# Supplementary Information

## Selective α-Me-C($sp^3$)-H Borylation of Methyl Sulfides Controlled by Substrate-Ligand Electrostatic Interaction

Rui-Mu Yu[1,2,#], Jin-Ping Li[1,2,#], Sumire Tobe[3], Shunsuke Yabu[3], Kanami Sugiyama[3], Li-Sheng Wang[2], Hirofumi Sato[3], Masahiro Higashi[4,*], Yoichiro Kuninobu[5,*], Hong-Liang Li[1,2,*]

[1] Guangxi Key Laboratory of Marine Natural Products and Combinatorial Biosynthesis Chemistry, Guangxi Academic of Marine Sciences, Guangxi Academy of Sciences, Nanning 530007, China

[2] School of Chemistry and Chemical Engineering, Guangxi University, Nanning 530005, China

[3] Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Kyoto 615-8510, Japan

[4] Department of Complex Systems Science, Graduate School of Informatics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8601, Japan

[5] Institute for Materials Chemistry and Engineering, Kyushu University, 6-1 Kasugakoen, Kasuga-shi, Fukuoka 816-8580, Japan

[#] These authors contributed to the work equally

* E-mail: Hongliang-Li@gxas.cn

* E-mail: kuninobu@cm.kyshu-u.ac.jp

* E-mail: Higashi@nagoya-u.jp

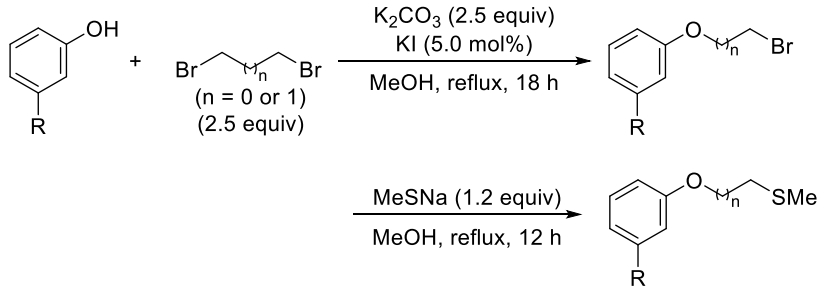
**Table of Contents**

## 1. General Information

All reactions were carried out in a dry and degassed solvent under $N_2$ atmosphere. Compounds **L1-L4, L11**, **5b**, **5c**, and **5d** were purchased from Aldrich, TCI, and Bide Pharmatech, and used without further purification unless otherwise noted. Reactions that require heating were carried out in an oil bath. Reactions were monitored by thin-layer chromatography (TLC) visualizing with UV-light (254 nm). Organic solutions were concentrated under reduced pressure using a rotary evaporator (30 °C, <50 torr). NMR spectra were recorded on 800 MHz (800 MHz for $^1$H NMR, 201 MHz for $^{13}$C NMR) spectrometers. In $^{13}$C NMR, signals of carbons adjacent to a boron atom were not observed because of the quadrupolar relaxation. HRMS/ESI were measured on Aglilent 6224 TOF LC/MS.

## 2. General procedure for the preparation of aryl substrates 1a to 1y

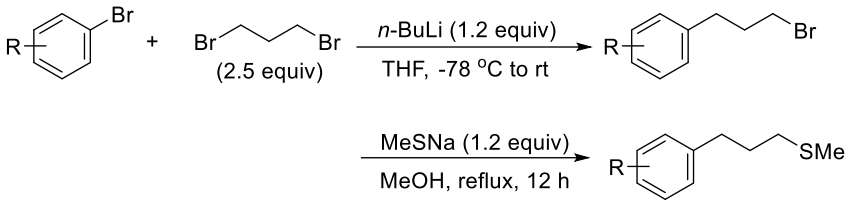
**Method-A:**[1]




**Step-1**: *meta*-Substituted-phenol (24.0 mmol) and potassium carbonate (60.0 mmol, 2.5 equiv) were dissolved in MeOH (50 mL). The mixture was refluxed for 0.5 h and dibromopropane (60.0 mmol, 2.5 equiv) and KI (1.20 mmol, 5.0 mol%) were added to the mixture, and then the reaction continued at reflux for 18 h. After removal of solvent, the crude mixture was extracted with ethyl acetate (2 x 30 mL). The organic layer was separated and dried over $Na_2SO_4$, filtered, and the solvent was removed in vacuo. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1).

**Step-2**: 1-(3-Bromopropoxy)-3-susbstituted aromatic compound (17.6 mmol) and sodium methanethiolate (1.49 g, 21.2 mmol, 1.2 equiv) in methanol (40 mL) was refluxed for overnight. The reaction mixture was diluted with ethyl acetate (60 mL) and washed with $H_2O$. The organic layer was separated, dried over $Na_2SO_4$, filtered, and the solvent was removed in vacuo. The crude product was purified by column chromatography on silica gel (hexane/ethyl acetate = 10:1).

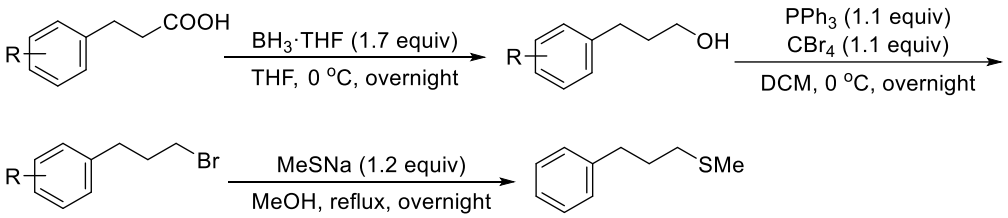
**Method-B**:[2]




**Step-1**: To a solution of substituted bromobenzene (27.0 mmol) was dissolved in dry THF (50 mL), a hexane solution of *n*-BuLi (1.6 M, 20.3 mL of in hexane, 34.4 mmol, 1.2 equiv) was added slowly at -78 °C. After stirring for 0.5 h at the same temperature, 1,3-dibromopropane (6.9 mL, 67.6 mmol, 2.5 equiv) was added dropwise. The mixture was then stirred for 2.5 h and slowly warmed to room temperature. The reaction was quenched with sat. aq. $NH_4Cl$ (20 mL) and extracted with ethyl acetate (2 x 50 mL). The organic layer was separated, dried over $Na_2SO_4$, filtered, and the solvent was removed in vacuo. The crude product was purified by column chromatography on silica gel with petroleum ether.

**Step-2**: The 1-Bromo-3-arylpropane (6.90 mmol) and sodium methanethiolate (0.575 g, 8.20 mmol, 1.2 equiv) was dissolved in methanol (20 mL) and refluxed for overnight. The work up process is the same as **method-A** (**step-2**).

**Method-C**:[3]

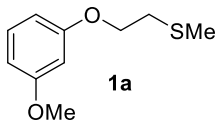



**Step-1:** The substituted hydrocinnamic acids (25.0 mmol) was dissolved in dried THF (50 mL) in a 100 mL round-bottom flask under $N_2$ atmosphere. The mixture was stirred at 0 °C and $BH_3$·THF (1.0 M, 42.5 mL, 1.7 equiv) was added slowly. After 8 h, the reaction mixture was quenched with $H_2O$ until no bubble generation. The solvent was removed under vacuum, and the residue was diluted with ethyl acetate (50 mL) and washed by brine. The organic layer was separated, dried over $Na_2SO_4$, filtered and concentrated. The crude product was directly used in next step without further purification.

**Step-2:** The crude product (23.5 mmol) and $CBr_4$ (8.59 g, 25.9 mmol, 1.1 equiv) were dissolved in DCM (50 mL) under $N_2$ atmosphere. The reaction mixture was cooled to 0 ℃ for 0.5 h, and then $PPh_3$ (6.79 g, 25.9 mmol, 1.1 equiv) was added slowly. After stirring overnight, the reaction mixture was washed with water. The organic layer was separated, dried over $Na_2SO_4$, filtered, and the solvent was removed in vacuo. The crude product was purified by column chromatography on silica gel with the mixture of petroleum ether and ethyl acetate (30:1) as an eluent.

**Step-3:** 1-Bromo-3-substituted-phenylpropane (20.0 mmol) and sodium methanethiolate (1.68 g, 24.0 mmol, 1.2 equiv) in methanol (40 mL) was refluxed overnight. The work up process is the same as **method-A** (**step-2**).

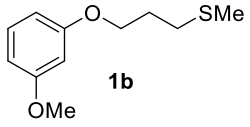
**(2-(3-Methoxyphenoxy)ethyl)(methyl)sulfane** (**1a**)



**1a**

Compound **1a** was prepared according to method A. Yield: 68%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.18 (dd, *J* = 8.2, 8.2 Hz, 1H), 6.54-6.49 (m, 2H), 6.48 (dd, *J* = 2.4, 2.4 Hz, 1H), 4.13 (t, *J* = 6.8 Hz, 2H), 3.78 (s, 3H), 2.87 (t, *J* = 6.8 Hz, 2H), 2.20 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.7, 159.6, 129.8, 106.4, 106.4, 100.9, 67.2, 55.1, 32.8, 16.0; HRMS ($ESI^+$) Calcd for $C_{10}H_{15}O_2S^+$ ($[M+H]^+$) 199.0787, Found 199.0783.

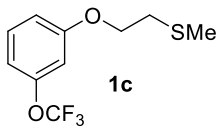
**(3-(3-Methoxyphenoxy)propyl)(methyl)sulfane** (**1b**)



**1b**

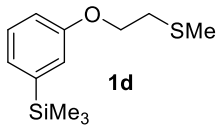
Compound **1b** was prepared according to method A. Yield: 54%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.18 (dd, *J* = 8.2, 8.2 Hz, 1H), 6.52 (d, *J* = 8.2 Hz, 2H), 6.49 (s, 1H), 4.06-4.03 (m, 2H), 3.78 (s, 3H), 2.71-2.66 (m, 2H), 2.12 (s, 3H), 2.09-2.04 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.8, 160.1, 129.9, 106.7, 106.3, 101.0, 66.2, 55.2, 30.7, 28.8, 15.6; HRMS ($ESI^+$) Calcd for $C_{11}H_{17}O_2S^+$ ($[M+H]^+$) 213.0944, Found 213.0940.

**Methyl(2-(3-(trifluoromethoxy)phenoxy)ethyl)sulfane** (**1c**)



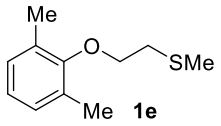

Compound **1c** was prepared according to method A. Yield: 72%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 8.3, 8.3 Hz, 1H), 6.85-6.81 (m, 2H), 6.76 (s, 1H), 4.15 (t, *J* = 6.8 Hz, 2H), 2.89 (t, *J* = 6.7 Hz, 2H), 2.22 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.5, 150.1 (q, *J* = 2.0 Hz), 130.2, 121.7 (q, *J* = 257 Hz), 113.2, 112.9, 107.7, 67.7, 32.9, 16.2; HRMS (ESI$^+$) Calcd for $C_{10}H_{11}F_3NaO_2S^+$ ([M+Na]$^+$) 275.0324, Found 275.0319.

**Trimethyl(3-(2-(methylthio)ethoxy)phenyl)silane** (**1d**)



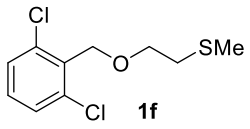

Compound **1d** was prepared according to method A. Yield: 57%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 8.3, 8.3 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 1H), 7.11 (s, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 4.21 (t, *J* = 6.9 Hz, 2H), 2.92 (t, *J* = 6.8 Hz, 2H), 2.25 (s, 3H), 0.31 (s, 9H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 157.8, 142.2, 128.9, 125.8, 119.5, 114.4, 67.1, 33.0, 16.1, -1.2; HRMS (ESI$^+$) Calcd for $C_{12}H_{20}NaOSSi^+$ ([M+Na]$^+$) 263.0896, Found 263.0891.

**(2-(2,6-Dimethylphenoxy)ethyl)(methyl)sulfane** (**1e**)




Compound **1e** was prepared according to method A. Yield: 66%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.04 (d, *J* = 7.6 Hz, 2H), 6.96 (t, *J* = 7.6 Hz, 1H), 3.99 (t, *J* = 6.8 Hz, 2H), 2.94 (t, *J* = 6.8 Hz, 2H), 2.34 (s, 6H), 2.24 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 155.4, 130.7, 128.7, 123.8, 71.1, 34.0, 16.2, 16.1; HRMS (ESI$^+$) Calcd for $C_{11}H_{16}NaOS^+$ ([M+Na]$^+$) 219.0814, Found 219.0811.

