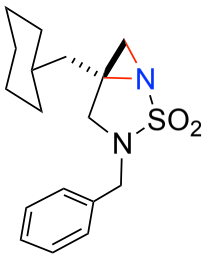
^{1}H NMR (*R*)-3-Benzyl-5-(cyclohexylmethyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2v



^{13}C NMR (*R*)-3-Benzyl-5-(cyclohexylmethyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2v



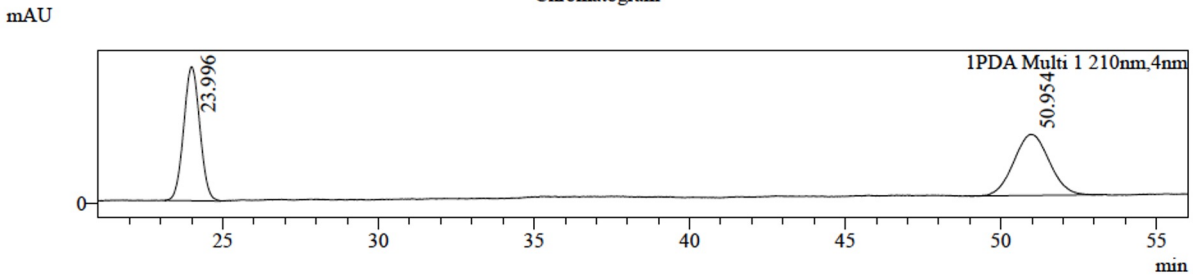
3-Benzyl-5-(cyclohexylmethyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2v



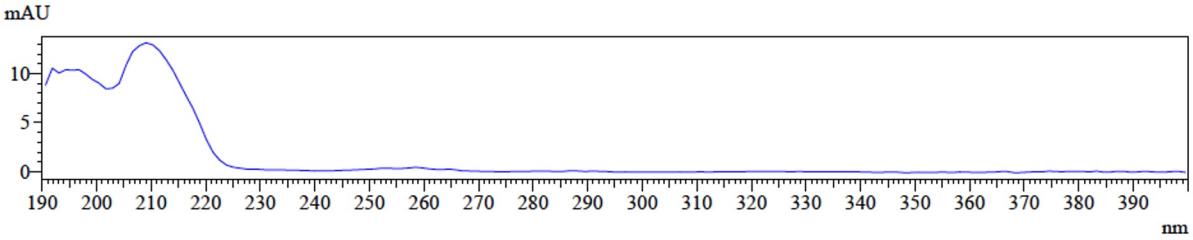
Sample Information

Data File	: H0X-0713_2--IC-20%1.0mL.lcd
Sample Name	: H0X-0713_2--IC-20%1.0mL
Sample ID	: H0X-0713_2--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

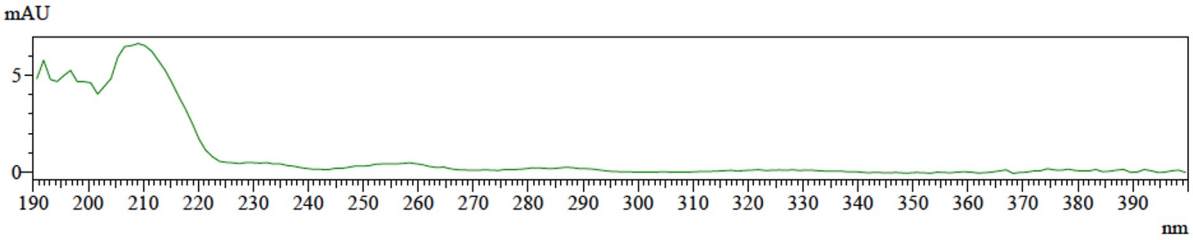
Chromatogram



UV Spectrum
Retention time = 23.996



UV Spectrum
Retention time = 50.954

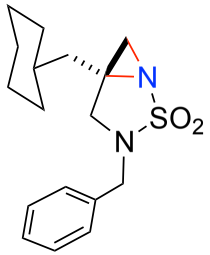


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	23.996	429800	49.974
2	50.954	430238	50.026
Total		860038	100.000

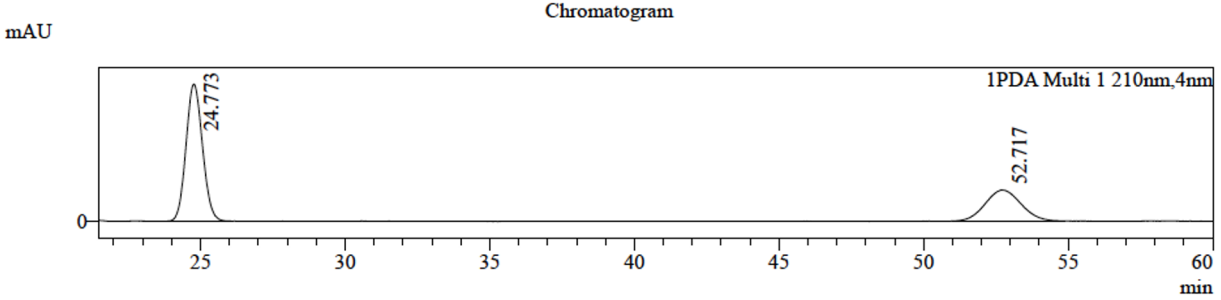
(*R*)-3-Benzyl-5-(cyclohexylmethyl)-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2v



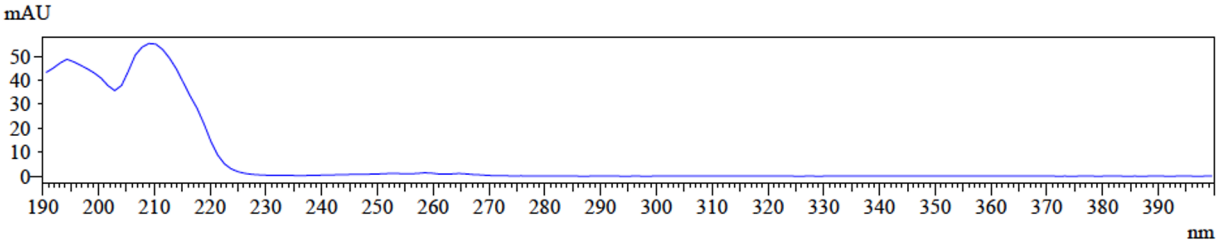
Sample Information

Data File	: H0X-841_F-IC-20%-1.0 mL.lc.lcd
Sample Name	: H0X-841_F-IC-20%-1.0 mL.lc
Sample ID	: H0X-841_F-IC-20%-1.0 mL.lc
Method File	: H0X-20%-1.0ml-60MIN.lcm

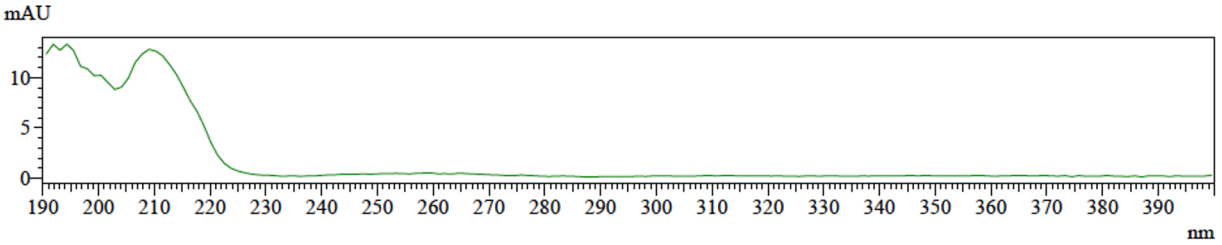
Chromatogram



UV Spectrum
Retention time = 24.773



UV Spectrum
Retention time = 52.717

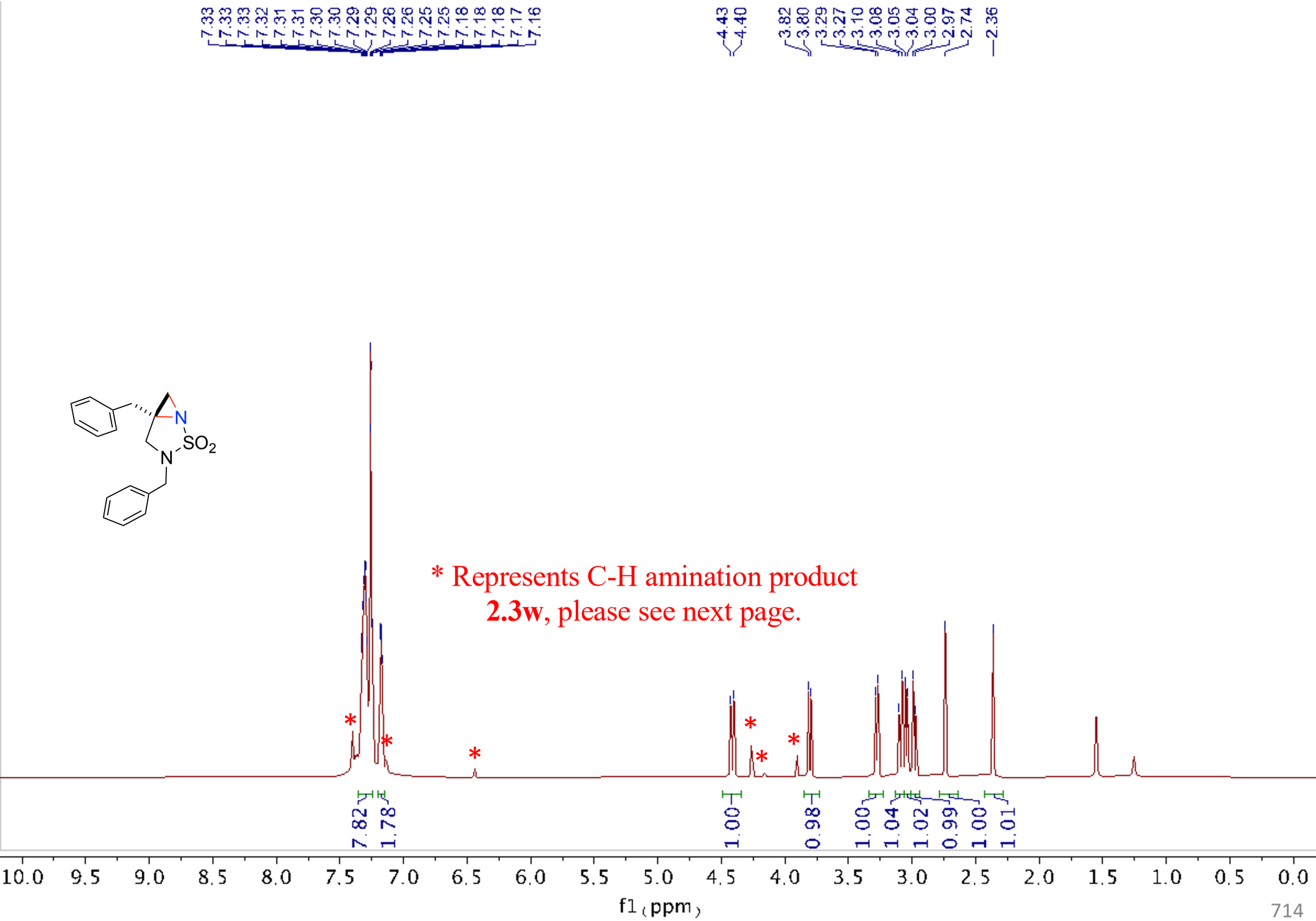


Peak Table

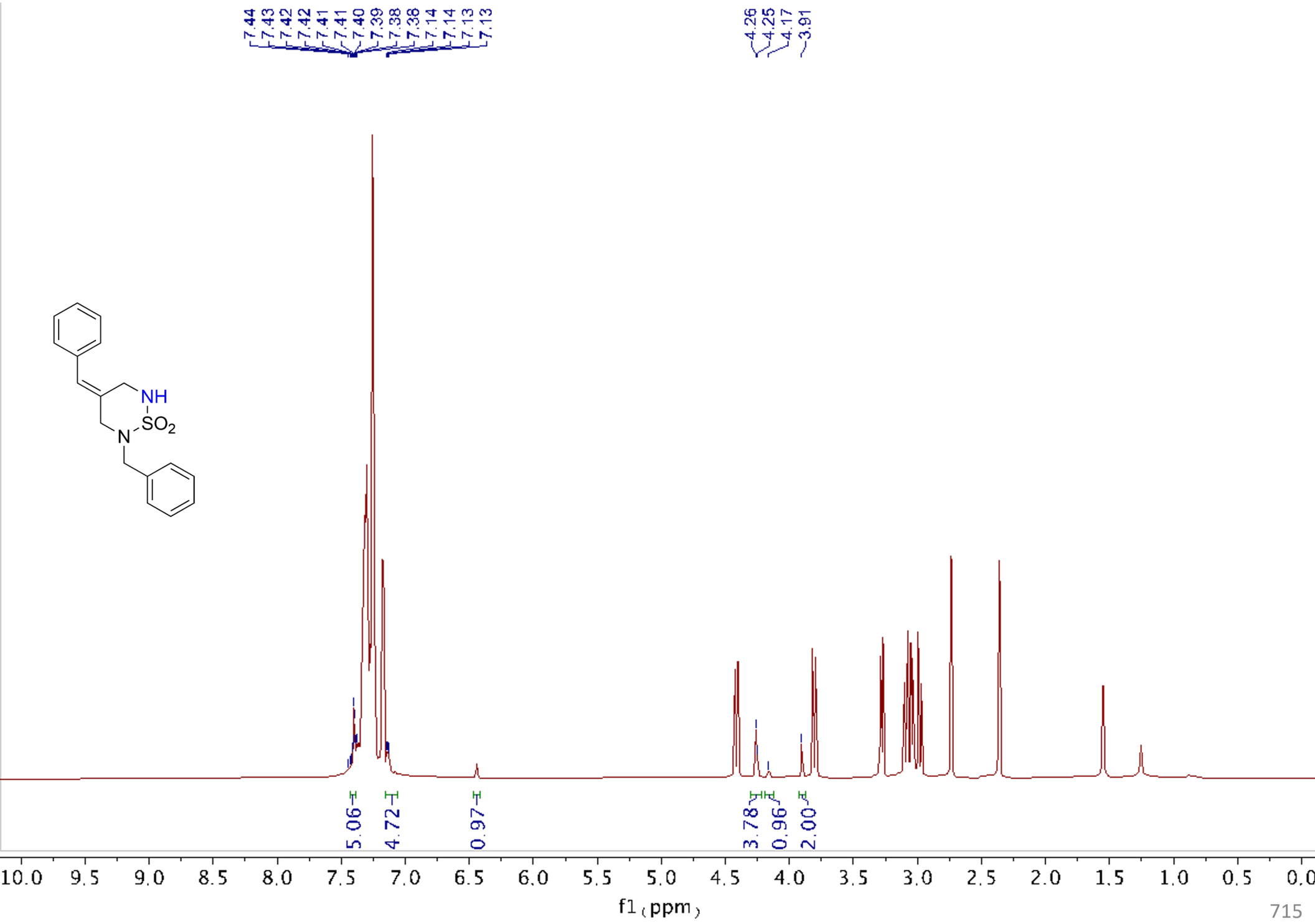
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	24.773	2042271	67.050
2	52.717	1003606	32.950
Total		3045877	100.000

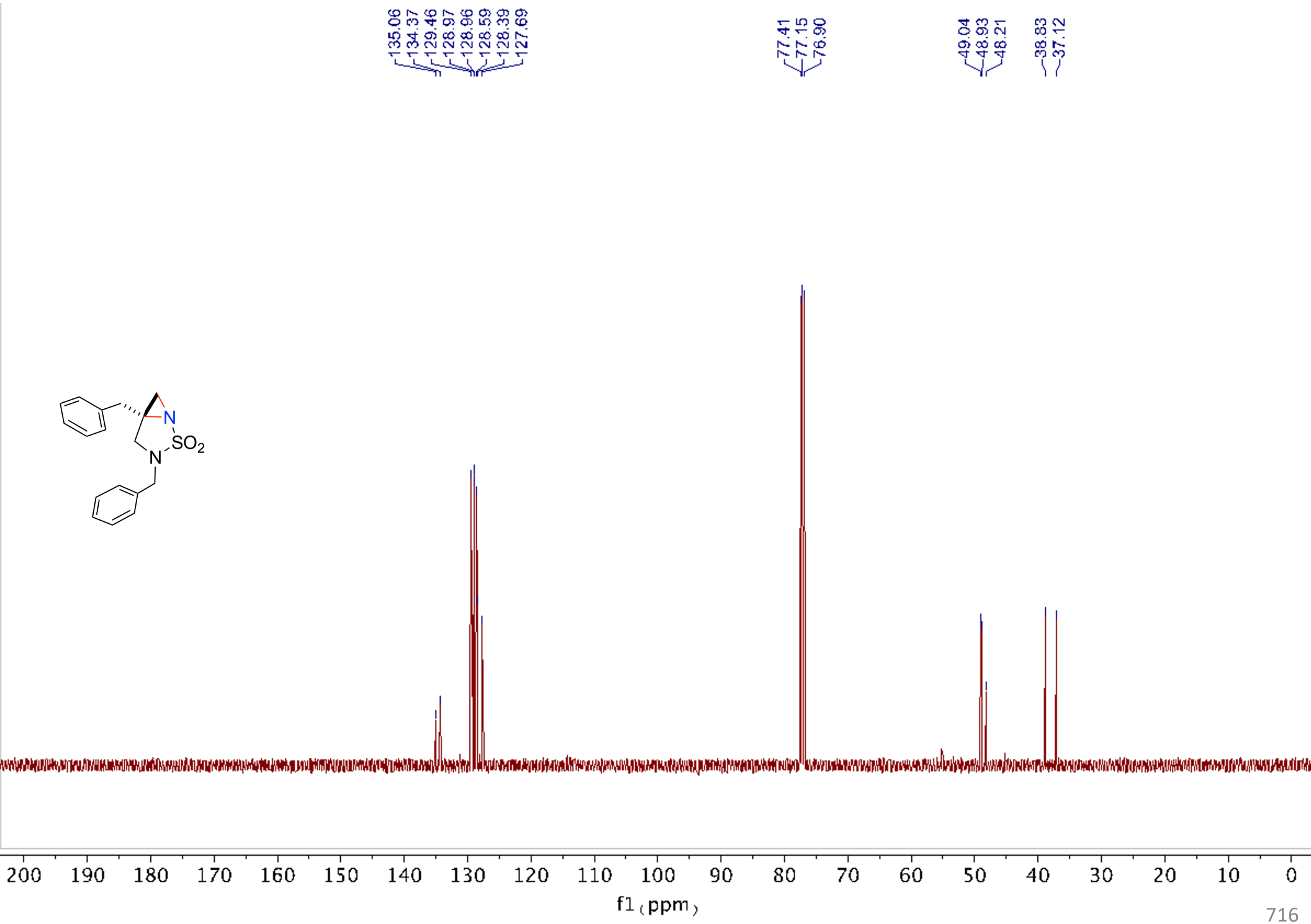
^{1}H NMR (*R*)-3,5-Dibenzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2w



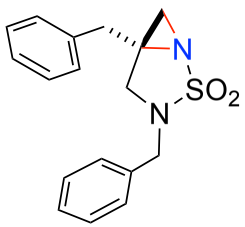
^{1}H NMR (*E*)-2-Benzyl-4-benzylidene-1,2,6-thiadiazinane 1,1-dioxide 2.3w



^{13}C NMR (*R*)-3,5-Dibenzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2w



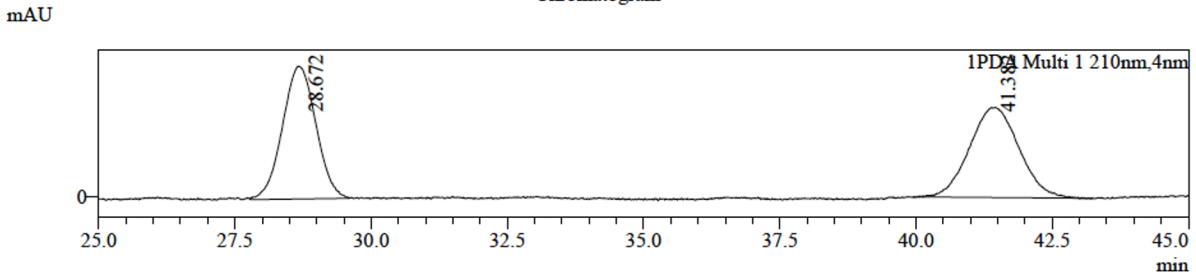
3,5-Dibenzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2w



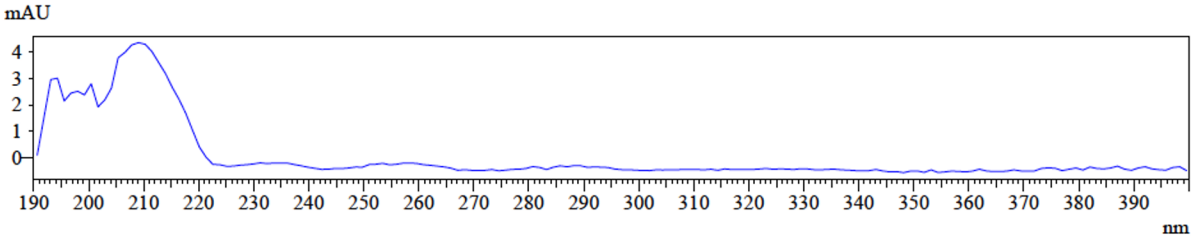
Sample Information

Data File	: H0X-0877_3-IC-20%-1.0 mL.lcd
Sample Name	: H0X-0877_3-IC-20%-1.0 mL
Sample ID	: H0X-0877_3-IC-20%-1.0 mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

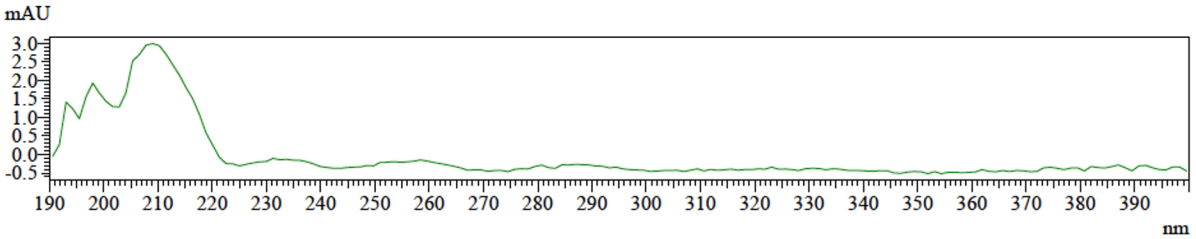
Chromatogram



UV Spectrum
Retention time = 28.672



UV Spectrum
Retention time = 41.382

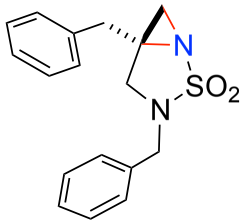


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	28.672	172390	49.948
2	41.382	172750	50.052
Total		345141	100.000

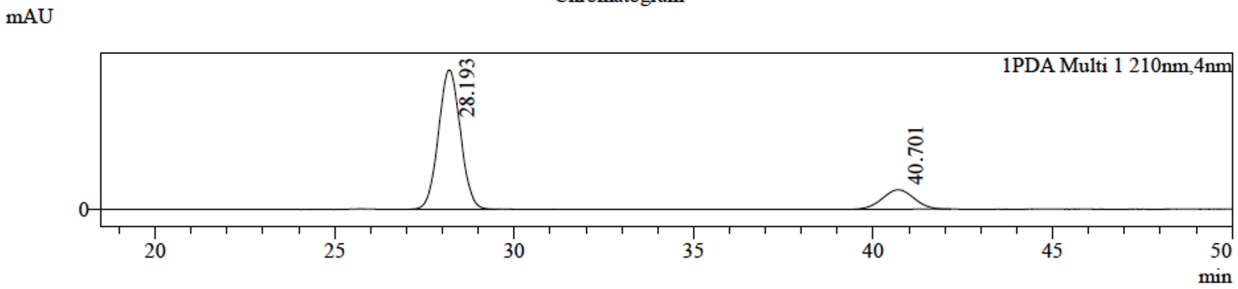
(*R*)-3,5-Dibenzyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2w



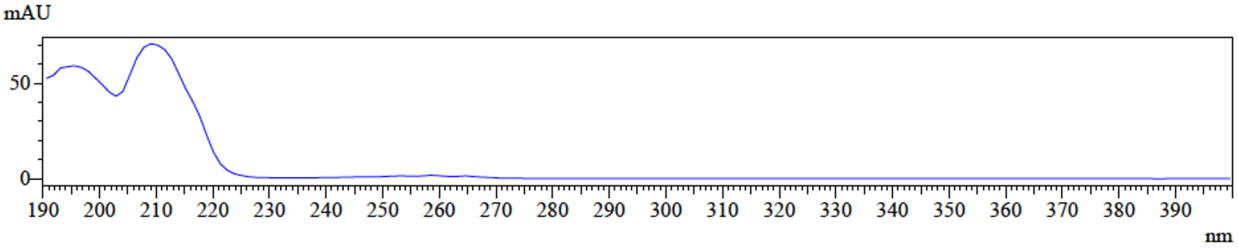
Sample Information

Data File	: H0X-839_F3-IC-20%-1.0 mL.lc.lcd
Sample Name	: H0X-839_F3-IC-20%-1.0 mL.lc
Sample ID	: H0X-839_F3-IC-20%-1.0 mL.lc
Method File	: H0X-20%-1.0ml-60MIN.lcm

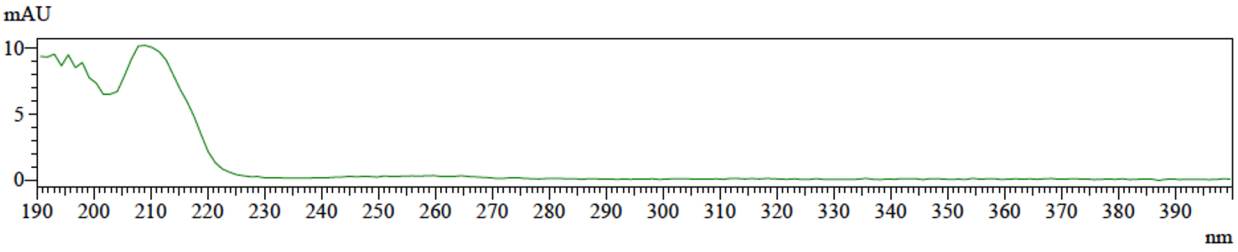
Chromatogram



UV Spectrum
Retention time = 28.193



UV Spectrum
Retention time = 40.701

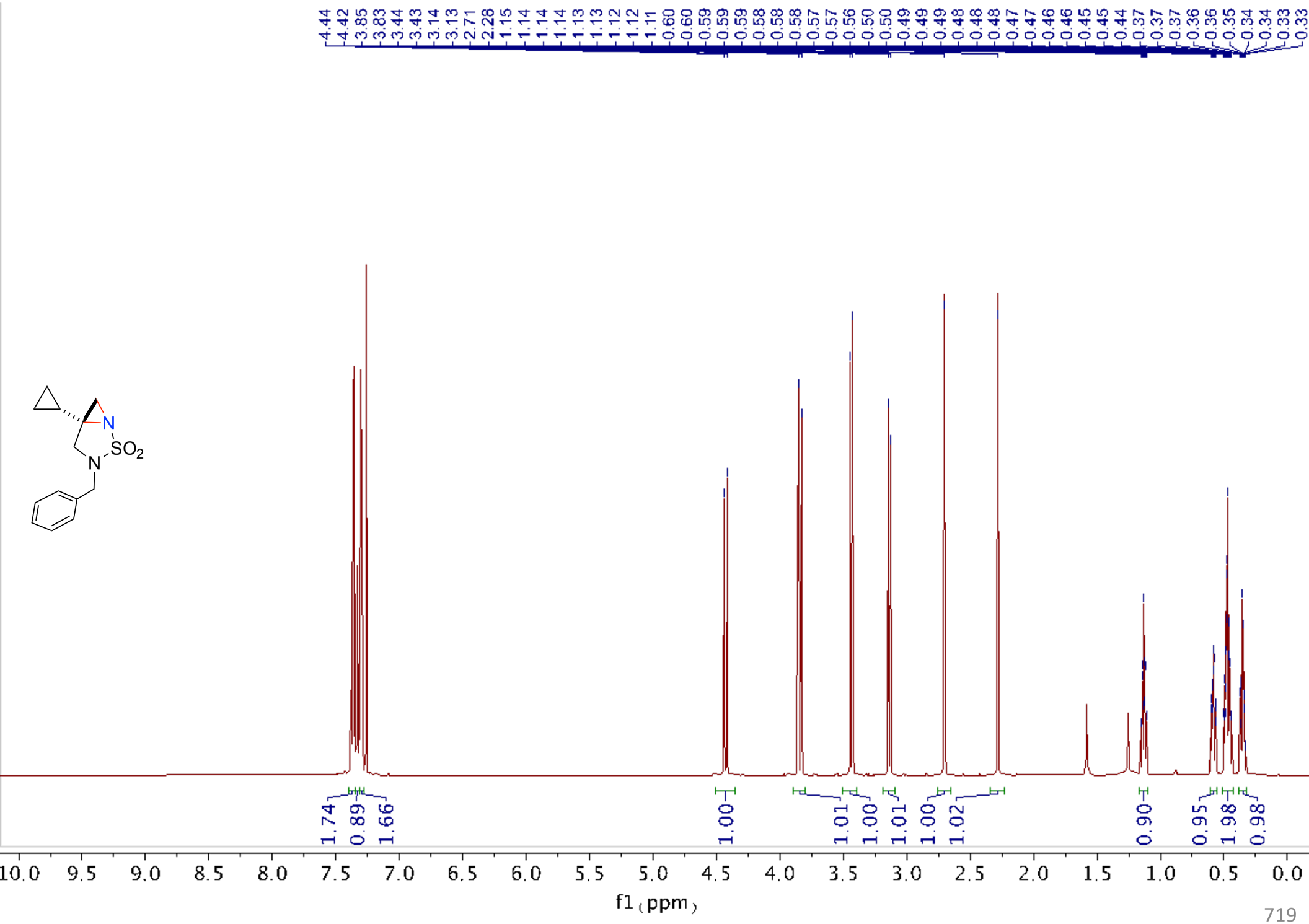


Peak Table

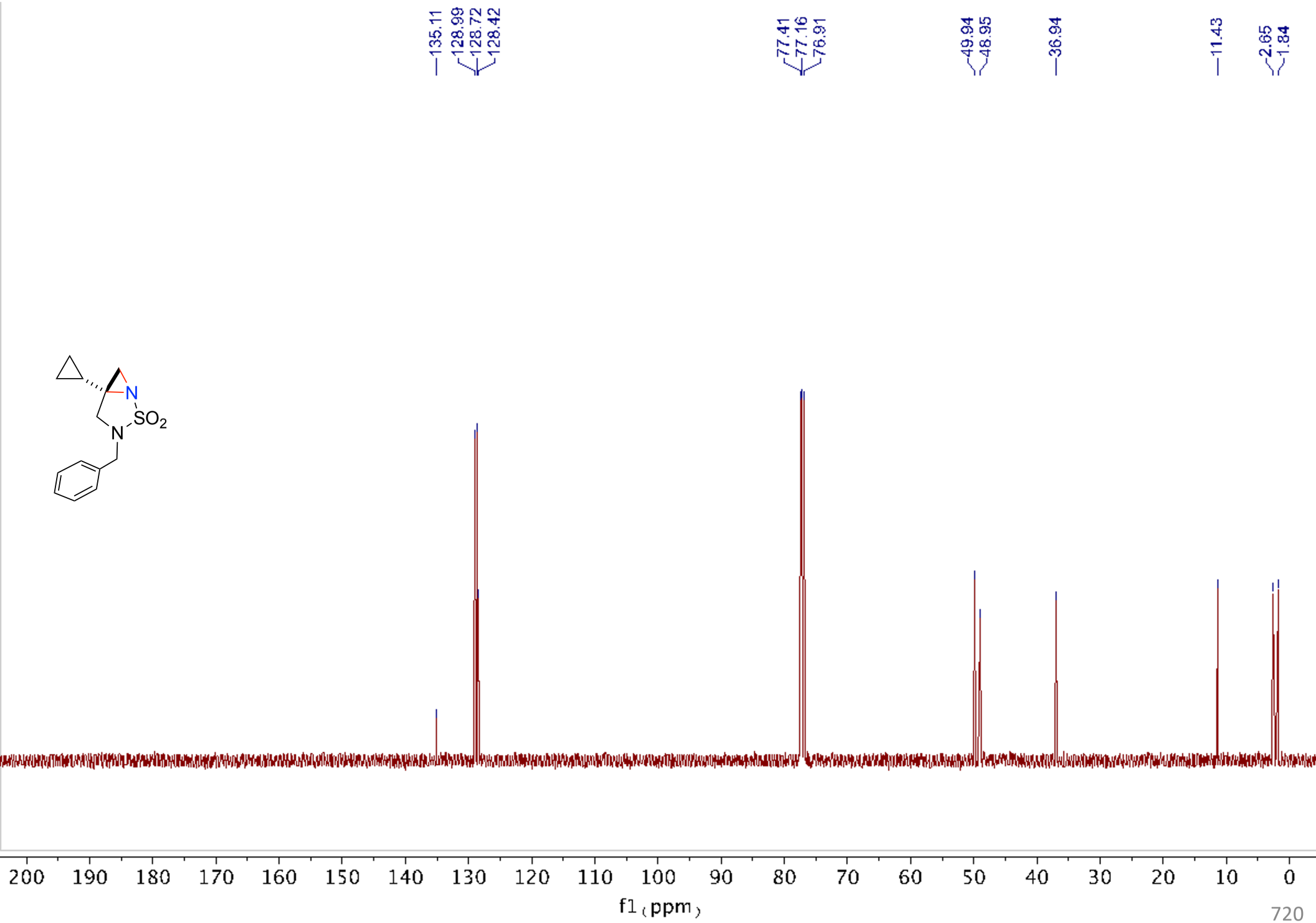
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	28.193	2772690	83.162
2	40.701	561374	16.838
Total		3334064	100.000

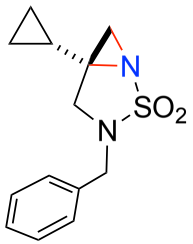
^{1}H NMR (*R*)-3-Benzyl-5-cyclopropyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2x



^{13}C NMR (*R*)-3-Benzyl-5-cyclopropyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2x



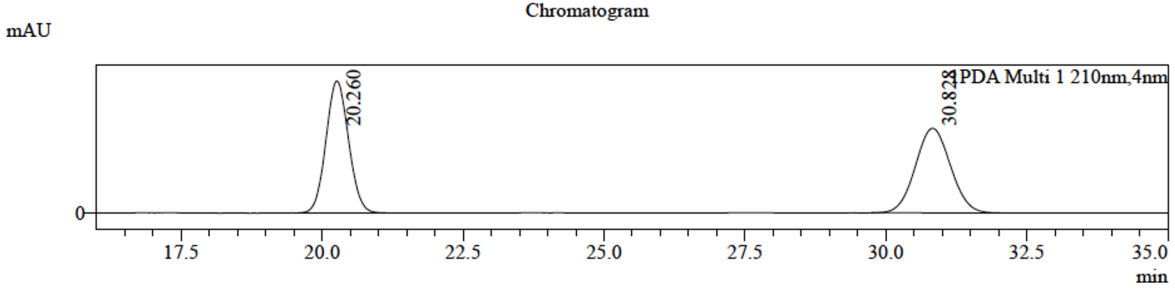
3-Benzyl-5-cyclopropyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2x



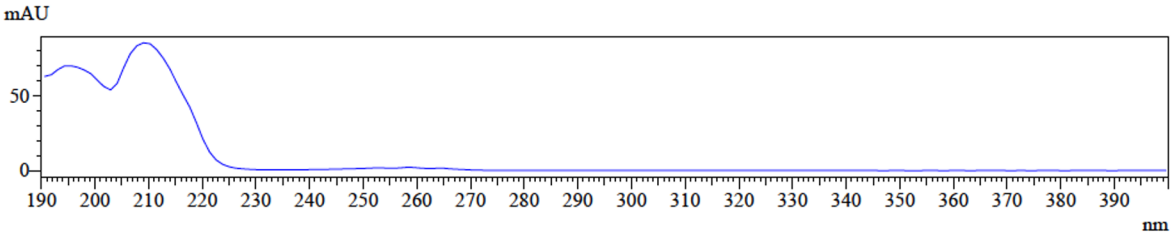
Sample Information

Data File	: H0X-0819-IC-20%1.0mL001.lcd
Sample Name	: H0X-0819-IC-20%1.0mL001
Sample ID	: H0X-0819-IC-20%1.0mL001
Method File	: H0X-20%-1.0ml-60MIN.lcm

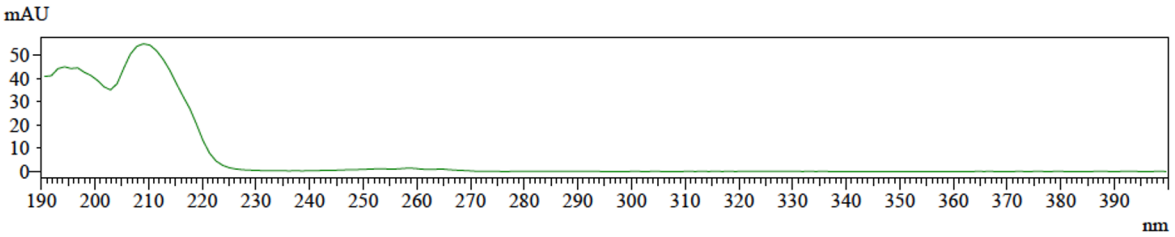
Chromatogram



UV Spectrum
Retention time = 20.260



UV Spectrum
Retention time = 30.828

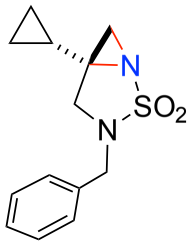


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	20.260	2220508	50.059
2	30.828	2215288	49.941
Total		4435797	100.000

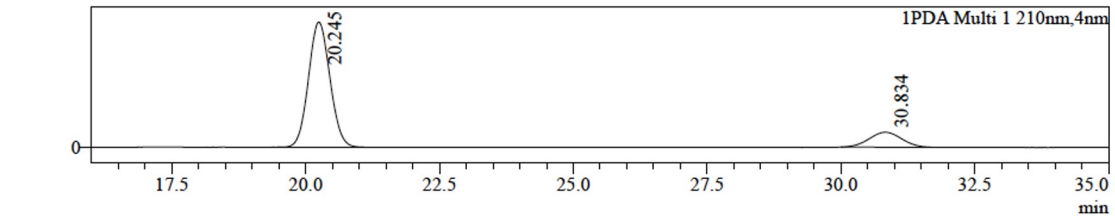
(*R*)-3-Benzyl-5-cyclopropyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2x



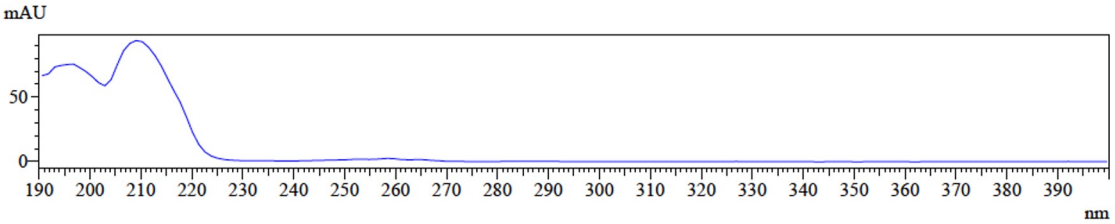
Sample Information

Data File	: H0X-0822-IC-20%1.0mL.lcd
Sample Name	: H0X-0822-IC-20%1.0mL
Sample ID	: H0X-0822-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

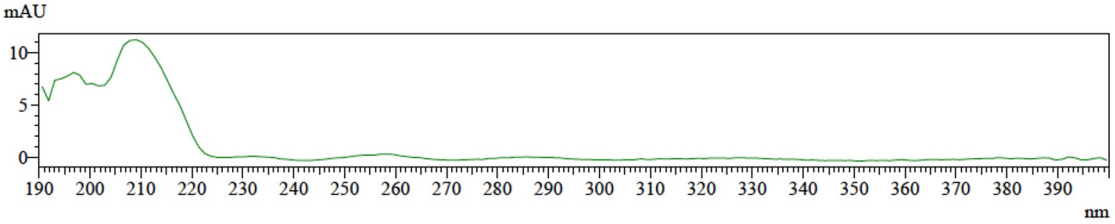
Chromatogram



UV Spectrum
Retention time = 20.245



UV Spectrum
Retention time = 30.834

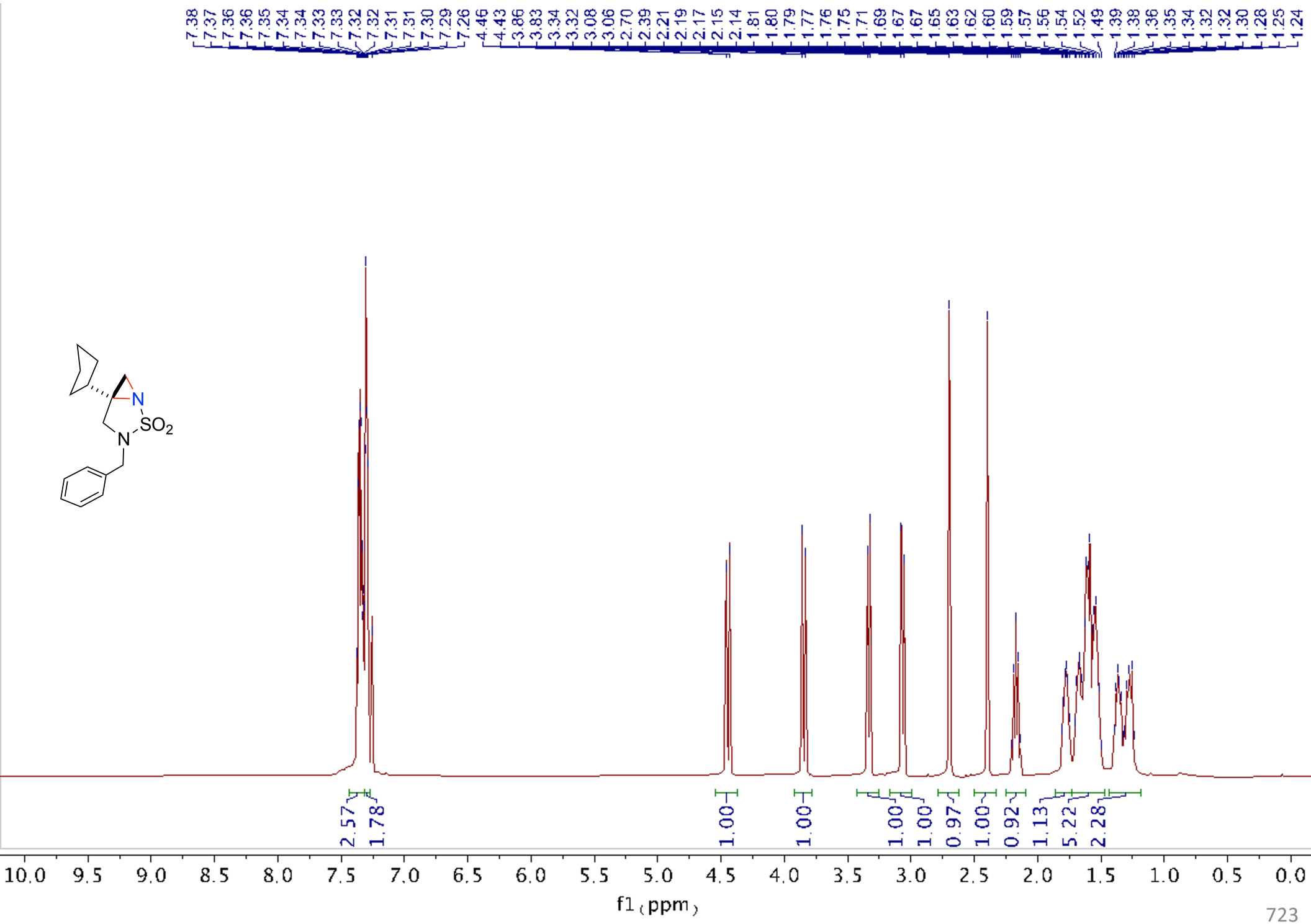


Peak Table

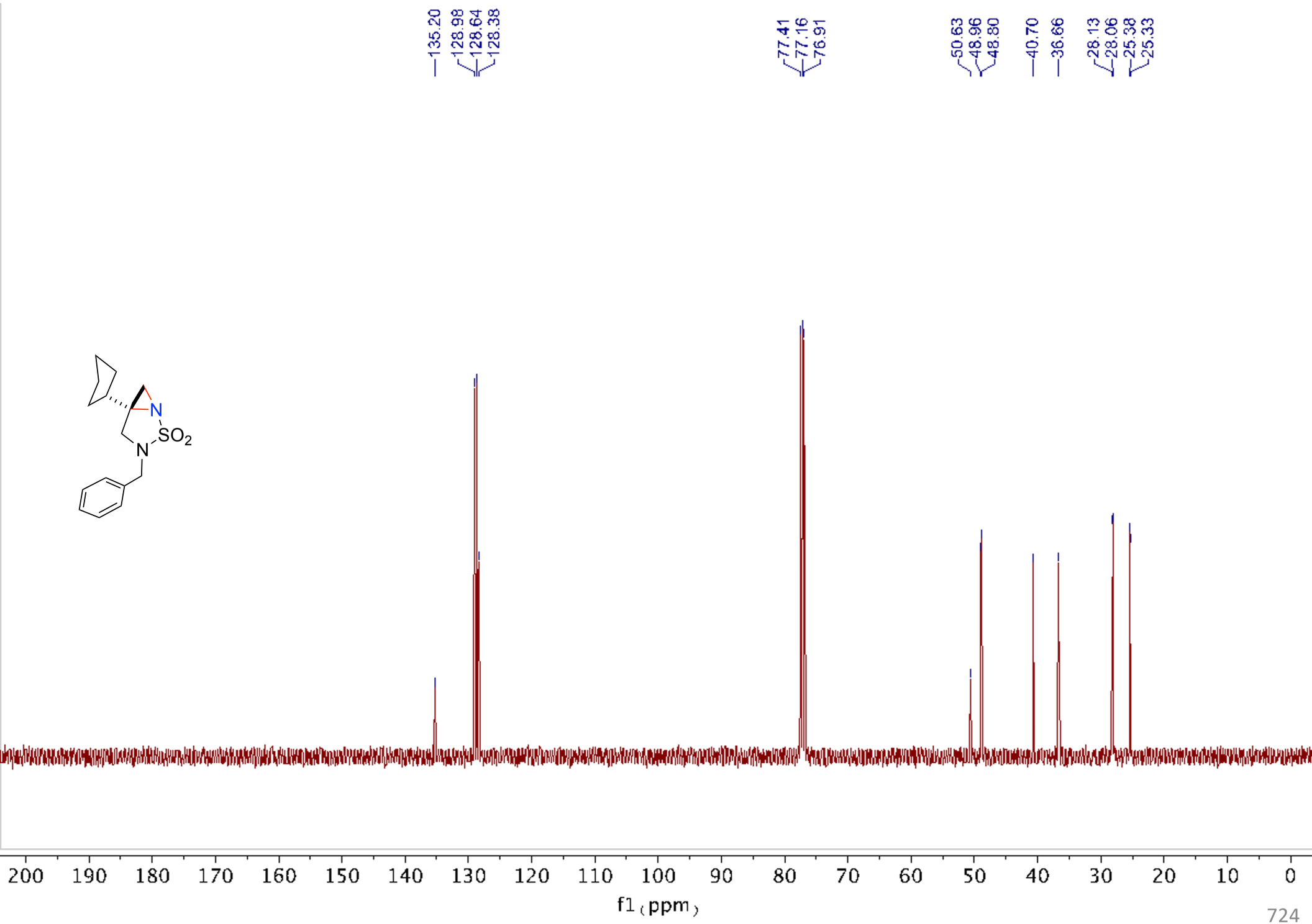
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	20.245	2438247	84.857
2	30.834	435118	15.143
Total		2873365	100.000

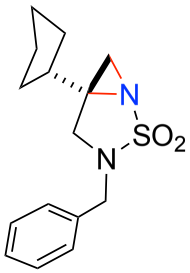
^{1}H NMR (*R*)-3-Benzyl-5-cyclopentyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2y



^{13}C NMR (*R*)-3-Benzyl-5-cyclopentyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2y



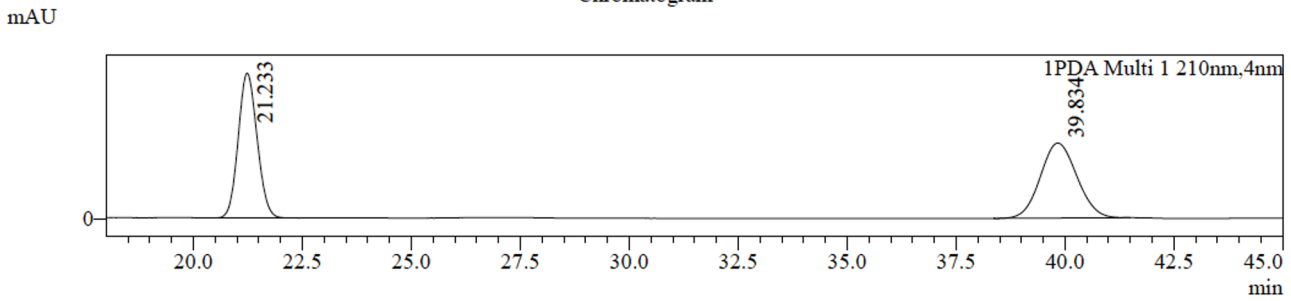
3-Benzyl-5-cyclopentyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2y



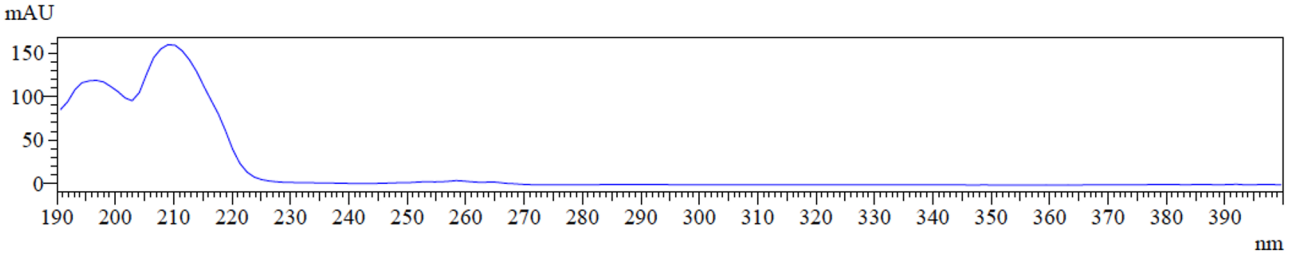
Sample Information

Data File	: H0X-0639-CYCLOPANTANE-IC-20%1.0mL.lcd
Sample Name	: H0X-0639-CYCLOPANTANE-IC-20%1.0mL
Sample ID	: H0X-0639-CYCLOPANTANE-IC-20%1.0
Method File	: H0X-20%-1.0ml-60MIN.lcm

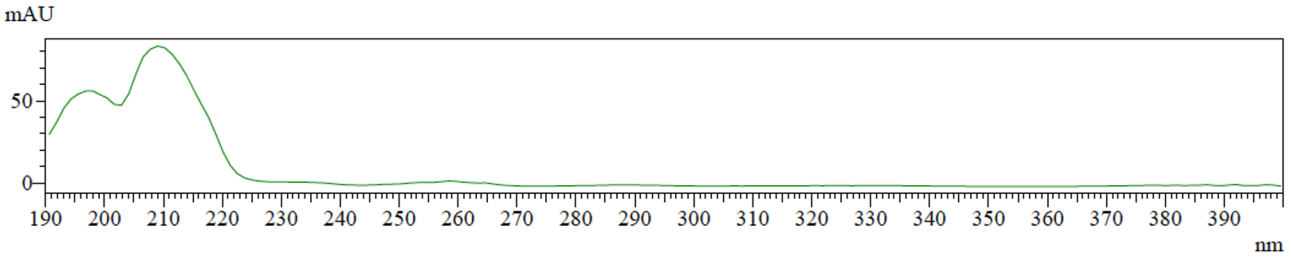
Chromatogram



UV Spectrum
Retention time = 21.233



UV Spectrum
Retention time = 39.834

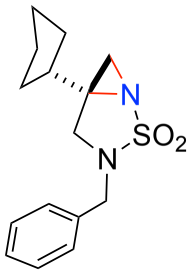


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	21.233	4467009	49.978
2	39.834	4471008	50.022
Total		8938016	100.000

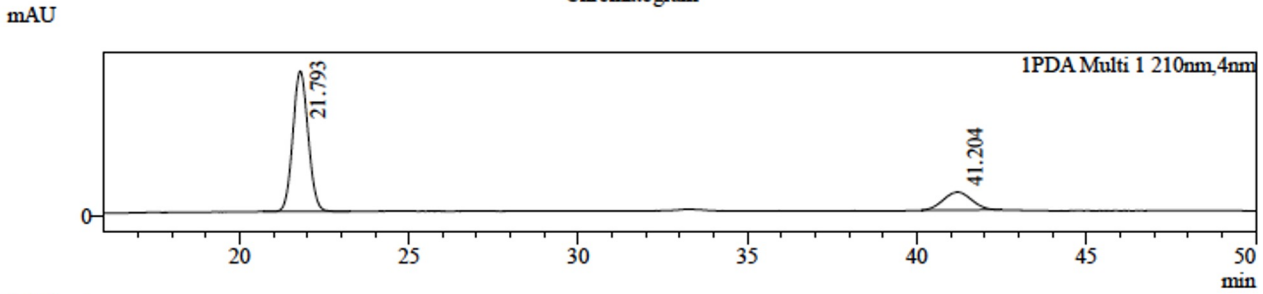
(*R*)-3-Benzyl-5-cyclopentyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2y



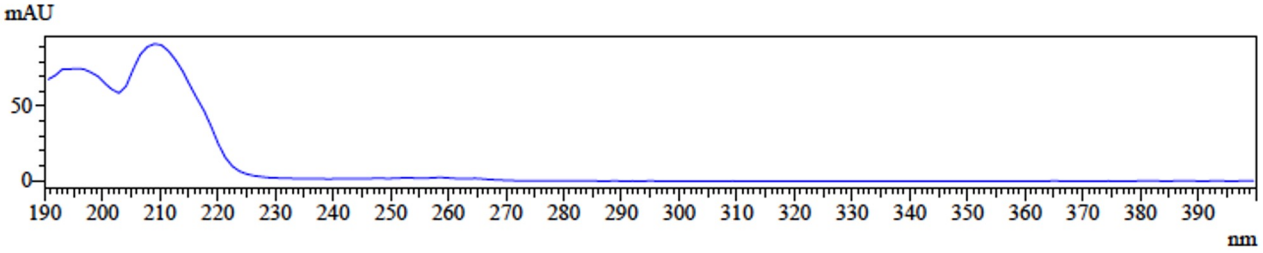
Sample Information

Data File	: H0X-0788-Final-IC-20%1.0mL.lcd
Sample Name	: H0X-0788-Final-IC-20%1.0mL
Sample ID	: H0X-0788-Final-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

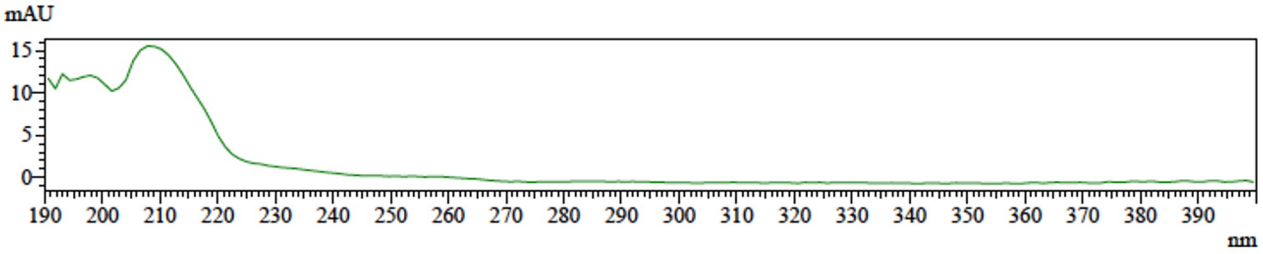
Chromatogram



UV Spectrum
Retention time = 21.793



UV Spectrum
Retention time = 41.204

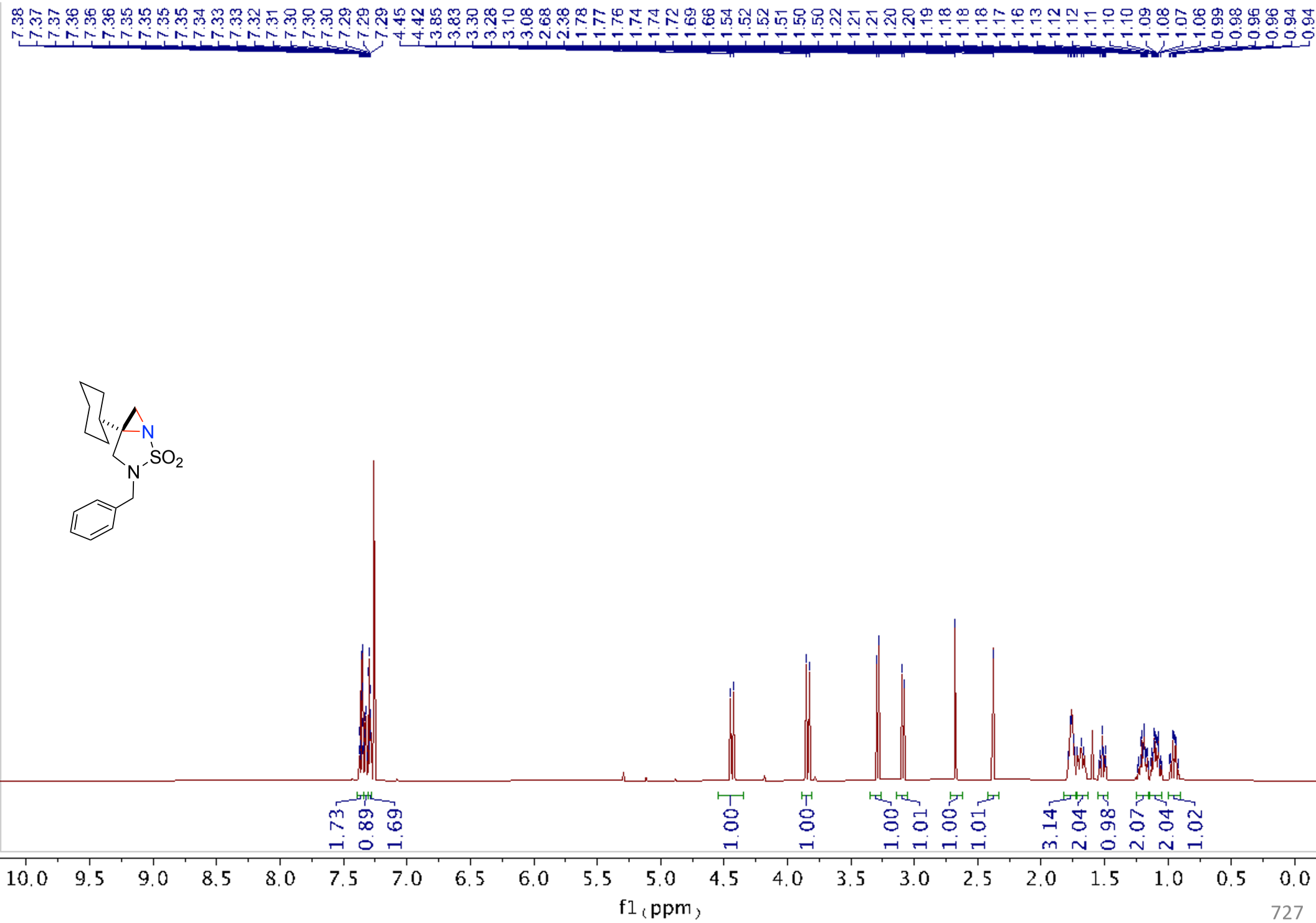


Peak Table

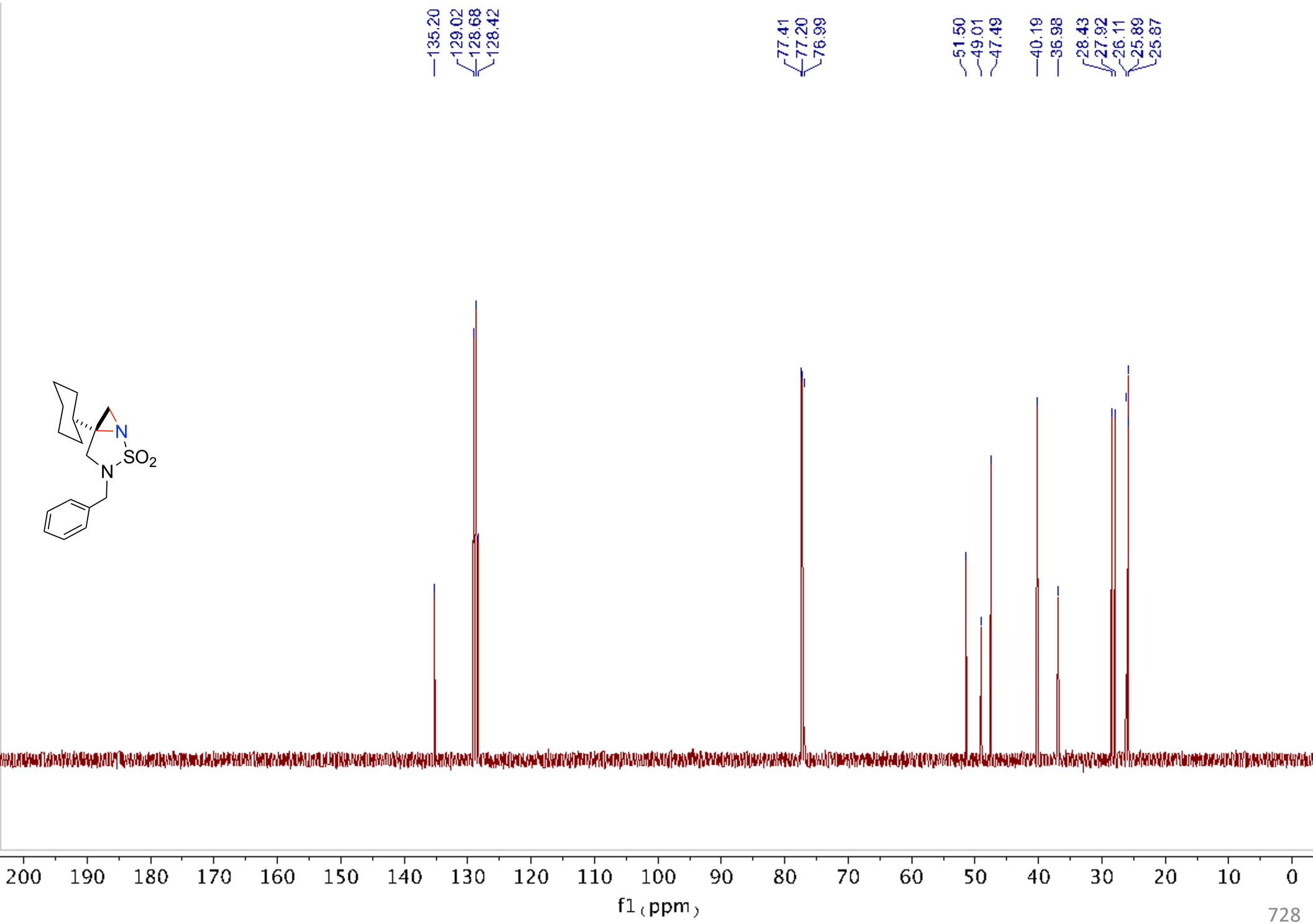
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	21.793	2592702	80.869
2	41.204	613351	19.131
Total		3206053	100.000

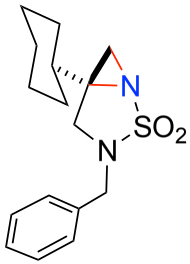
^{1}H NMR (*R*)-3-Benzyl-5-cyclohexyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2z



^{13}C NMR (*R*)-3-Benzyl-5-cyclohexyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2z



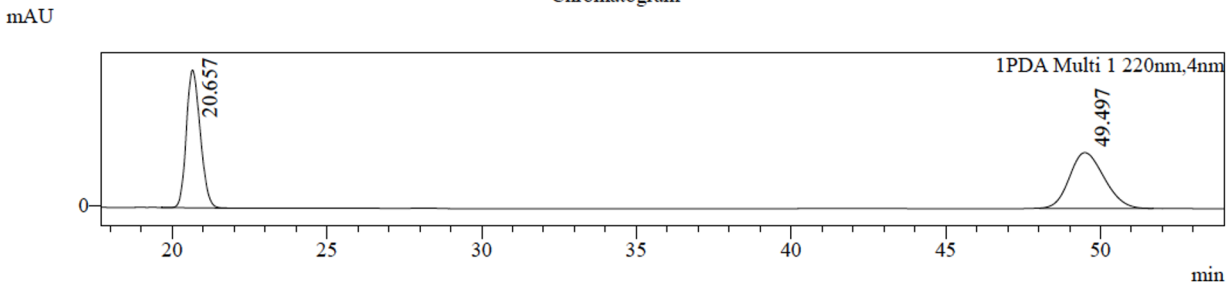
3-Benzyl-5-cyclohexyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2z



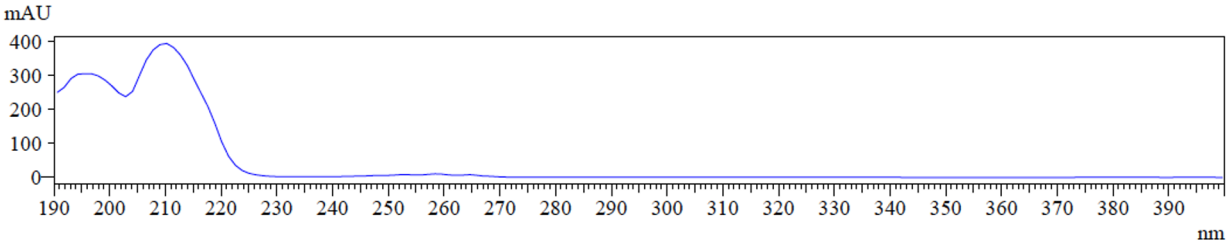
Sample Information

Data File	: H0X-0692-CYCLOHEXNAE-IC-20%1.0mL.lcd
Sample Name	: H0X-0692-CYCLOHEXNAE-IC-20%1.0mL
Sample ID	: H0X-0692-CYCLOHEXNAE-IC-20%1.0m
Method File	: H0X-20%-1.0ml-60MIN.lcm

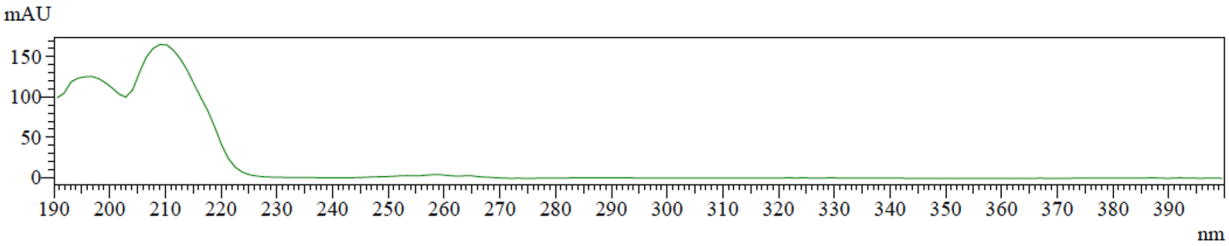
Chromatogram



UV Spectrum
Retention time = 20.657



UV Spectrum
Retention time = 49.497

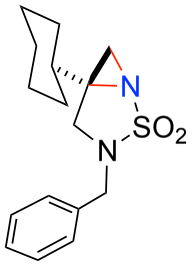


Peak Table

PDA Ch1 220nm

Peak#	Ret. Time	Area	Area%
1	20.657	3801498	49.836
2	49.497	3826569	50.164
Total		7628067	100.000

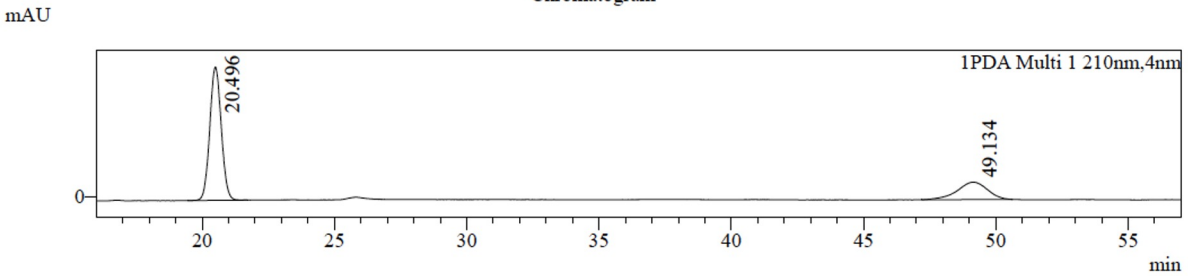
(*R*)-3-Benzyl-5-cyclohexyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2z



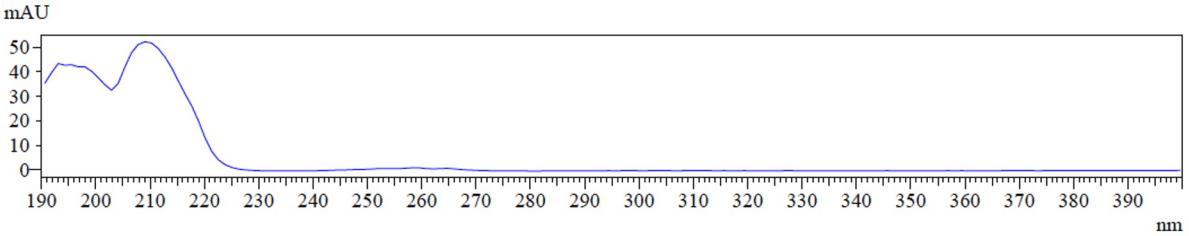
Sample Information

Data File	: H0X-0825-IC-20%1.0mL.lcd
Sample Name	: H0X-0825-IC-20%1.0mL
Sample ID	: H0X-0825-IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

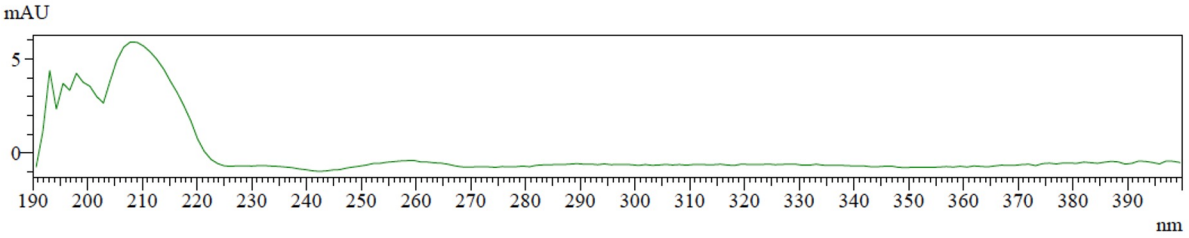
Chromatogram



UV Spectrum
Retention time = 20.496



UV Spectrum
Retention time = 49.134

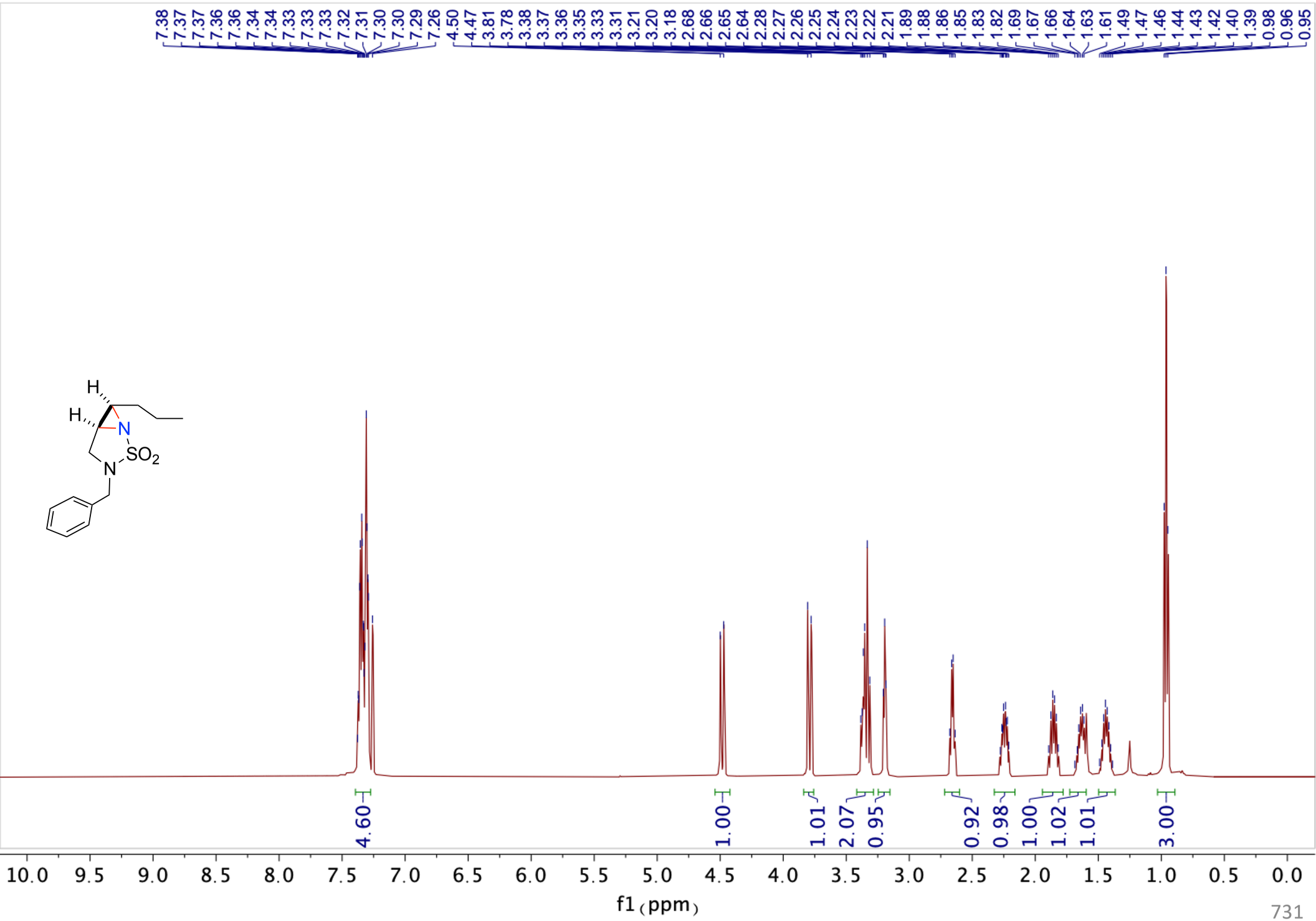


Peak Table

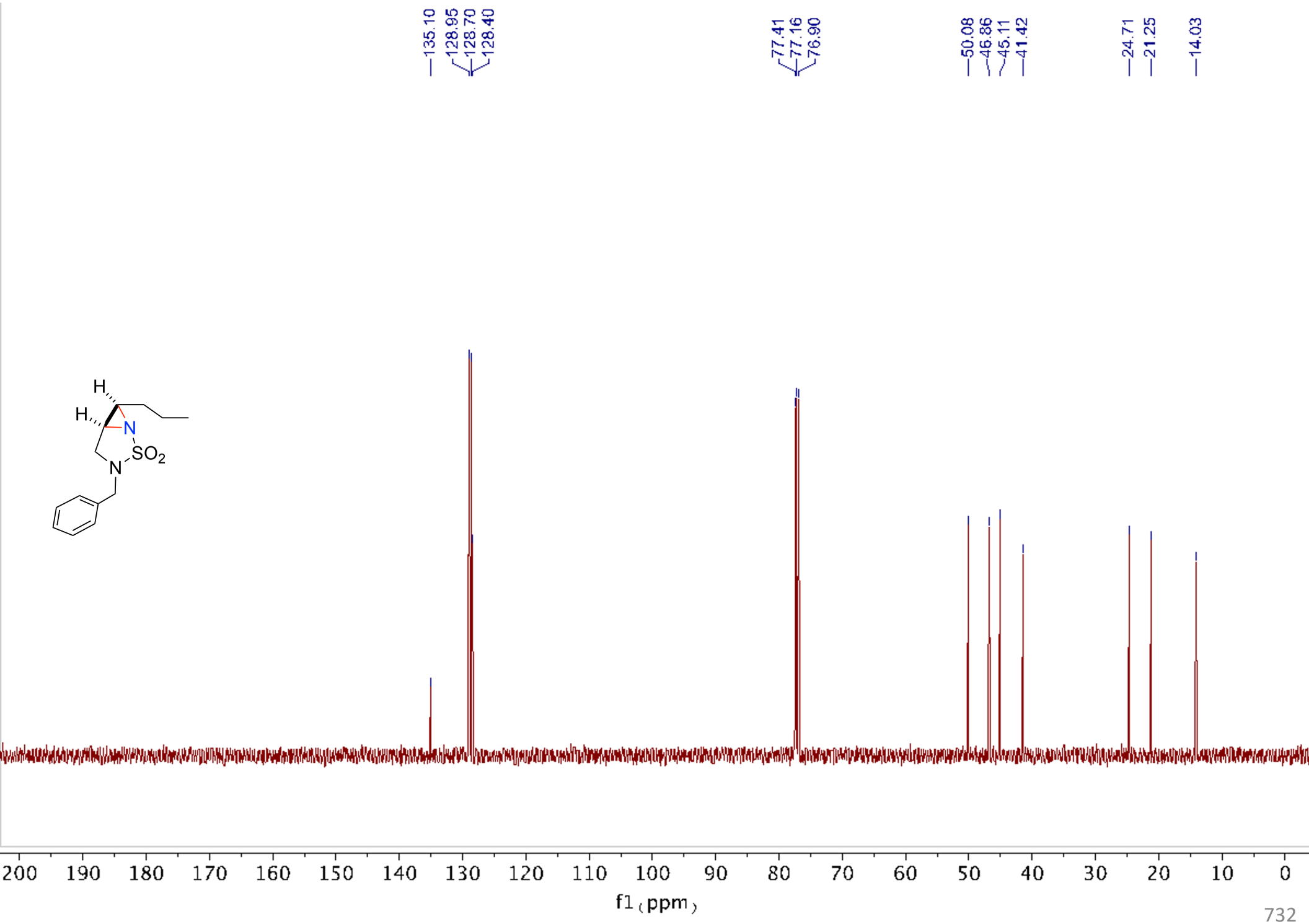
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	20.496	1512522	74.546
2	49.134	516456	25.454
Total		2028978	100.000

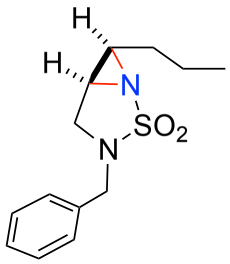
^{1}H NMR (5*S*)-3-Benzyl-6-propyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2aa



^{13}C NMR (5*S*)-3-Benzyl-6-propyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2aa



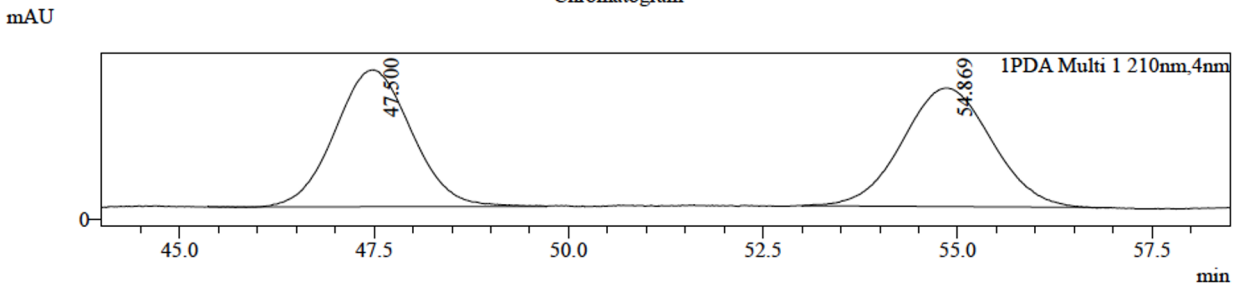
3-Benzyl-6-propyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2aa



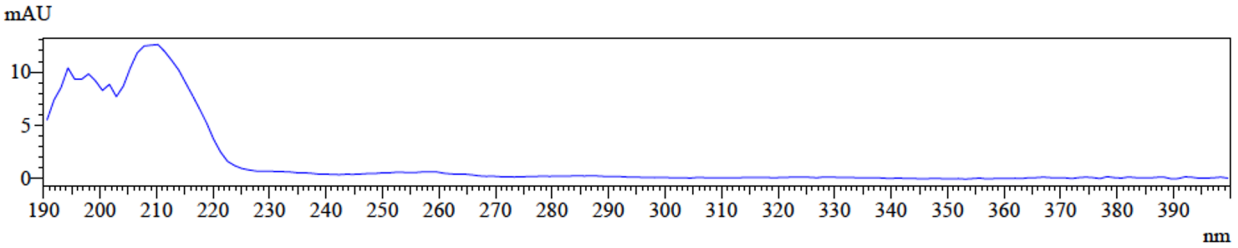
Sample Information

Data File	: H0X-0682--IC-20%1.0mL.lcd
Sample Name	: H0X-0715--IC-20%1.0mL
Sample ID	: H0X-0715--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

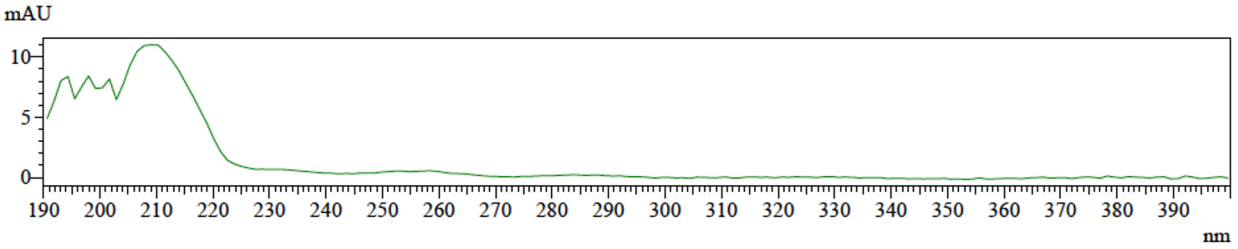
Chromatogram



UV Spectrum
Retention time = 47.500



UV Spectrum
Retention time = 54.869

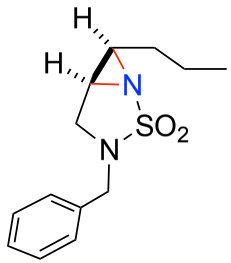


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	47.500	742575	49.826
2	54.869	747771	50.174
Total		1490346	100.000