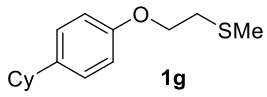
**(2-((2,6-Dichlorobenzyl)oxy)ethyl)(methyl)sulfane** (**1f**)



**1f**

Compound **1f** was prepared according to method A. Yield: 62%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.1 Hz, 2H), 7.14 (t, *J* = 8.1 Hz, 1H), 4.76 (s, 2H), 3.70 (t, *J* = 7.0 Hz, 2H), 2.68 (t, *J* = 7.0 Hz, 2H), 2.10 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 136.6, 133.0, 129.8, 128.2, 69.9, 67.0, 33.2, 15.8; HRMS (ESI$^+$) Calcd for $C_{10}H_{13}Cl_2OS^+$ ([M+H]$^+$) 251.0059, Found 251.0057.

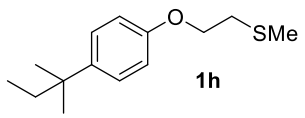
**(2-(4-Cyclohexylphenoxy)ethyl)(methyl)sulfane** (**1g**)



**1g**

Compound **1g** was prepared according to method A. Yield: 49%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.13 (d, *J* = 8.7 Hz, 2H), 6.85 (d, *J* = 8.7 Hz, 2H), 4.15 (t, *J* = 6.9 Hz, 2H), 2.88 (t, *J* = 6.9 Hz, 2H), 2.51-2.43 (m, 1H), 2.22 (s, 3H), 1.92-1.82 (m, 4H), 1.78-1.72 (m, 1H), 1.43-1.36 (m, 4H), 1.29-1.24 (m, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.5, 140.7, 127.6, 114.3, 67.4, 43.7, 34.7, 33.1, 26.9, 26.1, 16.7; HRMS (ESI$^+$) Calcd for $C_{15}H_{22}NaOS^+$ ([M+Na]$^+$) 273.1284, Found 273.1276.

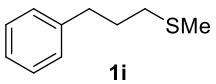
**Methyl(2-(4-(*tert*-pentyl)phenoxy)ethyl)sulfane** (**1h**)



**1h**

Compound **1h** was prepared according to method A. Yield: 70%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.9 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 4.16 (t, *J* = 6.8 Hz, 2H), 2.89 (t, *J* = 6.8 Hz, 2H), 2.22 (s, 3H), 1.63 (q, *J* = 7.5 Hz, 2H), 1.28 (s, 6H), 0.69 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.0, 141.8, 126.8, 113.8, 67.3, 37.2, 36.8, 33.0, 28.5, 16.1, 9.1; HRMS (ESI$^+$) Calcd for $C_{14}H_{22}NaOS^+$ ([M+Na]$^+$) 261.1284, Found 261.1280.

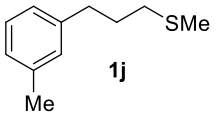
**Methyl(3-phenylpropyl)sulfane** (**1i**)




**1i**

Compound **1i** was prepared according to method B. Yield: 67%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.35-7.31 (m, 2H), 7.27-7.24 (m, 3H), 2.77 (t, *J* = 5.9 Hz, 2H), 2.57-2.53 (m, 2H), 2.14 (s, 3H), 2.00-1.95 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.5, 128.3, 128.2, 125.8, 34.6, 33.4, 30.5, 15.3; HRMS (ESI$^+$) Calcd for $C_{10}H_{15}S^+$ ([M+H]$^+$) 167.0889, Found 167.0889.

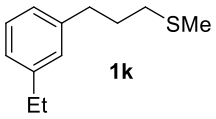
**Methyl(3-(m-tolyl)propyl)sulfane** (**1j**)




**1j**

Compound **1j** was prepared according to method B. Yield: 54%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.24 (s, 1H), 7.09-7.04 (m, 3H), 2.77-2.73 (m, 2H), 2.59-2.55 (m, 2H), 2.40 (s, 3H), 2.15 (s, 3H), 2.00-1.95 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.3, 137.7, 129.1, 128.1, 126.4, 125.3, 34.5, 33.4, 30.5, 21.2, 15.2; HRMS (ESI$^+$) Calcd for $C_{11}H_{17}S^+$ ([M+H]$^+$) 181.1045, Found 181.1044.

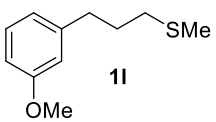
**(3-(3-Ethylphenyl)propyl)(methyl)sulfane** (**1k**)




**1k**

Compound **1k** was prepared according to method B. Yield: 40%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.13-7.11 (m, 2H), 7.09 (d, *J* = 6.1 Hz, 1H), 2.79 (t, *J* = 7.6, Hz, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 2.59 (t, *J* = 7.2 Hz, 2H), 2.17 (s, 3H), 2.03-1.97 (m, 2H), 1.35-1.31 (t, *J* = 8.0 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 144.1, 141.4, 128.2, 127.9, 125.6, 125.2, 34.6, 33.5, 30.6, 28.7, 15.5, 15.2; HRMS (ESI$^+$) Calcd for $C_{12}H_{19}S^+$ ([M+H]$^+$) 195.1202, Found 195.1198.

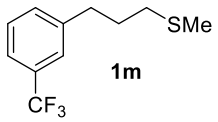
**(3-(3-Methoxyphenyl)propyl)(methyl)sulfane** (**1l**)




**1l**

Compound **1l** was prepared according to method C. Yield: 78%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 7.7, 7.7 Hz, 1H), 6.81 (d, *J* = 5.9 Hz, 1H), 6.78-6.75 (m, 2H), 3.80 (s, 3H), 2.72 (t, *J* = 7.7 Hz, 2H), 2.52 (t, *J* = 7.3 Hz, 2H), 2.11 (s, 3H), 1.94 (tt, *J* = 7.7, 7.3 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.5, 143.1, 129.2, 120.7, 114.1, 111.0, 54.9, 34.6, 33.4, 30.4, 15.3; HRMS (ESI$^+$) Calcd for $C_{11}H_{17}OS^+$ ([M+H]$^+$) 197.0995, Found 197.0992.

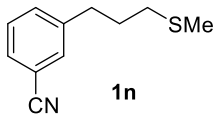
**Methyl(3-(3-(trifluoromethyl)phenyl)propyl)sulfane** (**1m**)



**1m**

Compound **1m** was prepared according to method C. Yield: 65%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.47-7.44 (m, 2H), 7.41-7.36 (m, 2H), 2.80-2.77 (m, 2H), 2.51 (t, *J* = 7.2 Hz, 2H), 2.10 (s, 3H), 1.96-1.91 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 142.4, 131.8, 130.8 (q, *J* = 32.0 Hz), 128.7, 125.5 (q, *J* = 271 Hz), 125.0 (q, *J* = 2.0 Hz), 122.7 (q, *J* = 2.0 Hz), 34.3, 33.3, 30.3, 15.2; HRMS (ESI$^+$) Calcd for $C_{11}H_{14}F_3S^+$ ([M+H]$^+$) 235.0763, Found 235.0761.

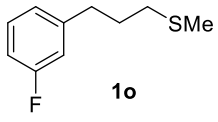
**3-(3-(Methylthio)propyl)benzonitrile** (**1n**)



**1n**

Compound **1n** was prepared according to method C. Yield: 50%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.46-7.42 (m, 2H), 7.40 (dd, *J* = 6.8, 6.8 Hz, 1H), 7.37-7.33 (m, 1H), 2.75-2.70 (m, 2H), 2.48-2.44 (m, 2H), 2.06 (s, 3H), 1.91-1.85 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 142.8, 132.9, 131.7, 129.5, 129.0, 118.8, 112.1, 33.9, 33.1, 29.9, 15.2; HRMS (ESI$^+$) Calcd for $C_{11}H_{14}NS^+$ ([M+H]$^+$) 192.0841, Found 192.0840.

**(3-(3-Fluorophenyl)propyl)(methyl)sulfane** (**1o**)

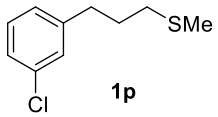


**1o**

Compound **1o** was prepared according to method C. Yield: 56%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.25-7.22 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.92-6.86 (m, 2H), 2.72 (t, *J* = 7.7 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.10 (s, 3H), 1.94-1.89 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 163.4 (d, *J* = 245 Hz), 144.1 (d, *J* = 6.0 Hz), 129.7 (d, *J* = 8.0 Hz), 124.0 (d, *J* = 4.0 Hz), 115.2 (d, *J* = 20.0

Hz), 112.7 (d, *J* = 22.0 Hz), 34.3, 33.3, 30.2, 15.3; HRMS (ESI$^+$) Calcd for $C_{10}H_{14}FS^+$ ([M+H]$^+$) 185.0795, Found 185.0784.

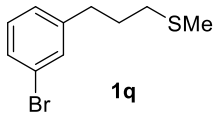
**(3-(3-Chlorophenyl)propyl)(methyl)sulfane** (**1p**)




**1p**

Compound **1p** was prepared according to method C. Yield: 63%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.22-7.15 (m, 3H), 7.07 (d, *J* = 7.6 Hz, 1H), 2.70 (t, *J* = 7.8 Hz, 2H), 2.49 (t, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.90 (tt, *J* = 7.8, 7.2 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.5, 134.0, 129.5, 128.4, 126.6, 126.0, 34.2, 33.3, 30.2, 15.3; HRMS (ESI$^+$) Calcd for $C_{10}H_{13}ClNaS^+$ ([M+Na]$^+$) 223.0319, Found 223.0318.

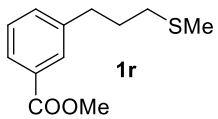
**(3-(3-Bromophenyl)propyl)(methyl)sulfane** (**1q**)




**1q**

Compound **1q** was prepared according to method C. Yield: 78%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.15 (dd, *J* = 7.8, 7.7 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 2.69 (t, *J* = 7.6 Hz, 2H), 2.49 (t, *J* = 7.3 Hz, 2H), 2.09 (s, 3H), 1.90 (tt, *J* = 7.6, 7.3 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.9, 131.4, 129.9, 128.9, 127.1, 122.4, 34.2, 33.3, 30.3, 15.4; HRMS (ESI$^+$) Calcd for $C_{10}H_{14}BrS^+$ ([M+H]$^+$) 244.9994, Found 244.9992.

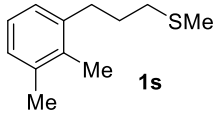
**Methyl 3-(3-(methylthio)propyl)benzoate** (**1r**)




**1r**

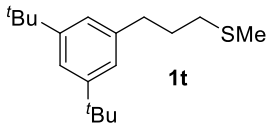
Compound **1r** was prepared according to method C. Yield: 62 %; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.87-7.84 (m, 2H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.34 (dd, *J* = 7.6, 7.5 Hz, 1H), 3.90 (s, 3H), 2.76 (t, *J* = 7.7 Hz, 2H), 2.49 (t, *J* = 7.3 Hz, 2H), 2.08 (s, 3H), 1.92 (tt, *J* = 7.7, 7.3 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 167.1, 141.8, 133.1, 130.1, 129.4, 128.3, 127.2, 52.0, 34.4, 33.4, 30.4, 15.4; HRMS (ESI$^+$) Calcd for $C_{12}H_{17}O_2S^+$ ([M+H]$^+$) 225.0944, Found 225.0942.

**(3-(2,3-Dimethylphenyl)propyl)(methyl)sulfane** (**1s**)



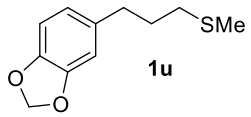

Compound **1s** was prepared according to method C. Yield: 55%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.15-7.09 (m, 3H), 2.87-2.82 (m, 2H), 2.65 (t, *J* = 7.3 Hz, 2H), 2.39 (s, 3H), 2.32 (s, 3H), 2.20 (s, 3H), 2.00-1.93 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 139.5, 136.7, 134.2, 127.7, 126.9, 125.2, 33.9, 32.8, 29.6, 20.6, 15.3, 14.8; HRMS (ESI$^+$) Calcd for $C_{12}H_{19}S^+$ ([M+H]$^+$) 195.1202, Found 195.1200.