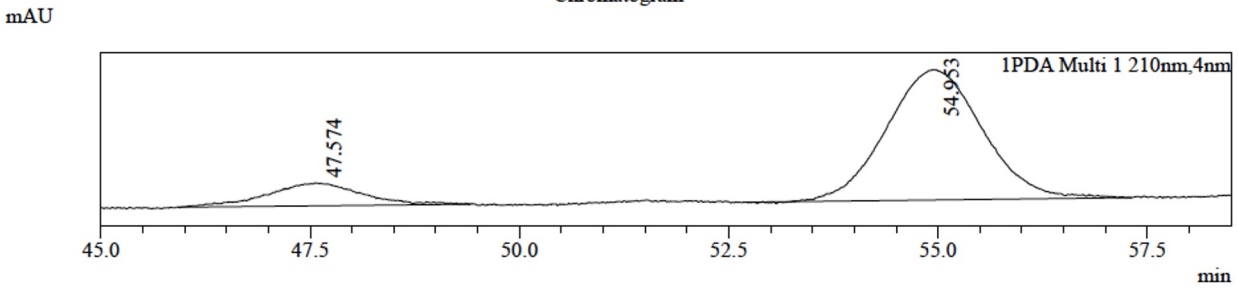
(5*S*)-3-Benzyl-6-propyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2aa



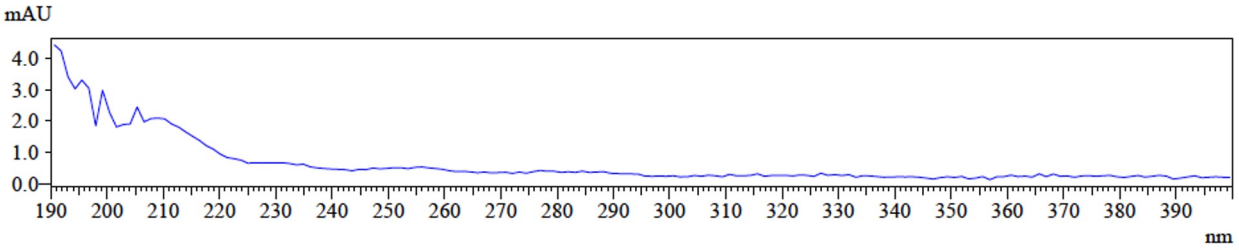
Sample Information

Data File	: H0X-0683--IC-20%1.0mL.lcd
Sample Name	: H0X-0716--IC-20%1.0mL
Sample ID	: H0X-0716--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

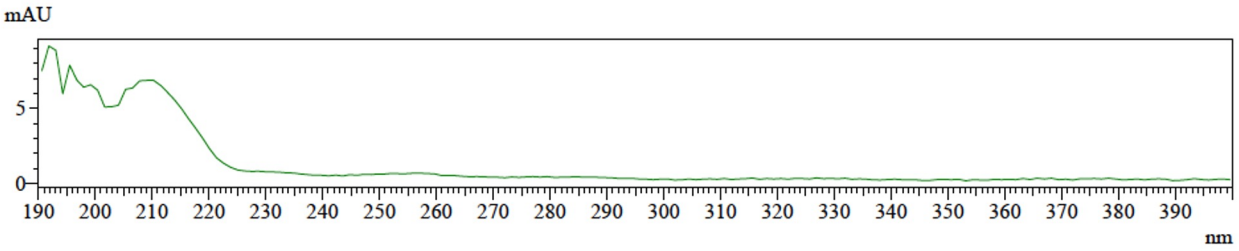
Chromatogram



UV Spectrum
Retention time = 47.574



UV Spectrum
Retention time = 54.953

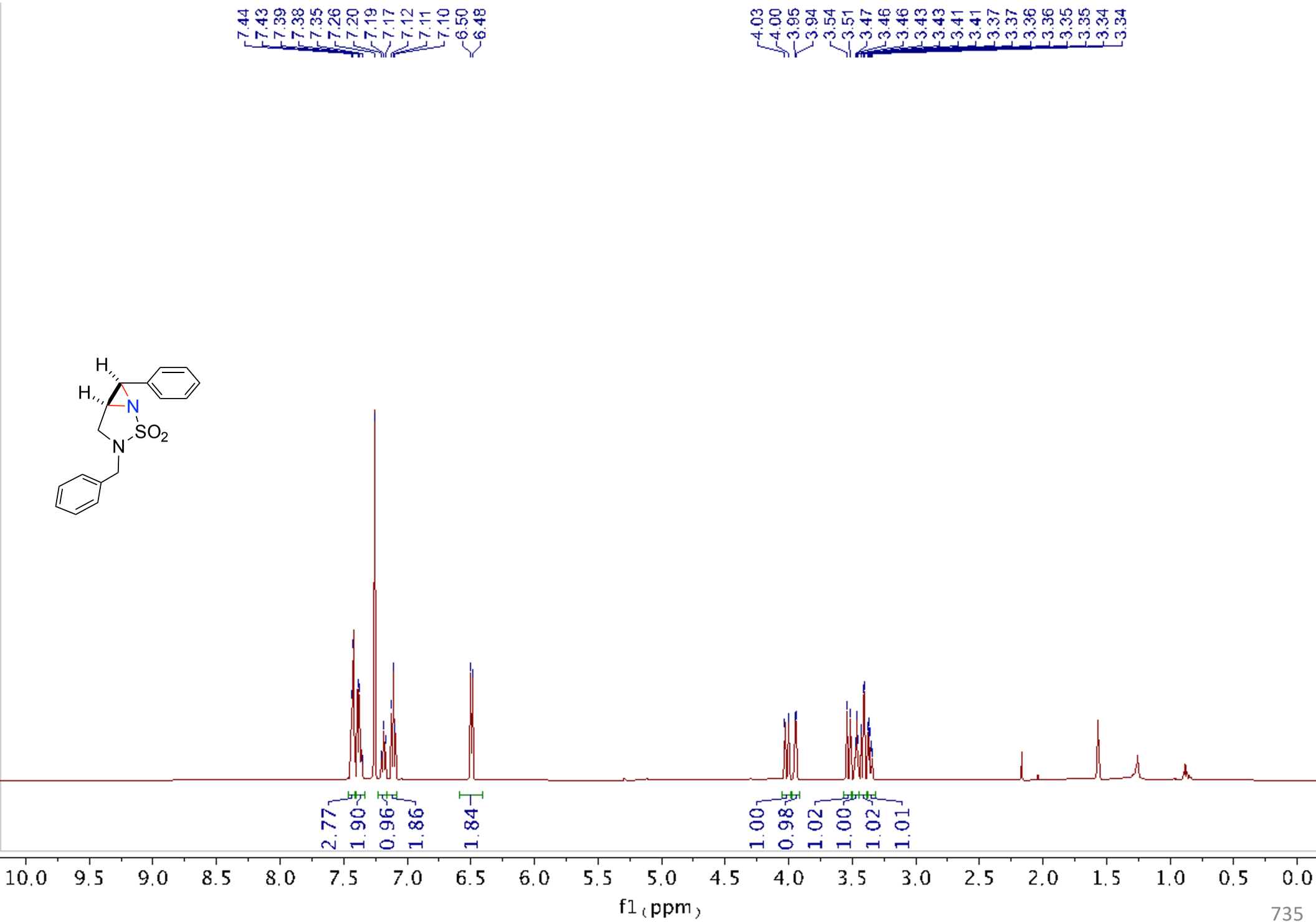


Peak Table

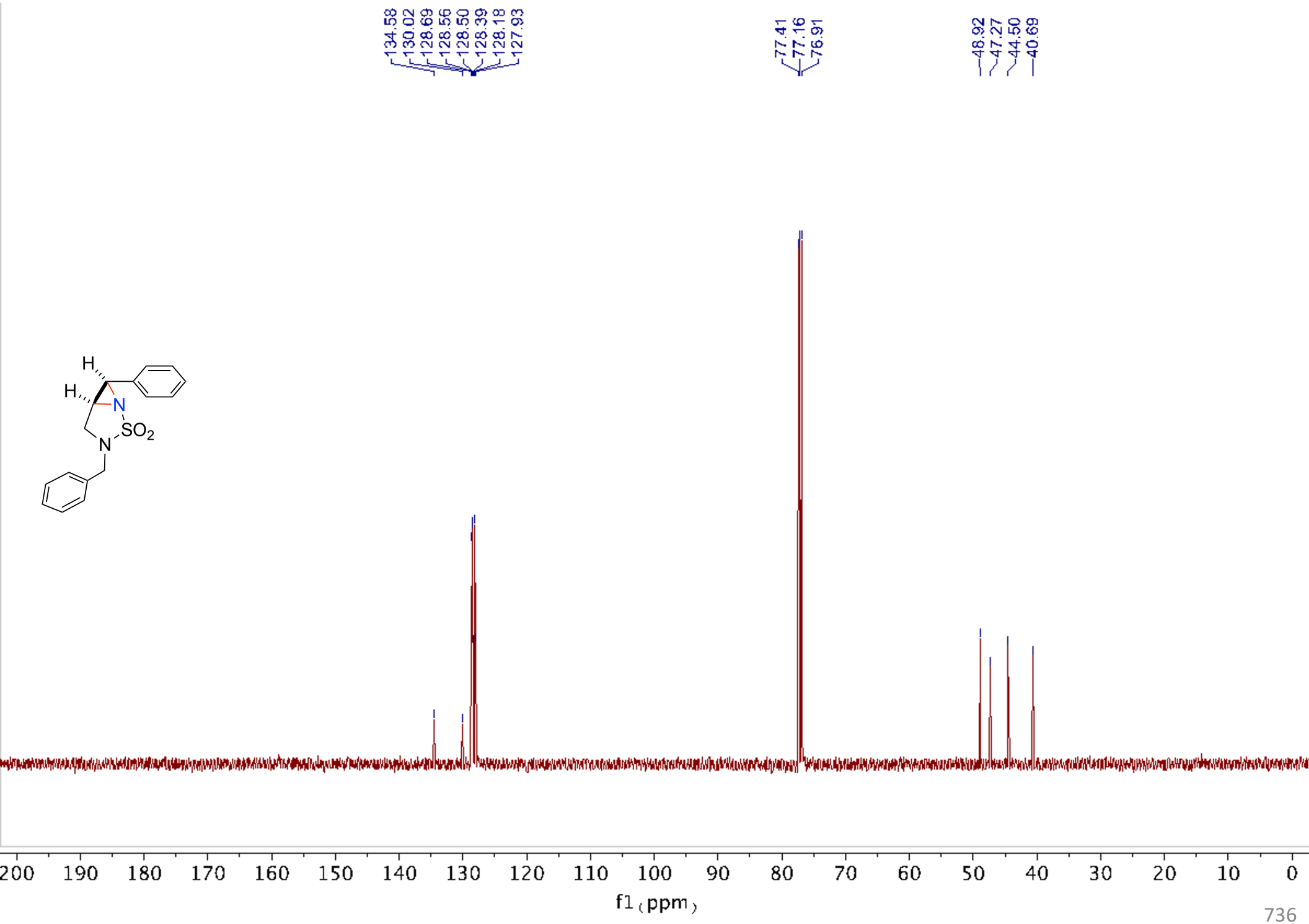
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	47.574	71409	14.746
2	54.953	412861	85.254
Total		484270	100.000

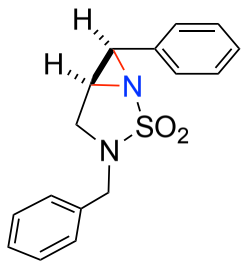
^{1}H NMR (5*S*)-3-Benzyl-6-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2ab



^{13}C NMR (5*S*)-3-Benzyl-6-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2ab



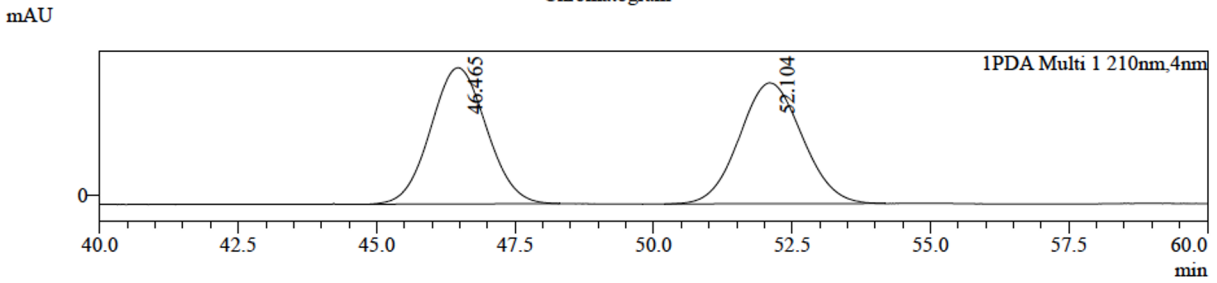
(5*S*)-3-Benzyl-6-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2ab



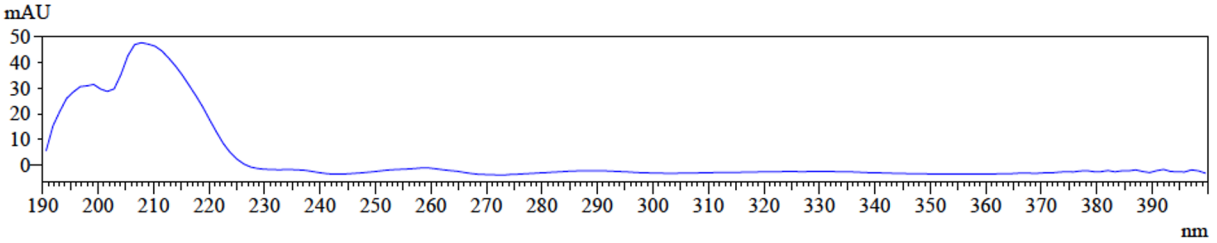
Sample Information

Data File	: H0X-0763_2--IC-20%1.0mL.lcd
Sample Name	: H0X-0763_2--IC-20%1.0mL
Sample ID	: H0X-0763_2--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

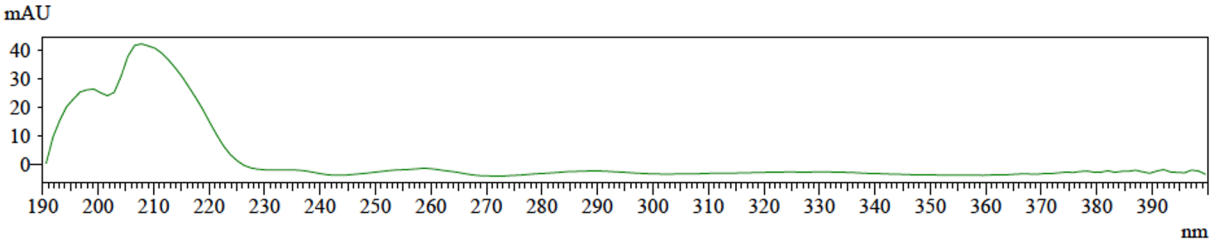
Chromatogram



UV Spectrum
Retention time = 46.465



UV Spectrum
Retention time = 52.104

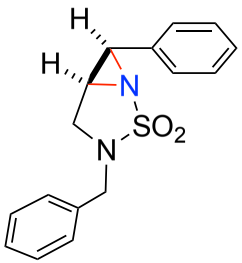


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	46.465	3372714	50.100
2	52.104	3359252	49.900
Total		6731965	100.000

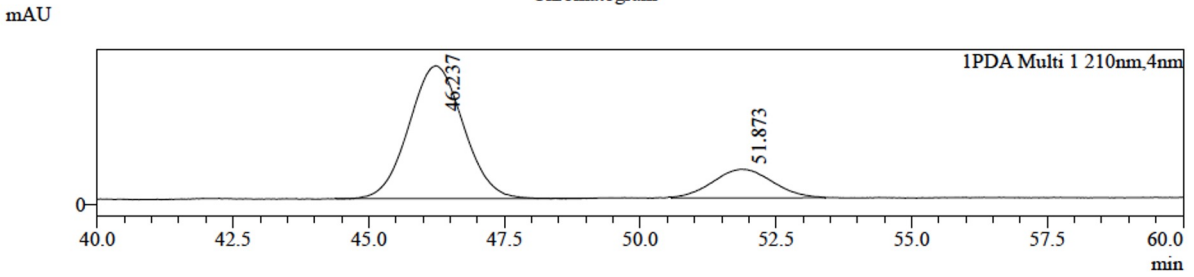
(5*S*)-3-Benzyl-6-phenyl-2-thia-1,3-diazabicyclo[3.1.0]hexane 2,2-dioxide 2.2ab



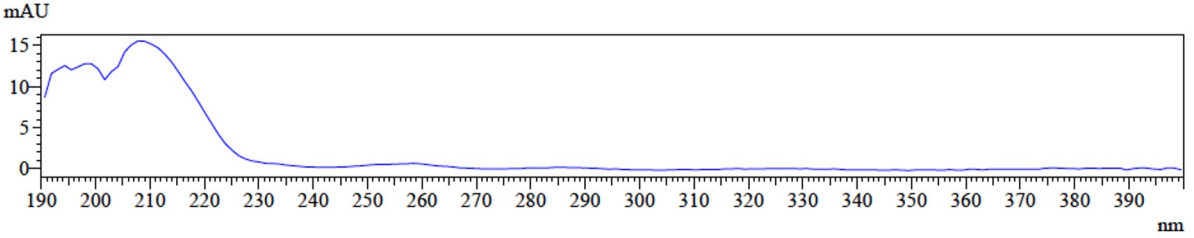
Sample Information

Data File	: H0X-0764--IC-20%1.0mL.lcd
Sample Name	: H0X-0764--IC-20%1.0mL
Sample ID	: H0X-0764--IC-20%1.0mL
Method File	: H0X-20%-1.0ml-60MIN.lcm

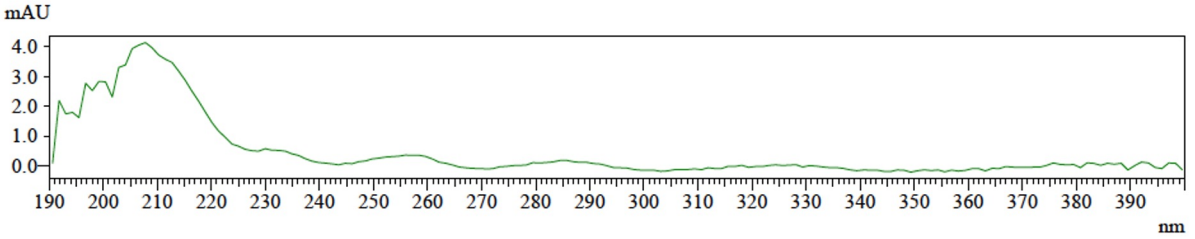
Chromatogram



UV Spectrum
Retention time = 46.237



UV Spectrum
Retention time = 51.873

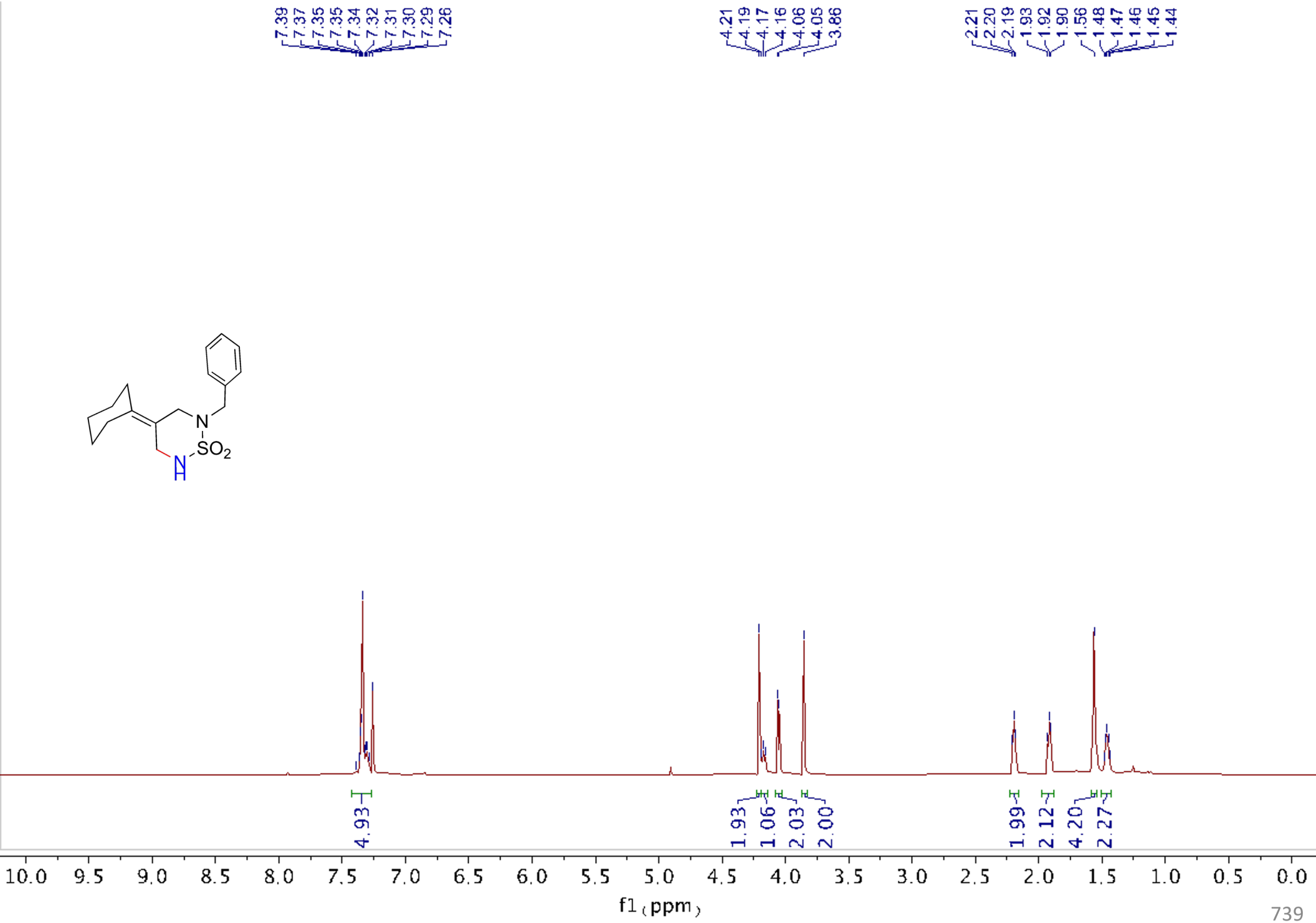


Peak Table

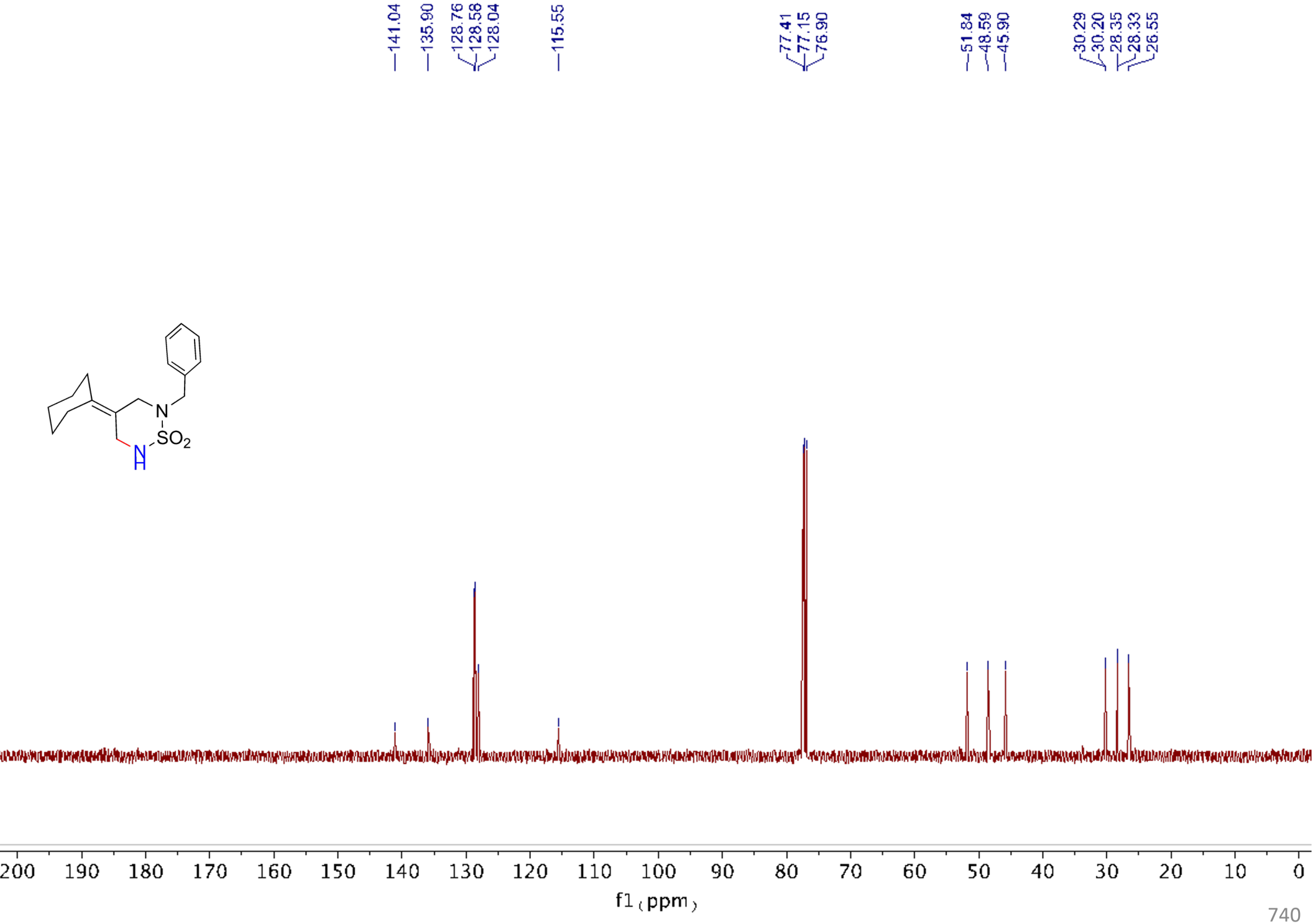
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	46.237	981853	80.893
2	51.873	231911	19.107
Total		1213764	100.000

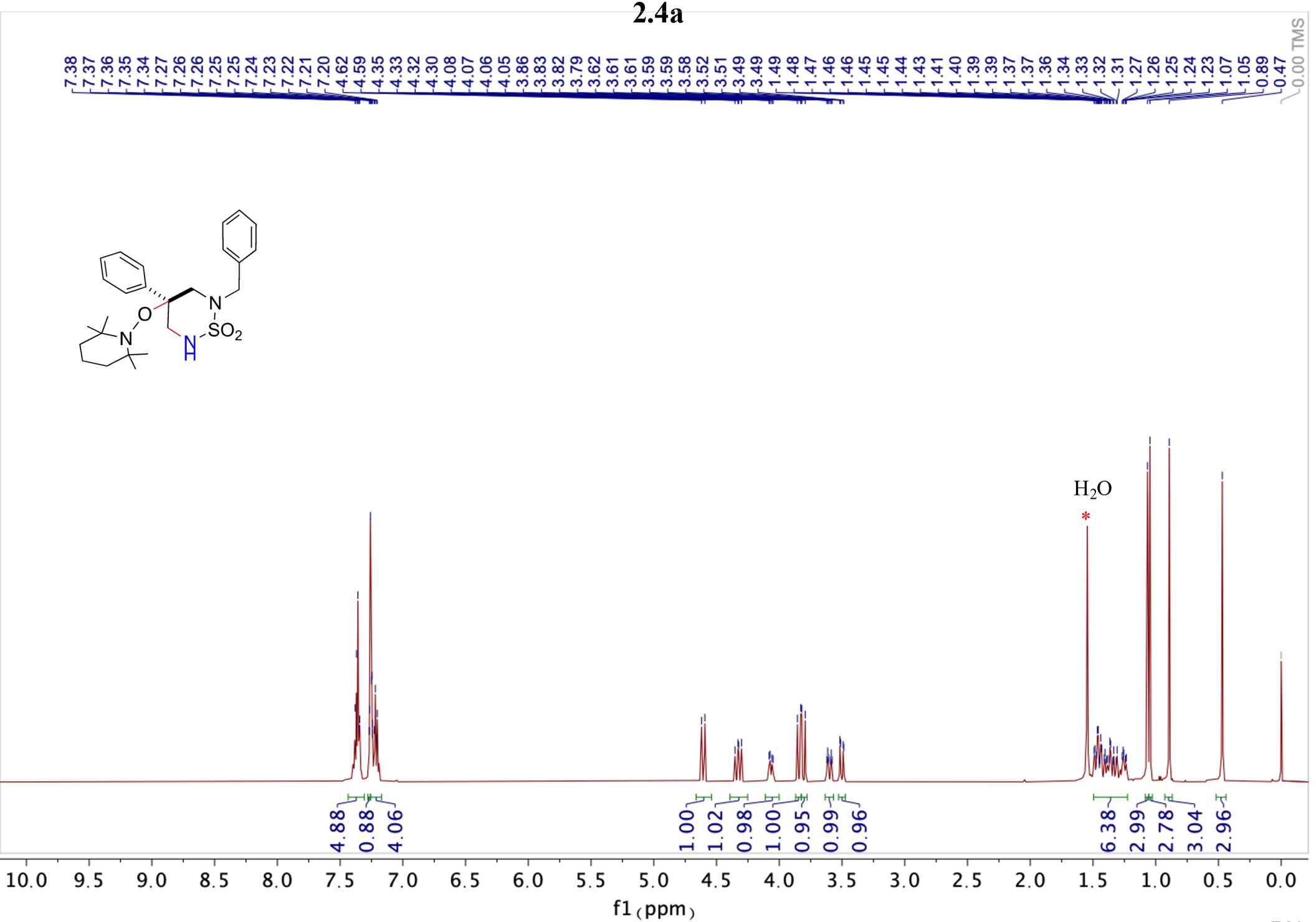
^{1}H NMR 2-Benzyl-4-cyclohexylidene-1,2,6-thiadiazinane 1,1-dioxide 2.3z



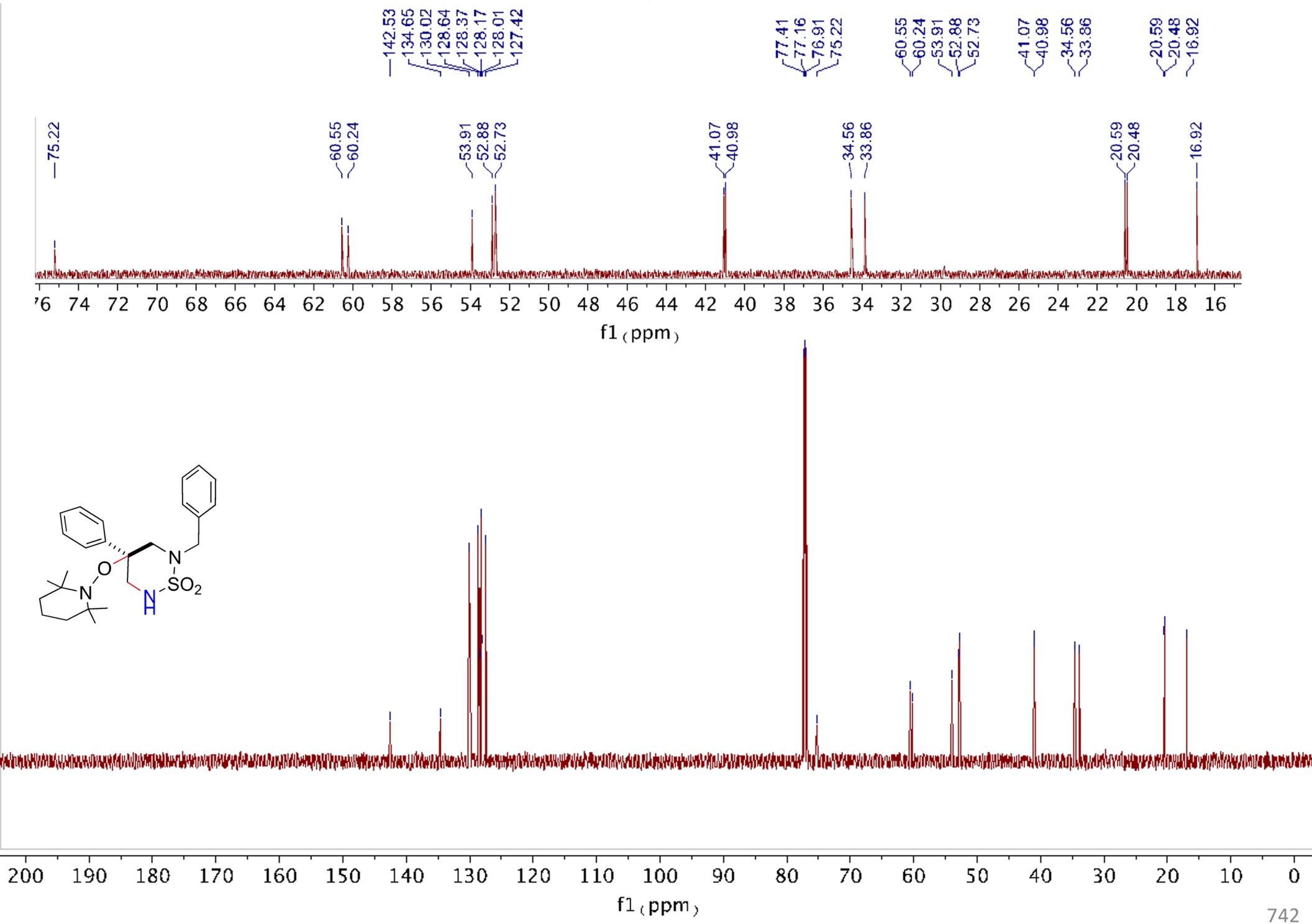
^{13}C NMR 2-Benzyl-4-cyclohexylidene-1,2,6-thiadiazinane 1,1-dioxide 2.3z



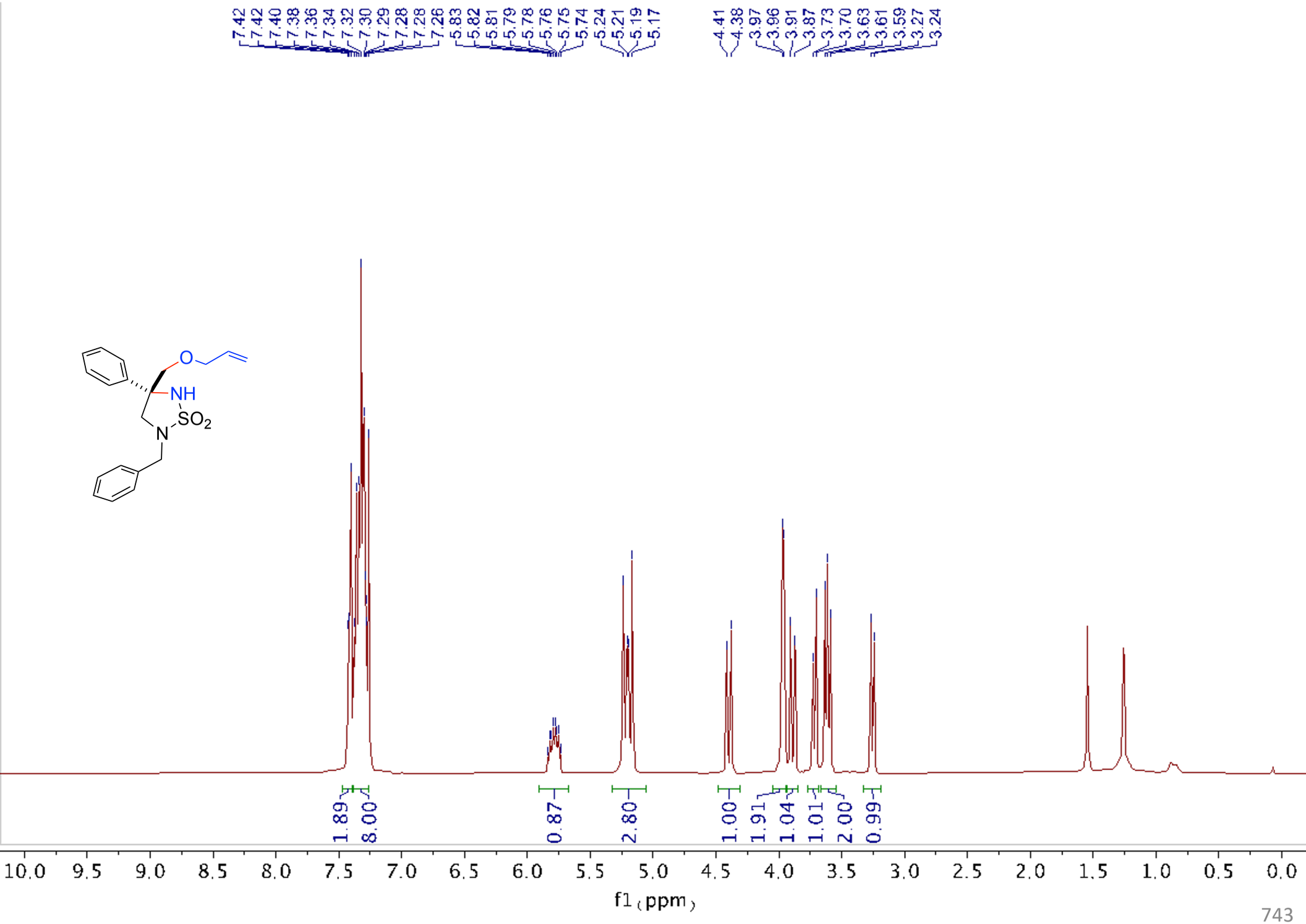
^{1}H NMR 2-Benzyl-4-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-1,2,6-thiadiazinane 1,1-dioxide 2.4a



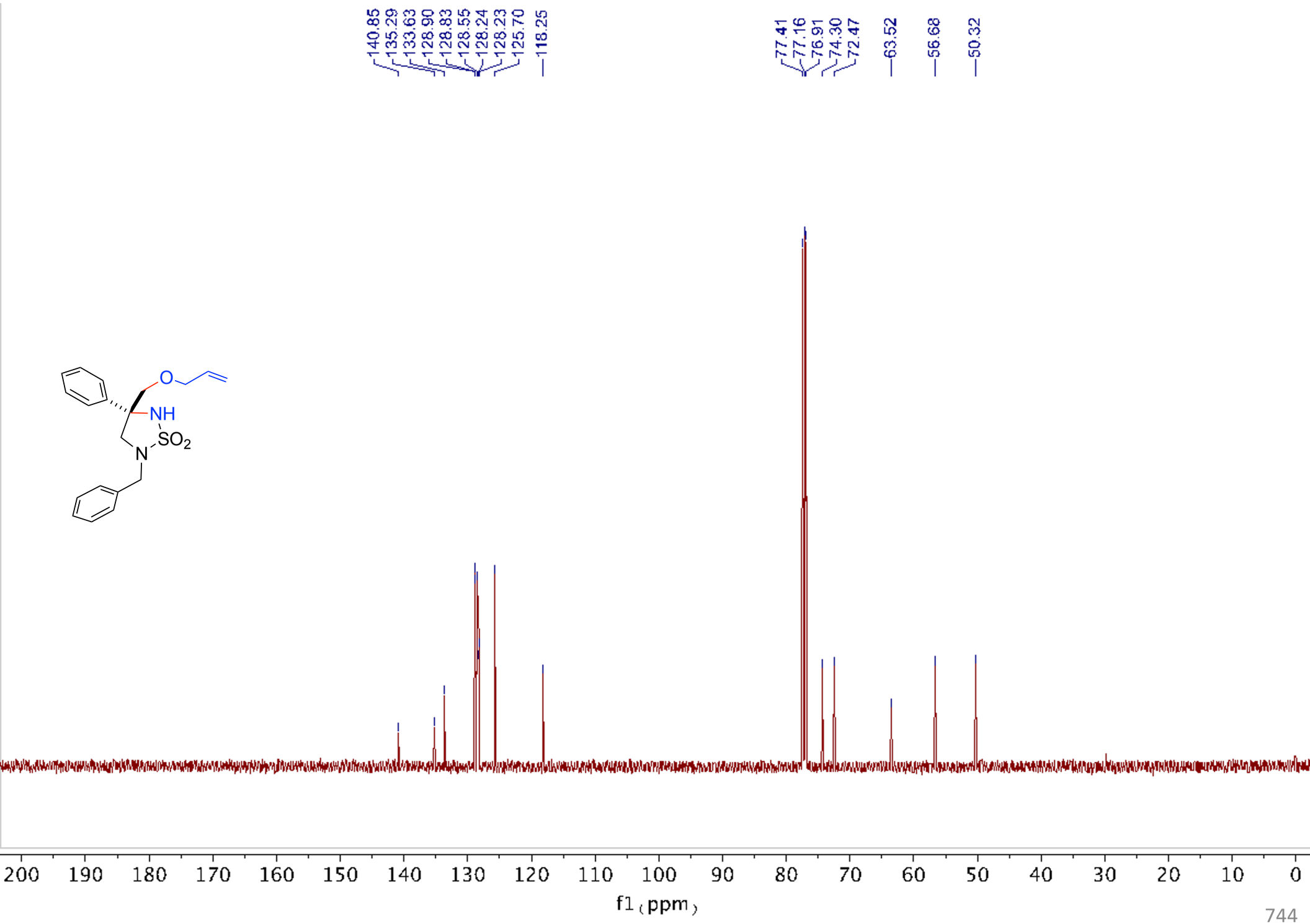
^{13}C NMR 2-Benzyl-4-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-1,2,6-thiadiazinane 1,1-dioxide 2.4a



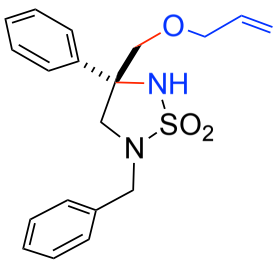
^{1}HNMR (*S*)-4-((Allyloxy)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6a



^{13}C NMR (*S*)-4-((Allyloxy)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6a



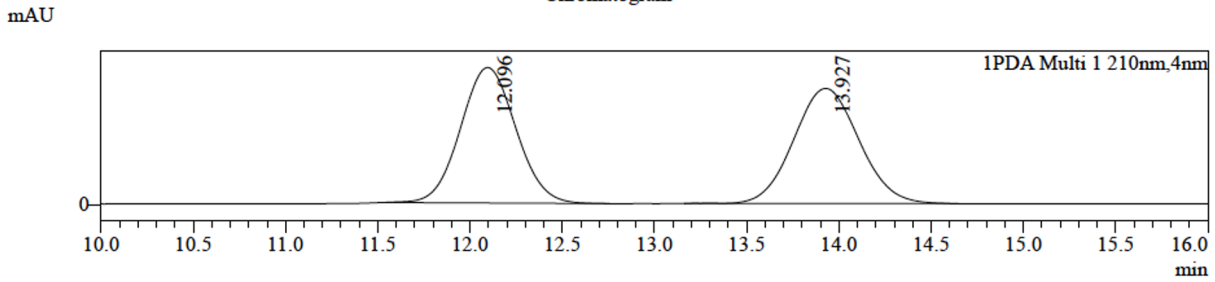
4-((Allyloxy)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6a



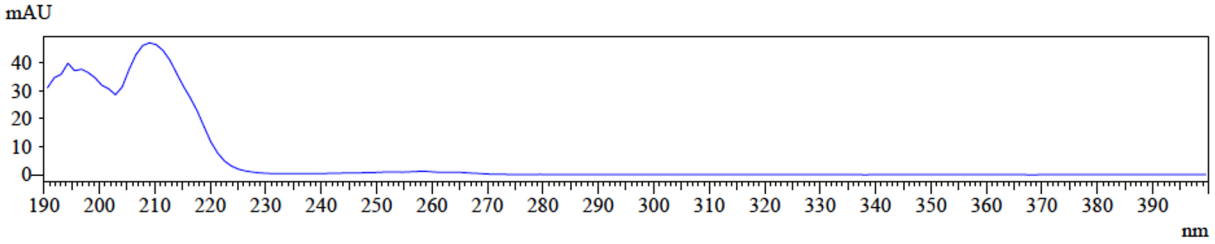
Sample Information

Data File	: H0X-TF-ALLOH--IC-30%1.0mL.lcd
Sample Name	: H0X-TF-ALLOH--IC-30%1.0mL
Sample ID	: H0X-TF-ALLOH--IC-30%1.0mL
Method File	: H0X-30%-1.0ml-90MIN.lcm

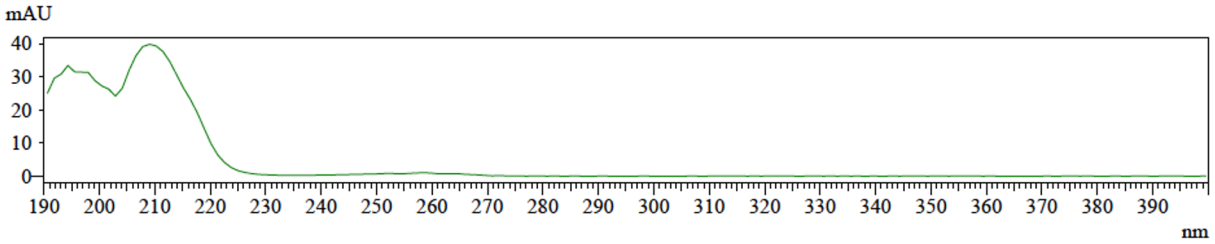
Chromatogram



UV Spectrum
Retention time = 12.096



UV Spectrum
Retention time = 13.927

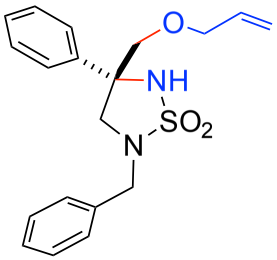


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	12.096	896543	49.983
2	13.927	897147	50.017
Total		1793690	100.000

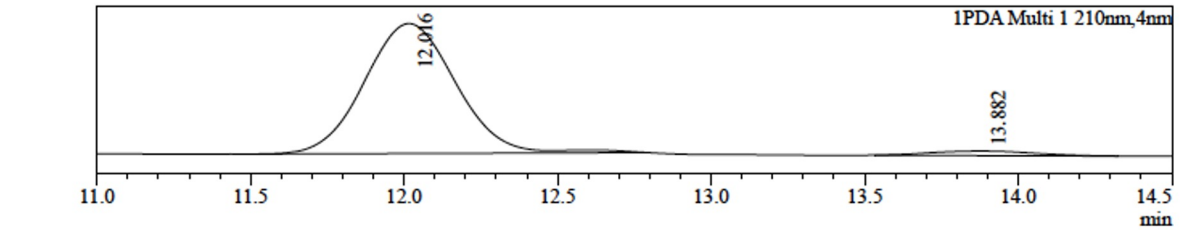
(*S*)-4-((Allyloxy)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6a



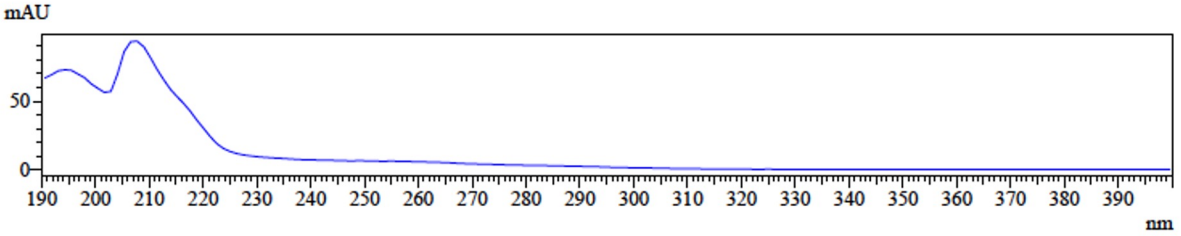
Sample Information

Data File	: H0X-TF-ALLOH-CH-IC-30%1.0mL001.lcd
Sample Name	: H0X-TF-ALLOH-CH-IC-30%1.0mL
Sample ID	: H0X-TF-ALLOH-CH-IC-30%1.0mL
Method File	: H0X-30%-1.0ml-20MIN.lcm

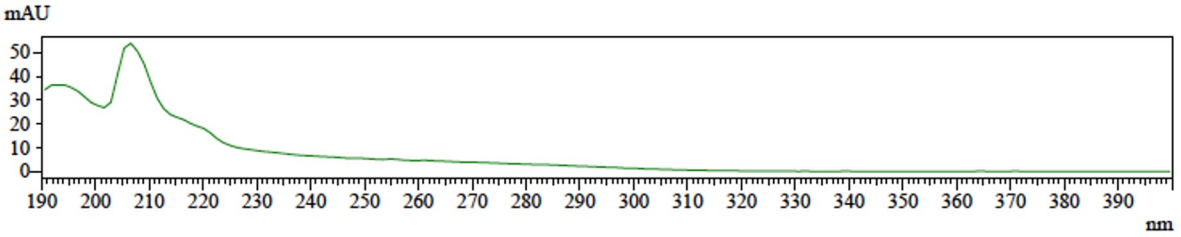
Chromatogram



UV Spectrum
Retention time = 12.016



UV Spectrum
Retention time = 13.882

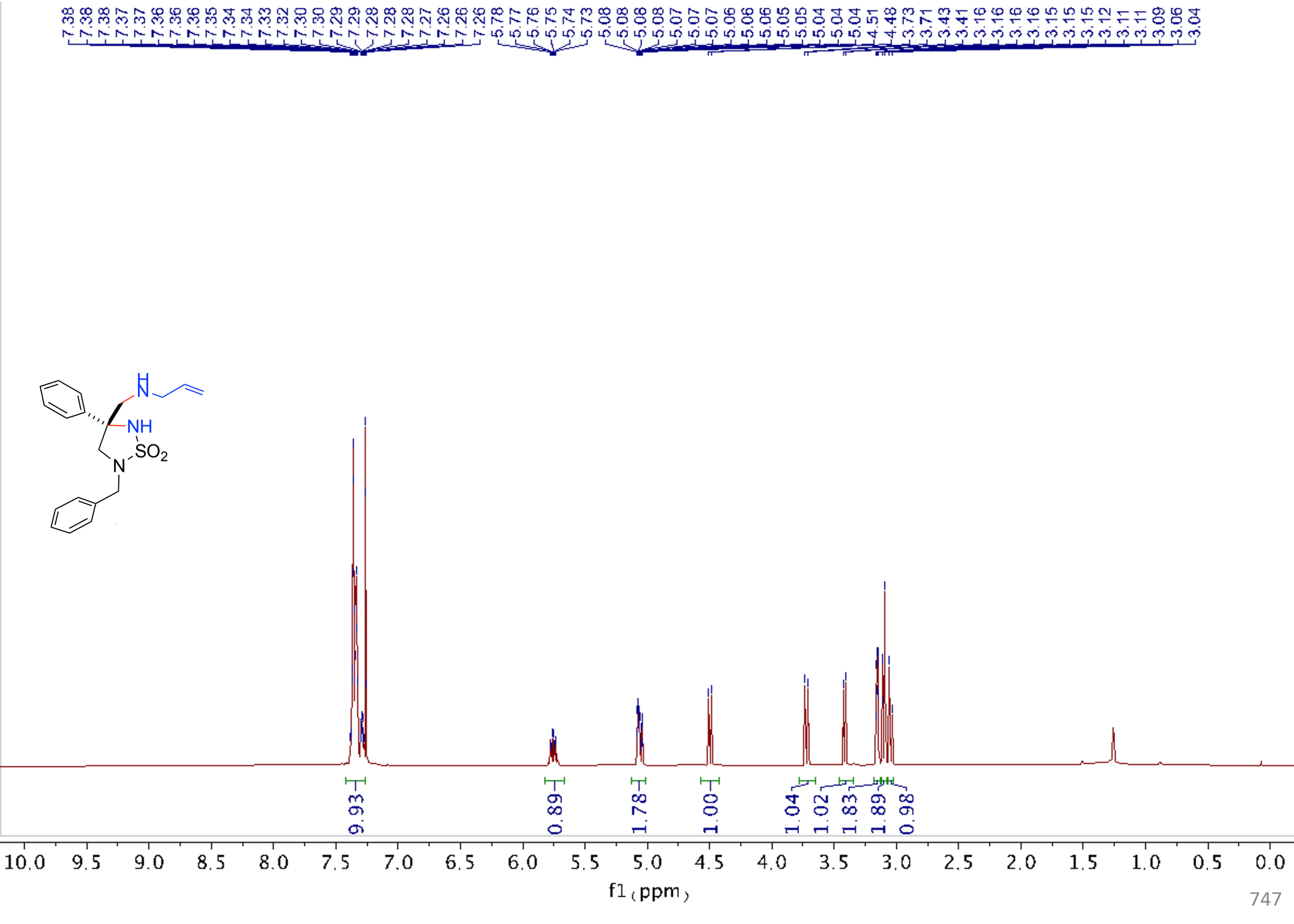


Peak Table

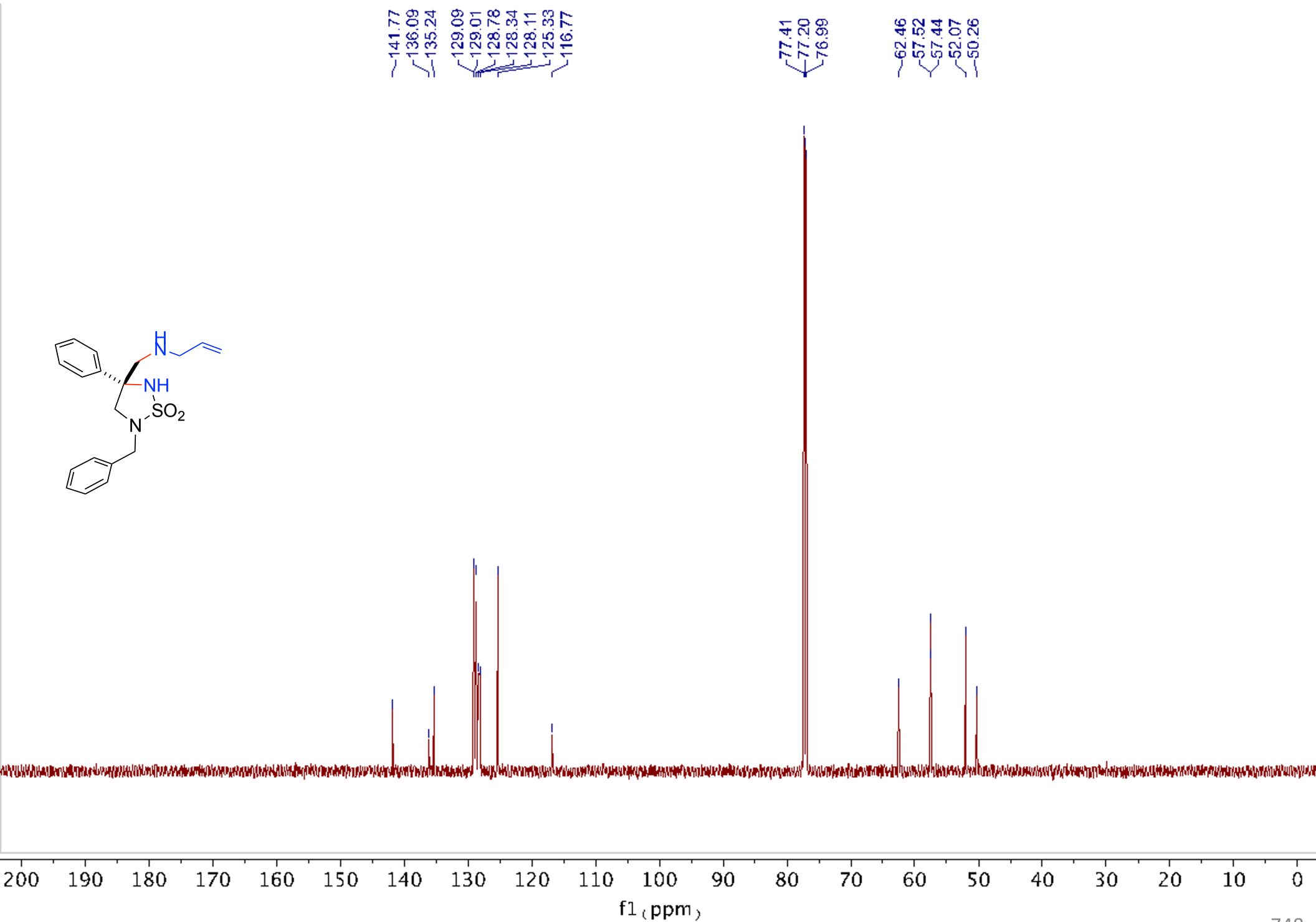
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	12.016	868400	96.320
2	13.882	33176	3.680
Total		901575	100.000

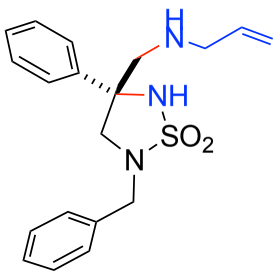
^{1}H NMR (*R*)-4-((Allylamino)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6b



^{13}C NMR (*R*)-4-((Allylamino)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6b



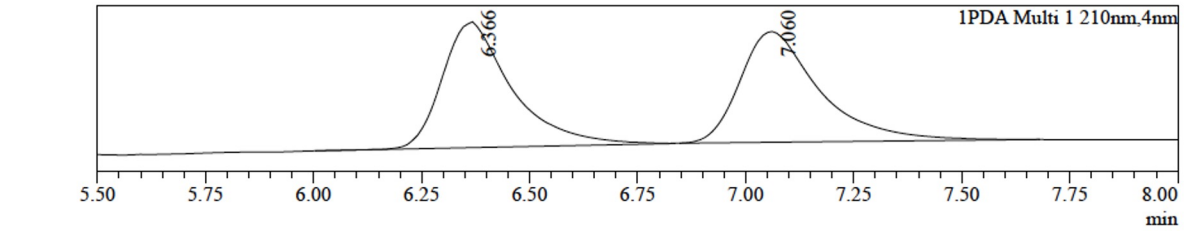
4-((Allylamino)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6b



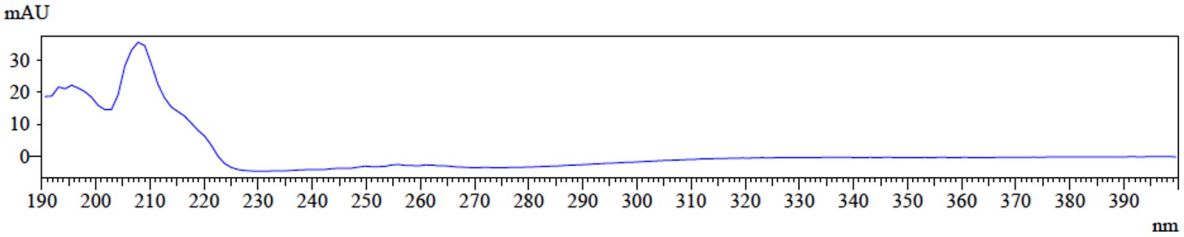
Sample Information

Data File	: H0X-TF-AllNH-RAC-IA-30%1.0mL.lcd
Sample Name	: H0X-TF-AllNH-RAC-IA-30%1.0mL
Sample ID	: H0X-TF-AllNH-RAC-IA-30%1.0mL
Method File	: H0X-30%-1.0ml-90MIN.lcm

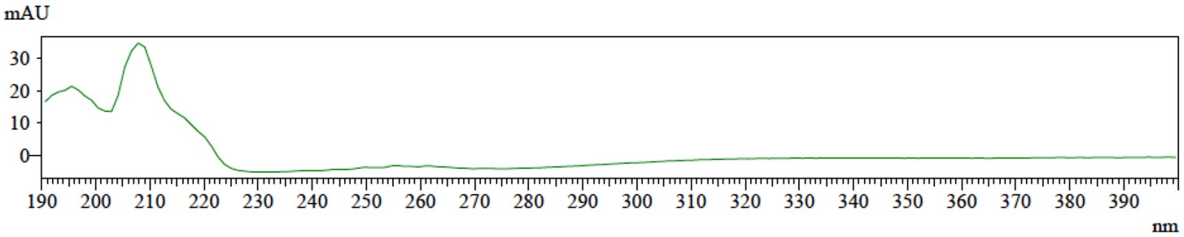
Chromatogram



UV Spectrum
Retention time = 6.366



UV Spectrum
Retention time = 7.060

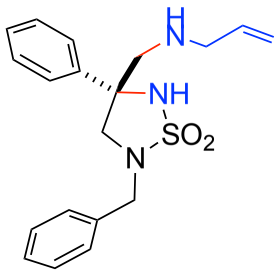


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	6.366	172892	49.914
2	7.060	173486	50.086
Total		346378	100.000

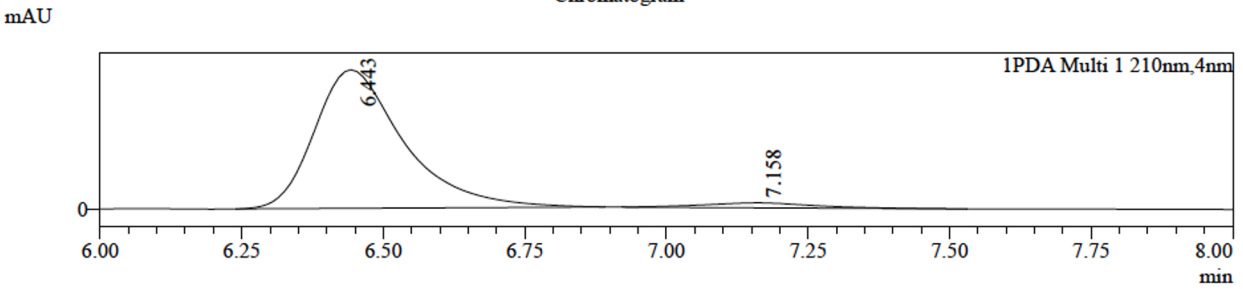
(*R*)-4-((Allylamino)methyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6b



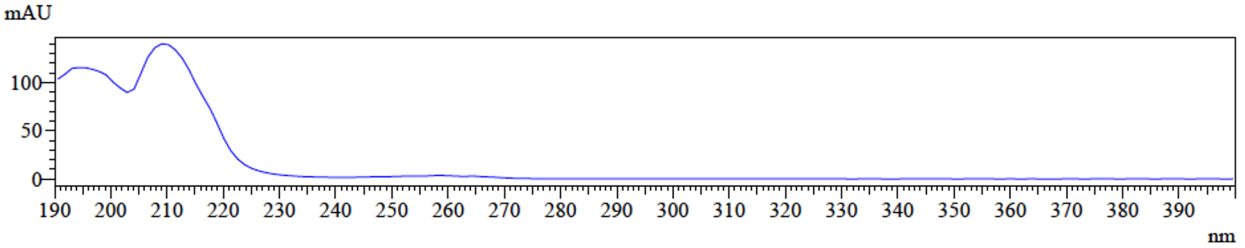
Sample Information

Data File	: H0X-TF-ALLNH2-CH-IA-30%1.0mL.lcd
Sample Name	: H0X-TF-ALLNH2-CH-IA-30%1.0mL
Sample ID	: H0X-TF-ALLNH2-CH-IA-30%1.0mL
Method File	: H0X-30%-1.0ml-20MIN.lcm

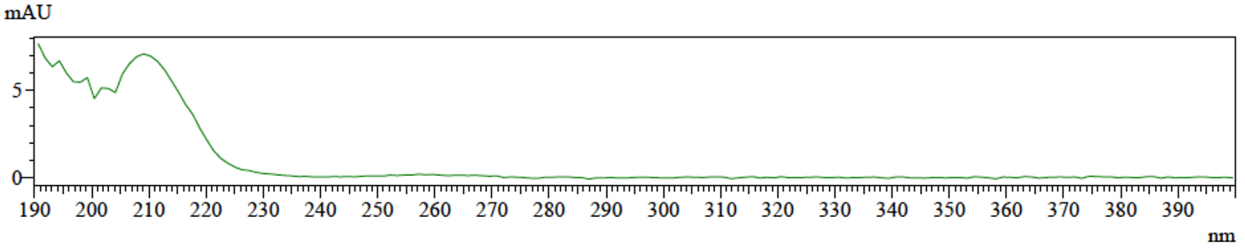
Chromatogram



UV Spectrum
Retention time = 6.443



UV Spectrum
Retention time = 7.158

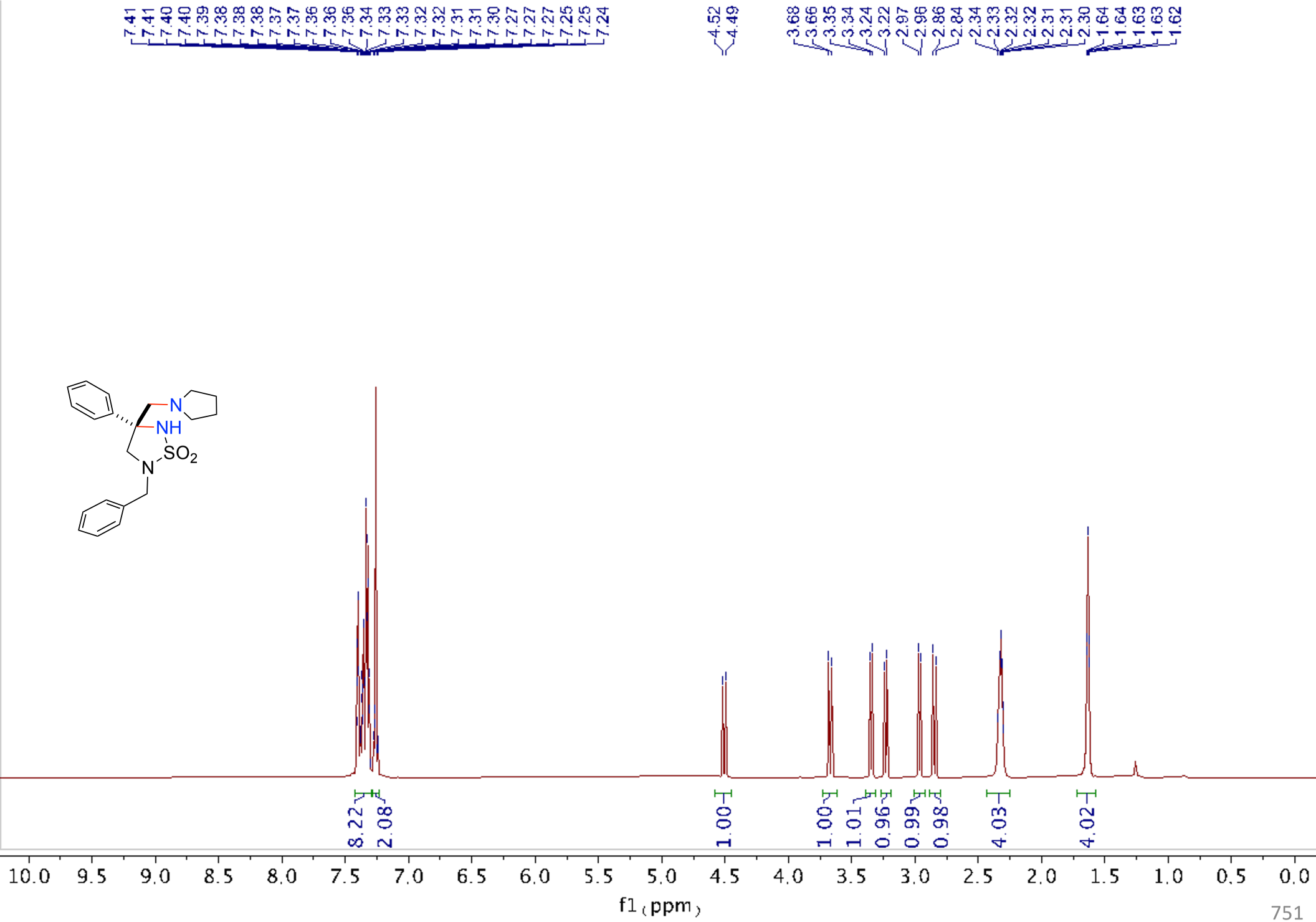


Peak Table

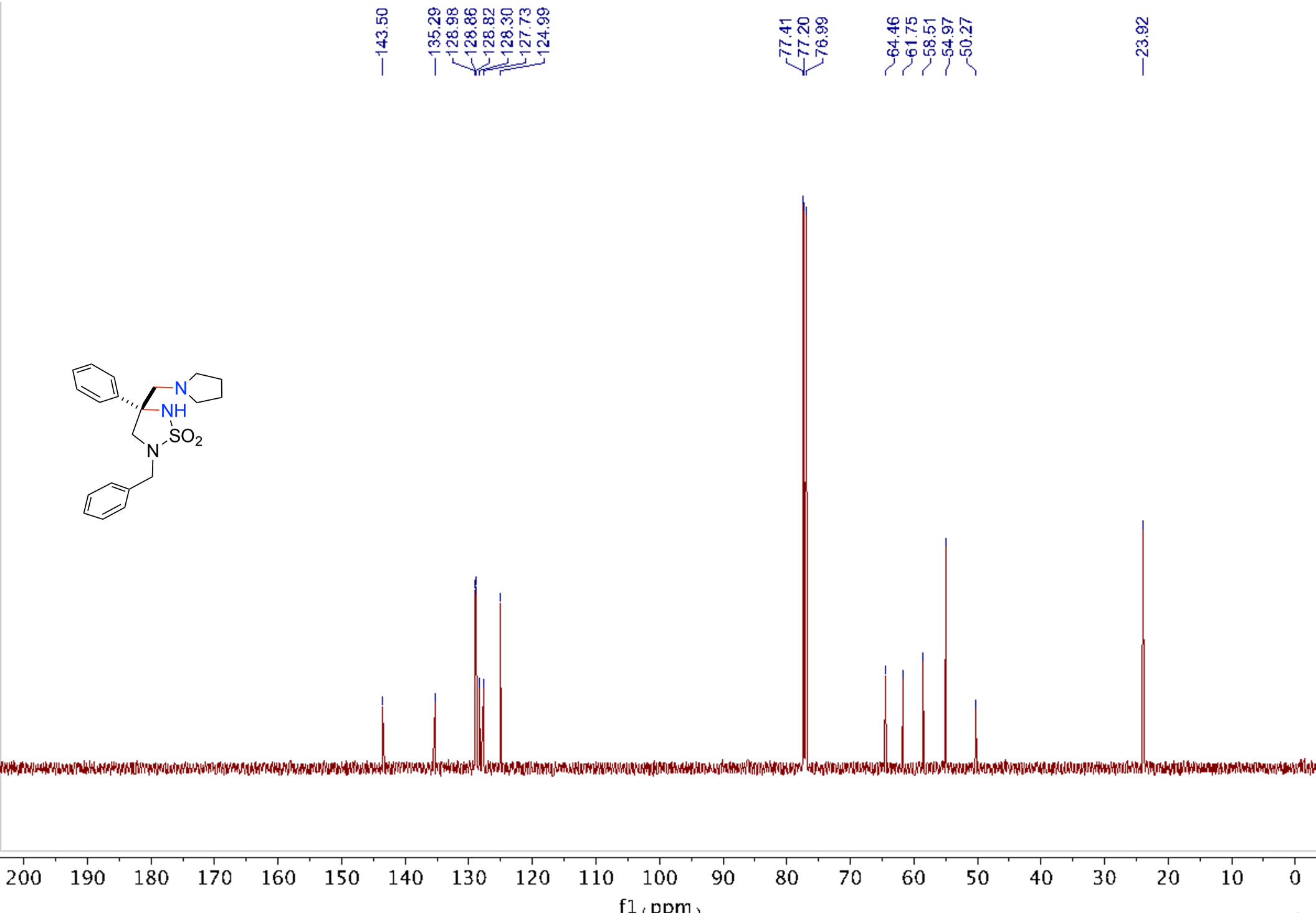
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	6.443	1412779	95.752
2	7.158	62675	4.248
Total		1475454	100.000

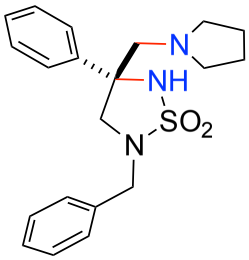
^{1}H NMR (*R*)-2-Benzyl-4-phenyl-4-(pyrrolidin-1-ylmethyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6c



$^{12.6c}$ NMR (*R*)-2-Benzyl-4-phenyl-4-(pyrrolidin-1-ylmethyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6c



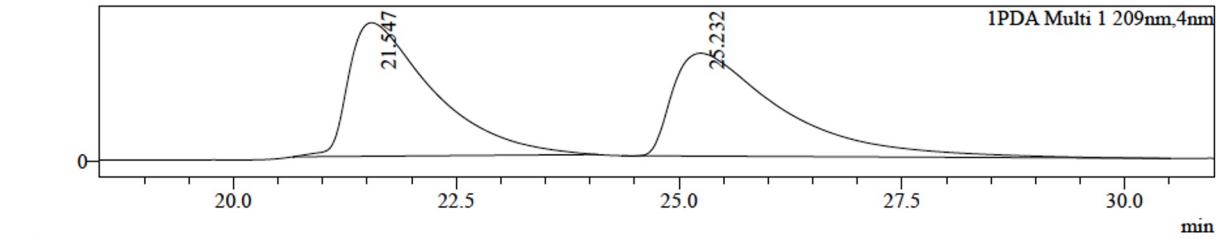
2-Benzyl-4-phenyl-4-(pyrrolidin-1-ylmethyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6c



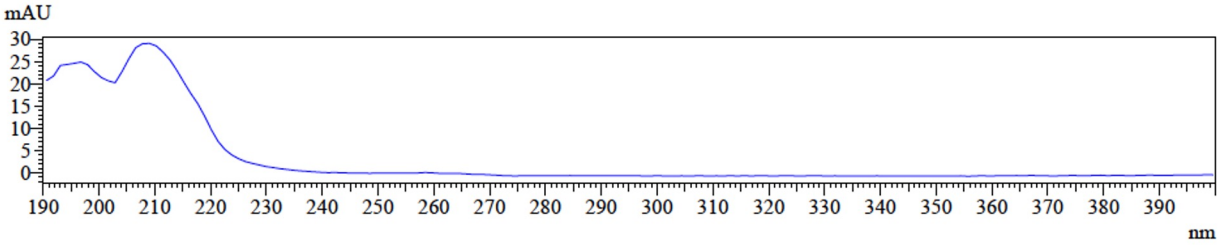
Sample Information

Data File	: H0X-TF-Py-RAC-ID-10%1.0mL.lcd
Sample Name	: H0X-TF-Py-RAC-ID-10%1.0mL
Sample ID	: H0X-TF-Py-RAC-ID-10%1.0mL
Method File	: H0X-10%-1.0ml-60MIN.lcm

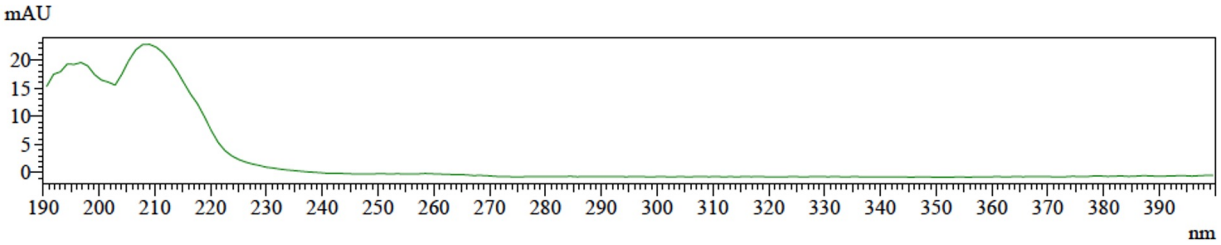
Chromatogram



UV Spectrum
Retention time = 21.547



UV Spectrum
Retention time = 25.232

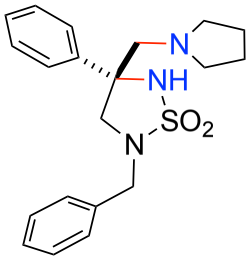


Peak Table

PDA Ch1 209nm

Peak#	Ret. Time	Area	Area%
1	21.547	1739750	50.147
2	25.232	1729521	49.853
Total		3469271	100.000

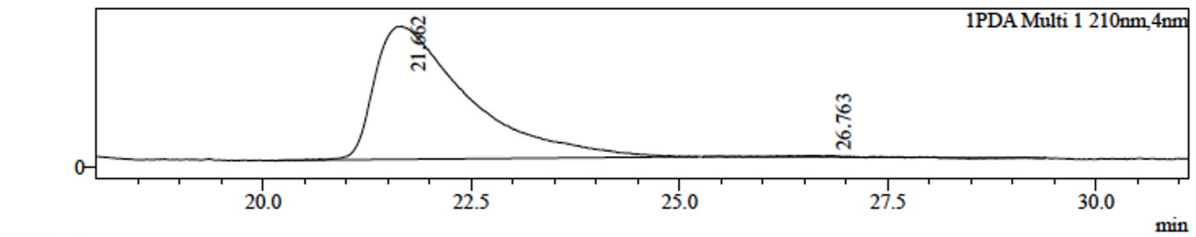
(*R*)-2-Benzyl-4-phenyl-4-(pyrrolidin-1-ylmethyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6c



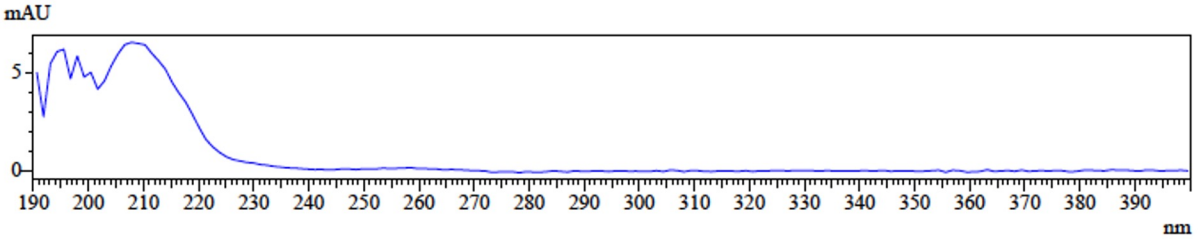
Sample Information

Data File	: H0X-TF-PY-CH3-ID-10%-1.0 mL.lcb.lcd
Sample Name	: H0X-TF-PY-CH3-ID-10%-1.0 mL.lcb
Sample ID	: H0X-TF-PY-CH3-ID-10%-1.0 mL.lcb
Method File	: H0X-10%-1.0ml-40MIN.lcm