**(3-(3,5-Di-*tert*-butylphenyl)propyl)(methyl)sulfane** (**1t**)



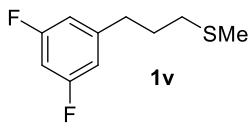

Compound **1t** was prepared according to method C. Yield: 76%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.14 (s, 2H), 2.81 (t, *J* = 7.6 Hz, 2H), 2.63 (t, *J* = 7.1 Hz, 2H), 2.19 (s, 3H), 2.06-2.00 (m, 2H), 1.42 (s, 18H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 150.5, 140.6, 122.6, 119.8, 35.3, 34.7, 33.8, 31.5, 30.9, 15.4; HRMS (ESI$^+$) Calcd for $C_{18}H_{31}S^+$ ([M+H]$^+$) 279.2141, Found 279.2137.

**5-(3-(Methylthio)propyl)benzo[*d*][1,3]dioxole** (**1u**)



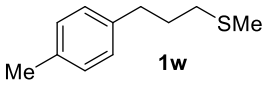

Compound **1u** was prepared according to method C. Yield: 62%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 6.72 (d, *J* = 7.9 Hz, 1H), 6.68 (s, 1H), 6.62 (d, *J* = 7.9 Hz, 1H), 5.89 (s, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 2.48 (t, *J* = 7.3 Hz, 2H), 2.08 (s, 3H), 1.86 (tt, *J* = 7.6, 7.3 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 147.4, 145.5, 135.2, 121.0, 108.7, 107.9, 100.6, 34.2, 33.2, 30.6, 15.2; HRMS (ESI$^+$) Calcd for $C_{11}H_{15}O_2S^+$ ([M+H]$^+$) 211.0787, Found 211.0785.

**Methyl 3-(3-(methylthio)propyl)benzoate** (**1v**)



Compound **1v** was prepared according to method C. Yield:70 %; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 6.72-6.68 (m, 2H), 6.62 (t, *J* = 9.0 Hz, 1H), 2.70 (t, *J* = 7.6 Hz, 2H), 2.49 (t, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.89 (tt, *J* = 7.6, 7.2 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 163.6 (dd, *J* = 248, 12.9 Hz), 145.5 (t, *J* = 9.0 Hz), 111.2 (dd, *J* = 20.1, 3.9 Hz), 101.4 (t, *J* = 25.3 Hz), 34.3, 33.2, 29.9, 15.3; HRMS (ESI$^+$) Calcd for $C_{10}H_{12}F_2NaS^+$ ([M+Na]$^+$) 225.0520, Found 225.0521.

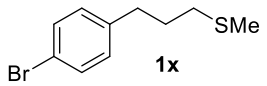
**(3-(2,3-Dimethylphenyl)propyl)(methyl)sulfane** (**1w**)




**1w**

Compound **1w** was prepared according to method C. Yield: 80%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.18-7.14 (m, 4H), 2.78-2.73 (m, 2H), 2.59-2.55 (m, 2H), 2.39 (s, 3H), 2.15 (s, 3H), 2.00-1.94 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 138.3, 135.1, 128.9, 128.2, 34.1, 33.4, 30.6, 20.9, 15.3; HRMS (ESI$^+$) Calcd for $C_{11}H_{16}NaS^+$ ([M+Na]$^+$) 230.0865, Found 230.0865.

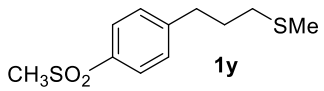
**(3-(4-Bromophenyl)propyl)(methyl)sulfane** (**1x**)




**1x**

Compound **1x** was prepared according to method C. Yield: 73%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.3 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 2.67 (t, *J* = 7.6 Hz, 2H), 2.49-2.46 (m, 2H), 2.08 (s, 3H), 1.90-1.86 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 140.4, 131.3, 130.1, 119.5, 33.9, 33.3, 30.3, 15.3; HRMS (ESI$^+$) Calcd for $C_{10}H_{14}BrS^+$ ([M+H]$^+$) 244.9994, Found 244.9986.

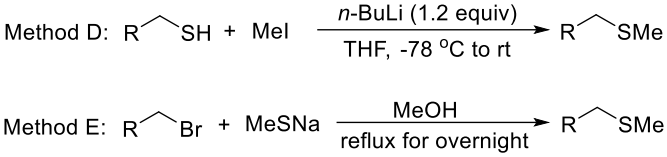
**Methyl(3-(*p*-tolyl)propyl)sulfane** (**1y**)




**1y**

Compound **1y** was prepared according to method C. Yield: 60%; white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 3.03 (s, 3H), 2.83-2.79 (m,, 2H), 2.51-2.47 (m, 2H), 2.09 (s, 3H), 1.95-1.90 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 148.2, 138.1, 129.4, 127.5, 44.5, 34.4, 33.3, 30.1, 15.4. HRMS (ESI$^+$) Calcd for $C_{11}H_{16}NaO_2S_2^+$ ([M+H]$^+$) 267.0484, Found 267.0478.

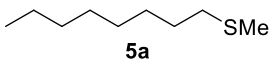
**3. General procedure for the preparation of aliphatic substrates 5a and 5c to 5j**




**Method D**:[4] To a solution of aliphatic mercaptan (10.0 mmol) in anhydrous THF (25 mL), a hexane solution of *n*-BuLi (2.5 M, 4.8 mL, 12 mmol, 1.2 equiv) was added slowly at -78 °C. After stirring for 0.5 h at the same temperature, 1-iodomethane (2.84 g, 20.0 mmol, 2.0 equiv) was added dropwise. The mixture was then stirred for 2.5 h and slowly warmed to room temperature. After removal of the solvent under vacuum, the mixture was extracted with dichloromethane (2 x 30 mL). The organic layer was separated, dried over $Na_2SO_4$, filtered, and the solvent was removed in vacuo. The crude product was purified by column chromatography on silica gel (petroleum/ethyl acetate = 20:1).

**Method E**: 1-Bromoalkane (5.00 mmol) and sodium methanethiolate (0.421 g, 6.00 mmol, 1.2 equiv) were dissolved in methanol (15 mL) and the mixture was refluxed for overnight. The work up process is the same as **method-A** (**step-2**).

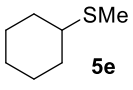
**Methyl(octyl)sulfane** (**5a**)




**5a**

Compound **5a** was prepared according to method D. Yield: 82%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 2.47-2.43 (m, 2H), 2.06 (s, 3H), 1.58-1.53 (m, 2H), 1.34 (t, *J* = 8.0 Hz, 2H), 1.29-1.19 (m, 8H), 0.85 (t, *J* = 7.1 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 34.2, 31.7, 29.3, 29.2, 29.1, 28.8, 22.6, 15.4, 14.0; HRMS (ESI$^+$) Calcd for $C_9H_{21}S^+$ ([M+H]$^+$) 161.1358, Found 161.1358.

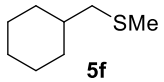
**Cyclohexyl(methyl)sulfane** (**5e**)




**5e**

Compound **5e** was prepared according to method E. Yield: 66%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 2.51-2.47 (m, 1H), 2.04 (s, 3H), 1.94-1.91 (m, 2H), 1.77-1.70 (m, 2H), 1.59-1.56 (m, 1H), 1.29-1.23 (m, 4H), 1.21-1.17 (m, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 44.7, 33.0, 26.0, 25.8, 13.1; HRMS (ESI$^+$) Calcd for $C_7H_{14}NaS^+$ ([M+Na]$^+$) 153.0708, Found 153.0714.

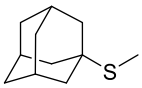
**(Cyclohexylmethyl)(methyl)sulfane** (**5f**)




**5f**

Compound **5f** was prepared according to method E. Yield: 54%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 2.35 (d, *J* = 6.9 Hz, 2H), 2.05 (s, 3H), 1.82 (d, *J* = 14.1 Hz, 2H), 1.69 (d, *J* = 15.4 Hz, 2H), 1.63 (d, *J* = 17.9 Hz, 1H), 1.48-1.42 (m, 1H), 1.24-1.17 (m, 2H), 1.16-1.09 (m, 1H), 0.95-0.88 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 42.1, 37.4, 32.7, 26.3, 26.0, 16.2; HRMS ($ESI^+$) Calcd for $C_8H_{17}S^+$ ($[M+H]^+$) 145.1045, Found 145.1043.

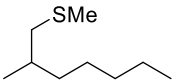
**Adamantan-1-yl-methyl sulfane** (**5g**)




**5g**

Compound **5g** was prepared according to method E. Yield: 46%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 2.04-2.00 (m, 3H), 1.99-1.97 (m, 3H), 1.83-1.80 (m, 6H), 1.71-1.67 (m, 3H), 1.66-1.62 (m, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 42.7, 36.3, 29.5, 8.7; HRMS ($ESI^+$) Calcd for $C_{11}H_{18}NaS^+$ ($[M+Na]^+$) 205.1021, Found 205.1019.

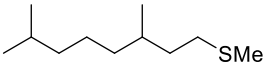
**Methyl(2-methylheptyl)sulfane** (**5h**)




**5h**

Compound **5h** was prepared according to method E. Yield: 52%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 2.41 (q, *J* = 5.6 Hz, 2H), 2.02 (s, 3H), 1.48-1.42 (m, 1H), 1.41-1.30 (m, 3H), 1.30-1.17 (m, 5H), 0.88-0.79 (m, 6H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 39.0, 38.8, 32.2, 28.7, 25.4, 22.9, 16.1, 13.9, 10.6; HRMS ($ESI^+$) Calcd for $C_9H_{21}S^+$ ($[M+H]^+$) 161.1358, Found 161.1358.

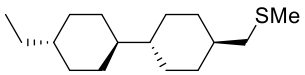
**(3,7-Dimethyloctyl)(methyl)sulfane** (**5i**)




**5i**

Compound **5i** was prepared according to method E. Yield: 60%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 2.50-2.46 (m, 1H), 2.45-2.41 (m, 1H), 2.06 (s, 3H), 1.59-1.55 (m, 1H), 1.51-1.47 (m, 2H), 1.41-1.34 (m, 1H), 1.32-1.19 (m, 3H), 1.14-1.09 (m, 3H), 0.88-0.81 (m, 9H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 39.2, 36.9, 36.3, 32.1, 32.0, 27.9, 24.6, 22.6, 22.5, 19.3, 15.4; HRMS (ESI$^+$) Calcd for $C_{11}H_{25}S^+$ ([M+H]$^+$) 189.1671, Found 189.1675.

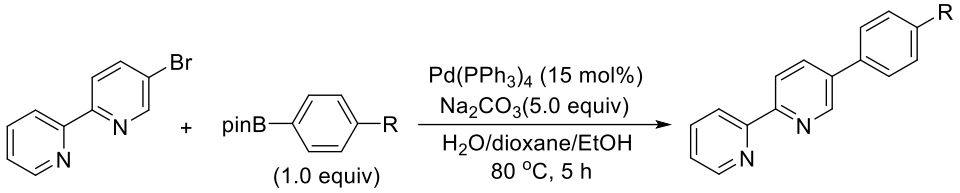
**(((1r,1'r,4R,4'R)-4'-ethyl-[1,1'-bi(cyclohexan)]-4-yl)methyl)(methyl)sulfane** (**5j**)




**5j**

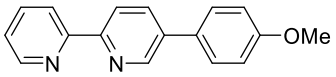
Compound **5j** was prepared according to method E. Yield: 38%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 2.37 (d, *J* = 6.9 Hz, 2H), 2.08 (s, 3H), 1.89 (d, *J* = 11.8 Hz, 2H), 1.77-1.71 (m, 4H), 1.69 (d, *J* = 13.0 Hz, 2H), 1.43-1.37 (m, 1H), 1.18 (p, *J* = 7.3 Hz, 2H), 1.04-0.88 (m, 9H), 0.87-0.79 (m, 5H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 43.3, 43.2, 42.1, 39.7, 37.8, 33.2, 33.0, 30.1, 30.0, 29.8, 16.3, 11.5; HRMS (ESI$^+$) Calcd for $C_{16}H_{31}S^+$ ([M+H]$^+$) 255.2141, Found 255.2136.