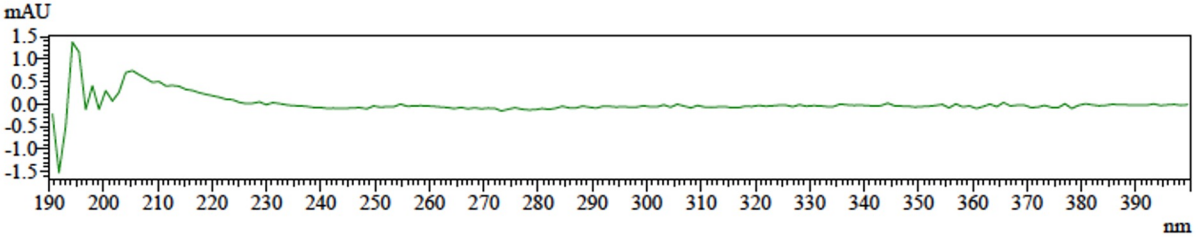
Chromatogram



UV Spectrum
Retention time = 21.662



UV Spectrum
Retention time = 26.763

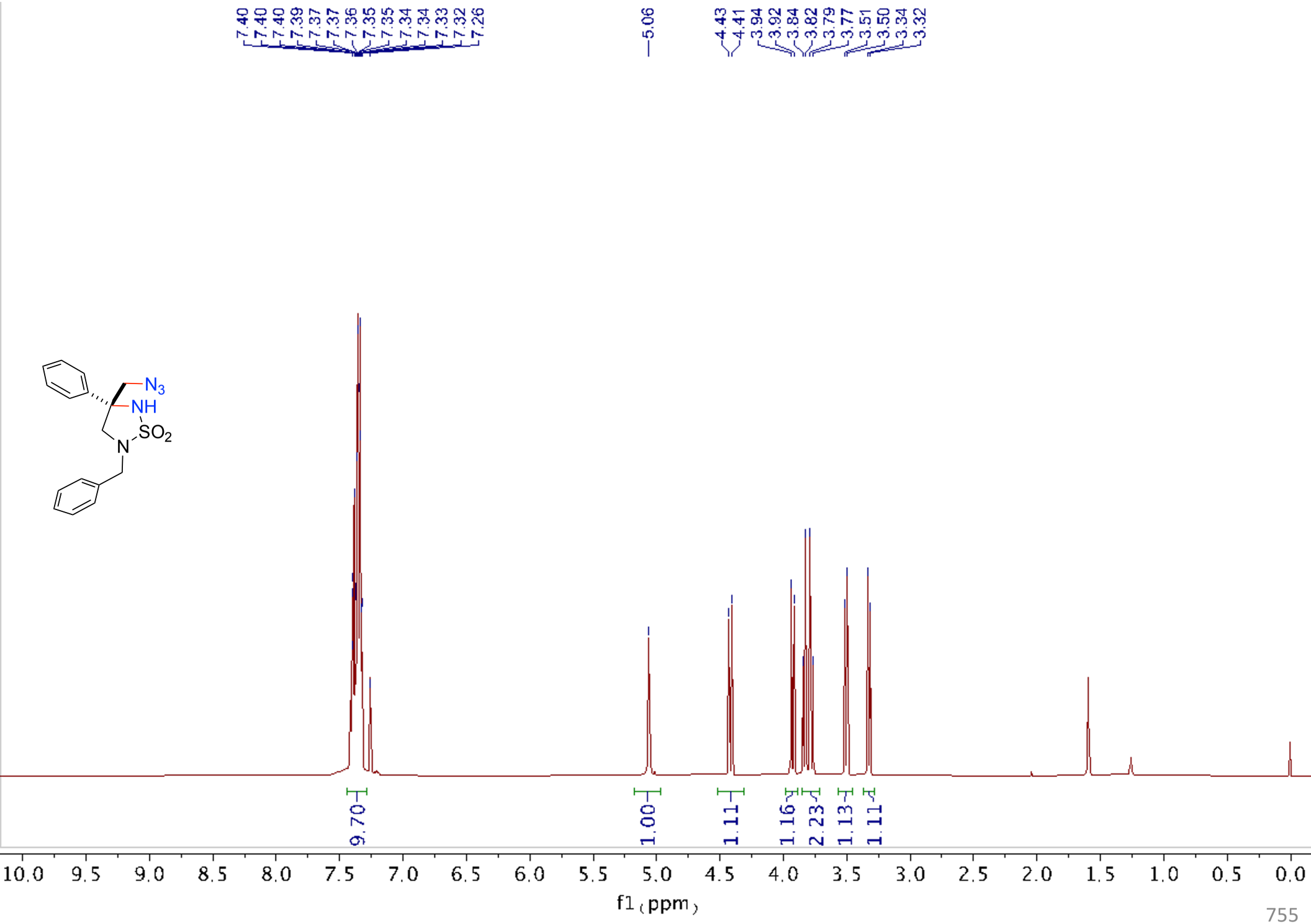


Peak Table

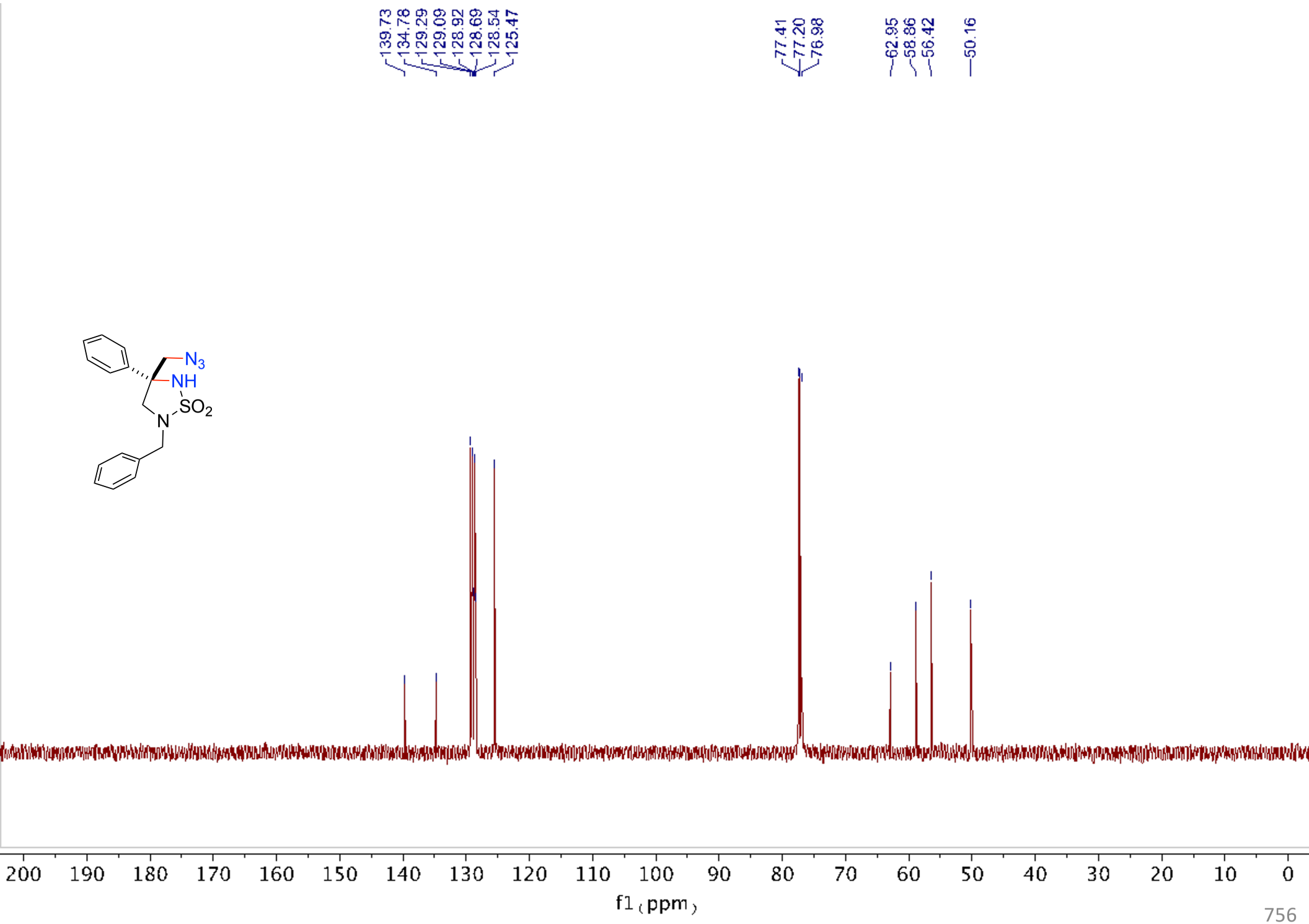
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	21.662	447878	99.380
2	26.763	2793	0.620
Total		450671	100.000

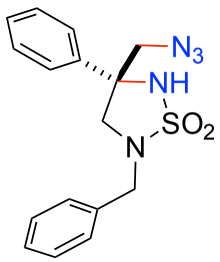
^{1}H NMR (*R*)-4-(Azidomethyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6d



^{13}C NMR (*R*)-4-(Azidomethyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6d



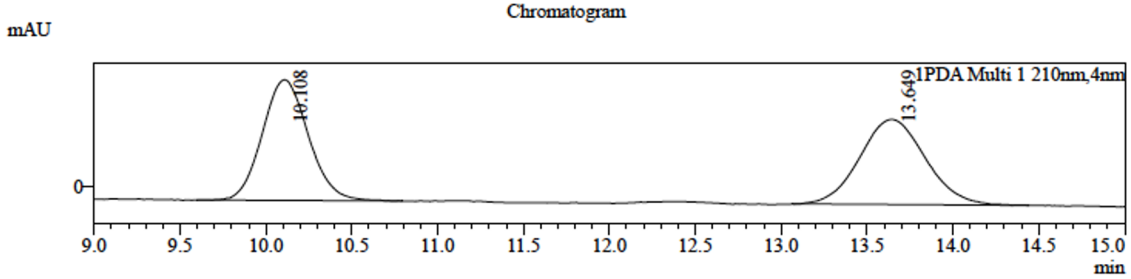
4-(Azidomethyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6d



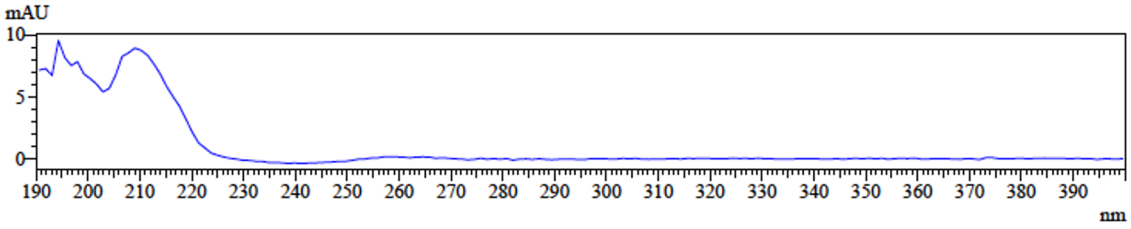
Sample Information

Data File	: H0X-TF-N3-RAC-IC-30%1.0mL.lcd
Sample Name	: H0X-TF-N3-RAC-IC-30%1.0mL
Sample ID	: H0X-TF-N3-RAC-IC-30%1.0mL
Method File	: H0X-30%-1.0ml-60MIN.lcm

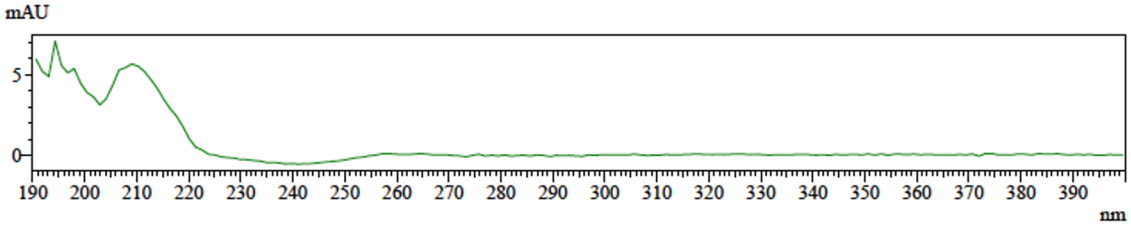
Chromatogram



UV Spectrum
Retention time = 10.108



UV Spectrum
Retention time = 13.649

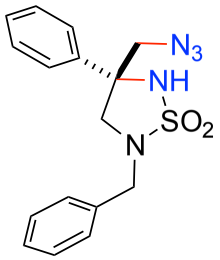


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	10.108	173370	49.924
2	13.649	173894	50.076
Total		347264	100.000

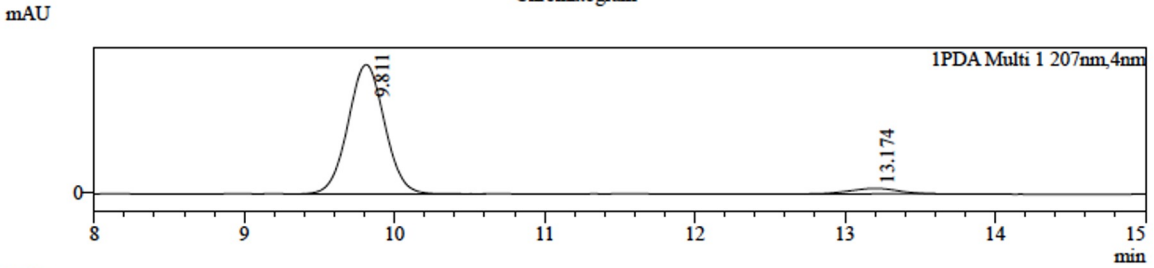
(*R*)-4-(Azidomethyl)-2-benzyl-4-phenyl-1,2,5-thiadiazolidine 1,1-dioxide 2.6d



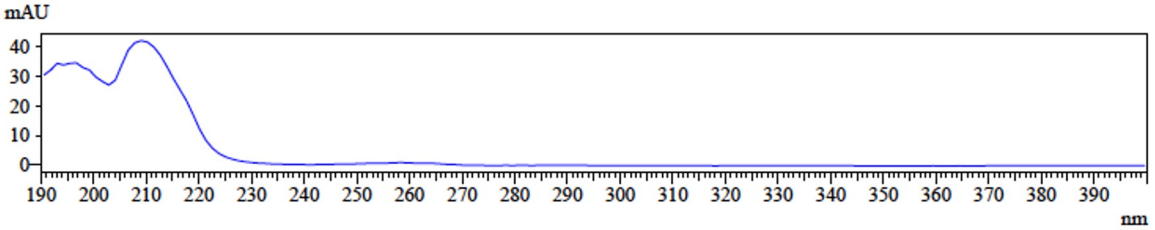
Sample Information

Data File	: H0X-TF3-N3-CH-IC-30%1.0mL.lcd
Sample Name	: H0X-TF3-N3-CH-IC-30%1.0mL
Sample ID	: H0X-TF3-N3-CH-IC-30%1.0mL
Method File	: H0X-30%-1.0ml-20MIN.lcm

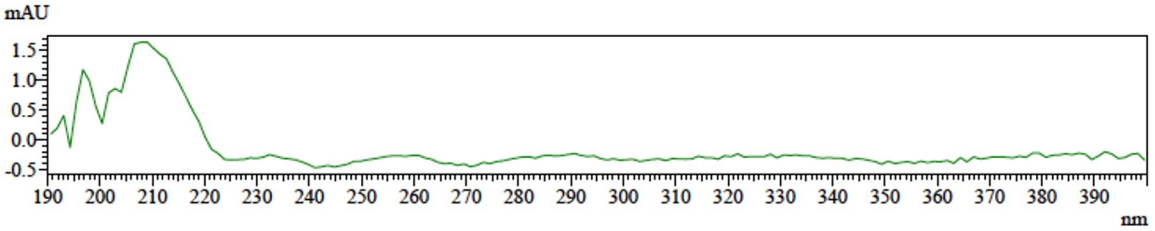
Chromatogram



UV Spectrum
Retention time = 9.811



UV Spectrum
Retention time = 13.174

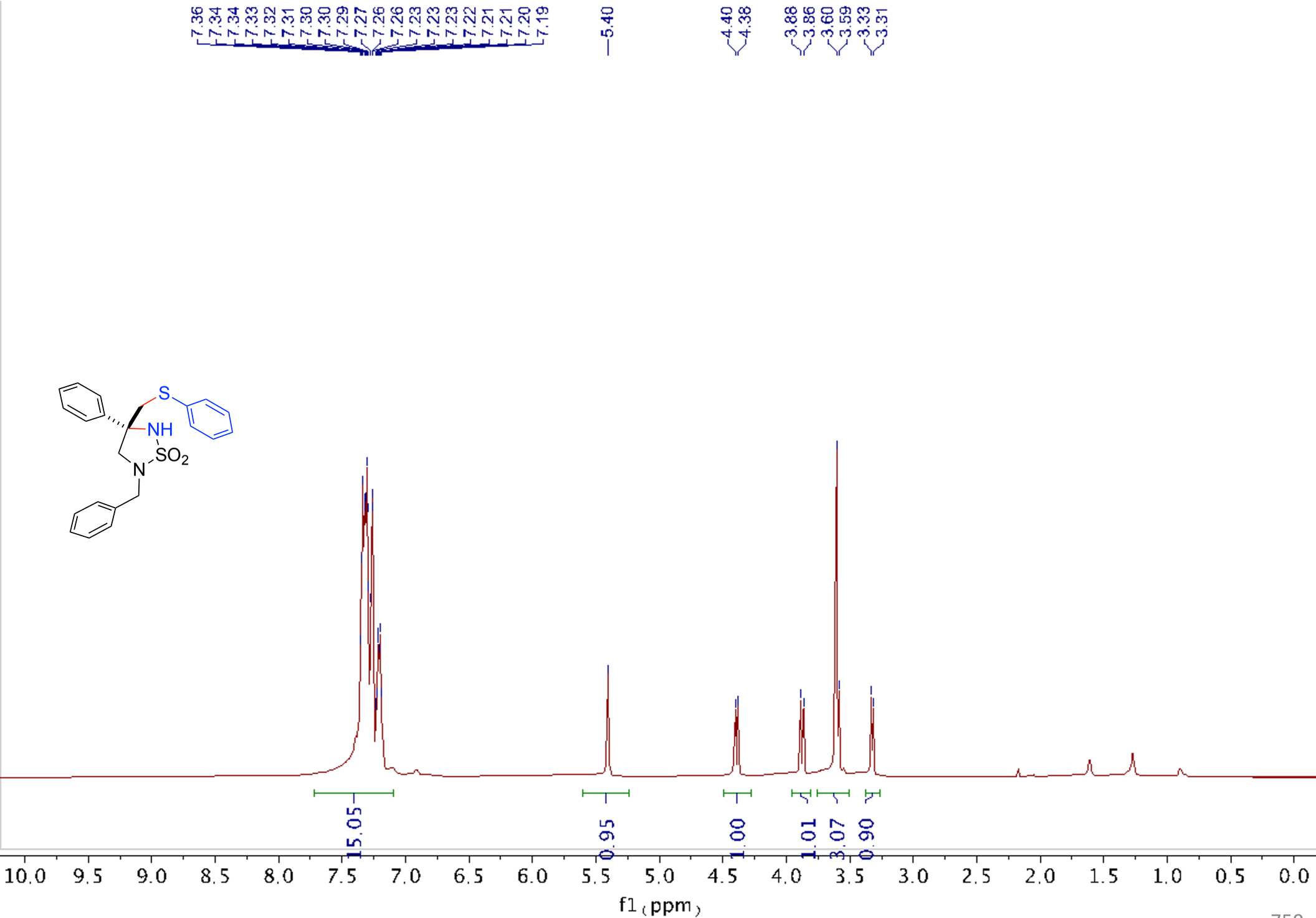


Peak Table

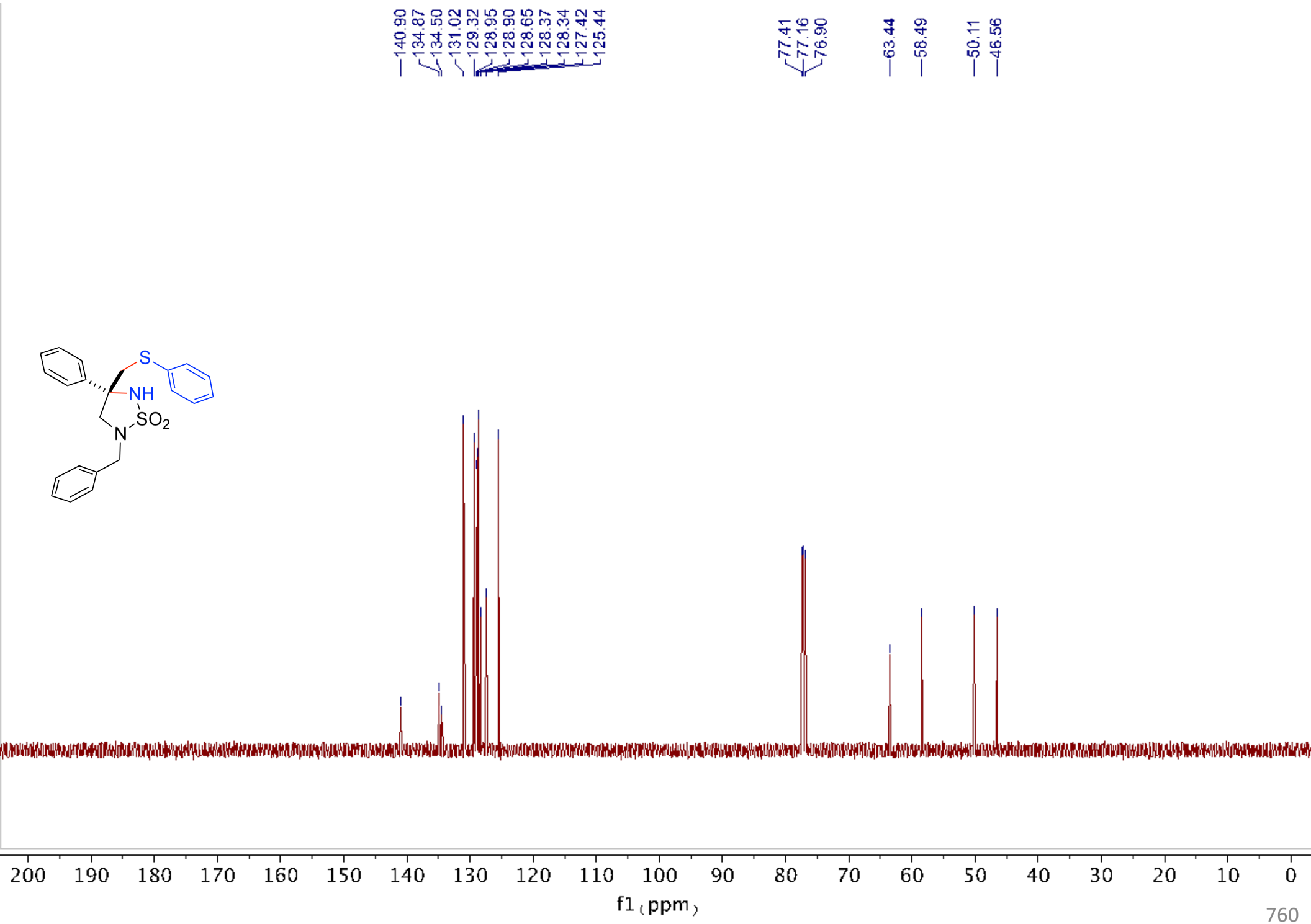
PDA Ch1 207nm

Peak#	Ret. Time	Area	Area%
1	9.811	646284	94.814
2	13.174	35351	5.186
Total		681635	100.000

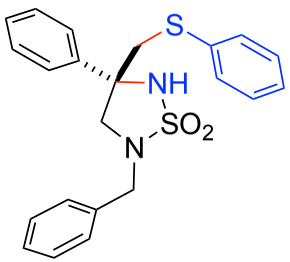
^{1}H NMR (*S*)-2-Benzyl-4-phenyl-4-((phenylthio)methyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6e



^{13}C NMR (*S*)-2-Benzyl-4-phenyl-4-((phenylthio)methyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6e



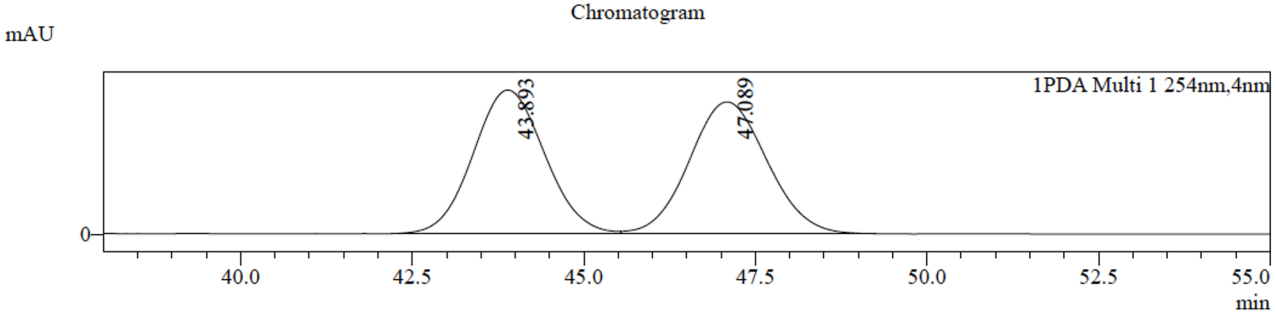
2-Benzyl-4-phenyl-4-((phenylthio)methyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6e



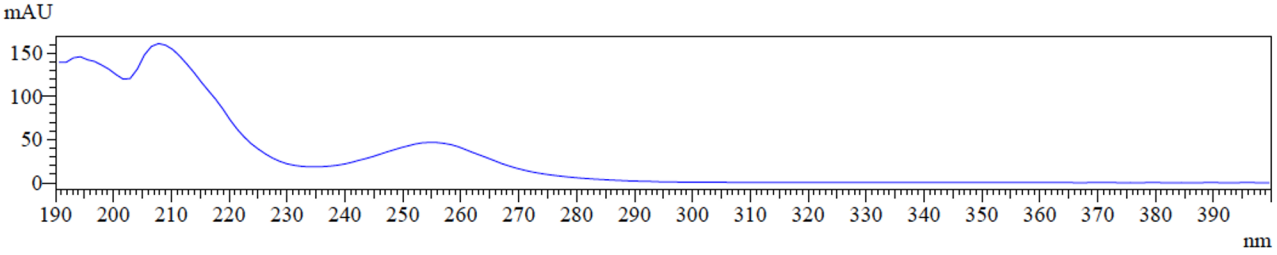
Sample Information

Data File	: H0X-TF-SPh-RAC-IC-10%1.0mL.lcd
Sample Name	: H0X-TF-SPh-RAC-IC-10%1.0mL
Sample ID	: H0X-TF-SPh-RAC-IC-10%1.0mL
Method File	: H0X-10%-1.0ml-60MIN.lcm

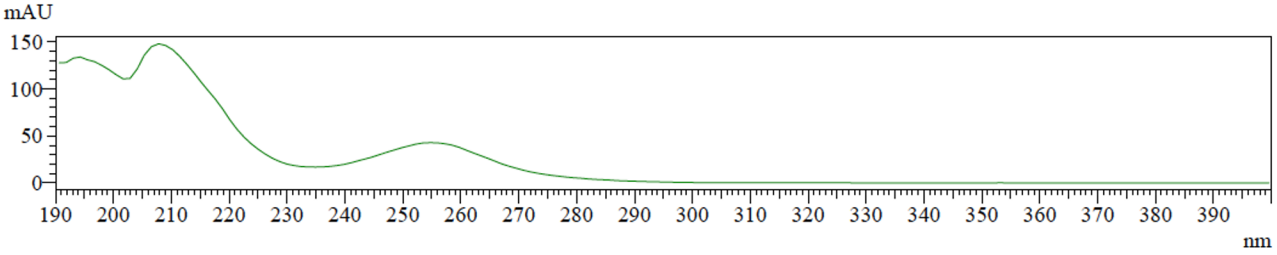
Chromatogram



UV Spectrum
Retention time = 43.893



UV Spectrum
Retention time = 47.089

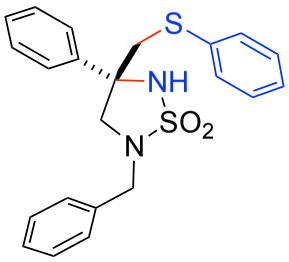


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	43.893	3288855	50.064
2	47.089	3280400	49.936
Total		6569255	100.000

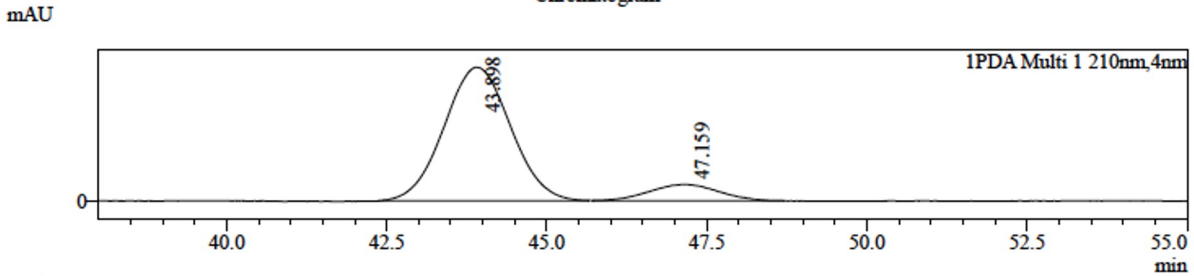
(*S*)-2-Benzyl-4-phenyl-4-((phenylthio)methyl)-1,2,5-thiadiazolidine 1,1-dioxide 2.6e



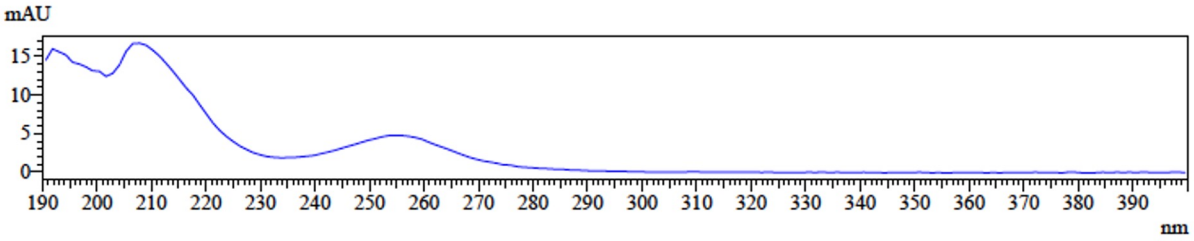
Sample Information

Data File	: H0X-TF-SPh-Ch-IC-10%1.0ml.lcd
Sample Name	: H0X-TF-SPh-Ch-IC-10%1.0ml
Sample ID	: H0X-TF-SPh-Ch-IC-10%1.0ml
Method File	: H0X-10%-1.0ml-60MIN.lcm

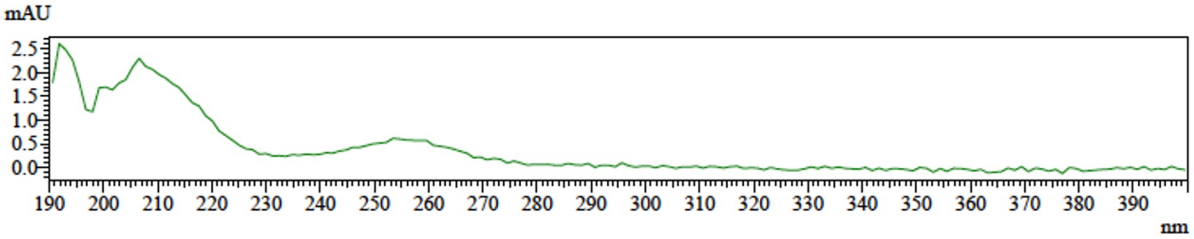
Chromatogram



UV Spectrum
Retention time = 43.898



UV Spectrum
Retention time = 47.159

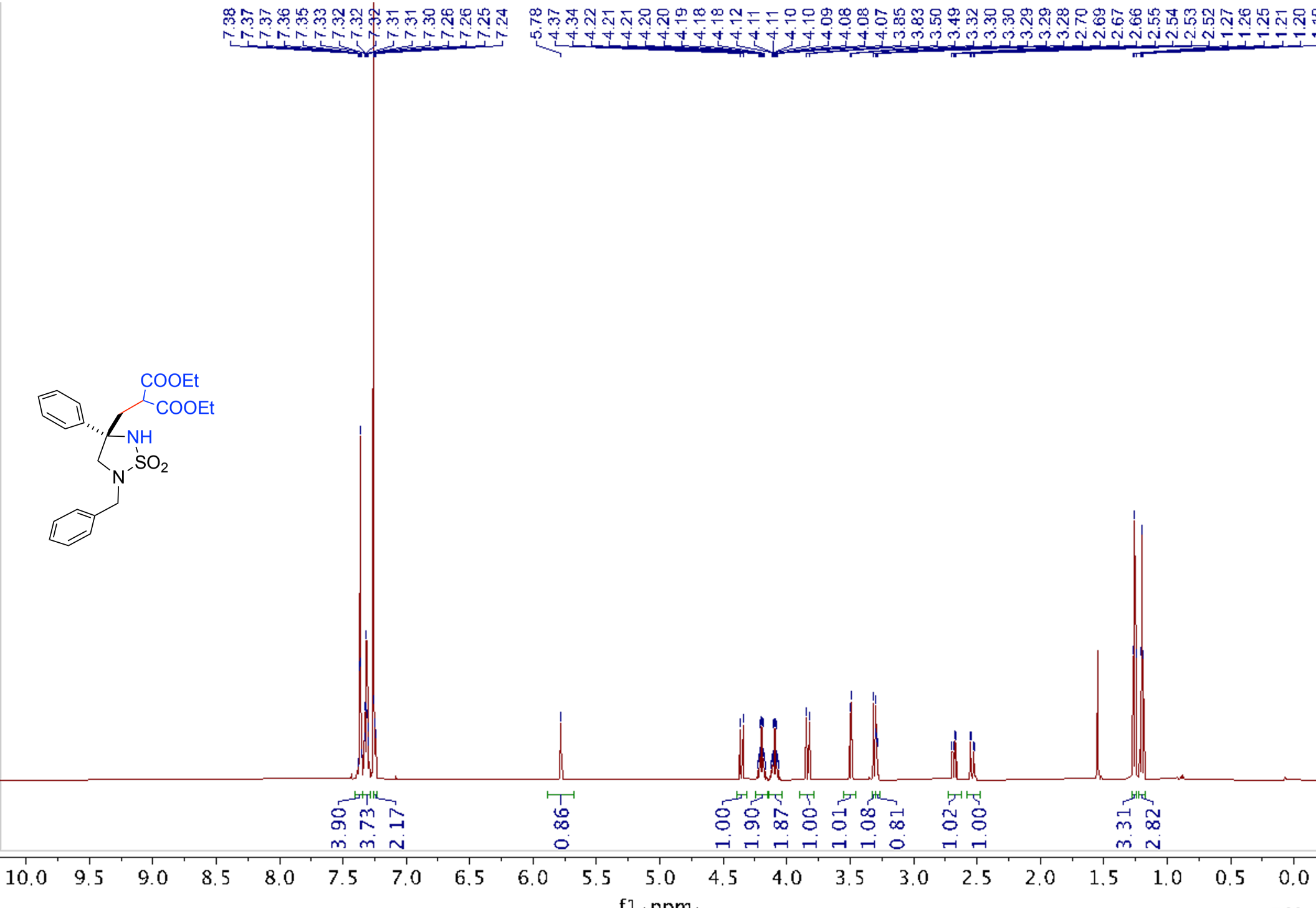


Peak Table

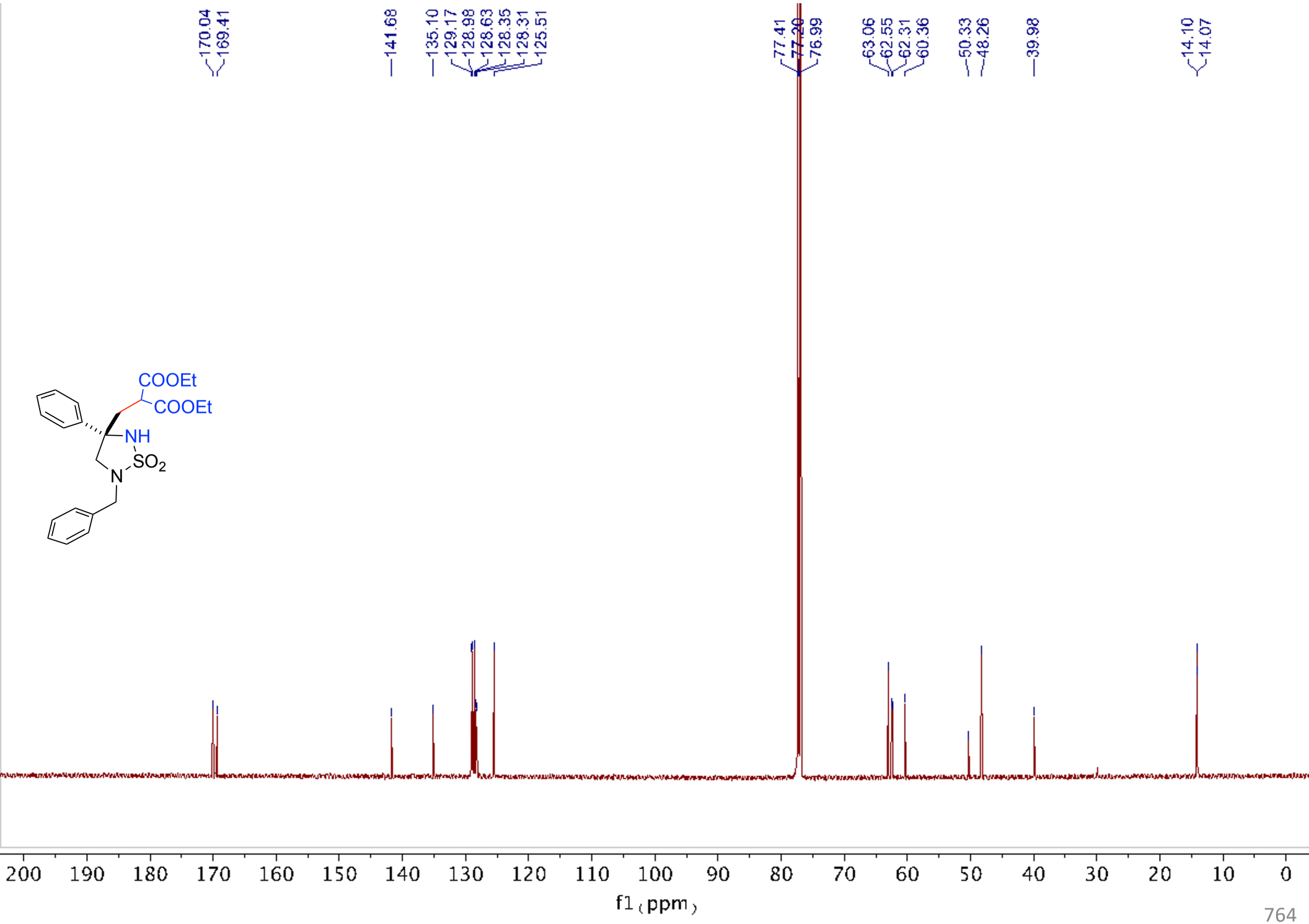
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	43.898	1106920	88.776
2	47.159	139943	11.224
Total		1246862	100.000

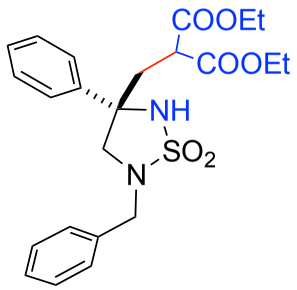
^{1}H NMR Diethyl (*S*)-2-((5-benzyl-1,1-dioxido-3-phenyl-1,2,5-thiadiazolidin-3-yl)methyl)malonate 2.6f



^{13}C NMR Diethyl (*S*)-2-((5-benzyl-1,1-dioxido-3-phenyl-1,2,5-thiadiazolidin-3-yl)methyl)malonate 2.6f



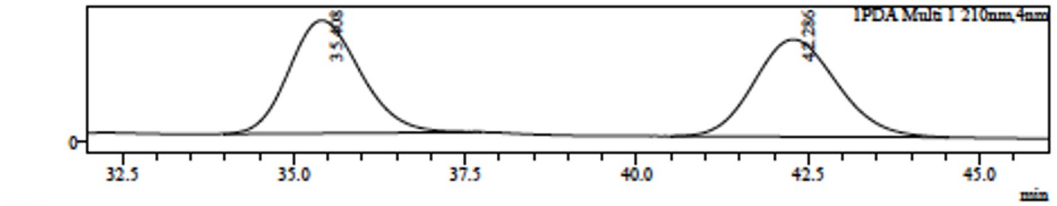
Diethyl 2-((5-benzyl-1,1-dioxido-3-phenyl-1,2,5-thiadiazolidin-3-yl)methyl)malonate 2.6f



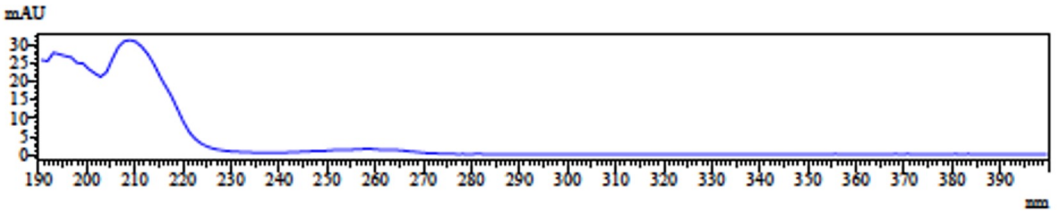
Sample Information

Data File	: H0X-TF-DM-IC-20%-0.8 mL.lcd
Sample Name	: H0X-TF-DM-IC-20%-0.8 mL
Sample ID	: H0X-TF-DM-IC-20%-0.8 mL
Method File	: H0X-20%-0.8ml-90MIN.lcm

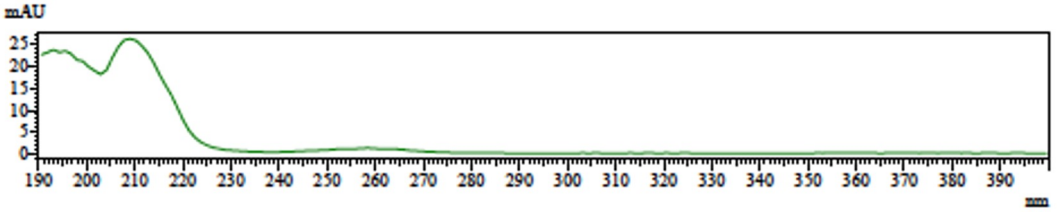
Chromatogram



UV Spectrum
Retention time = 35.408



UV Spectrum
Retention time = 42.286

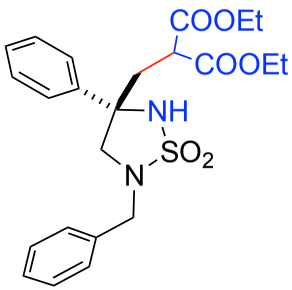


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	35.408	1949899	49.940
2	42.286	1954572	50.060
Total		3904471	100.000

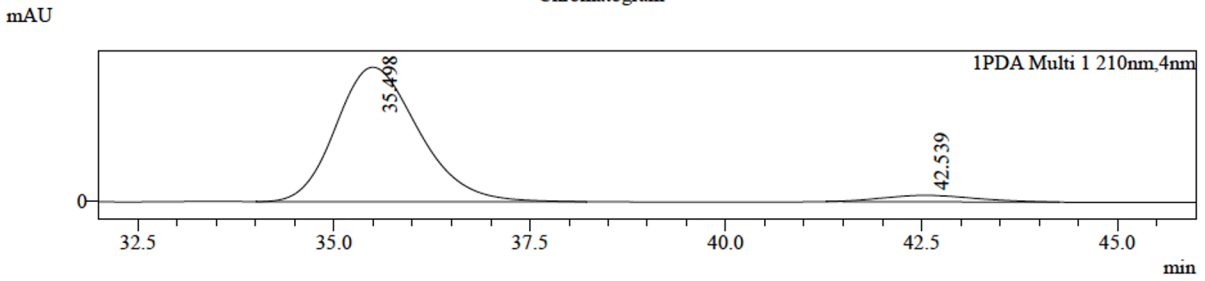
Diethyl (*S*)-2-((5-benzyl-1,1-dioxido-3-phenyl-1,2,5-thiadiazolidin-3-yl)methyl)malonate 2.6f



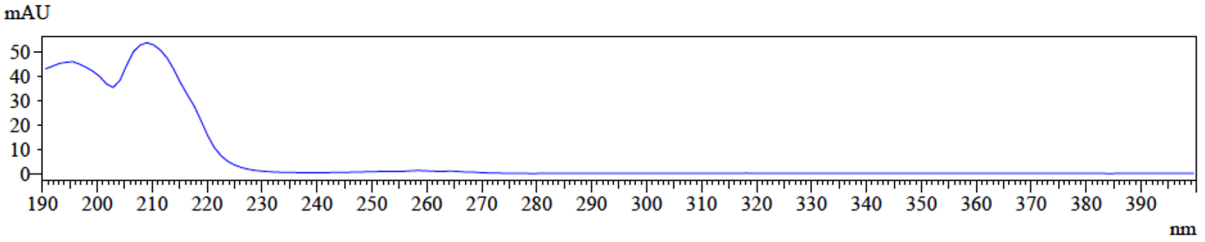
Sample Information

Data File	: H0X-884-IC-20%-0.8 mL002.lcd
Sample Name	: H0X-884-IC-20%-0.8 mL002
Sample ID	: H0X-884-IC-20%-0.8 mL002
Method File	: H0X-20%-0.8ml-90MIN.lcm

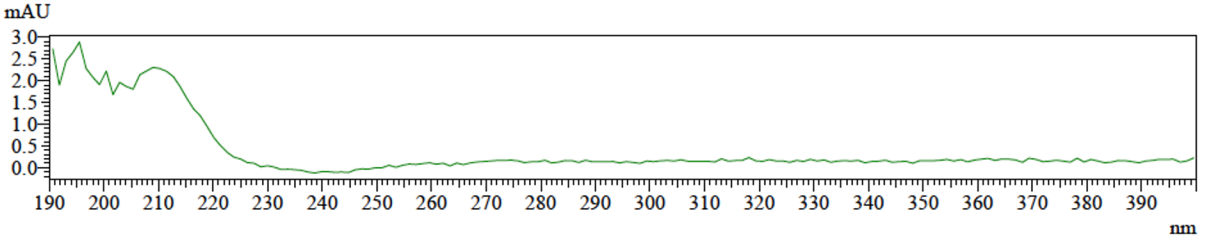
Chromatogram



UV Spectrum
Retention time = 35.498



UV Spectrum
Retention time = 42.539

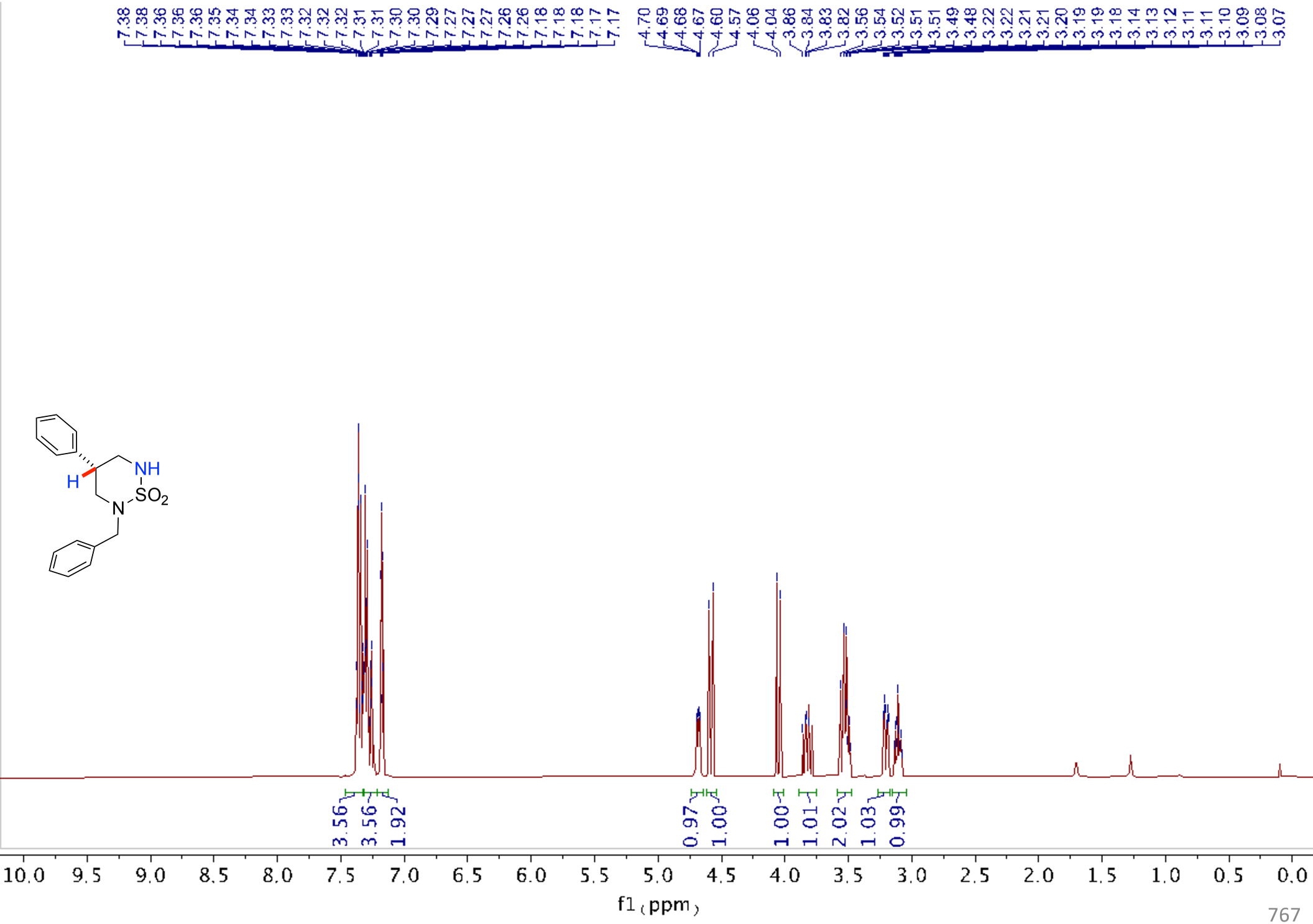


Peak Table

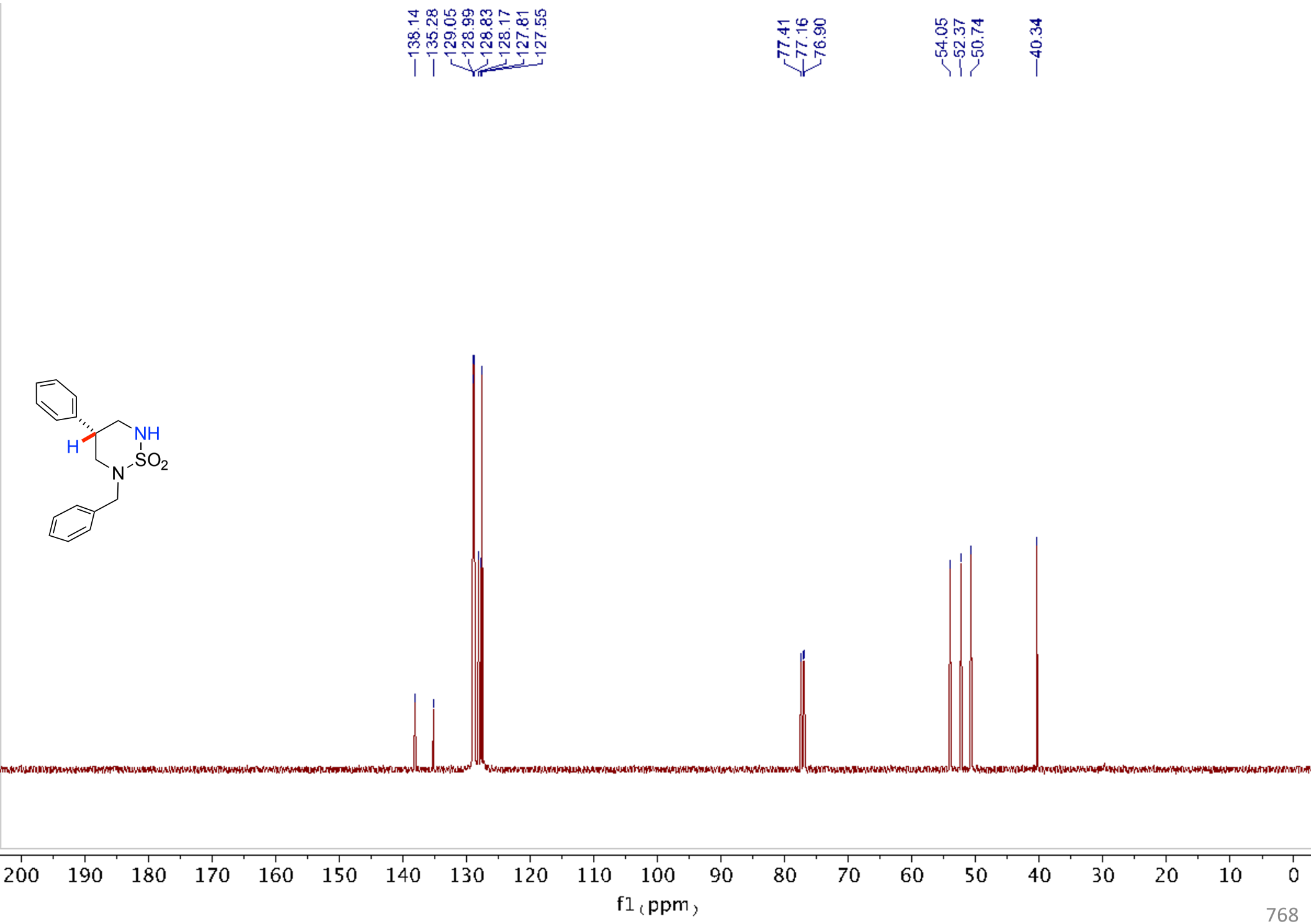
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	35.498	3721472	94.866
2	42.539	201382	5.134
Total		3922853	100.000

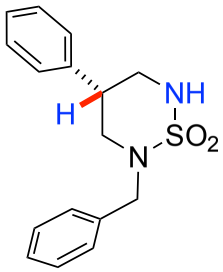
^{1}H NMR (*R*)-2-Benzyl-4-phenyl-1,2,6-thiadiazinane 1,1-dioxide 2.6g



^{13}C NMR (*R*)-2-Benzyl-4-phenyl-1,2,6-thiadiazinane 1,1-dioxide 2.6g



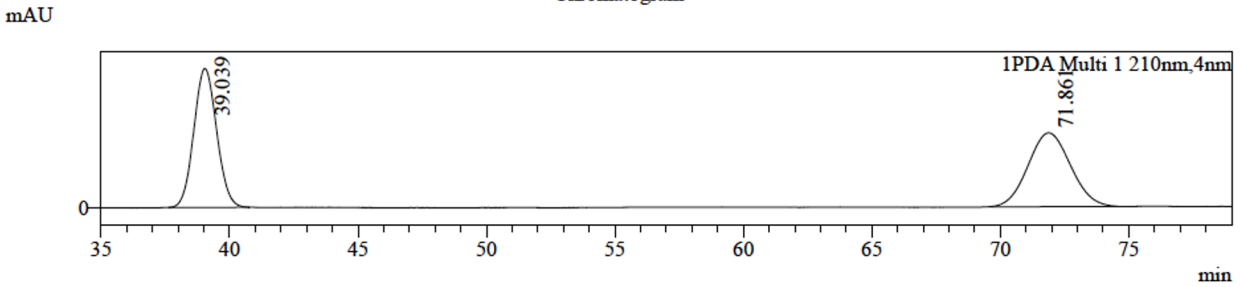
2-Benzyl-4-phenyl-1,2,6-thiadiazinane 1,1-dioxide 2.6g



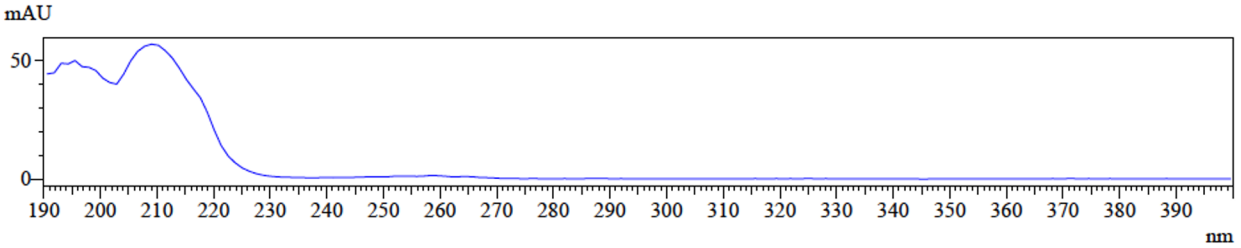
Sample Information

Data File	: H0X-1067-IC-10%-0.8 mL001.lcd
Sample Name	: H0X-1067-IC-10%-0.8 mL001
Sample ID	: H0X-1067-IC-10%-0.8 mL001
Method File	: H0X-10%-0.8ml-90MIN.lcm

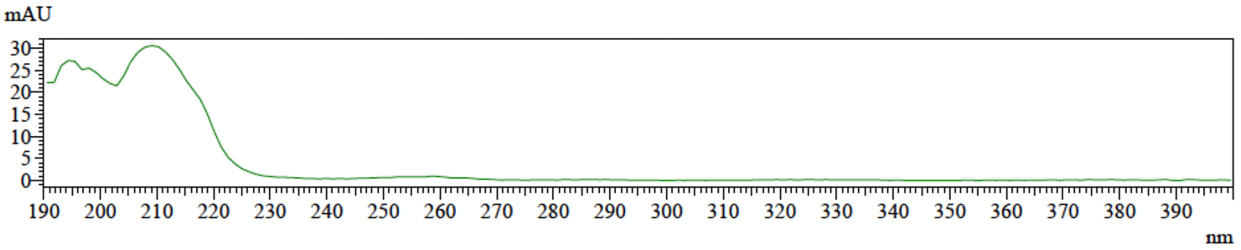
Chromatogram



UV Spectrum
Retention time = 39.039



UV Spectrum
Retention time = 71.861

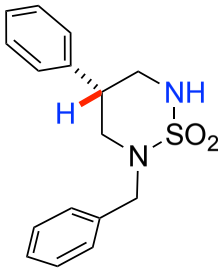


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	39.039	3280032	50.257
2	71.861	3246455	49.743
Total		6526487	100.000

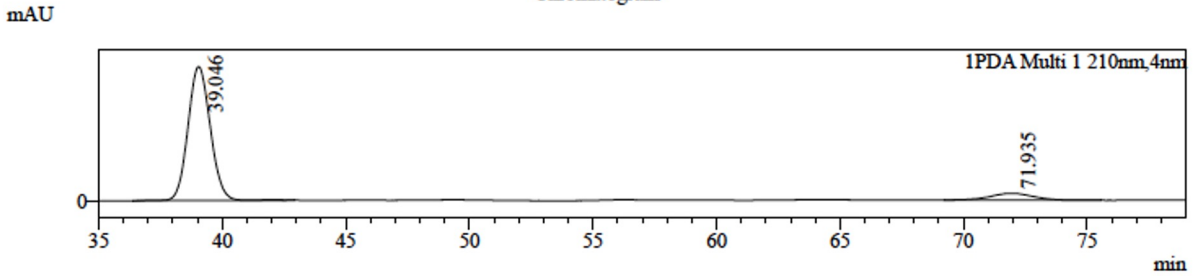
(*R*)-2-Benzyl-4-phenyl-1,2,6-thiadiazinane 1,1-dioxide 2.6g



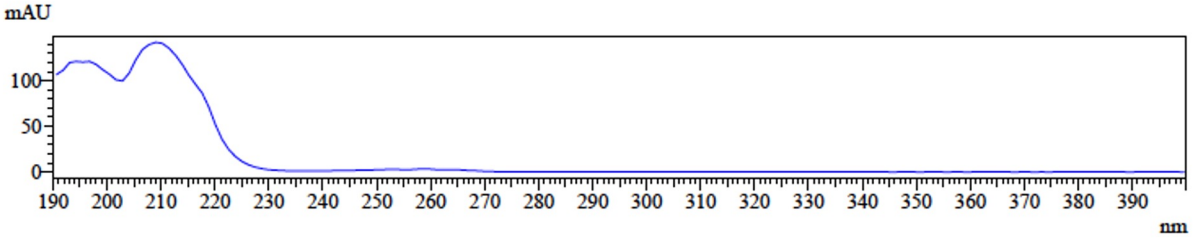
Sample Information

Data File	: H0X-1075-IC-10%-0.8 mL001.lcd
Sample Name	: H0X-1075-IC-10%-0.8 mL001
Sample ID	: H0X-1075-IC-10%-0.8 mL001
Method File	: H0X-10%-0.8ml-90MIN.lcm

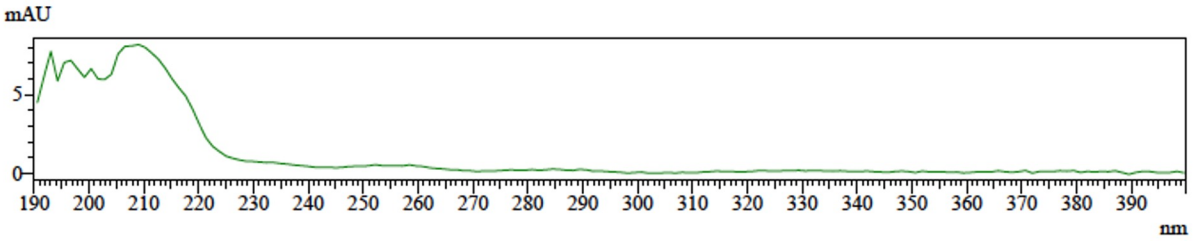
Chromatogram



UV Spectrum
Retention time = 39.046



UV Spectrum
Retention time = 71.935

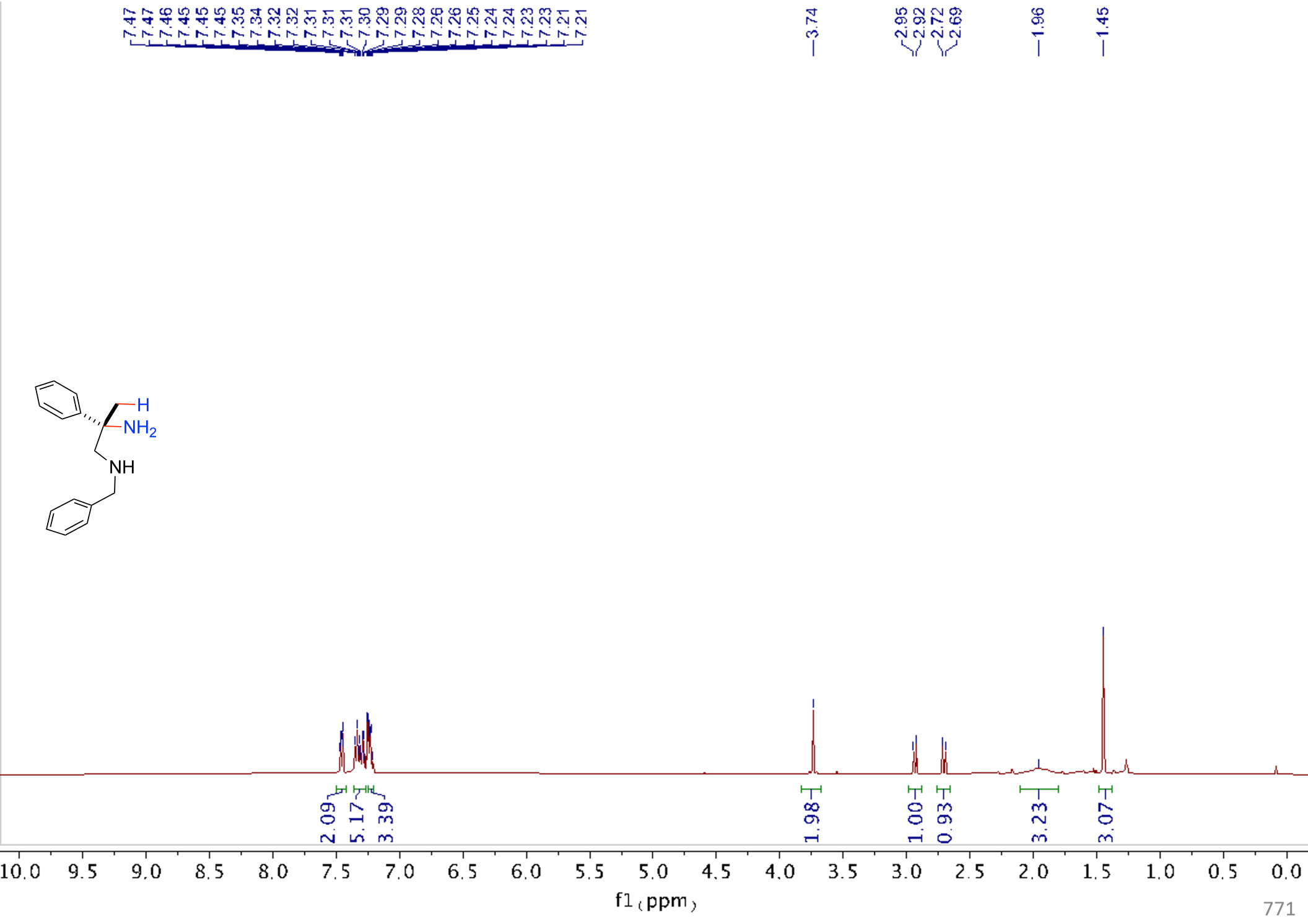


Peak Table

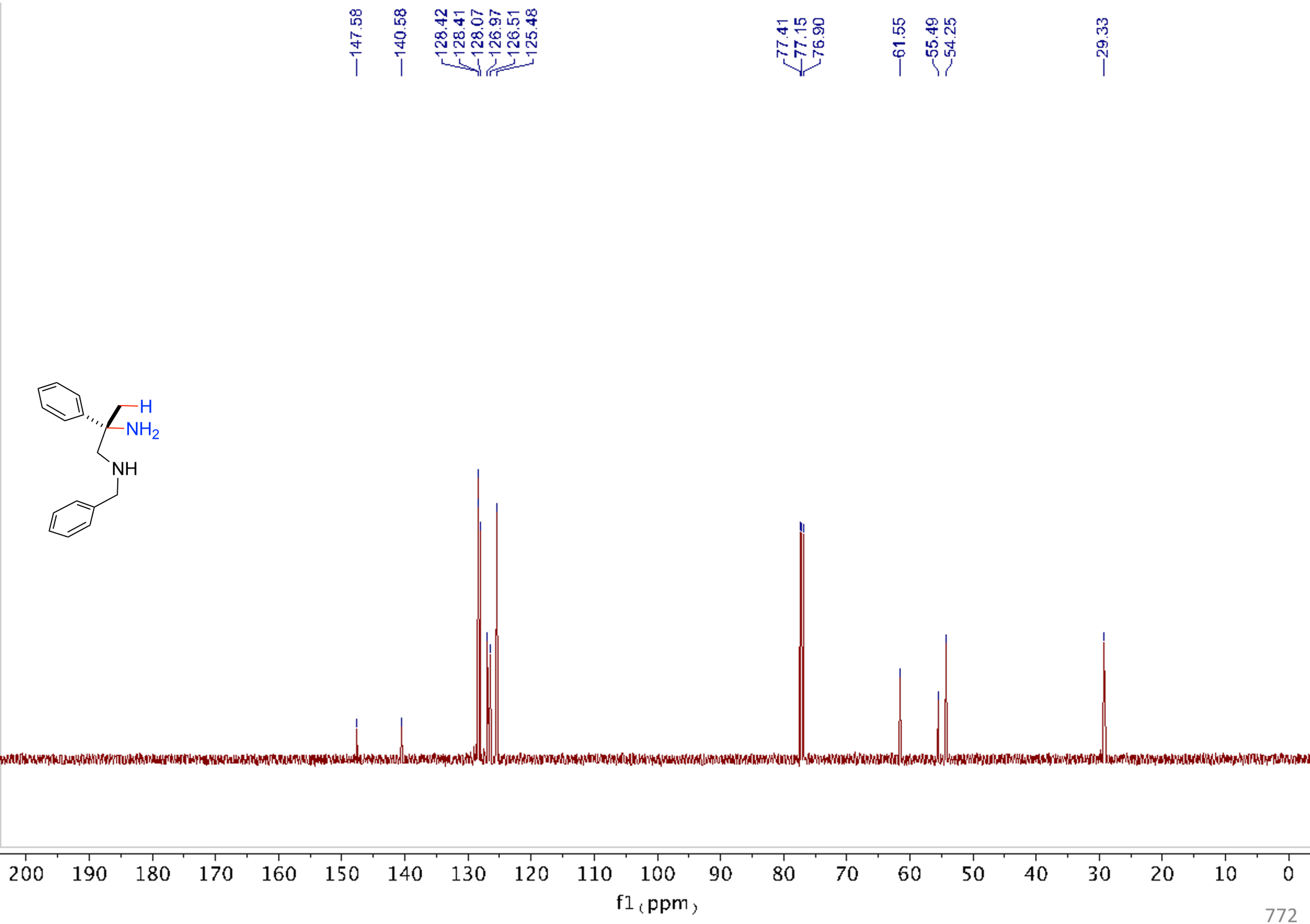
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	39.046	8417083	91.074
2	71.935	824916	8.926
Total		9241999	100.000

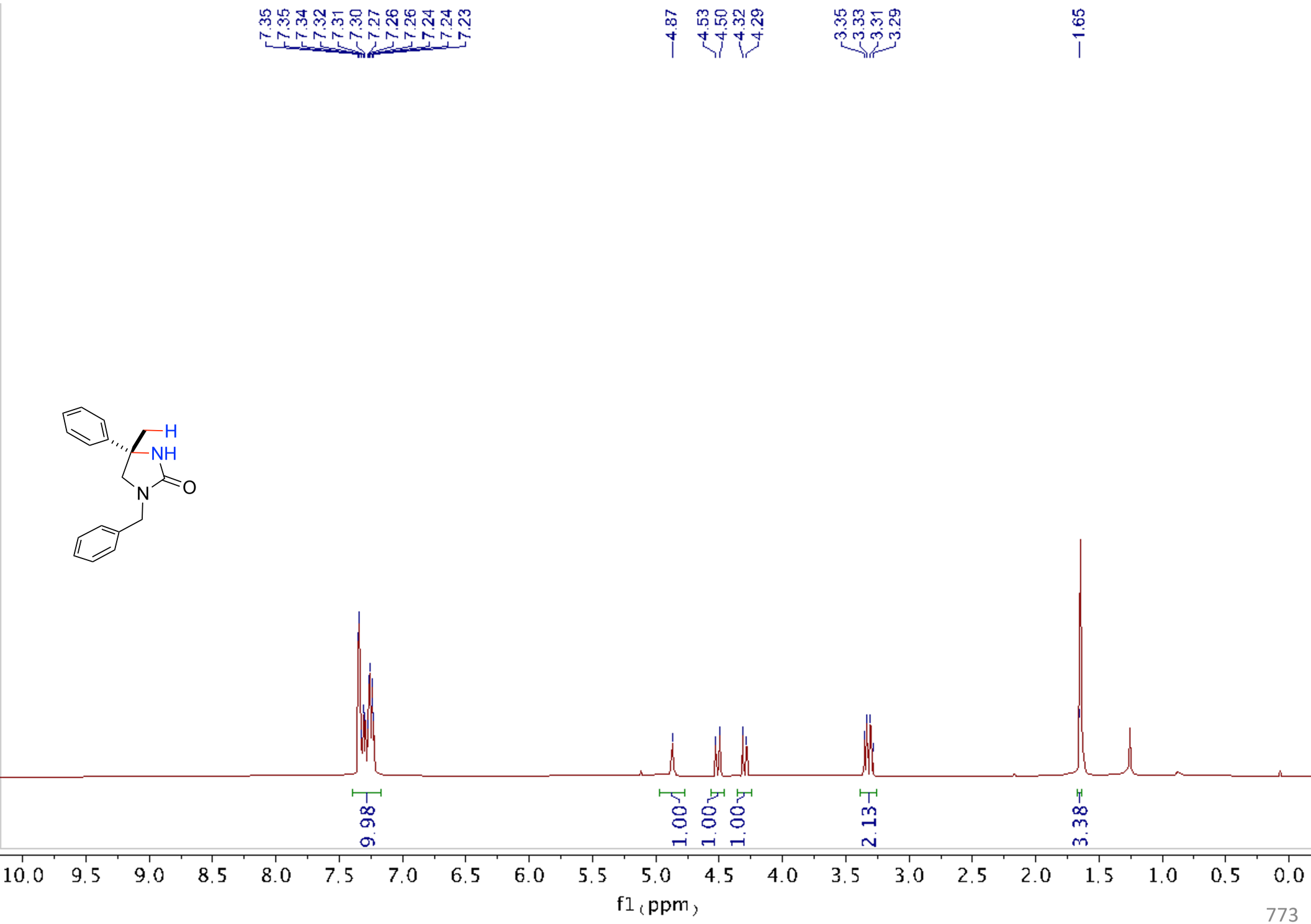
^{1}H NMR (*S*)-*N*1-benzyl-2-phenylpropane-1,2-diamine 2.6h



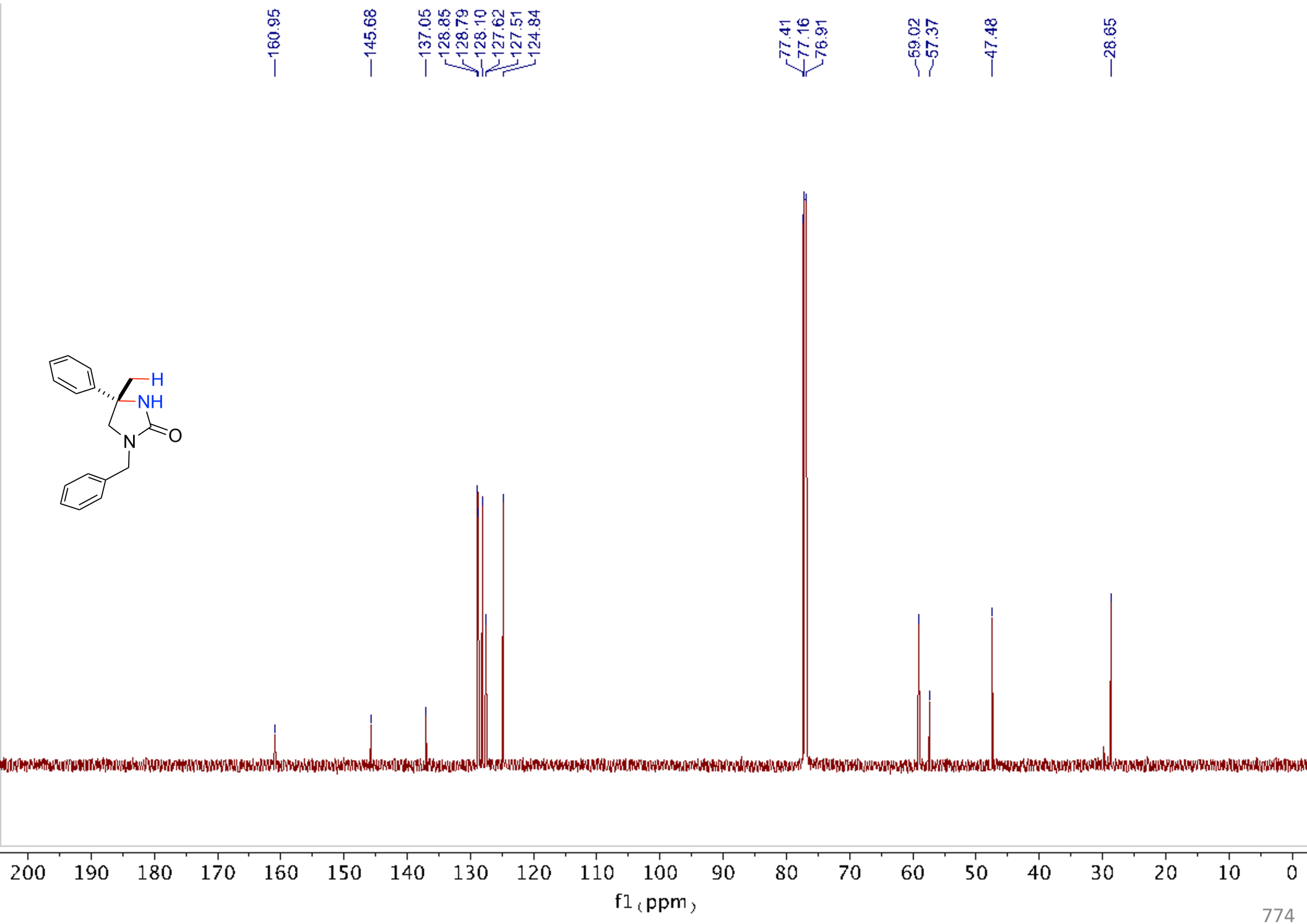
^{13}C NMR (*S*)-*N*1-benzyl-2-phenylpropane-1,2-diamine 2.6h



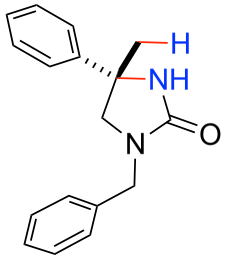
^{1}H NMR (*S*)-1-Benzyl-4-methyl-4-phenylimidazolidin-2-one 2.6i



^{13}C NMR (*S*)-1-Benzyl-4-methyl-4-phenylimidazolidin-2-one 2.6i



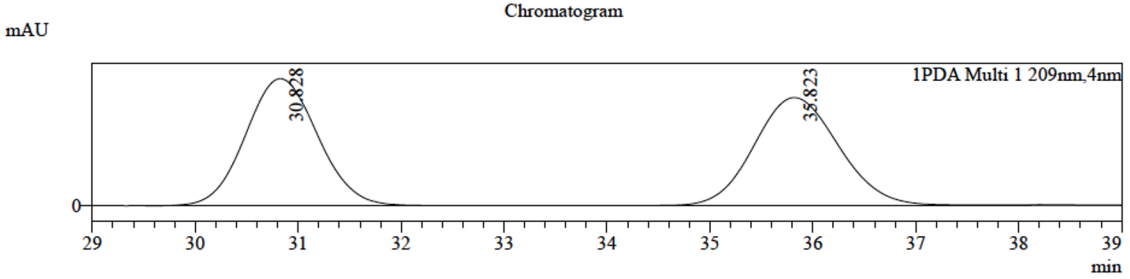
1-Benzyl-4-methyl-4-phenylimidazolidin-2-one 2.6i



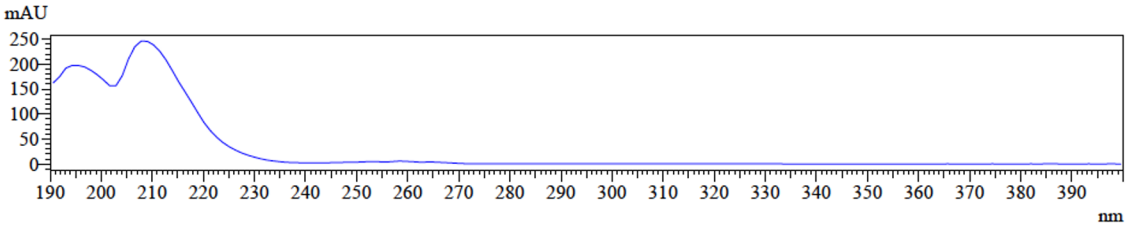
Sample Information

Data File	: H0X-1296-IC-10%0.8mL001.lcd
Sample Name	: H0X-1296-IC-10%0.8mL001
Sample ID	: H0X-1296-IC-10%0.8mL001
Method File	: H0X-10%-0.8ml-90MIN.lcm

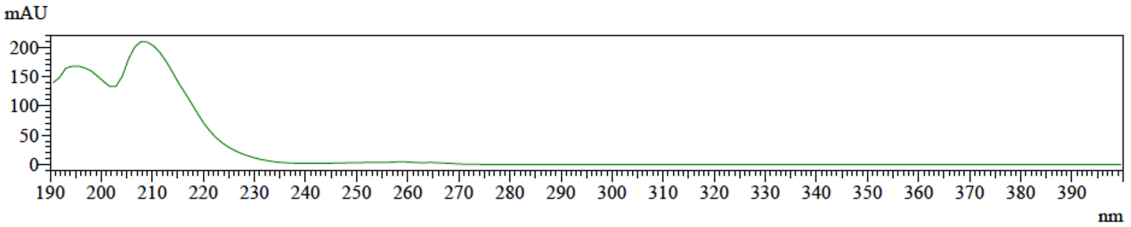
Chromatogram



UV Spectrum
Retention time = 30.828



UV Spectrum
Retention time = 35.823

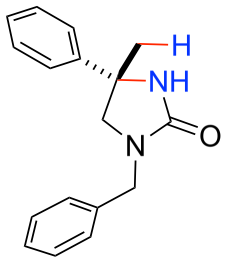


Peak Table

PDA Ch1 209nm

Peak#	Ret. Time	Area	Area%
1	30.828	11220793	49.960
2	35.823	11238808	50.040
Total		22459601	100.000

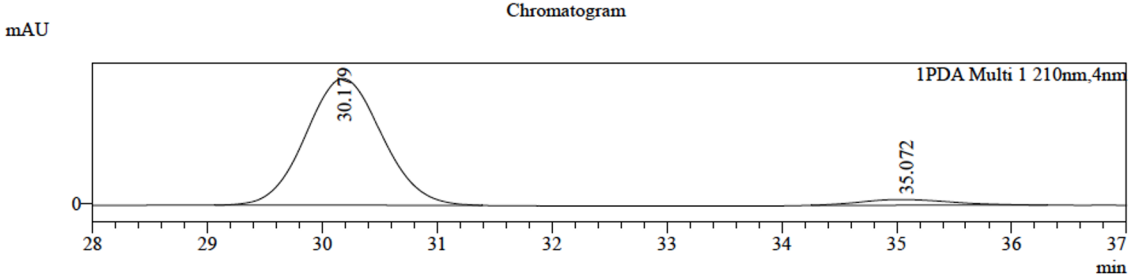
(*S*)-1-Benzyl-4-methyl-4-phenylimidazolidin-2-one 2.6i



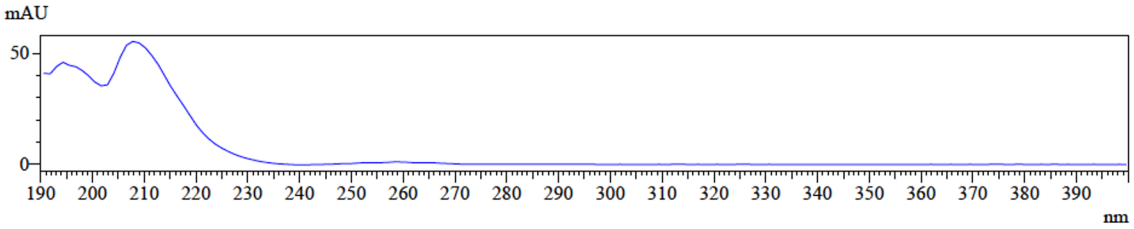
Sample Information

Data File	: H0X-1092-IC-10%-0.8 mL.lcd
Sample Name	: H0X-1092-IC-10%-0.8 mL
Sample ID	: H0X-1092-IC-10%-0.8 mL
Method File	: H0X-10%-0.8ml-75MIN.lcm

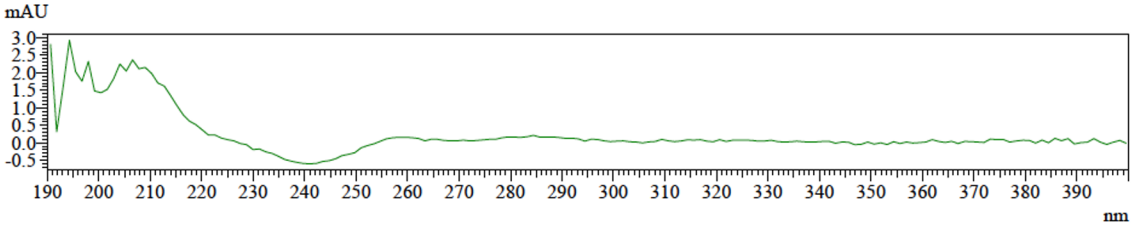
Chromatogram



UV Spectrum
Retention time = 30.179



UV Spectrum
Retention time = 35.072



Peak Table

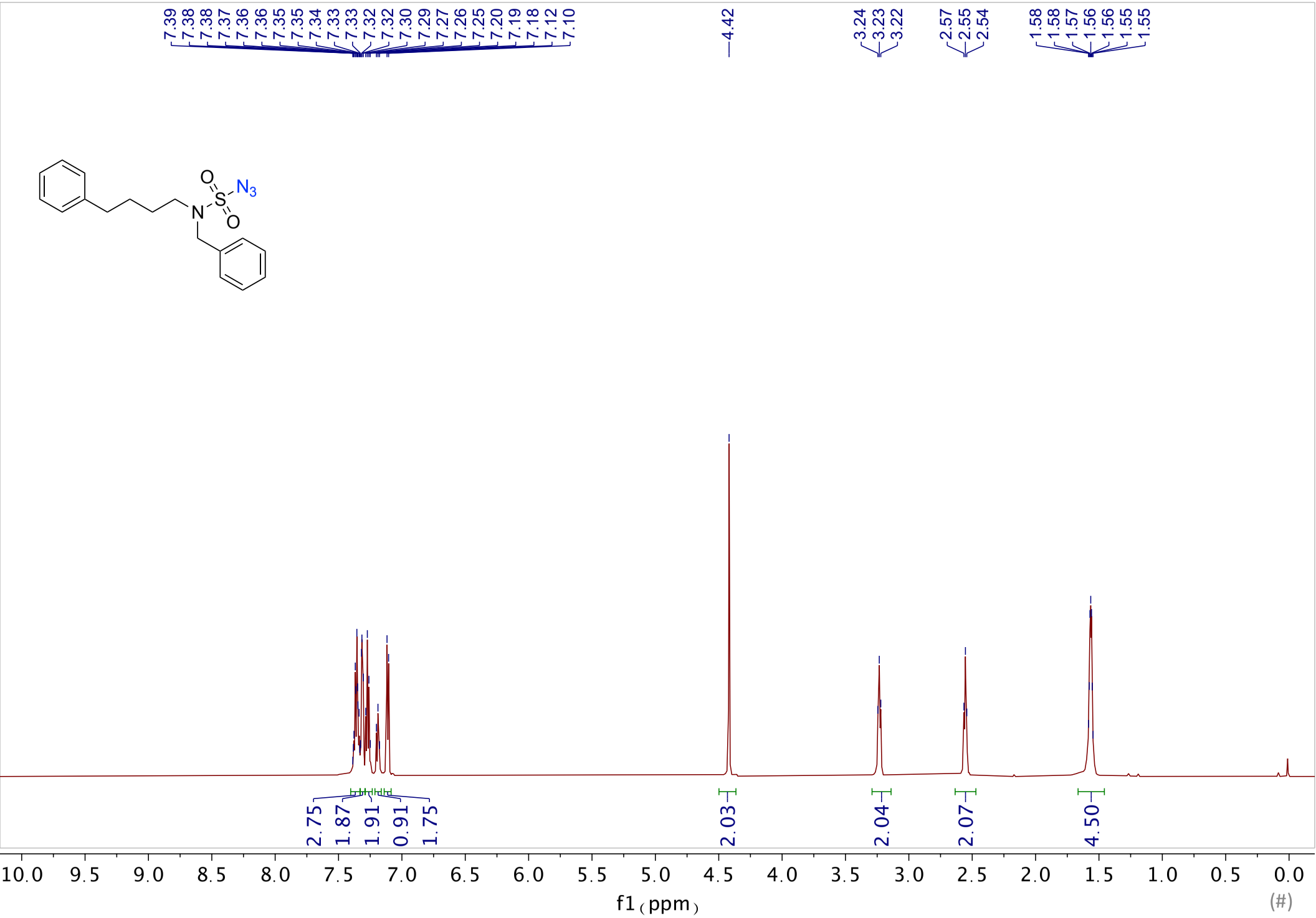
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	30.179	2327396	94.910
2	35.072	124815	5.090
Total		2452211	100.000