**4. General procedure for the synthesis of ligands L5-L11**.[5]




5-Bromo-2,2'-bipyridine (1.00 g, 4.27 mmol), *para*-substituted 4,4,5,5-tetramethyl-2-phenyl-1,3,2-dioxaborolane (4.27 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (745 mg, 0.640 mmol, 15 mol%), and sodium carbonate (2.30 g, 21.5 mmol, 5.0 equiv) were added into a 50 mL two-necked flask quipped with a reflux condenser. After addition of 1,4-dioxane (20 mL), EtOH (12 mL), and water (12 mL), the mixture was refluxed for 4 h. The reaction mixture was cooled to room temperature and extracted with EtOAc (2 x 20 mL). The organic phase was separated and washed with $H_2O$ (30 mL), and dried over anhydrous $Na_2SO_4$. The mixture was filtered, and the solvent was removed under vacuum and the mixture was purified by column chromatography on silica gel.

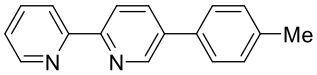
**5-(4-MethoxyphenylMethoxyphenyl)-2,2'-bipyridine** (**L5**)




**L5**

Yield: 80%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.71-8.68 (m, 1H), 8.45 (d, *J* = 8.2 Hz, 1H), 8.43-8.41 (m, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.83 (t, *J* = 6.8 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.34-7.30 (m, 1H), 7.03 (d, *J* = 8.7 Hz, 2H), 3.87 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.8, 155.9, 154.2, 149.2, 147.2, 145.0, 137.0, 136.1, 134.7, 129.9, 128.2, 123.6, 121.0, 114.6, 55.4; HRMS (ESI$^+$) Calcd for $C_{17}H_{14}N_2NaO^+$ ([M+Na]$^+$) 285.0998, Found 285.0994.

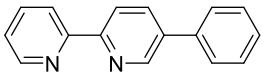
**5-(*p*-Tolyl)-2,2'-bipyridine** (**L6**)




**L6**

Yield: 66%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.72-8.69 (m, 1H), 8.46 (d, *J* = 8.1 Hz, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.84-7.80 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.31-7.28 (m, 3H), 2.42 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 155.9, 154.6, 149.2, 147.4, 138.2, 136.9, 136.4, 135.0, 134.6, 129.8, 126.9, 123.6, 121.0, 120.9, 21.2; HRMS (ESI$^+$) Calcd for $C_{17}H_{15}N_2^+$ ([M+H]$^+$) 247.1230, Found 247.1227.

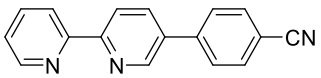
**5-Phenyl-2,2'-bipyridine** (**L7**)




**L7**

Yield: 72%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.72-8.68 (m, 1H), 8.48 (d, *J* = 8.3 Hz, 1H), 8.44 (d, *J* = 7.2 Hz, 1H), 8.04-7.99 (m, 1H), 7.86-7.80 (m, 1H), 7.67-7.62 (m, 2H), 7.51-7.47 (m, 2H), 7.43-7.39 (m, 1H), 7.33-7.29 (m, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 155.8, 154.9, 149.2, 147.6, 137.6, 136.9, 136.5, 135.2, 129.1, 128.2, 127.1, 123.7, 121.0, 120.9; HRMS (ESI$^+$) Calcd for $C_{16}H_{12}N_2Na^+$ ([M+Na]$^+$) 255.0893, Found 255.0886.

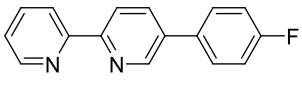
**4-(2,2'-Bipyridin]-5-yl)benzonitrile** (**L8**)




**L8**

Yield: 45%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.72 (d, *J* = 6.3 Hz, 1H), 8.54 (d, *J* = 8.2 Hz, 1H), 8.46 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.86 (dd, *J* = 8.5, 8.5 Hz, 1H), 7.80 (d, *J* = 7.9 Hz, 2H), 7.77 (d, *J* = 8.5 Hz, 2H), 7.36 (dd, *J* = 7.5, 4.7 Hz, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.1, 155.3, 149.3, 147.6, 142.1, 137.1, 135.4, 134.5, 132.9, 127.7, 124.1, 121.3, 121.2, 118.6, 111.9; HRMS ($ESI^+$) Calcd for $C_{17}H_{11}N_3Na^+$ ($[M+Na]^+$) 280.0845, Found 280.0842.

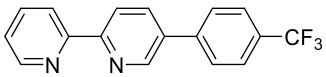
**5-(4-Fluorophenyl)-2,2'-bipyridine** (**L9**)




**L9**

Yield: 69%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.87 (s, 1H), 8.71-8.69 (m, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.00-7.96 (m, 1H), 7.86-7.82 (m, 1H), 7.63-7.60 (m, 2H), 7.34-7.31 (m, 1H), 7.21-7.17 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 170.3, 163.6 (d, *J* = 248 Hz), 155.7, 154.9, 149.2, 147.4, 137.0, 135.5, 135.1, 133.7 (d, *J* = 3.4 Hz), 128.7 (d, *J* = 8.2 Hz), 123.8, 121.0 (d, *J* = 10.9 Hz), 116.2 (d, *J* = 21.5 Hz); HRMS ($ESI^+$) Calcd for $C_{16}H_{11}FN_2Na^+$ ($[M+Na]^+$) 273.0798, Found 273.0792.

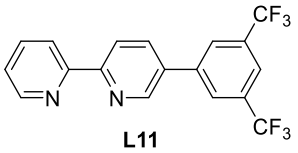
**5-(4-(Trifluoromethyl)phenyl)-2,2'-bipyridine** (**L10**)




**L10**

Yield: 84%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.71-8.69 (m, 1H), 8.53-8.49 (m, 1H), 8.47-8.43 (m, 1H), 8.04-7.99 (m, 1H), 7.86-7.82 (m, 1H), 7.77-7.73 (m, 4H), 7.35-7.32 (m, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 155.8, 155.5, 149.3, 147.6, 141.2, 137.0, 135.4, 135.0, 130.3 (q, *J* = 32.0 Hz), 127.4, 126.0, 124.1 (q, *J* = 271 Hz), 123.4, 121.2, 121.1; HRMS ($ESI^+$) Calcd for $C_{17}H_{11}F_3N_2Na^+$ ($[M+Na]^+$) 323.0767, Found 323.0761.

**5-(3,5-Bis(trifluoromethyl)phenyl)-2,2'-bipyridine** (**L11**)

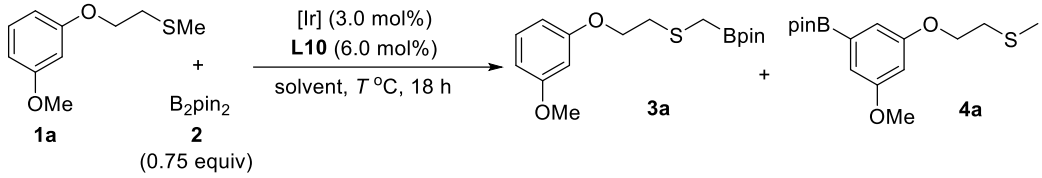



**L11**

Yield: 70%; white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.73-8.70 (m, 1H), 8.58-8.54

(m, 1H), 8.47 (d, $J$ = 6.8 Hz, 1H), 8.08-8.04 (m, 3H), 7.93 (s, 1H), 7.87-7.83 (m, 1H), 7.37-7.34 (m, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.4, 155.2, 149.3, 147.5, 139.9, 137.1, 135.4, 133.6, 132.8 (q, $J$ = 32.0 Hz), 127.1, 124.5 (q, $J$ = 271 Hz), 124.2, 121.8, 121.3, 121.2; HRMS ($ESI^+$) Calcd for $C_{18}H_{10}F_6N_2Na^+$ ($[M+Na]^+$) 391.0640, Found 391.0633.

**5. Optimization of reaction conditions**




A mixture of [Ir] (3.0 mol%), **L10** (6.0 mol%), and $B_2pin_2$ (0.75 equiv) were added to a solution of (2-(3-methoxyphenoxy)ethyl)(methyl)sulfane (**1a**, 49.6 mg, 0.250 mmol) in a solvent (1.5 mL). The mixture was then heated and stirred for 18 h. Then, the solvent was removed under vacuum and the yield of **3a** was isolated yield.

**Table S1. Screening of iridium catalysts in *p*-xylene**

| Entry | [Ir] | Yield (%)[a] | Ratio (**3a**:**4a**) |
|---|---|---|---|
| 1 | $[Ir(BF_4)(cod)]_2$ | 42 | 86:14 r.r. |
| 2 | $[Ir(OMe)(cod)]_2$ | 60 | 93:7 r.r |
| 3 | $[Ir(Cl)(cod)]_2$ | 65 | 99:1 r.r. |
| 4 | $[Ir(OH)(cod)]_2$ | - | - |

[a]Isolated yield of **3a** + **4a**.

**Table S2. Screening of catalytic amounts in *p*-xylene**

| Entry | $[Ir(Cl)(cod)]_2$ (X mol%) | **L10** (2X mol%) | Yield (%)[a] | Ratio (**3a**:**4a**) |
|---|---|---|---|---|
| 1 | 1.5 | 3.0 | 47 | 99:1 r.r. |
| 2 | 3.0 | 6.0 | 69 | 99:1 r.r. |
| 3 | 5.0 | 10.0 | 34 | 92:8 r.r. |
| 4 | 8.0 | 16.0 | 60 | 90:10 r.r. |

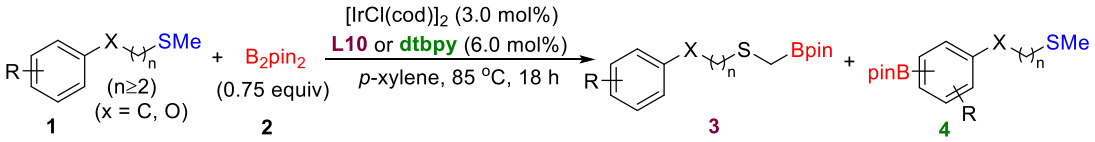
[a]Isolated yield of **3a** + **4a**.

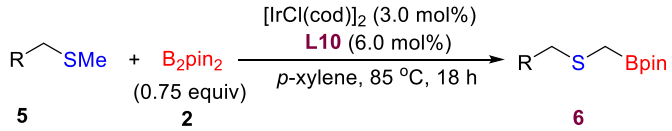
**Table S3. Screening of solvents and temperature**[a]

| Entry | solvent | Temperature (°C) | Yield (%)[b] | Ratio (**3a**:**4a**) |
|---|---|---|---|---|
| 1 | THF | 85 °C | 40 | 80:20 r.r. |
| 2 | cyclohexane | 85 °C | 36 | 94:6 r.r. |
| 3 | dioxane | 85 °C | - | - |
| 4 | $^t$BuOMe | 85 °C | - | - |
| 5 | DME | 85 °C | - | - |
| 6 | *p*-xylene | 70 °C | 33 | 98:2 r.r. |
| 7 | *p*-xylene | 100 °C | 68 | 96:4 r.r. |
| 8 | *p*-xylene | 115 °C | 62 | 55:45 r.r. |

[a][Ir(Cl)(cod)]$_2$ (3.0 mol%), **L10** (6.0 mol%). [b]Isolated yield of **3a** + **4a**.

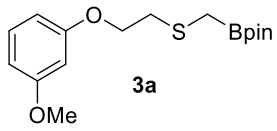
## 6. General procedure for α-C(sp$^3$)-H borylation of methyl sulfides 1a-y and 5a-j




A mixture of [Ir(Cl)(cod)]$_2$ (5.03 mg, 0.00750 mmol, 3.0 mol%), **L10** (4.50 mg, 0.0150 mmol, 6.0 mol%), and $B_2pin_2$ (47.7 mg, 0.188 mmol, 0.75 equiv) were added to a solution of methyl sulfides (**1** or **5**, 0.250 mmol) in *p*-xylene (1.5 mL) under $N_2$ atmosphere in a 10 mL sealed tube. The mixture was stirred at 85 °C for 18 h. Then, the solvent was removed under vacuum and borylation products **3**, **4**, and **6** were separated by column chromatography on silica gel using a mixture of hexane and ethyl acetate as an eluent.