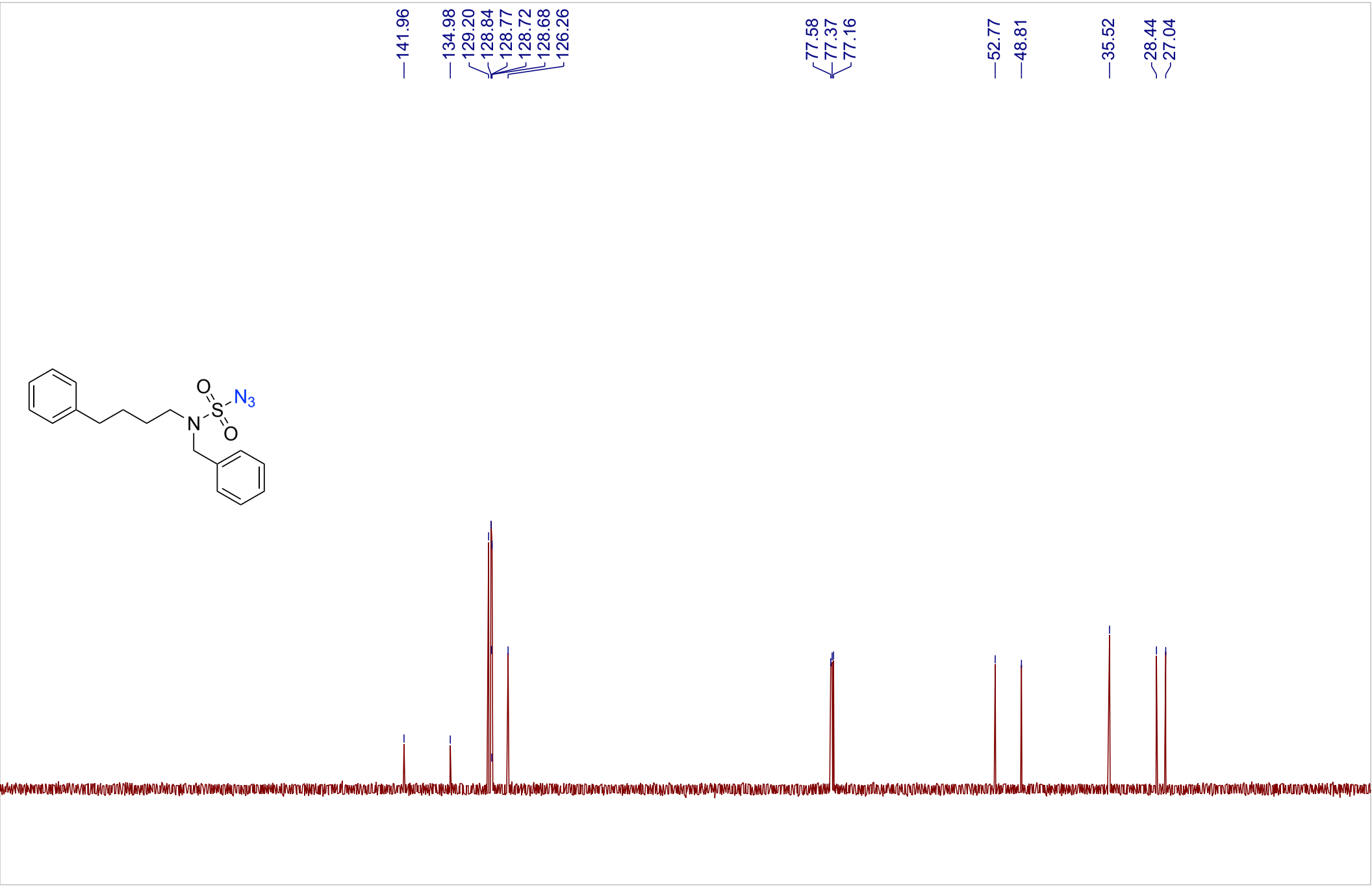
CHAPTER 3

Catalytic Radical *N*-Heterocyclization by Metalloradical C–H Amination involving 1,7-Hydrogen Atom Abstraction

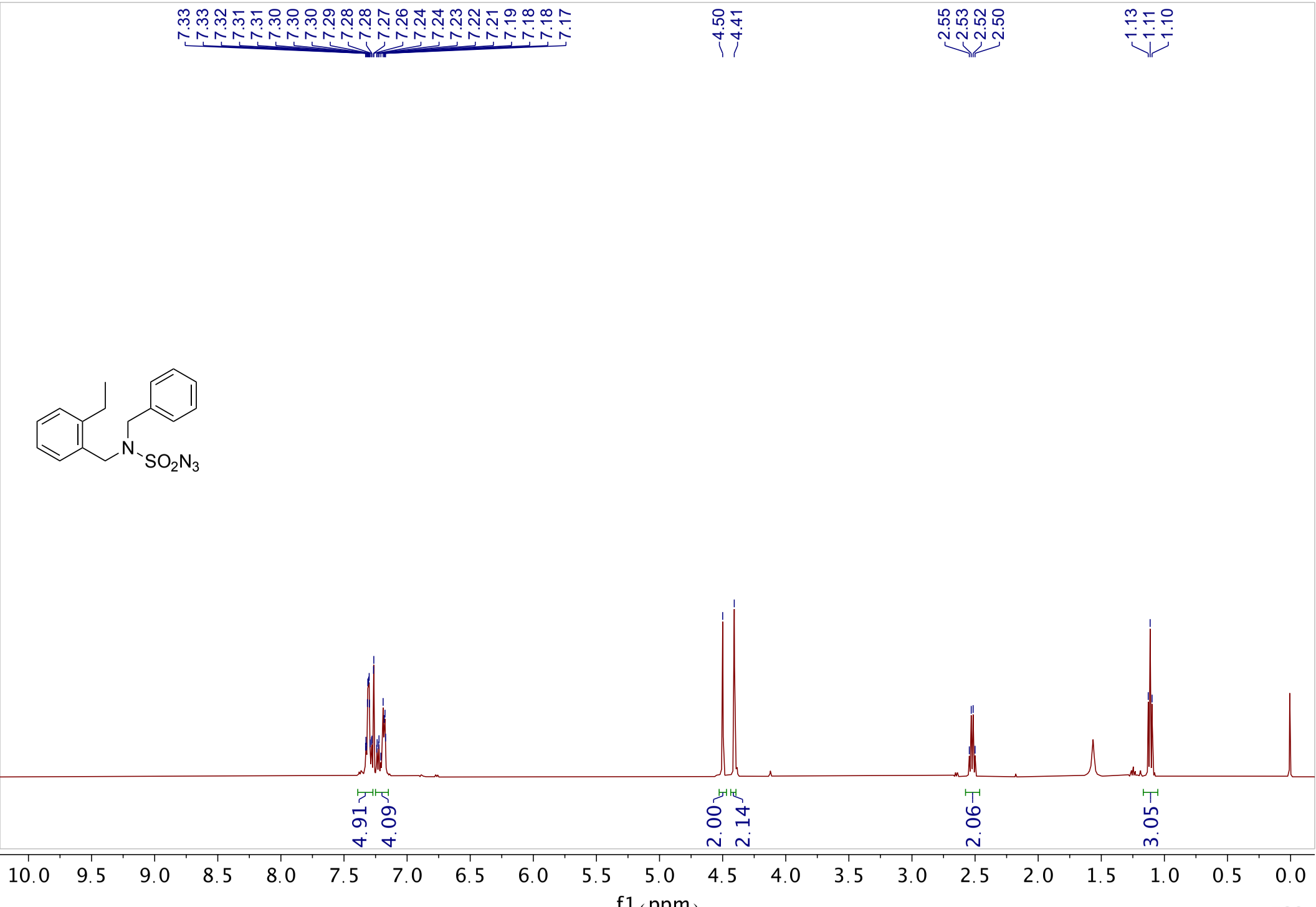
^{1}HNMR (((Azidosulfonyl)(4-phenylbutyl)amino)methyl)benzene 3.1a



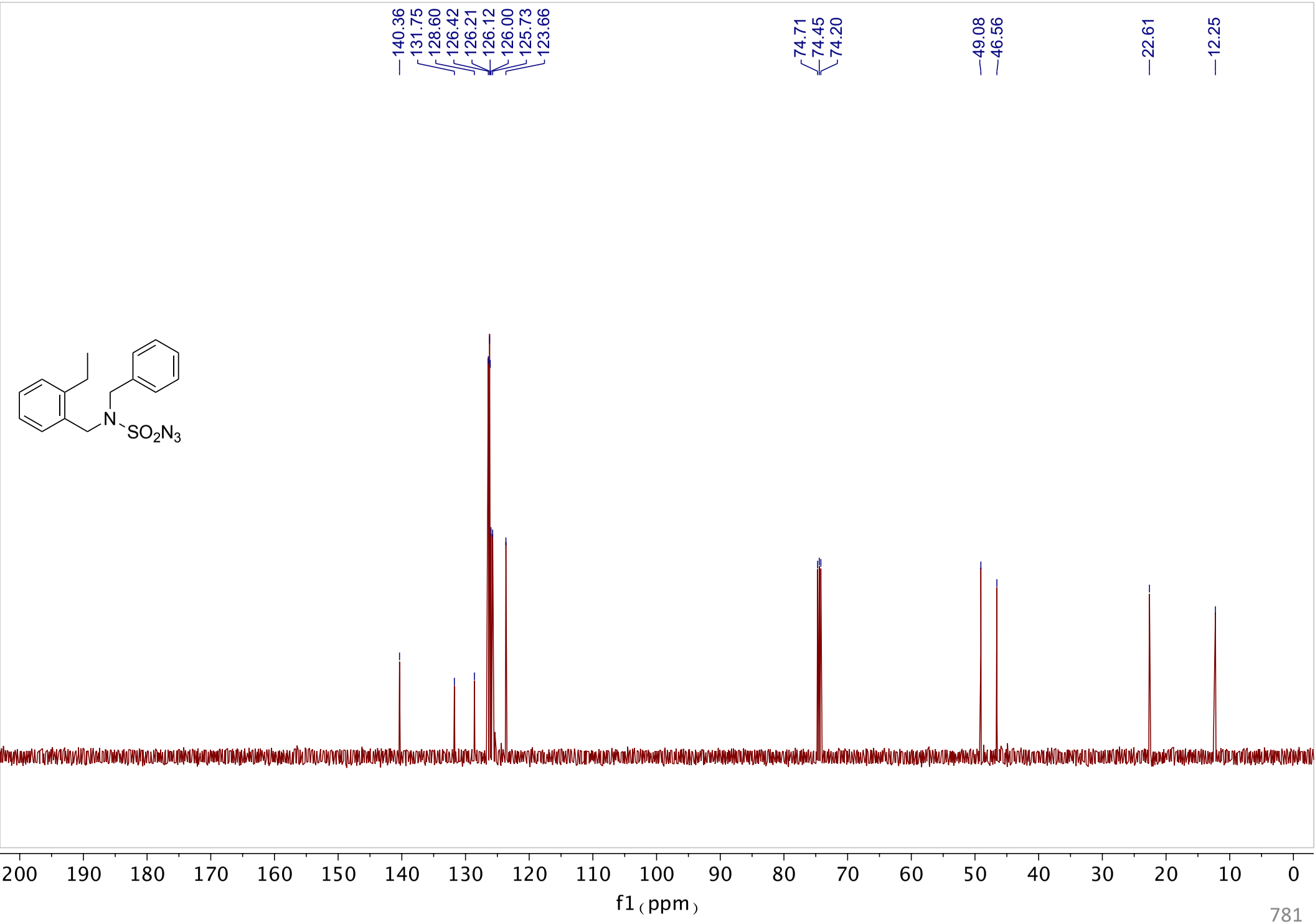
^{13}CNMR (((Azidosulfonyl)(4-phenylbutyl)amino)methyl)benzene 3.1a



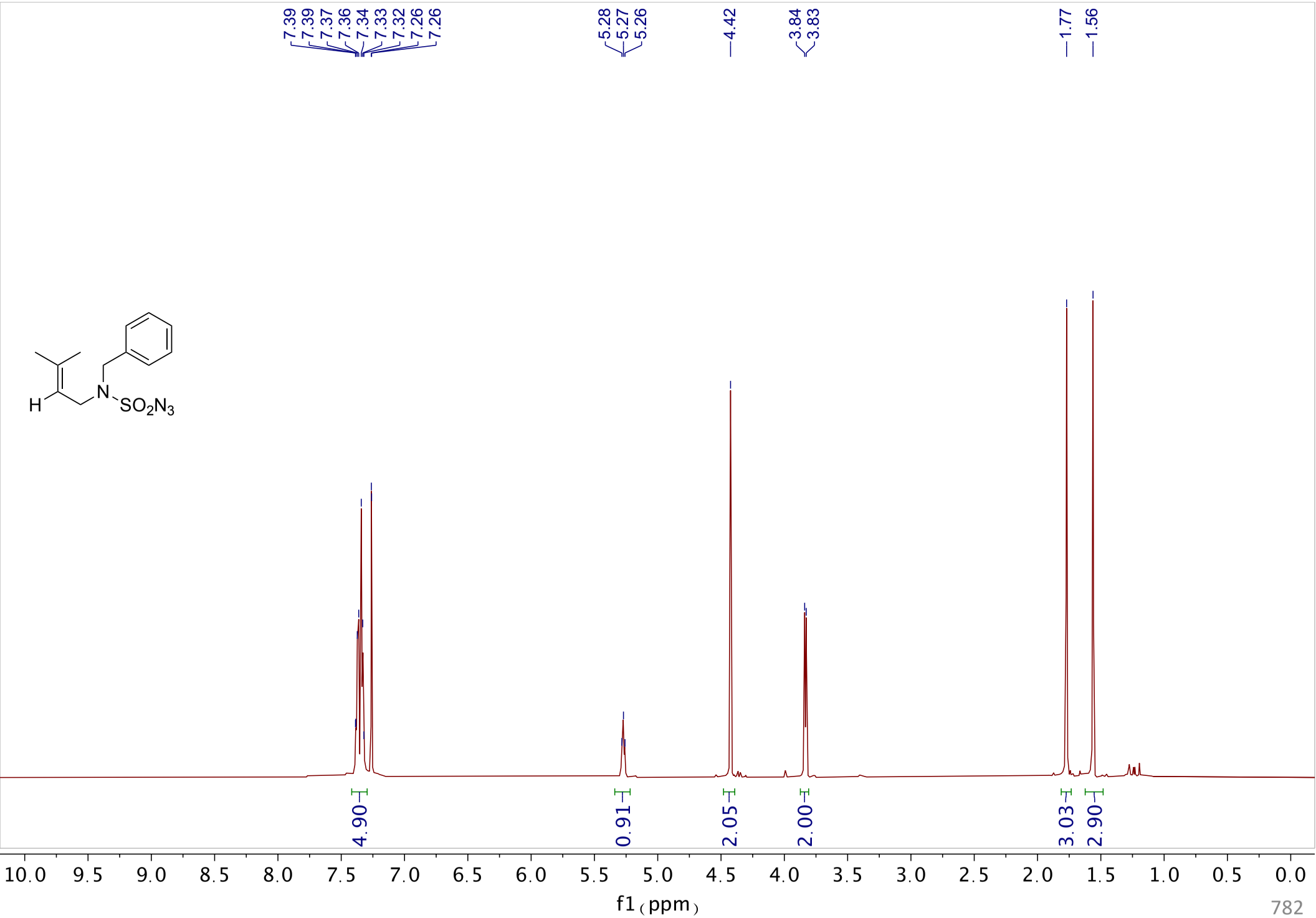
^{1}HNMR 1-(((Azidosulfonyl)(benzyl)amino)methyl)-2-ethylbenzene 3.1b



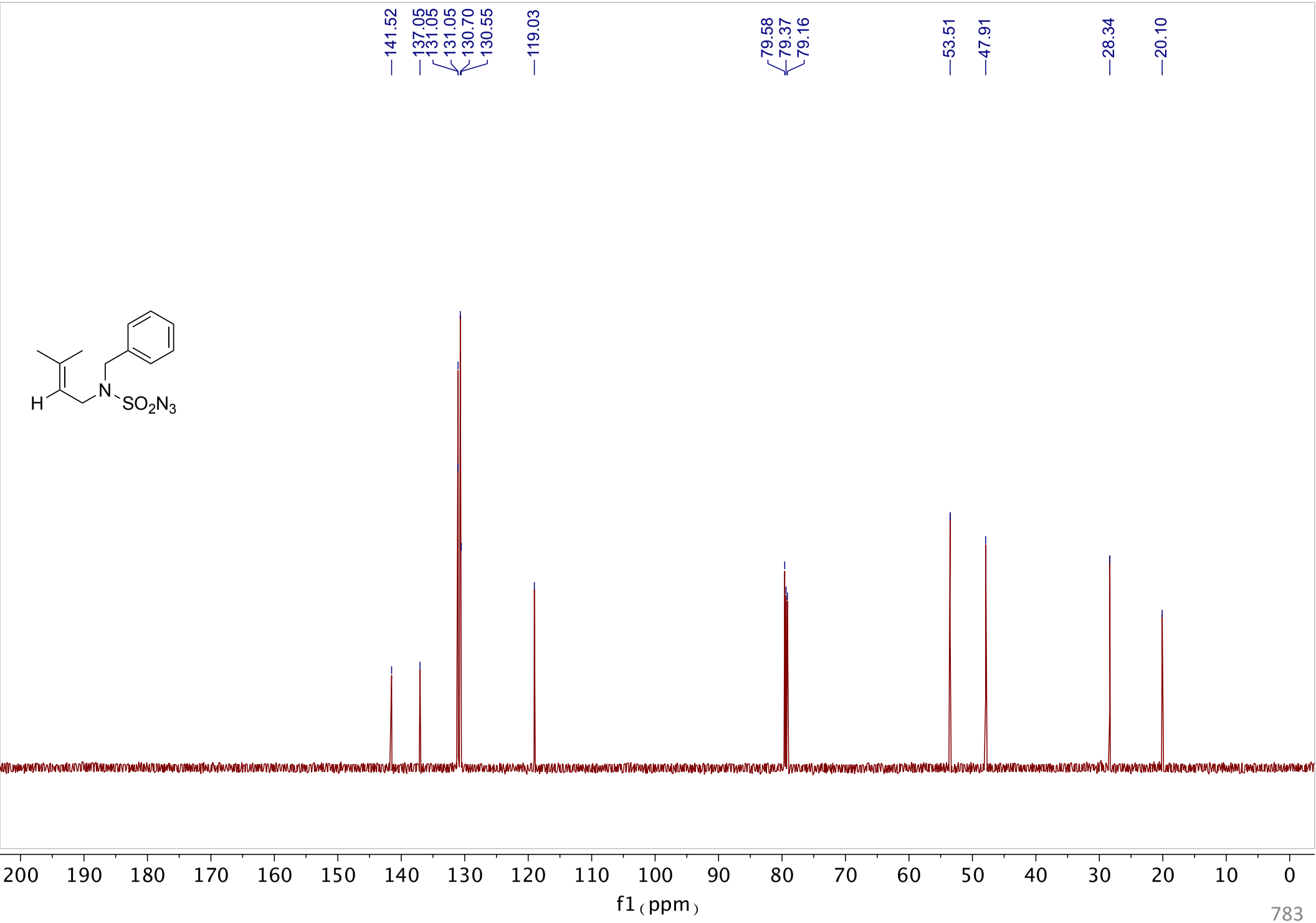
^{13}CNMR 1-(((Azidosulfonyl)(benzyl)amino)methyl)-2-ethylbenzene 3.1b



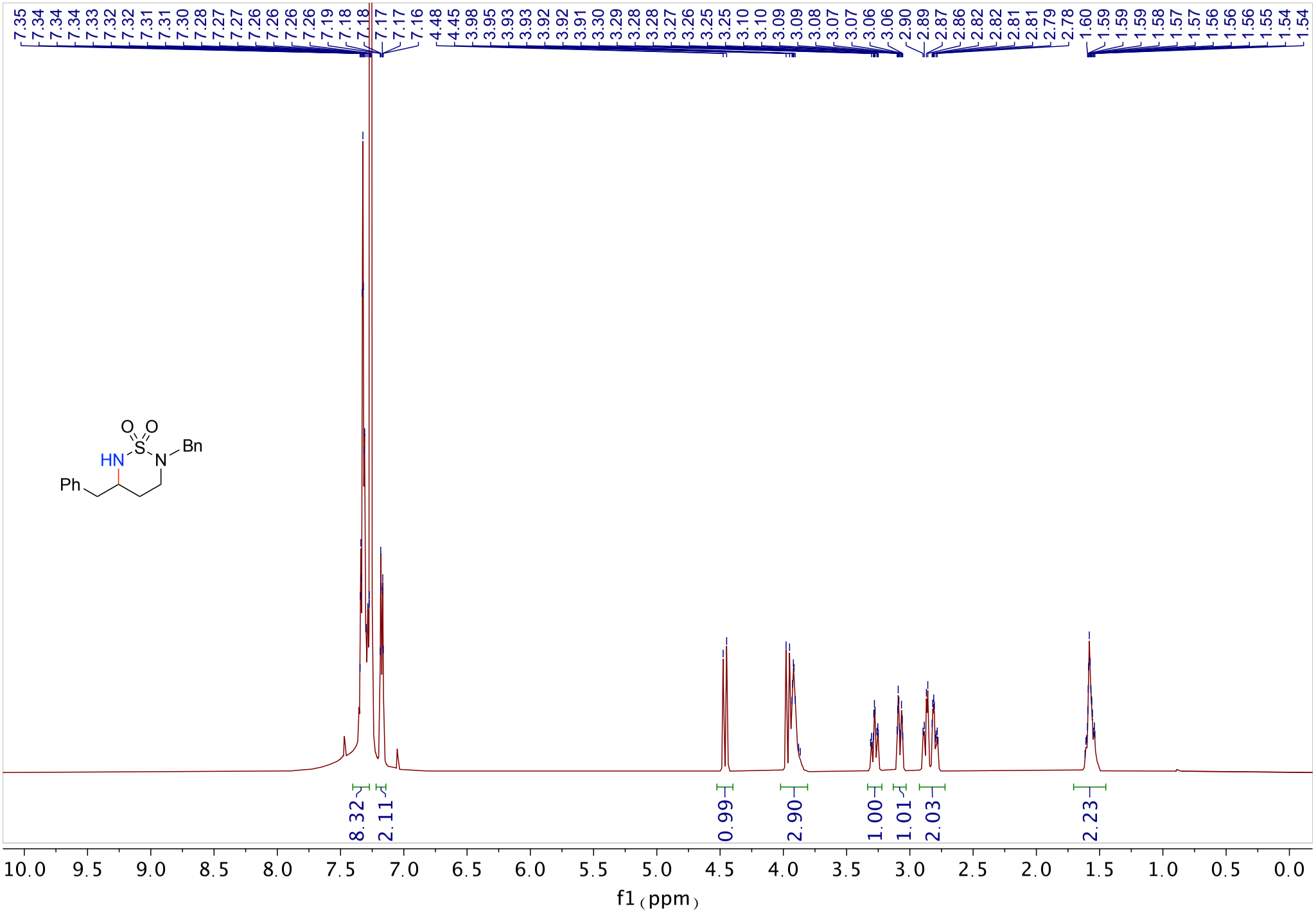
^{1}HNMR (((Azidosulfonyl)(3-methylbut-2-en-1-yl)amino)methyl)benzene 3.1c



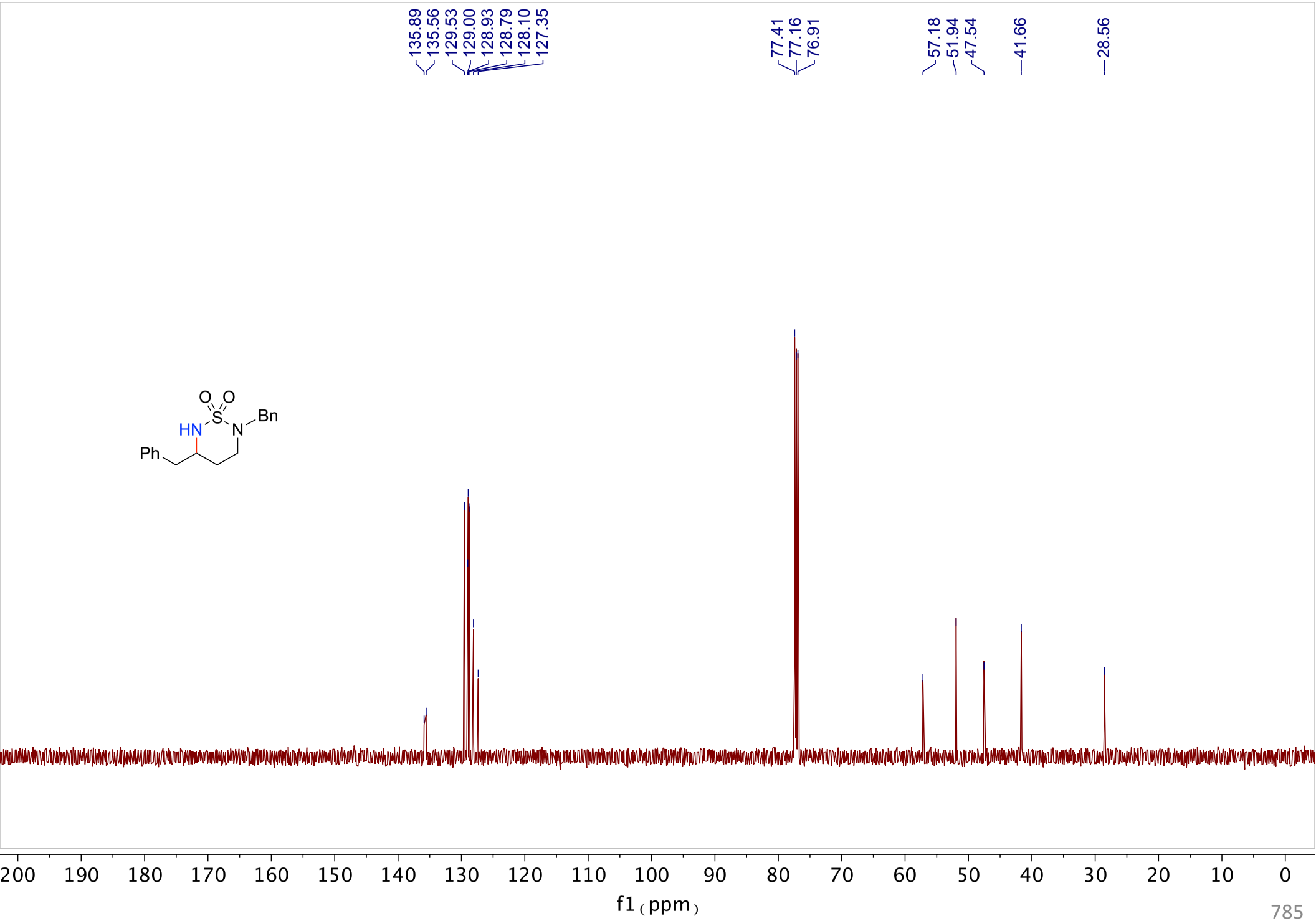
^{13}CNMR (((Azidosulfonyl)(3-methylbut-2-en-1-yl)amino)methyl)benzene 3.1c



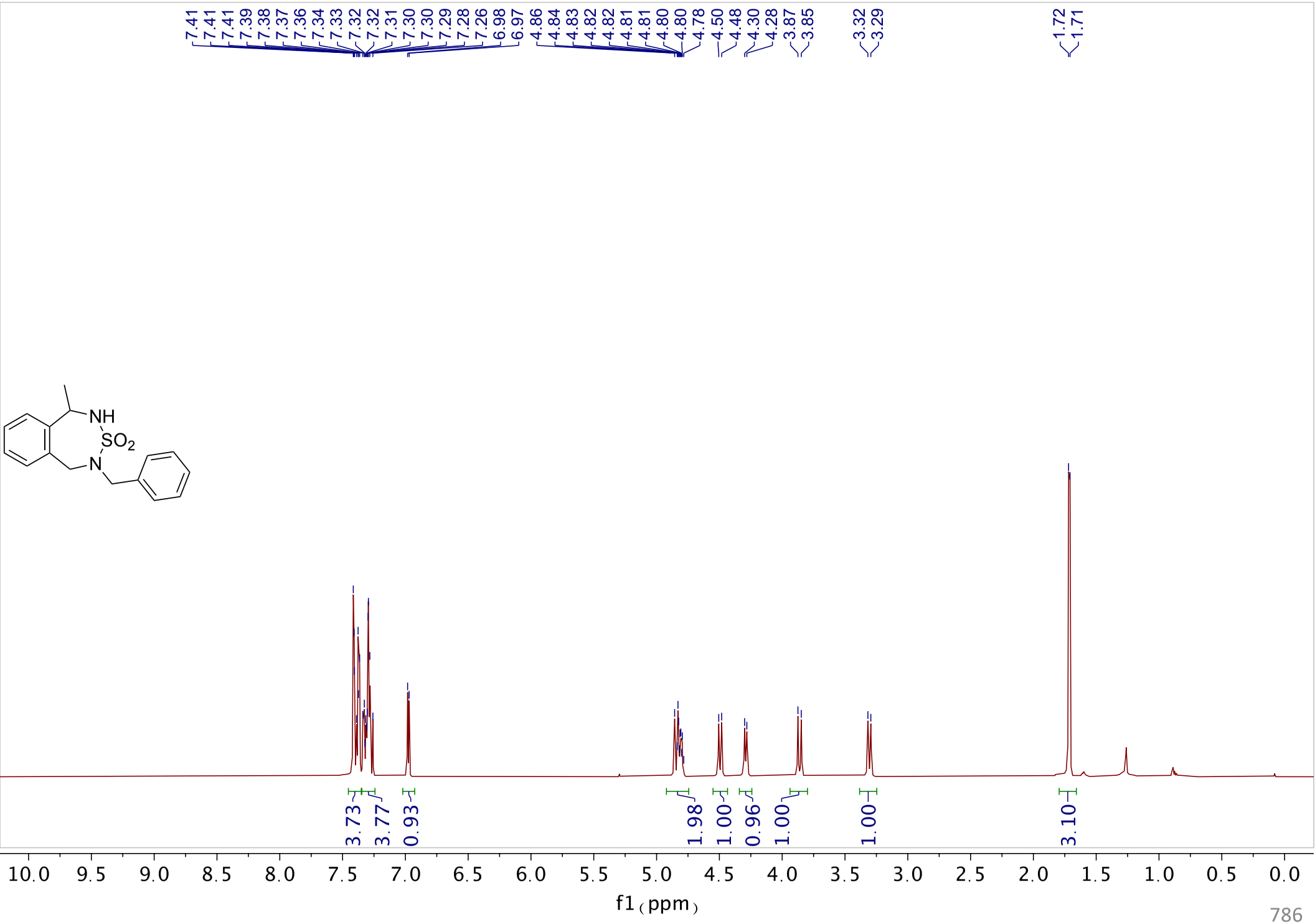
[1]HNMR 2,5-Dibenzyl-1,2,6-thiadiazinane 1,1-dioxide 3.3a



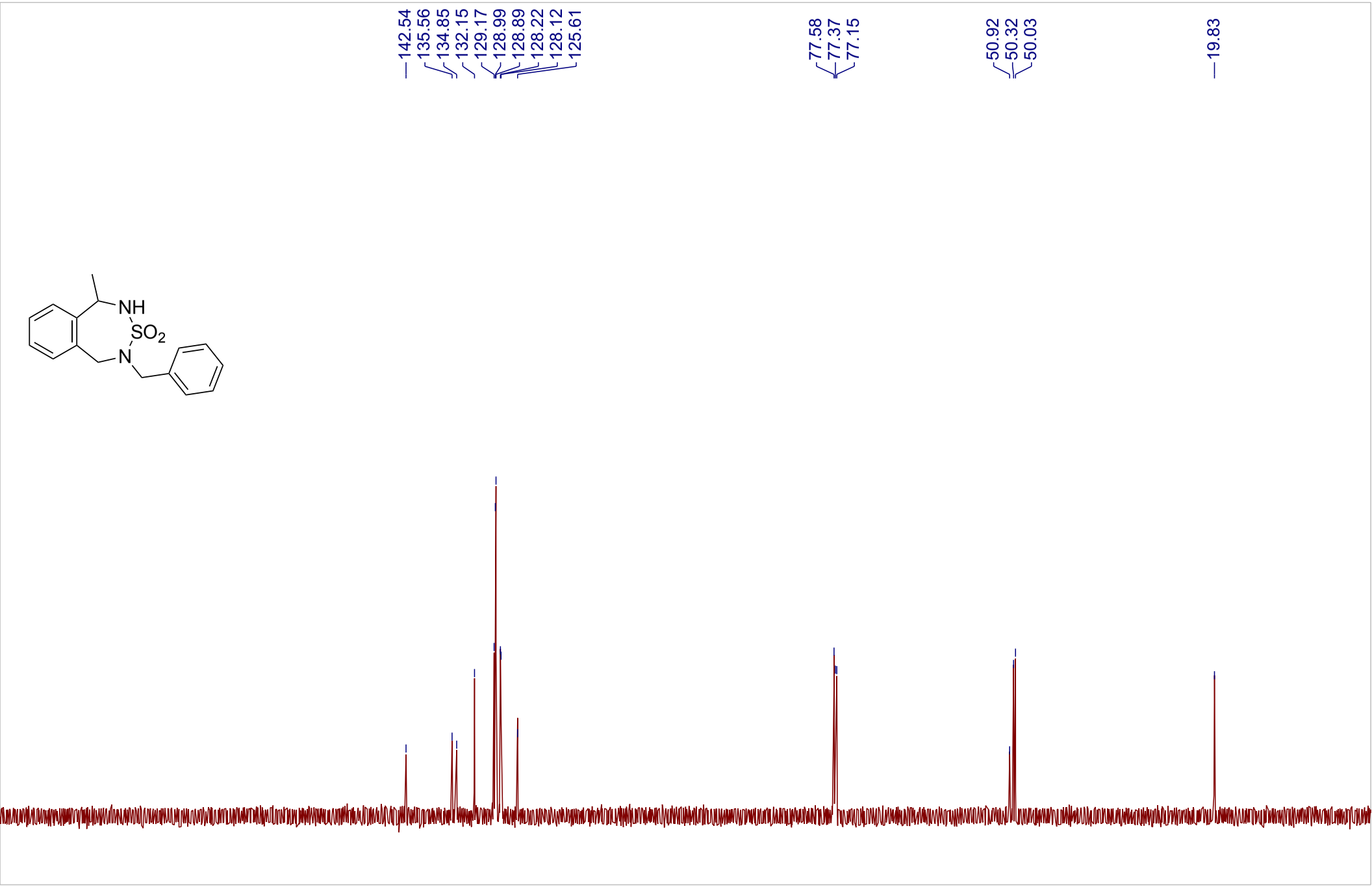
^{13}CNMR 2,5-Dibenzyl-1,2,6-thiadiazinane 1,1-dioxide 3.3a



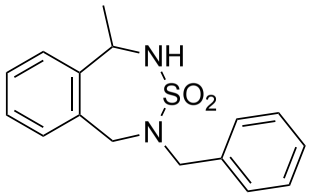
^{1}HNMR Methyl-1,2,4,5-tetrahydrobenzo[*d*][1,2,7]thiadiazepine 3,3-dioxide 3.2b



^{13}CNMR Methyl-1,2,4,5-tetrahydrobenzo[*d*][1,2,7]thiadiazepine 3,3-dioxide 3.2b



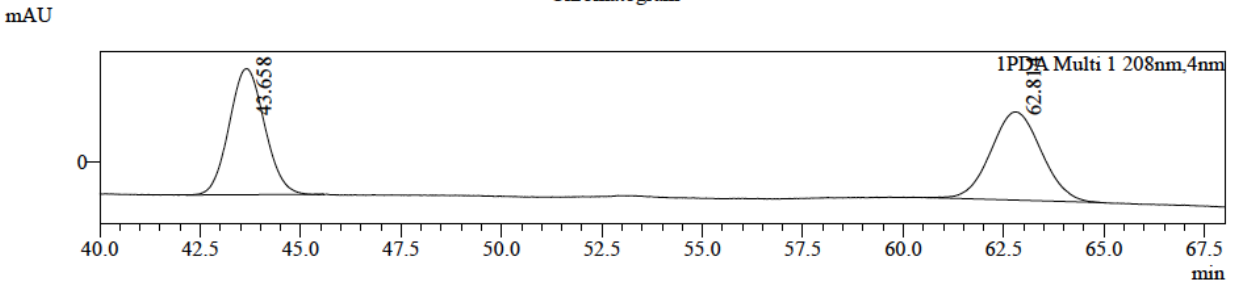
Methyl-1,2,4,5-tetrahydrobenzo[*d*][1,2,7]thiadiazepine 3,3-dioxide 2b



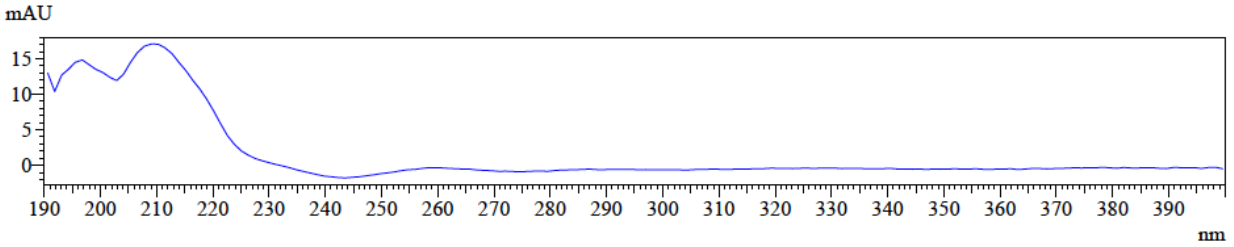
Sample Information

Data File	: H0X-0951-IC-10%-0.8 mL.lcd
Sample Name	: H0X-0951-IC-10%-0.8 mL
Sample ID	: H0X-0951-IC-10%-0.8 mL
Method File	: H0X-10%-0.8ml-90MIN.lcm

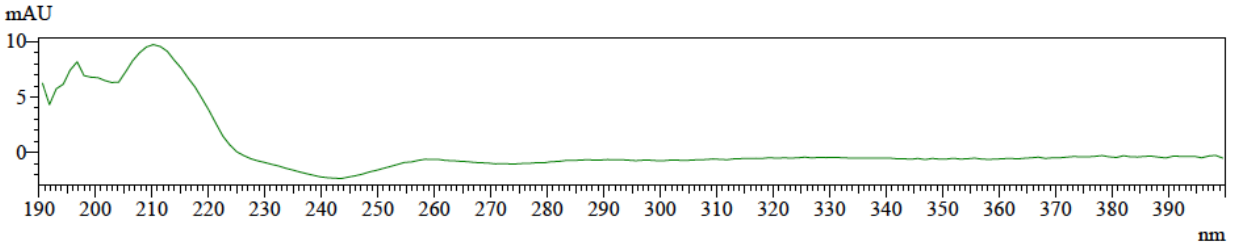
Chromatogram



UV Spectrum
Retention time = 43.658



UV Spectrum
Retention time = 62.814

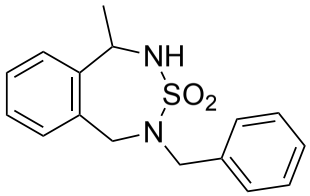


Peak Table

PDA Ch1 208nm

Peak#	Ret. Time	Area	Area%
1	43.658	1302921	50.020
2	62.814	1301868	49.980
Total		2604789	100.000