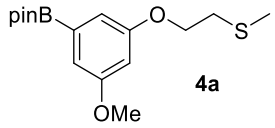
**2-(((2-(3-Methoxyphenoxy)ethyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane** (**3a**).




**3a**

**L10**: The mixture of product (53.0 mg, 65% yield, ratio of C($sp^3$)–H borylated product **3a** to C($sp^2$)–H borylated product **4a** =99:1 r.r.); yellow solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 8.2, 8.2 Hz, 1H), 6.52-6.49 (m, 2H), 6.47 (s, 1H), 4.14 (t, *J* = 7.2 Hz, 2H), 3.78 (s, 3H), 2.92 (t, *J* = 7.2 Hz, 2H), 2.08 (s, 2H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.8, 159.7, 129.8, 106.6, 106.5, 101.0, 84.0, 67.2, 55.2, 33.0, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{26}BO_4S^+$ ([M+H]$^+$) 325.1639, Found 325.1633.

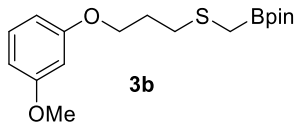
**2-(3-Methoxy-5-(2-(methylthio)ethoxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane** (**4a**)




**4a**

**dtbpy**: The mixture of product (50.4 mg, 62% yield, ratio of C($sp^3$)–H borylated product **3a** to C($sp^2$)-H borylated product **4a** = 32:68 r.r.); C($sp^2$)–H borylated product **4a** was obtained by further purification (32.2 mg); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 6.96 (s, 1H), 6.95 (s, 1H), 6.57 (s, 1H), 4.17 (t, *J* = 6.8 Hz, 2H), 3.81 (s, 3H), 2.87 (t, *J* = 6.8 Hz, 2H), 2.21 (s, 3H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.4, 159.3, 112.2, 112.0, 105.0, 83.9, 67.5, 55.4, 33.1, 24.8, 16.2; HRMS (ESI$^+$) Calcd for $C_{16}H_{25}BNaO_4S^+$ ([M+Na]$^+$) 347.1459, Found 347.1454.

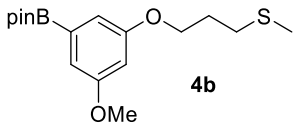
**2-(((3-(3-Methoxyphenoxy)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane** (**3b**)




**3b**

**L10**: The mixture of product (53.3 mg, 66% yield, ratio of C($sp^3$)–H borylated product **3b** to C($sp^2$)–H borylated product **4b** = 95:5 r.r.); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 8.3, 8.3 Hz, 1H), 6.49 (d, *J* = 8.3 Hz, 2H), 6.45 (s, 1H), 4.03 (t, *J* = 6.2 Hz, 2H), 3.78 (s, 3H), 2.72 (t, *J* = 7.1 Hz, 2H), 2.06 (tt, *J* = 7.1, 6.2 Hz, 2H), 1.98 (s, 2H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.7, 160.1, 129.8, 106.6, 106.3, 100.9, 83.9, 66.3, 55.2, 31.0, 28.6, 24.7; HRMS (ESI$^+$) Calcd for $C_{17}H_{28}BO_4S^+$ ([M+H]$^+$) 339.1796, Found 339.1791.

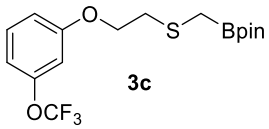
**2-(3-Methoxy-5-(3-(methylthio)propoxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane** (**4b**)




**4b**

**dtbpy**: The mixture of product (60.8 mg, 72% yield, ratio of C($sp^3$)–H borylated **3b** to C($sp^2$)–H borylated product **4b** = 34:66 r.r.); C($sp^2$)–H borylated product **4b** was obtained by further purification (38.9 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 6.95 (s, 1H), 6.94 (s, 1H), 6.56 (s, 1H), 4.08 (t, *J* = 6.0 Hz, 2H), 3.81 (s, 3H), 2.67 (t, *J* = 6.4 Hz, 2H), 2.12 (s, 3H), 2.05 (tt, *J* = 6.4, 6.0 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.4, 159.6, 112.4, 111.6, 104.8, 83.9, 66.2, 55.4, 30.7, 28.8, 24.8, 15.6; HRMS (ESI$^+$) Calcd for $C_{17}H_{27}BNaO_4S^+$ ([M+Na]$^+$) 361.1615, Found 361.1611.

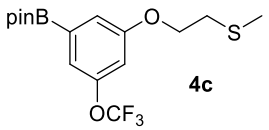
**4,4,5,5-Tetramethyl-2-(((2-(3-(trifluoromethoxy)phenoxy)ethyl)thio)methyl)-1,3,2-dioxaborolane (3c)**




**3c**

**L10**: The mixture of product (63.5 mg, 78% yield, ratio of C($sp^3$)–H borylated product **3c** to C($sp^2$)–H borylated product **4c** = 89:11 r.r.); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.28-7.24 (m, 1H), 6.84-6.79 (m, 2H), 6.75 (s, 1H), 4.15 (t, *J* = 6.9 Hz, 2H), 2.92 (t, *J* = 6.9 Hz, 2H), 2.08 (s, 2H), 1.26 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.5, 150.8 (q, *J* = 2.0 Hz), 130.2, 121.7 (q, *J* = 257 Hz), 113.1, 112.9, 107.7, 84.0, 67.7, 32.9, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{23}BF_3O_4S^+$ ([M+H]$^+$) 379.1357, Found 379.1342.

**4,4,5,5-Tetramethyl-2-(3-(2-(methylthio)ethoxy)-5-(trifluoromethoxy)phenyl)-1,3,2-dioxaborolane (4c)**

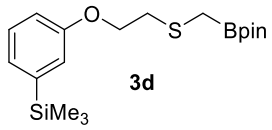



**4c**

**dtbpy**: The mixture of product (58.6 mg, 62% yield, ratio of C($sp^3$)–H borylated product **3c** to C($sp^2$)–H borylated product **4c** = 38:62 r.r.); C($sp^2$)–H borylated product **4c** was obtained by further purification (35.7 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.25-7.23 (m, 2H), 6.85 (s, 1H), 4.18 (t, *J* = 7.1 Hz, 2H), 2.88 (t, *J* = 7.1 Hz, 2H), 2.22 (s, 3H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.0, 149.7 (q, *J* = 2.0 Hz), 121.7 (q, *J* = 257 Hz), 119.8, 118.0, 111.1, 84.3,

67.8, 33.0, 24.8, 16.3; HRMS (ESI$^+$) Calcd for $C_{16}H_{22}BF_3NaO_4S^+$ ([M+Na]$^+$) 401.1176, Found 401.1164.

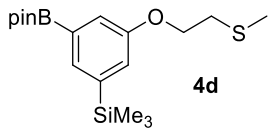
**Trimethyl(3-(2-(((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)thio)ethoxy)phenyl)silane (3d)**



**3d**

**L10**: The mixture of product (58.0 mg, 65% yield, ratio of C(sp$^3$)–H borylated product **3d** to C(sp$^2$)–H borylated product **4d** = 98:2 r.r.); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 8.3, 7.5 Hz, 1H), 7.10 (d, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 2.5 Hz, 1H), 6.88 (dd, *J* = 8.3, 2.5 Hz, 1H), 4.17 (t, *J* = 7.0 Hz, 2H), 2.94 (t, *J* = 7.0 Hz, 2H), 2.10 (s, 2H), 1.28 (s, 12H), 0.26 (s, 9H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 157.9, 142.2, 128.9, 125.7, 119.6, 114.4, 84.0, 67.0, 33.1, 24.7, -1.2; HRMS (ESI$^+$) Calcd for $C_{18}H_{32}BO_3SSi^+$ ([M+H]$^+$) 367.1929, Found 367.1915.

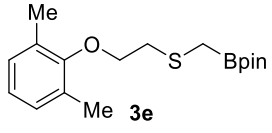
**Trimethyl(3-(2-(methylthio)ethoxy)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)silane (4d)**



**4d**

**dtbpy**: The mixture of product (52.2 mg, 57% yield, ratio of C(sp$^3$)–H borylated product **3d** to C(sp$^2$)–H borylated product **4d** = 19:81 r.r.); C(sp$^2$)–H borylated product **4d** was obtained by further purification (40.3 mg); white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.31 (s, 1H), 7.17 (s, 1H), 4.20 (t, *J* = 6.9 Hz, 2H), 2.89 (t, *J* = 6.9 Hz, 2H), 2.23 (s, 3H), 1.35 (s, 12H), 0.27 (s, 9H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 157.4, 141.7, 132.3, 123.6, 119.4, 83.8, 67.2, 33.2, 24.8, 16.2, -1.1; HRMS (ESI$^+$) Calcd for $C_{18}H_{31}BNaO_3SSi^+$ ([M+Na]$^+$) 389.1748, Found 389.1743.

**2-(((2-(2,6-Dimethylphenoxy)ethyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3e)**

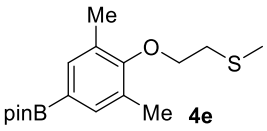


**3e**

**L10**: The mixture of product (54.5 mg, 69% yield, ratio of C(sp$^3$)–H borylated product **3e** to C(sp$^2$)–H borylated product **4e** = 98:2 r.r.); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.00 (d, *J*

= 7.5 Hz, 2H), 6.91 (t, *J* = 7.5 Hz, 1H), 3.96 (t, *J* = 7.1 Hz, 2H), 2.96 (t, *J* = 7.1 Hz, 2H), 2.29 (s, 6H), 2.07 (s, 2H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 155.6, 130.8, 128.7, 123.8, 83.9, 71.1, 33.9, 24.7, 16.3; HRMS ($ESI^+$) Calcd for $C_{17}H_{28}BO_3S^+$ ($[M+H]^+$) 323.1847, Found 323.1832.

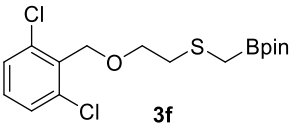
**2-(3,5-Dimethyl-4-(2-(methylthio)ethoxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4e)**



**4e**

**dtbpy**: The mixture of product (51.5 mg, 64% yield, ratio of C($sp^3$)–H borylated product **3e** to C($sp^2$)–H borylated product **4e** = 37:63 r.r.); C($sp^2$)–H borylated product **4e** was obtained by further purification (30.5 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.50-7.45 (s, 2H), 3.96 (t, *J* = 6.9 Hz, 2H), 2.90 (t, *J* = 6.9 Hz, 2H), 2.30 (s, 6H), 2.20 (s, 3H), 1.33 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 158.4, 135.6, 130.3, 83.7, 71.1, 34.1, 24.8, 16.2, 16.1; HRMS ($ESI^+$) Calcd for $C_{17}H_{27}BNaO_3S^+$ ($[M+Na]^+$) 345.1666, Found 345.1661.

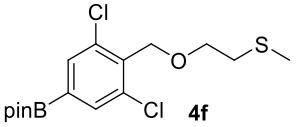
**2-(((2-((2,6-Dichlorobenzyl)oxy)ethyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3f)**



**3f**

**L10**: The mixture of product (77.1 mg, 82% yield, ratio of C($sp^3$)–H borylated product **3f** to C($sp^2$)–H borylated product **4f** = 18:82 r.r.); C($sp^3$)–H borylated product **3f** was obtained by further purification (12.5 mg); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.2 Hz, 2H), 7.17 (t, *J* = 8.1 Hz, 1H), 4.78 (s, 2H), 3.72 (t, *J* = 7.2 Hz, 2H), 2.76 (t, *J* = 7.2 Hz, 2H), 2.02 (s, 2H), 1.25 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 136.8, 133.2, 129.9, 128.3, 83.9, 69.8, 67.1, 33.4, 24.7; HRMS ($ESI^+$) Calcd for $C_{16}H_{24}BCl_2O_3S^+$ ($[M+H]^+$) 377.0911, Found 377.0909.

**2-(3,5-Dichloro-4-((2-(methylthio)ethoxy)methyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4f)**

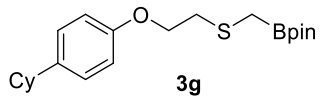


**4f**

**dtbpy**: The mixture of product (62.0 mg, 69% yield, ratio of C($sp^3$)–H borylated product **3f** to C($sp^2$)–H borylated product **4f** = 5:95 r.r.); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.69 (s,

2H), 4.79 (s, 2H), 3.69 (t, *J* = 7.4 Hz, 2H), 2.67 (t, *J* = 7.4 Hz, 2H), 2.11 (s, 3H), 1.32 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 136.5, 135.5, 134.1, 84.5, 70.0, 67.1, 33.3, 24.8, 16.0; HRMS ($ESI^+$) Calcd for $C_{16}H_{23}BCl_2NaO_3S^+$ ($[M+Na]^+$) 399.0730, Found 399.0726.

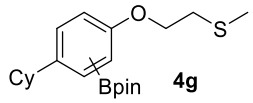
**2-(((2-(4-Cyclohexylphenoxy)ethyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3g)**




**3g**

**L10**: The mixture of product (61.1 mg, 65% yield, ratio of C($sp^3$)–H borylated product **3g** to C($sp^2$)–H borylated product **4g** = 89:11 r.r.); C($sp^3$)–H borylated product **3g** was obtained by further purification (50.3 mg); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.11 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 4.14 (t, *J* = 7.0 Hz, 2H), 2.91 (t, *J* = 7.0 Hz, 2H), 2.46-2.41 (m, 1H), 2.08 (s, 2H), 1.85-1.81 (m, 4H), 1.76-1.71 (m, 1H), 1.40-1.35 (m, 4H), 1.27 (s, 12H), 1.25-1.20 (m, 1H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.5, 140.6, 127.6, 114.3, 84.0, 67.3, 43.6, 34.7, 33.1, 26.9, 26.1, 24.7; HRMS ($ESI^+$) Calcd for $C_{21}H_{34}BO_3S^+$ ($[M+H]^+$) 377.2316, Found 377.2325.

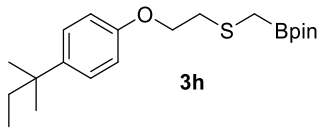
**Product of borylation at C($sp^2$)-H bond of (2-(4-cyclohexylphenoxy)ethyl)(methyl)sulfane (4g)**




**4g**

**dtbpy**: The mixture of product (56.4 mg, 60% yield, ratio of C($sp^3$)–H borylated product **3g** to C($sp^2$)–H borylated product **4g** = 67:33 r.r.); we did not isolate single C($sp^2$)–H borylated product.

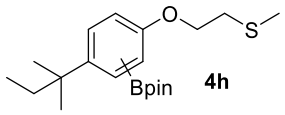
**2-(((2-(4-(*tert*-Pentyl)phenoxy)ethyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3h)**




**3h**

**L10**: The mixture of product (70.1 mg, 77% yield, ratio of C($sp^3$)–H borylated product **3h** to C($sp^2$)–H borylated product **4h** = 91:9 r.r.); C($sp^3$)–H borylated product **3h** was obtained by further purification (62.9 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.7 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 4.15 (t, *J* = 6.9 Hz, 2H), 2.92 (t, *J* = 6.9 Hz, 2H), 2.09 (s, 2H), 1.60 (q, *J* = 7.4 Hz, 3H), 1.27 (s, 12H), 1.25 (s, 6H), 0.67 (t, *J* = 7.4 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.1, 141.7, 126.9, 113.9, 84.0, 67.2, 37.2, 36.9, 33.1, 28.6, 24.7, 9.1; HRMS ($ESI^+$) Calcd for $C_{20}H_{34}BO_3S^+$ ($[M+H]^+$) 365.2316, Found 365.2312.

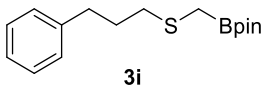
**Product of borylation at C($sp^2$)-H bond of methyl(2-(4-(tert-pentyl)phenoxy)ethyl)sulfane (4h)**




**4h**

**dtbpy**: The mixture of product (60.0 mg, 66% yield, ratio of C($sp^3$)–H borylated product **3h** to C($sp^2$)–H borylated product **4h** = 74:26 r.r.); we did not isolate single C($sp^2$)–H borylated product.

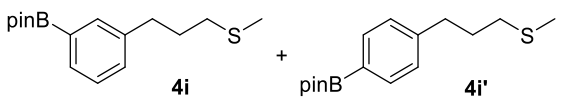
**2-(((3-Phenylpropyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3i)**




**3i**

**L10**: The mixture of product (54.1 mg, 74% yield, ratio of C($sp^3$)–H borylated product **3i** to C($sp^2$)–H borylated product (**4i** + **4i′**) = 94:6 r.r.); C($sp^3$)–H borylated product **3i** was obtained by further purification (48.8 mg); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.26 (dd, *J* = 7.7, 7.7 Hz, 2H), 7.18-7.15 (m, 3H), 2.71 (t, *J* = 7.8 Hz, 2H), 2.54 (t, *J* = 7.3 Hz, 2H), 1.95 (s, 2H), 1.91 (tt, *J* = 7.8, 7.3 Hz, 2H), 1.25 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.6, 128.4, 128.3, 125.8, 83.8, 34.7, 33.9, 30.5, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{26}BO_2S^+$ ([M+H]$^+$) 293.1741, Found 293.1734.

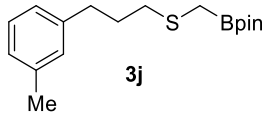
**2-(3 or 4-(3-(Methylthio)propyl)phenyl)-4,4,5,5-Tetramethyl-1,3,2-dioxaborolane (4i + 4i′)**




**4i** **4i'**

**dtbpy**: The mixture of product (46.4 mg, 63% yield, ratio of C($sp^3$)–H borylated product **3i** to C($sp^2$)–H borylated product (**4i** + **4i′**) = 5:95 r.r.); C($sp^2$)–H borylated product **4i** (28.7 mg) and **4i′** (15.4 mg) was obtained by further purification; ***meta*-isomer 4i:** colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.66-7.63 (m, 2H), 7.30-7.27 (m, 2H), 2.72 (t, *J* = 7.8 Hz, 2H), 2.51 (t, *J* = 7.5 Hz, 2H), 2.11 (s, 3H), 1.93 (tt, *J* = 7.8, 7.5 Hz, 2H), 1.35 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 140.8, 134.7, 132.4, 131.4, 127.8, 83.7, 34.7, 33.7, 30.8, 24.8, 15.4; ***para*-isomer 4i′**: colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.2 Hz, 2H), 2.74 (t, *J* = 7.7 Hz, 2H), 2.50 (t, *J* = 7.4 Hz, 2H), 2.09 (s, 3H), 1.92 (tt, *J* = 7.7, 7.4 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 145.0, 134.9, 127.9, 83.6, 34.9, 33.5, 30.4, 24.8, 15.4; HRMS (ESI$^+$) Calcd for $C_{16}H_{25}BNaO_2S^+$ ([M+Na]$^+$) 315.1561, Found 315.1557.

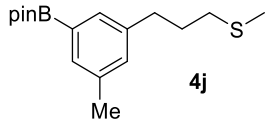
**2-(((3-(m-Tolyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3j)**




**3j**

**L10**: The mixture of product (49.5 mg, 68% yield, ratio of C($sp^3$)–H borylated product **3j** to C($sp^2$)–H borylated product **4j** = 98:2 r.r.); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.01-6.97 (m, 3H), 2.68 (t, *J* = 7.6 Hz, 2H), 2.56 (t, *J* = 7.3 Hz, 2H), 2.32 (s, 3H), 1.97 (s, 2H), 1.93-1.89 (m, 2H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.6, 137.8, 129.3, 128.2, 126.5, 125.5, 83.8, 34.7, 33.9, 30.5, 24.7, 21.4; HRMS ($ESI^+$) Calcd for $C_{17}H_{28}BO_2S^+$ ($[M+H]^+$) 307.1898, Found 307.1883.

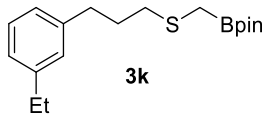
**2-(3-Methyl-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4j)**




**4j**

**dtbpy**: The mixture of product (55.9 mg, 73% yield, ratio of C($sp^3$)–H borylated product **3j** to C($sp^2$)–H borylated product **4j** = 15:85 r.r.); C($sp^2$)–H borylated product **4j** was obtained by further purification (45.2 mg); colorless solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.44 (s, 1H), 7.11 (s, 1H), 2.69 (t, *J* = 7.7 Hz, 2H), 2.50 (t, *J* = 7.3 Hz, 2H), 2.33 (s, 3H), 2.10 (s, 3H), 1.92 (tt, *J* = 7.7, 7.3 Hz, 2H), 1.35 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 140.9, 137.2, 133.0, 132.3, 131.8, 83.7, 34.7, 33.7, 30.8, 24.8, 21.2, 15.4; HRMS ($ESI^+$) Calcd for $C_{17}H_{27}BNaO_2S^+$ ($[M+Na]^+$) 329.1717, Found 329.1712.

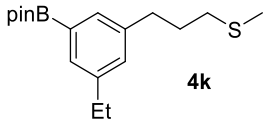
**2-(((3-(3-Ethylphenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3k)**




**3k**

**L10**: The mixture of product (58.5 mg, 75% yield, ratio of C($sp^3$)–H borylated product **3k** to C($sp^2$)–H borylated product **4k** = 98:2 r.r.); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.19 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.03-6.99 (m, 3H), 2.70 (t, *J* = 7.6 Hz, 2H), 2.62 (tt, *J* = 7.6, 7.2 Hz, 2H), 2.56 (t, *J* = 7.2 Hz, 2H), 1.97 (s, 2H), 1.92 (q, *J* = 7.6 Hz, 2H), 1.26 (s, 12H), 1.23 (t, *J* = 7.6 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 144.2, 141.7, 128.3, 128.1, 125.7, 125.3, 83.8, 34.8, 34.0, 30.6, 28.8, 24.7, 15.6; HRMS ($ESI^+$) Calcd for $C_{18}H_{30}BO_2S^+$ ($[M+H]^+$) 321.2054, Found 321.2043.

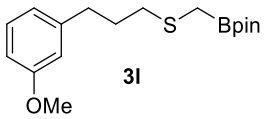
**2-(3-Ethyl-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4k)**




**4k**

**dtbpy**: The mixture of product (52.0 mg, 65% yield, ratio of C($sp^3$)–H borylated product **3k** to C($sp^2$)–H borylated product **4k** = 9:91 r.r.); C($sp^2$)–H borylated product **4k** was obtained by further purification (45.5 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.47 (s, 1H), 7.13 (s, 1H), 2.70 (t, *J* = 7.7 Hz, 2H), 2.63 (tt, *J* = 7.7, 7.3 Hz, 2H), 2.51 (t, *J* = 7.3 Hz, 2H), 2.1 (s, 3H), 1.93 (q, *J* = 7.5 Hz, 2H), 1.35 (s, 12H), 1.23 (t, *J* = 7.6 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.7, 141.0, 132.1, 131.9, 131.2, 83.7, 34.8, 33.8, 30.9, 28.7, 24.8, 15.8, 15.5; HRMS ($ESI^+$) Calcd for $C_{18}H_{29}BNaO_2S^+$ ($[M+Na]^+$) 343.1874, Found 343.1867.

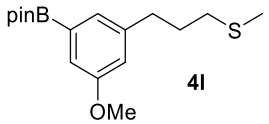
**2-(((3-(3-Methoxyphenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3l)**




**3l**

**L10**: The mixture of product (54.3 mg, 70% yield, ratio of C($sp^3$)–H borylated product **3l** to C($sp^2$)–H borylated product **4l** = 98:2 r.r.); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.18 (dd, *J* = 7.6, 7.6 Hz, 1H), 6.78 (d, *J* = 7.6 Hz, 1H), 6.74-6.71 (m, 2H), 3.79 (s, 3H), 2.69 (t, *J* = 7.7 Hz, 2H), 2.55 (t, *J* = 7.2 Hz, 2H), 1.96 (s, 2H), 1.91 (tt, *J* = 7.7, 7.2 Hz, 2H), 1.26 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.6, 143.2, 129.2, 120.8, 114.1, 111.1, 83.8, 55.0, 34.7, 33.8, 30.4, 24.7; HRMS ($ESI^+$) Calcd for $C_{17}H_{28}BO_3S^+$ ($[M+H]^+$) 323.1847, Found 323.1838.