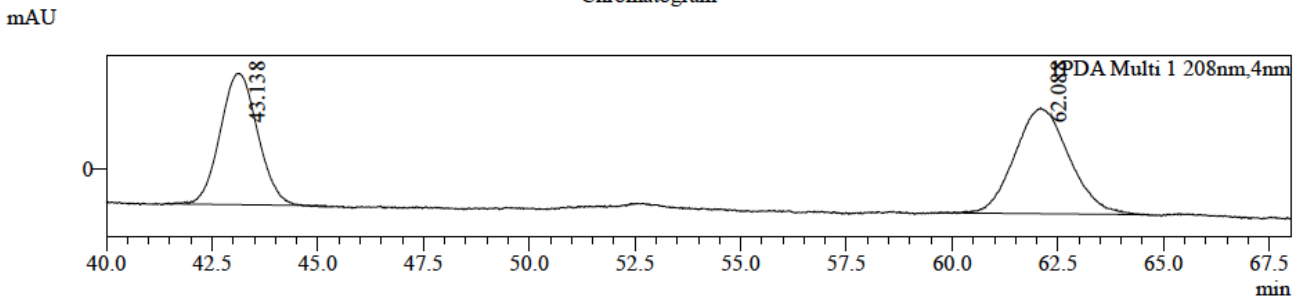
Methyl-1,2,4,5-tetrahydrobenzo[*d*][1,2,7]thiadiazepine 3,3-dioxide (–)-2b



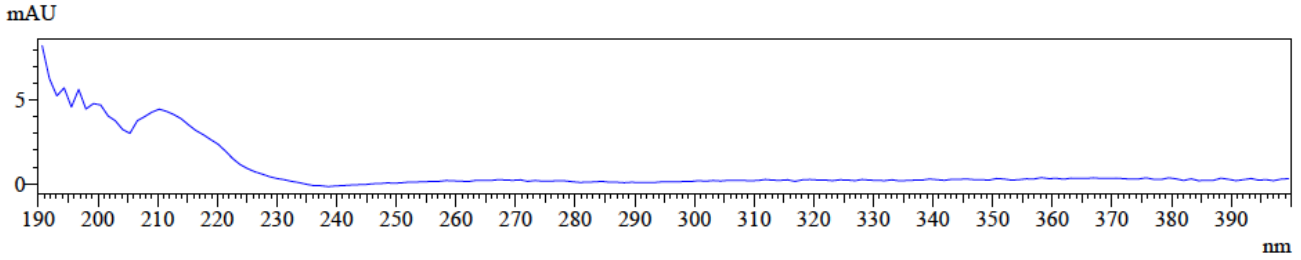
Sample Information

Data File : H0X-0952-IC-10%-0.8 mL.lcd
Sample Name : H0X-0952-IC-10%-0.8 mL
Sample ID : H0X-0952-IC-10%-0.8 mL
Method File : H0X-10%-0.8ml-90MIN.lcm

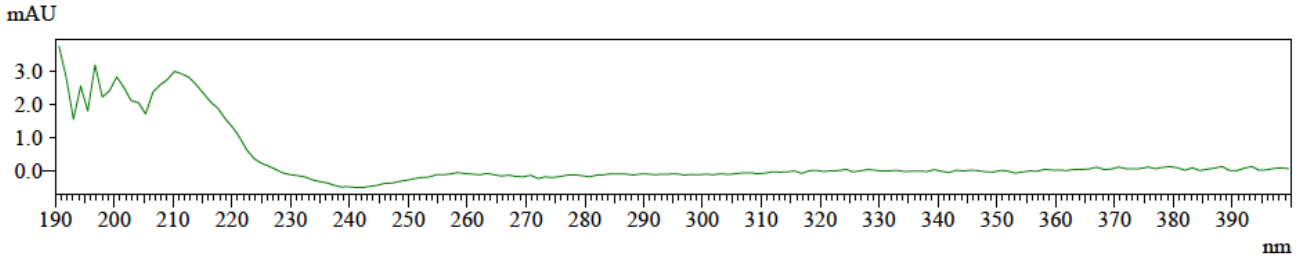
Chromatogram



UV Spectrum
Retention time = 43.138



UV Spectrum
Retention time = 62.088

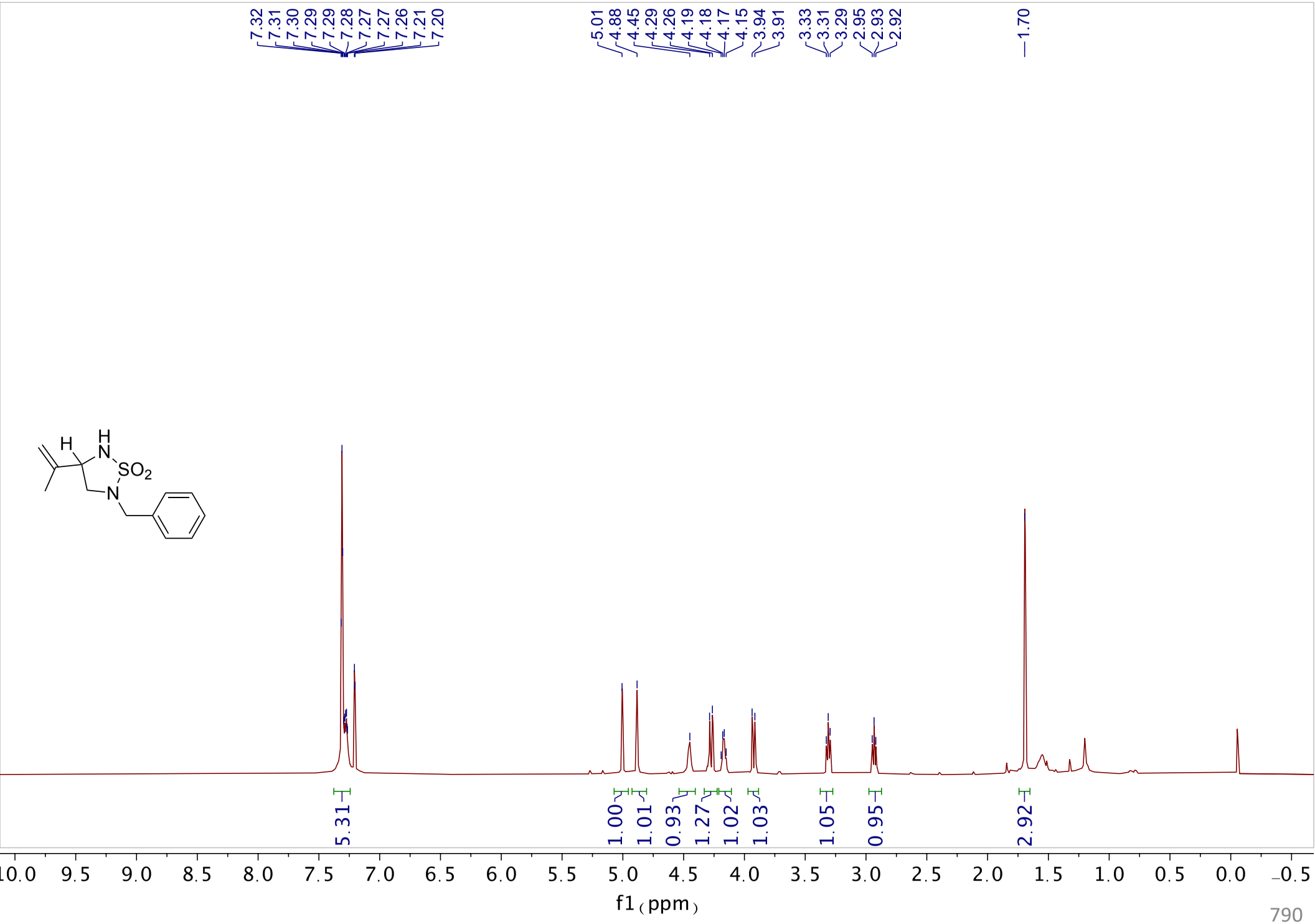


Peak Table

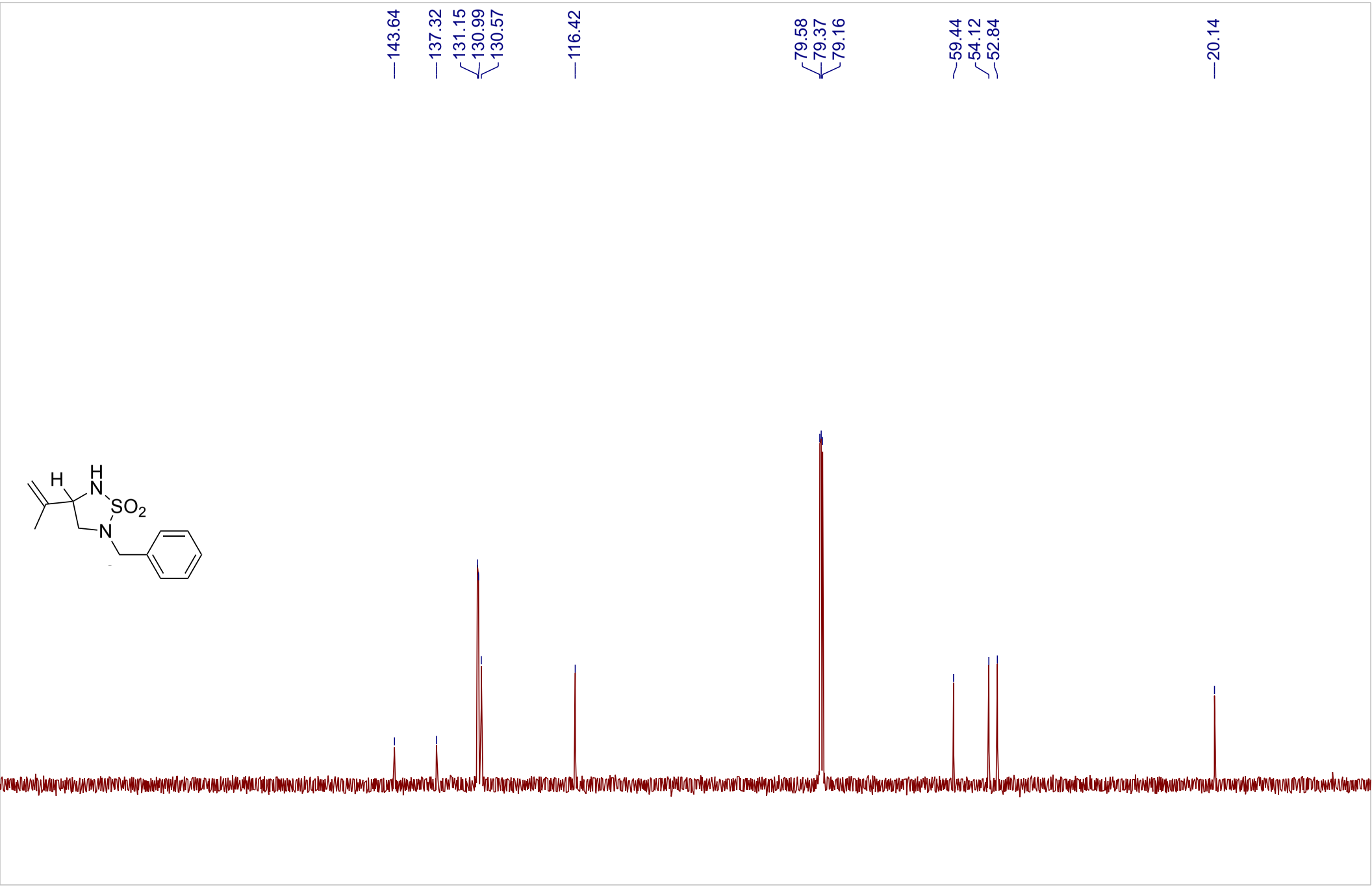
PDA Ch1 208nm

Peak#	Ret. Time	Area	Area%
1	43.138	326268	46.124
2	62.088	381104	53.876
Total		707372	100.000

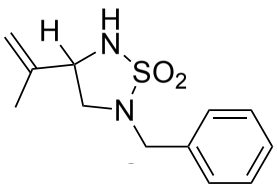
^{1}HNMR 2-benzyl-4-(prop-1-en-2-yl)-1,2,5-thiadiazolidine 1,1-dioxide 3.6c



^{13}CNMR 2-benzyl-4-(prop-1-en-2-yl)-1,2,5-thiadiazolidine 1,1-dioxide 3.6c



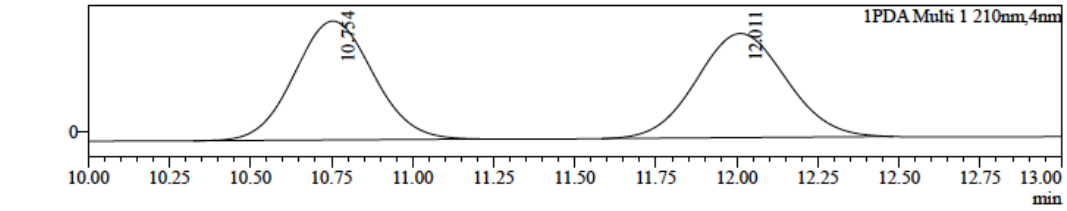
2-benzyl-4-(prop-1-en-2-yl)-1,2,5-thiadiazolidine 1,1-dioxide 3.6c



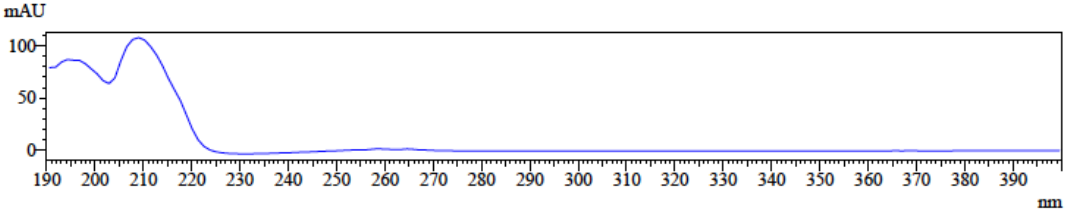
Sample Information

Data File	: H0X-0864-IC-30%1.0mL.lcd
Sample Name	: H0X-0864-IC-30%1.0mL
Sample ID	: H0X-0864-IC-30%1.0mL
Method File	: H0X-30%-1.0ml-20MIN.lcm

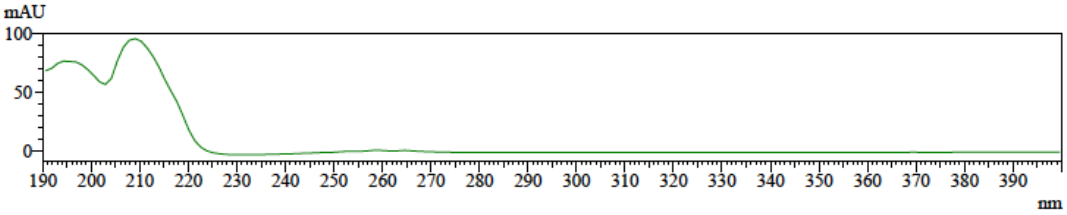
Chromatogram



UV Spectrum
Retention time = 10.754



UV Spectrum
Retention time = 12.011

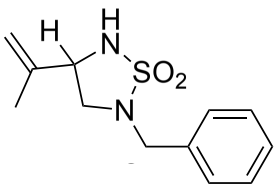


Peak Table

PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	10.754	1795779	50.107
2	12.011	1788110	49.893
Total		3583889	100.000

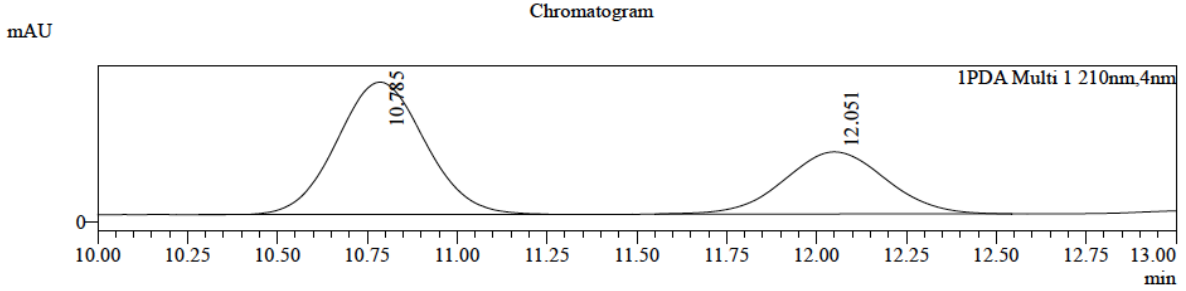
2-benzyl-4-(prop-1-en-2-yl)-1,2,5-thiadiazolidine 1,1-dioxide (–)-3.6c



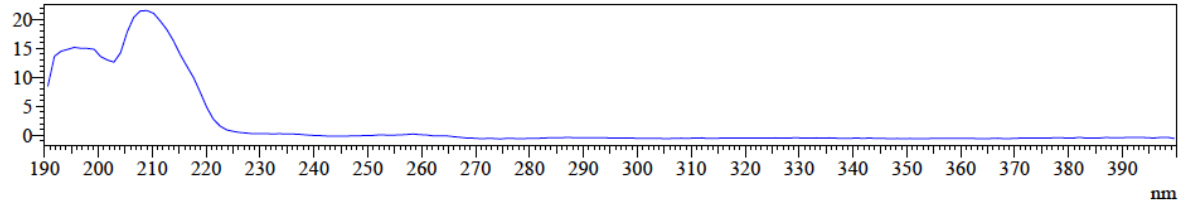
Sample Information

Data File : H0X-2-IC-30%1.0mL.lcd
Sample Name : H0X-2-IC-30%1.0mL
Sample ID : H0X-2-IC-30%1.0mL
Method File : H0X-30%-1.0ml-20MIN.lcm

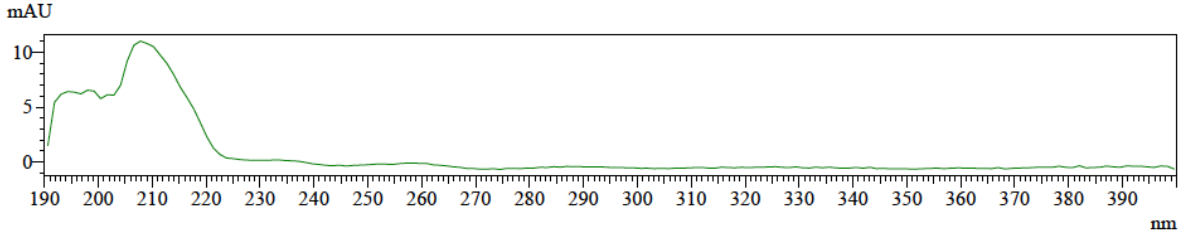
Chromatogram



UV Spectrum
Retention time = 10.785



UV Spectrum
Retention time = 12.051

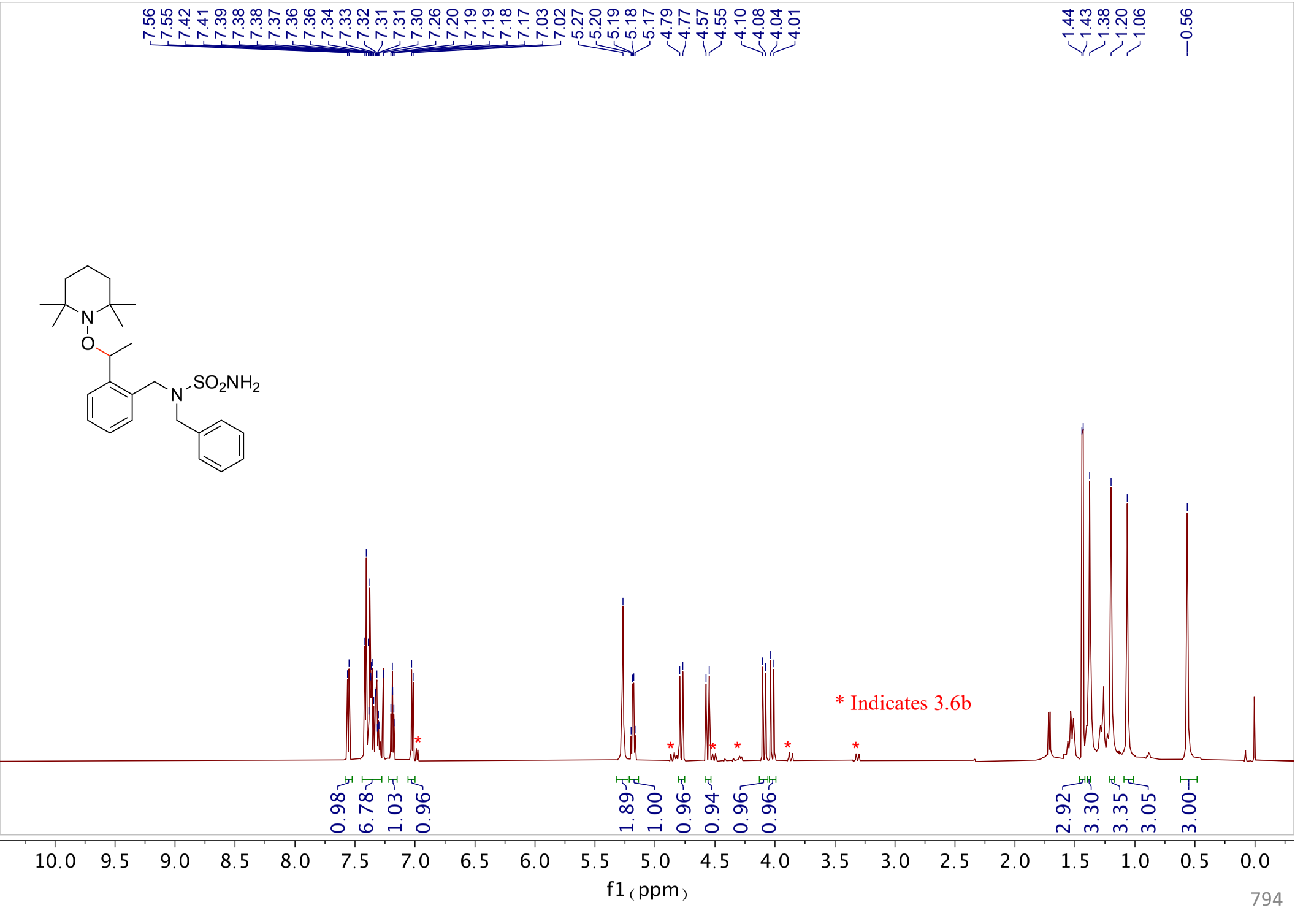


Peak Table

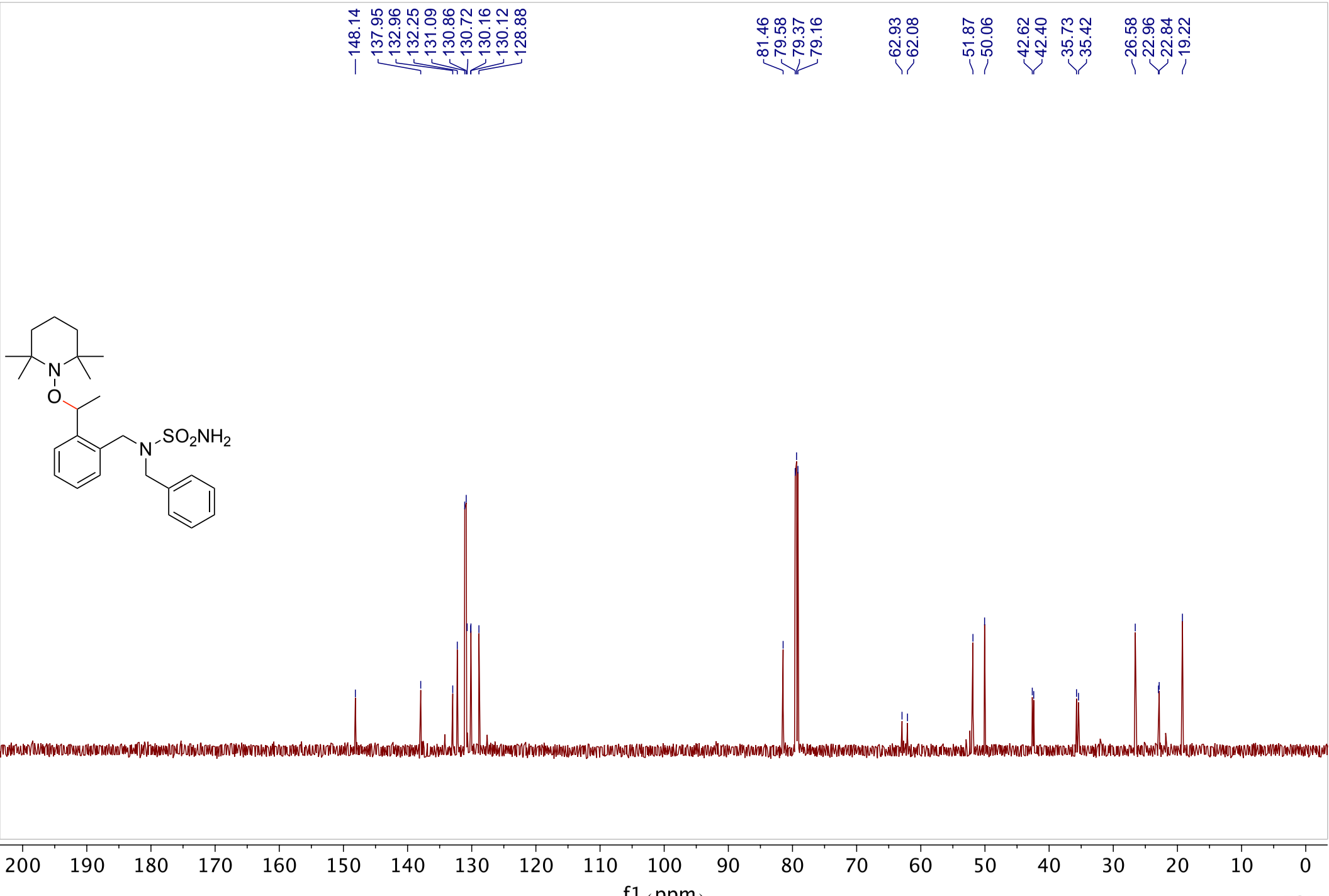
PDA Ch1 210nm

Peak#	Ret. Time	Area	Area%
1	10.785	320328	64.826
2	12.051	173811	35.174
Total		494138	100.000

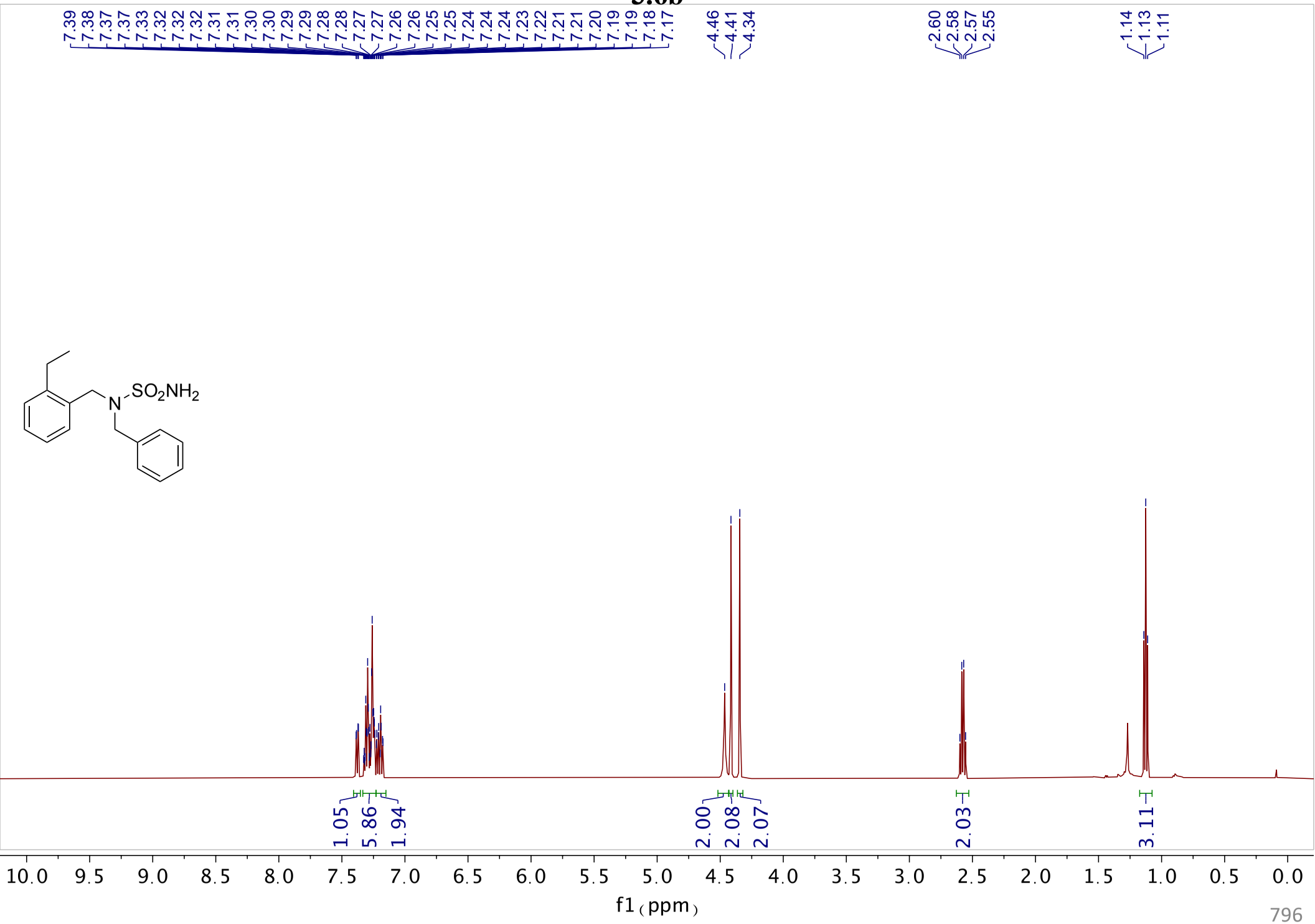
^{1}HNMR *N*-benzyl-*N*-(2-(1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethyl)benzyl)-λ2-azanesulfonamide 3.5b



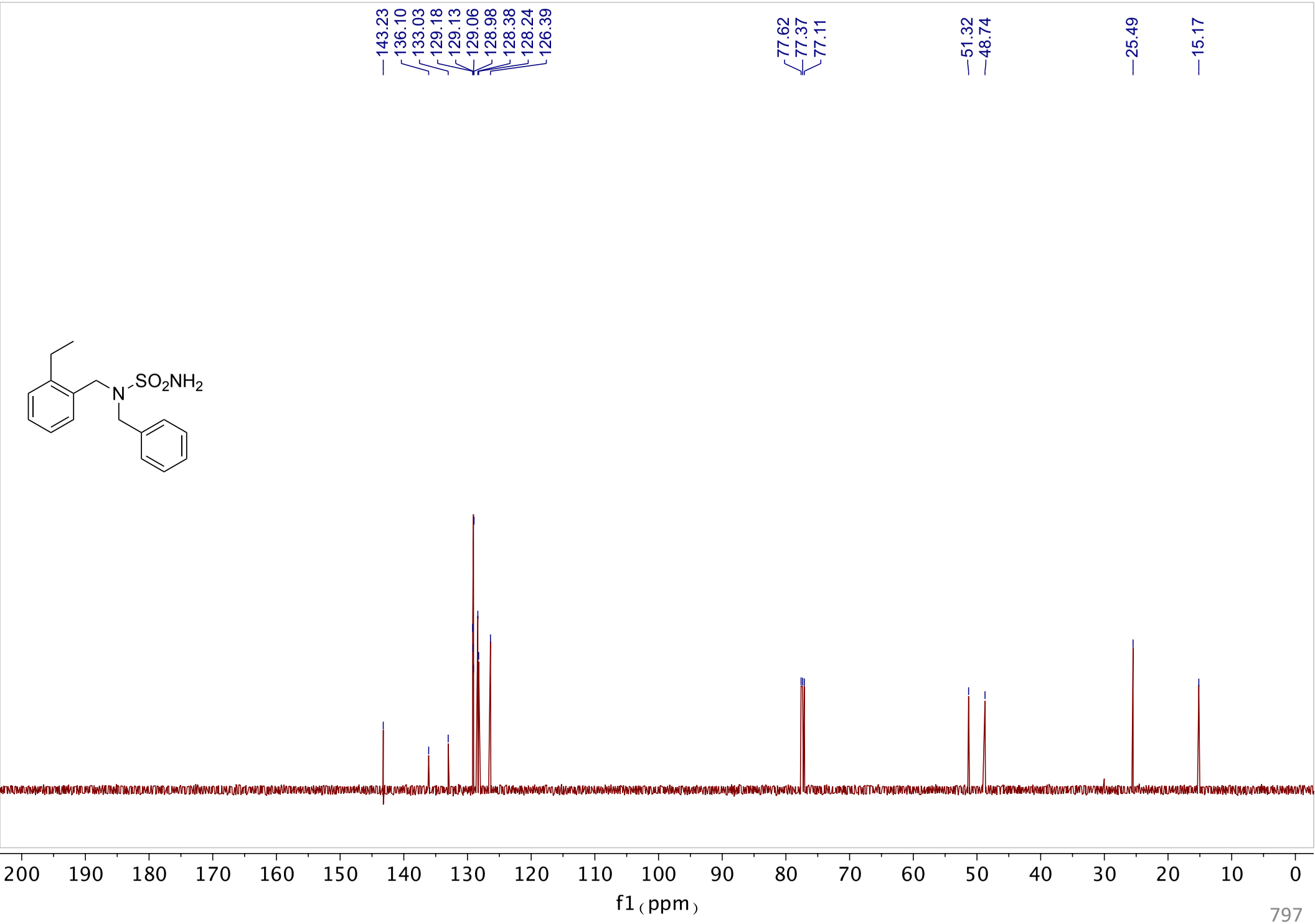
^{1}HNMR *N*-benzyl-*N*-(2-(1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethyl)benzyl)-λ2-azanesulfonamide 3.5b



^{1}HNMR *N*-benzyl-*N*-(2-(1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethyl)benzyl)-λ2-azanesulfonamide 3.6b



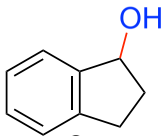
^{13}CNMR *N*-benzyl-*N*-(2-(1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethyl)benzyl)-λ2-azanesulfonamide 3.6b



CHAPTER 4

Metalloradical Activation of Alkyl Hydroperoxides for Catalytic Radical C–H Hydroxylation

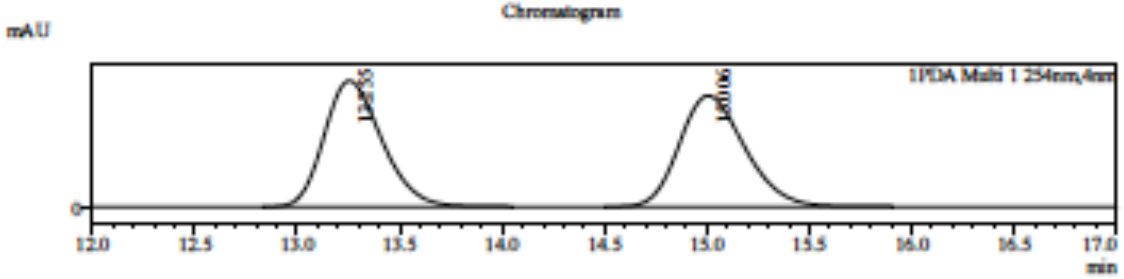
2,3-dihydro-1*H*-inden-1-ol (±)-4.3a



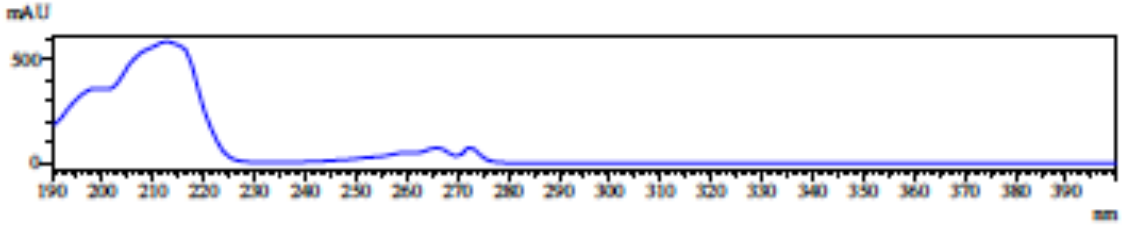
Sample Information

Data File : X1W-RACE-OD-H-4%0.8mL4.lcd
Sample Name : X1W-RACE-OD-H-4%0.8mL
Sample ID : X1W-RACE-OD-H-4%0.8mL
Method File : X1W-4%0.8mL30MIN.lcm

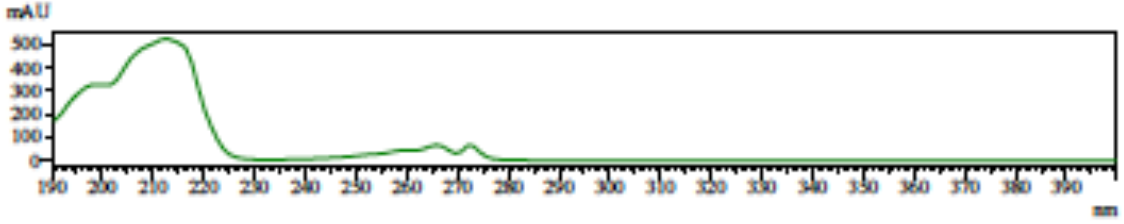
Chromatogram



UV Spectrum
Retention time = 13.255



UV Spectrum
Retention time = 15.006

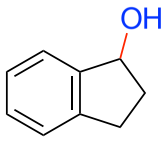


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	13.255	625737	49.985
2	15.006	626119	50.015
Total		1251856	100.000

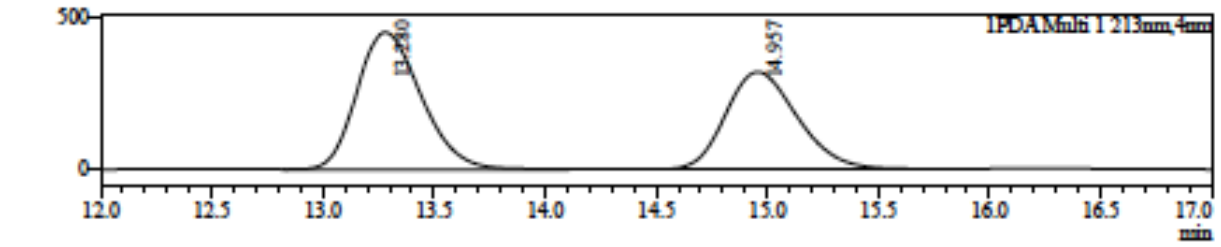
2,3-dihydro-1*H*-inden-1-ol (+)-4.3a



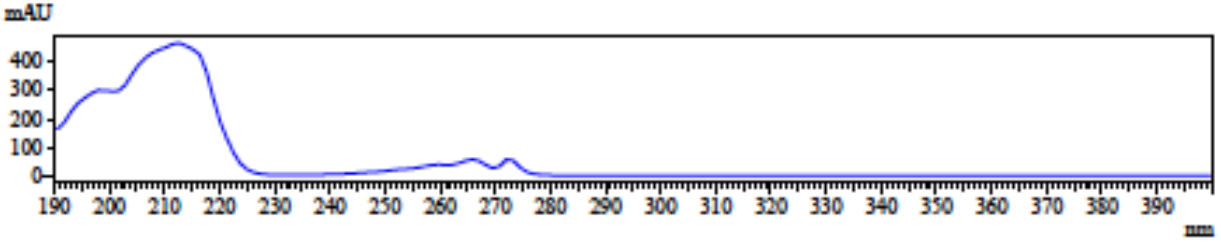
Sample Information

Data File	: X1W-0091-OD-H-4%0.8mL001.lcd
Sample Name	: X1W-0091-OD-H-4%0.8mL001
Sample ID	: X1W-0091-OD-H-4%0.8mL001
Method File	: X1W-4%0.8mL30MIN.lcm

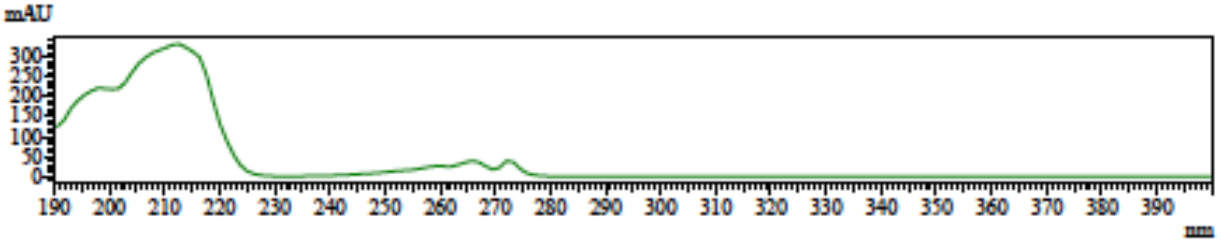
Chromatogram



UV Spectrum
Retention time = 13.280



UV Spectrum
Retention time = 14.957



Peak Table

PDA Ch1 213nm

Peak#	Ret. Time	Area	Area%
1	13.280	9133277	55.917
2	14.957	7200214	44.083
Total		16333490	100.000