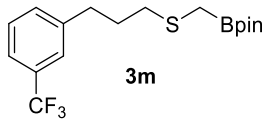
**2-(3-Methoxy-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4l)**




**4l**

**dtbpy**: The mixture of product (57.5 mg, 76% yield, ratio of C($sp^3$)–H borylated product **3l** to C($sp^2$)–H borylated product **4l** =5:95 r.r.); colorless solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.24 (s, 1H), 7.16 (s, 1H), 6.85 (s, 1H), 3.82 (s, 3H), 2.69 (t, *J* = 7.8 Hz, 2H), 2.50 (t, *J* = 7.3 Hz, 2H), 2.09 (s, 3H), 1.92 (tt, *J* = 7.8, 7.3 Hz, 2H), 1.35 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 159.2, 142.7, 127.4, 118.3, 115.9, 83.8, 55.2, 34.7, 33.7, 30.6, 24.8, 15.4; HRMS ($ESI^+$) Calcd for $C_{17}H_{27}BNaO_3S^+$ ($[M+Na]^+$) 345.1666, Found 345.1658.

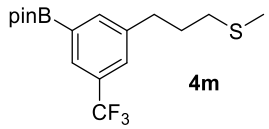
**2-(((3-(3-(Trifluoromethyl)phenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3m)**




3m

**L10**: The mixture of product (58.6 mg, 65% yield, ratio of C($sp^3$)–H borylated product **3m** to C($sp^2$)–H borylated product **4m** = 90:10 r.r.); C($sp^3$)–H borylated product **3m** was obtained by further purification (49.0 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.44-7.41 (m, 2H), 7.39-7.34 (m, 2H), 2.77 (t, *J* = 7.7 Hz, 2H), 2.55 (t, *J* = 7.2 Hz, 2H), 1.95 (s, 2H), 1.92 (tt, *J* = 7.7, 7.2 Hz, 2H), 1.24 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 142.5, 131.9, 130.8 (q, *J* = 32.0 Hz), 128.7, 125.1 (q, *J* = 2.0 Hz), 124.2 (q, *J* = 271 Hz), 122.7 (q, *J* = 4.0 Hz), 83.9, 34.4, 33.7, 30.3, 24.1; HRMS (ESI$^+$) Calcd for $C_{17}H_{25}BF_3O_2S^+$ ([M+H]$^+$) 361.1615, Found 361.1608.

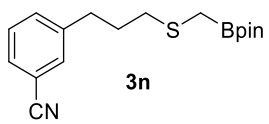
**2-(3-(3-(Methylthio)propyl)-5-(trifluoromethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4m)**




4m

**dtbpy**: The mixture of product (55.8 mg, 62% yield, ratio of C($sp^3$)–H borylated product **3m** to C($sp^2$)–H borylated product **4m** = 12:88 r.r.); C($sp^2$)–H borylated product **4m** was obtained by further purification (47.3 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.80 (s, 1H), 7.51 (s, 1H), 2.78 (t, *J* = 7.8 Hz, 2H), 2.51 (t, *J* = 7.2 Hz, 2H), 2.10 (s, 3H), 1.94 (tt, *J* = 7.8, 7.2 Hz, 2H), 1.36 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.7, 138.1, 130.3 (q, *J* = 32.0 Hz), 129.1 (q, *J* = 4.0 Hz), 127.8 (q, *J* = 2.0 Hz), 124.3 (q, *J* = 273 Hz), 84.2, 34.5, 33.6, 30.6, 24.8, 15.5; HRMS (ESI$^+$) Calcd for $C_{17}H_{24}BF_3NaO_2S^+$ ([M+H]$^+$) 383.1434, Found 383.1425.

**3-(3-(((4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)thio)propyl)benzonitrile (3n)**

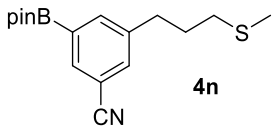



3n

**L10**: The mixture of product (48.2 mg, 67% yield, ratio of C($sp^3$)–H borylated product **3n** to C($sp^2$)–H borylated product **4n** = 92:8 r.r.); C($sp^3$)–H borylated product **3n** was obtained by further purification (48.0 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.48-7.45 (m, 2H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.38-7.35 (m, 1H), 2.75 (t, *J* = 7.7 Hz, 2H), 2.53 (t, *J* = 7.1 Hz, 2H), 1.94 (s,

2H), 1.90 (tt, *J* = 7.7, 7.1 Hz, 2H), 1.25 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.0, 133.1, 132.0, 129.7, 129.1, 118.9, 112.3, 83.9, 34.1, 33.5, 30.0, 24.7; HRMS ($ESI^+$) Calcd for $C_{17}H_{25}BNO_2S^+$ ($[M+H]^+$) 318.1694, Found 318.1690.

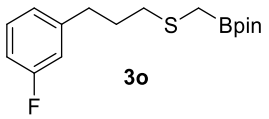
**3-(3-(Methylthio)propyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzonitrile (4n)**



**4n**

**dtbpy**: The mixture of product (50.7 mg, 64% yield, ratio of C($sp^3$)–H borylated product **3n** to C($sp^2$)–H borylated product **4n** = 14:86 r.r.); C($sp^2$)–H borylated product **4n** was obtained by further purification (42.7 mg); white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.82 (s, 1H), 7.54 (s, 1H), 2.75 (t, *J* = 7.7 Hz, 2H), 2.48 (t, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.91 (tt, *J* = 7.7, 7.2 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 142.1, 139.0, 136.0, 134.2, 118.9, 112.0, 84.4, 34.1, 33.4, 30.3, 24.8, 15.4; HRMS ($ESI^+$) Calcd for $C_{17}H_{24}BNNaO_2S^+$ ($[M+Na]^+$) 340.1513, Found 340.1508.

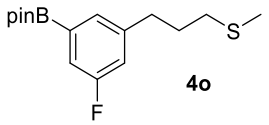
**2-(((3-(3-Fluorophenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3o)**



**3o**

**L10**: The mixture of product (47.8 mg, 74% yield, ratio of C($sp^3$)–H borylated product **3o** to C($sp^2$)–H borylated product **4o** = 90:10 r.r.); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.23-7.19 (m, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.89-6.84 (m, 2H), 2.71 (t, *J* = 7.7 Hz, 2H), 2.53 (t, *J* = 7.2 Hz, 2H), 1.95 (s, 2H), 1.90 (tt, *J* = 7.7, 7.2 Hz, 2H), 1.25 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 163.4 (d, *J* = 245 Hz), 144.2 (d, *J* = 6.0 Hz), 129.6 (d, *J* = 8.0 Hz), 124.1 (d, *J* = 2.0 Hz), 115.3 (d, *J* = 20.0 Hz), 112.7 (d, *J* = 20.0 Hz), 83.9, 34.3, 33.6, 30.1, 24.7; HRMS ($ESI^+$) Calcd for $C_{16}H_{25}BFO_2S^+$ ($[M+H]^+$) 311.1647, Found 311.1632.

**2-(3-Fluoro-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4o)**

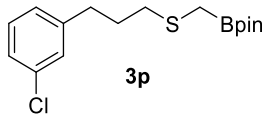


**4o**

**dtbpy**: The mixture of product (53.5 mg, 69% yield, ratio of C($sp^3$)–H borylated product **3o** to C($sp^2$)–H borylated product **4o** = 11:89 r.r.); C($sp^2$)–H borylated product **4o** was obtained by

further purification (45.5 mg); yellow oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 6.98 (d, *J* = 9.7 Hz, 1H), 2.73-2.70 (t, *J* = 7.5 Hz, 2H), 2.50-2.48 (t, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.94-1.89 (tt, *J* = 7.5, 7.2 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 163.2 (d, *J* = 245 Hz), 143.6 (d, *J* = 6.0 Hz), 130.3 (d, *J* = 4.0 Hz), 118.5 (d, *J* = 20.0 Hz), 118.2 (d, *J* = 20.0 Hz), 84.1, 34.4, 33.5, 30.5, 24.8, 15.5; HRMS (ESI$^+$) Calcd for $C_{16}H_{24}BFNaO_2S^+$ ([M+Na]$^+$) 333.1466, Found 333.1469.

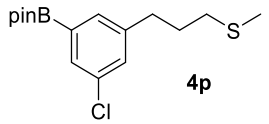
**2-(((3-(3-Chlorophenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3p)**



**3p**

**L10**: The mixture of product (48.5 mg, 63% yield, ratio of C(sp$^3$)–H borylated product **3p** to C(sp$^2$)–H borylated product **4p** = 95:5 r.r.); white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.21-7.11 (m, 3H), 7.05 (s, 1H), 2.68 (t, *J* = 7.9 Hz, 2H), 2.53 (t, *J* = 6.9 Hz, 2H), 1.94 (s, 2H), 1.89 (tt, *J* = 7.9, 6.9 Hz, 2H), 1.24 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.7, 134.1, 129.5, 128.6, 126.7, 126.0, 83.9, 34.3, 33.7, 30.2, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{25}BClO_2S^+$ ([M+H]$^+$) 327.1351, Found 327.1358.

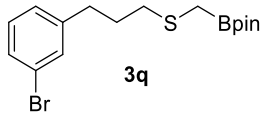
**2-(3-Chloro-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4p)**



**4p**

**dtbpy**: The mixture of product (52.7 mg, 70% yield, ratio of C(sp$^3$)–H borylated product **3p** to C(sp$^2$)–H borylated product **4p** = 6:94 r.r.); white solid; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.49 (s, 1H), 7.26 (s, 1H), 2.69 (t, *J* = 7.8 Hz, 2H), 2.49 (t, *J* = 7.3 Hz, 2H), 2.09 (s, 3H), 1.93 (tt, *J* = 7.8, 7.3 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.0, 133.9, 132.8, 132.1, 131.3, 84.1, 34.3, 33.5, 30.5, 24.8, 15.4; HRMS (ESI$^+$) Calcd for $C_{16}H_{24}BClNaO_2S^+$ ([M+Na]$^+$) 349.1171, Found 349.1163.

**2-(((3-(3-Bromophenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3q)**

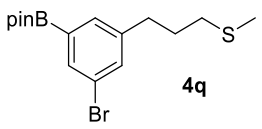


**3q**

**L10**: The mixture of product (60.0 mg, 65% yield, ratio of C(sp$^3$)–H borylated product **3q** to

C($sp^2$)–H borylated product **4q** = 93:7 r.r.); C($sp^3$)–H borylated product **3q** was obtained by further purification (54.9 mg); white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.33-7.27 (m, 2H), 7.12-7.08 (m, 2H), 2.67 (t, *J* = 7.4 Hz, 2H), 2.52 (t, *J* = 7.6 Hz, 2H), 1.96 (s, 2H), 1.91 (tt, *J* = 7.6, 7.4 Hz , 2H), 1.24 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 144.0, 131.4, 129.8, 128.9, 127.1, 122.3, 83.8, 34.2, 33.6, 30.2, 24.7; HRMS (ESI$^+$) Calcd for $C_{10}H_{15}S^+$ ([M+H]$^+$) 371.0846, Found 371.0857.

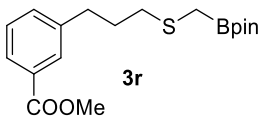
**2-(3-Bromo-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4q)**



**4q**

**dtbpy**: The mixture of product (63.0 mg, 68% yield, ratio of C($sp^3$)–H borylated product **3q** to C($sp^2$)–H borylated product **4q** = 9:91 r.r.); C($sp^2$)–H borylated product **4q** was obtained by further purification (56.8 mg); white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.54 (s, 1H), 7.43 (s, 1H), 2.71 ((t, *J* = 7.7 Hz, 2H), 2.50 ((t, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.93 (tt, *J* = 7.7, 7.2 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 143.3, 135.0, 134.2, 133.2, 122.4, 84.1, 34.3, 33.5, 30.5, 24.8, 15.5; HRMS (ESI$^+$) Calcd for $C_{16}H_{24}BBrNaO_2S^+$ ([M+Na]$^+$) 393.0666, Found 393.0652.

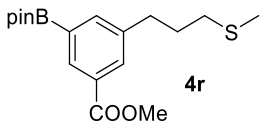
**Methyl 3-(3-(((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)thio)propyl)benzoate (3r)**



**3r**

**L10**: The mixture of product (59.5 mg, 68% yield, ratio of C($sp^3$)–H borylated product **3r** to C($sp^2$)–H borylated product **4r** = 92:8 r.r.); C($sp^3$)–H borylated product **3r** was obtained by further purification (53.7 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.85-7.83 (m, 2H), 7.36 (d, *J* = 7.7 Hz, 1H), 7.34-7.31 (m, 1H), 3.89 (s, 3H), 2.75 (t, *J* = 8.0 Hz, 2H), 2.55 (t, *J* = 7.3 Hz, 2H), 1.94 (s, 2H), 1.91 (tt, *J* = 8.0, 7.3 Hz, 2H), 1.23 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 167.1, 141.9, 133.1, 130.1, 129.5, 128.3, 127.1, 83.8, 52.0, 34.4, 33.7, 30.3, 24.7; HRMS (ESI$^+$) Calcd for $C_{18}H_{28}BO_4S^+$ ([M+H]$^+$) 351.1796, Found 351.1792.

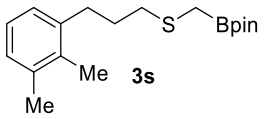
**Methyl 3-(3-(methylthio)propyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (4r)**




**4r**

**dtbpy**: The mixture of product (66.0 mg, 75% yield, ratio of C($sp^3$)–H borylated product **3r** to C($sp^2$)–H borylated product **4r** = 8:92 r.r.); C($sp^2$)–H borylated product **4r** was obtained by further purification (58.8 mg); white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.96 (s, 1H), 7.81 (s, 1H), 3.91 (s, 3H), 2.78 (t, *J* = 8.8 Hz, 2H), 2.50 (t, *J* = 7.3 Hz, 2H), 2.09 (s, 3H), 1.94 (tt, *J* = 8.8, 7.3 Hz, 2H), 1.35 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 167.3, 141.3, 139.3, 133.6, 132.3, 129.7, 84.1, 52.0, 34.5, 33.6, 30.6, 24.9, 15.5; HRMS (ESI$^+$) Calcd for $C_{18}H_{27}BNaO_4S^+$ ([M+Na]$^+$) 373.1615, Found 373.1606.

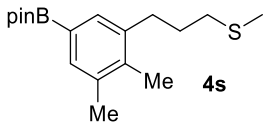
**2-(((3-(2,3-Dimethylphenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3s)**




**3s**

**L10**: The mixture of product (52.9 mg, 70% yield, ratio of C($sp^3$)–H borylated product **3s** to C($sp^2$)–H borylated product **4s** = 98:2 r.r.); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.04-6.98 (m, 3H), 2.73 (t, *J* = 7.7 Hz, 2H), 2.62 (t, *J* = 6.9 Hz, 2H), 2.28 (s, 3H), 2.21 (s, 3H), 1.98 (s, 2H), 1.88 (tt, *J* = 7.7, 6.9 Hz, 2H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 139.7, 136.8, 134.4, 127.7, 127.0, 125.3, 83.9, 34.3, 33.0, 29.6, 24.7, 20.7, 15.0; HRMS (ESI$^+$) Calcd for $C_{18}H_{30}BO_2S^+$ ([M+H]$^+$) 321.2054, Found 321.2044.

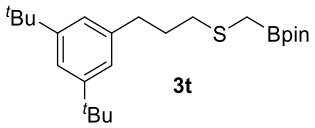
**2-(3,4-Dimethyl-5-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4s)**




**4s**

**dtbpy**: The mixture of product (45.0 mg, 56% yield, ratio of C($sp^3$)–H borylated product **3s** to C($sp^2$)–H borylated product **4s** = 12:88 r.r.); C($sp^2$)-H borylated product **4s** was obtained by further purification (38.9 mg); white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.44 (s, 1H), 2.76 (t, *J* = 8.2 Hz, 2H), 2.55 (t, *J* = 7.3 Hz, 2H), 2.29 (s, 3H), 2.23 (s, 3H), 2.11 (s, 3H), 1.88 (tt, *J* = 8.2, 7.3 Hz, 2H), 1.34 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 139.2, 138.2, 136.4, 134.2, 133.4, 83.6, 34.2, 33.1, 30.1, 24.8, 20.5, 15.5, 15.3; HRMS (ESI$^+$) Calcd for $C_{18}H_{29}BNaO_2S^+$ ([M+Na]$^+$) 343.1874, Found 343.1866.

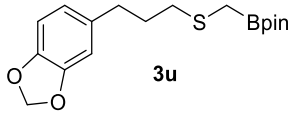
**2-(((3-(3,5-Di-tert-butylphenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3t)**




**3t**

**L10**: The C($sp^3$)–H borylated product (76.2 mg, 75% yield); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.25 (s, 1H), 7.03 (s, 2H), 2.73 (t, *J* = 8.0 Hz, 2H), 2.59 (t, *J* = 7.7 Hz, 2H), 1.99 (s, 2H), 1.96 (tt, *J* = 8.0, 7.7 Hz, 2H), 1.32 (s, 18H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 150.6, 140.7, 122.6, 119.8, 83.8, 35.4, 34.7, 34.3, 31.5, 30.9, 24.7; HRMS (ESI$^+$) Calcd for $C_{23}H_{40}BO_3S^+$ ([M+H]$^+$) 407.2786, Found 407.2780.

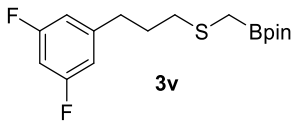
**2-(((3-(Benzo[d][1,3]dioxol-5-yl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3u)**




**3u**

**L10**: The C($sp^3$)–H borylated product (53.8 mg, 64% yield); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 6.72-6.69 (m, 1H), 6.66 (d, *J* = 4.9 Hz, 1H), 6.61 (d, *J* = 8.3 Hz, 1H), 5.91 (s, 2H), 2.65 (t, *J* = 6.9 Hz, 2H), 2.54 (t, *J* = 6.3 Hz, 2H), 1.94 (s, 2H), 1.88 (tt, *J* = 6.9, 6.3 Hz, 2H), 1.25 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 147.5, 145.6, 135.5, 121.2, 108.9, 108.1, 100.7, 83.9, 34.4, 33.7, 30.7, 24.7; HRMS (ESI$^+$) Calcd for $C_{17}H_{26}BO_4S^+$ ([M+H]$^+$) 337.1639, Found 337.1642.

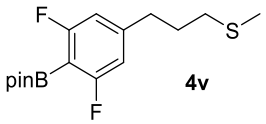
**2-(((3-(3,5-Difluorophenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3v)**




**3v**

**L10**: The mixture of product (54.1 mg, 66% yield, ratio of C($sp^3$)–H borylated product **3v** to C($sp^2$)–H borylated product **4v** = 52:48 r.r.); C($sp^3$)–H borylated product **3v** was obtained by further purification (24.5 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 6.70 (d, *J* = 8.3 Hz, 2H), 6.61 (t, *J* = 9.1 Hz, 1H), 2.70 (t, *J* = 7.5 Hz, 2H), 2.53 (t, *J* = 6.6 Hz, 2H), 1.95 (s, 2H), 1.90 (tt, *J* = 7.5, 6.6 Hz, 2H), 1.26 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 163.6 (dd, *J* = 247, 12 Hz), 146.0, 111.2 (dd, *J* = 20, 4.0 Hz), 101.4 (t, *J* = 26.0 Hz), 83.9, 34.3, 33.5, 29.8, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{24}BF_2O_2S^+$ ([M+H]$^+$) 329.1553, Found 329.1551.

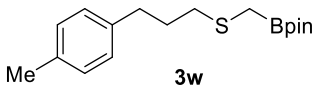
**2-(2,6-Difluoro-4-(3-(methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4v)**



**4v**

**dtbpy**: The mixture of product (59.1 mg, 72% yield, ratio of C($sp^3$)–H borylated product **3v** to C($sp^2$)–H borylated product **4v** = 7:93 r.r.); C($sp^2$)–H borylated product **4v** was obtained by further purification (53.2 mg); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 6.68 (d, *J* = 8.2 Hz, 1H), 2.69 (t, *J* = 7.6 Hz, 2H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.07 (s, 3H), 1.87 (tt, *J* = 7.6, 7.2 Hz, 2H), 1.36 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 167.3 (dd, *J* = 14, 251 Hz), 148.4 (t, *J* = 10.0 Hz), 111.1 (dd, *J* = 4.0, 24 Hz), 84.0, 34.3, 33.2, 29.7, 24.7, 15.4; HRMS (ESI$^+$) Calcd for $C_{16}H_{23}BF_2NaO_2S^+$ ([M+Na]$^+$) 351.1372, Found 351.1364.

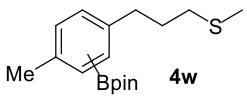
**2-(4-(3-(Methylthio)propyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3w)**



**3w**

**L10**: The mixture of product (46.0 mg, 60% yield, ratio of C($sp^3$)–H borylated product **3w** to C($sp^2$)–H borylated product **4w** = 89:11 r.r.); C($sp^3$)–H borylated product **3w** was obtained by further purification (38.8 mg); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.10-7.06 (m, 4H), 2.68 (t, *J* = 7.7 Hz, 2H), 2.57 (t, *J* = 7.4 Hz, 2H), 2.31 (s, 3H), 1.96 (s, 2H), 1.90 (tt, *J* = 7.7, 7.4 Hz, 2H), 1.26 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 138.5, 135.1, 128.9, 128.3, 83.8, 34.3, 33.8, 30.6, 24.7, 20.9; HRMS (ESI$^+$) Calcd for $C_{17}H_{28}BO_2S^+$ ([M+H]$^+$) 307.1898, Found 307.1903.

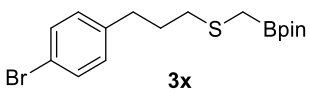
**Borylation at C($sp^2$)-H bond of methyl(3-(p-tolyl)propyl)sulfane (4w)**



**4w**

**dtbpy**: The mixture of product (42.9 mg, 56% yield, ratio of C($sp^3$)–H borylated product **3w** to C($sp^2$)–H borylated product **4w** = 76:24 r.r.); we did not isolate single C($sp^2$)–H borylated product.

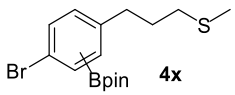
**2-(((3-(4-Bromophenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3x)**



**3x**

**L10**: The mixture of product (50.5 mg, 55% yield, ratio of C($sp^3$)–H borylated product **3x** to C($sp^2$)–H borylated product **4x** = 90:10 r.r.); C($sp^3$)–H borylated product **3x** was obtained by further purification (44.7 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 2.66 (t, *J* = 7.6 Hz, 2H), 2.51 (t, *J* = 7.3 Hz, 2H), 1.93 (s, 2H), 1.87 (tt, *J* = 7.6, 7.3 Hz, 2H), 1.24 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 140.5, 131.3, 130.2, 119.5, 83.8, 34.0, 33.6, 30.2, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{25}BBrO_2S^+$ ([M+H]$^+$) 371.0846, Found 371.0850.

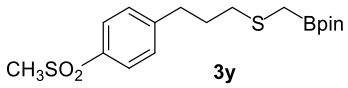
**Borylation at C($sp^2$)-H bond of (3-(4-bromophenyl)propyl)(methyl)sulfane (4x)**



**4x**

**dtbpy**: The mixture of product (55.5 mg, 60% yield, ratio of C($sp^3$)–H borylated product **3x** to C($sp^2$)–H borylated product **4x** = 71:29 r.r.); we did not isolate single C($sp^2$)–H borylated product.

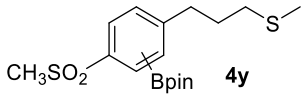
**2-(((3-(4-(Methylsulfonyl)phenyl)propyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3y)**



**3y**

**L10**: The mixture of product (48.3 mg, 63% yield, ratio of C($sp^3$)–H borylated product **3y** to C($sp^2$)–H borylated product **4y** = 85:15 r.r.); C($sp^3$)–H borylated product **3y** was obtained by further purification (53.2 mg); yellow oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 3.02 (s, 3H), 2.80 (t, *J* = 7.5 Hz, 2H), 2.56 (t, *J* = 7.7 Hz, 2H), 1.95 (tt, *J* = 7.7, 7.5 Hz, 2H), 1.92 (s, 2H), 1.24 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 148.3, 138.1, 129.4, 127.5, 83.9, 44.5, 34.5, 33.6, 30.0, 24.7; HRMS (ESI$^+$) Calcd for $C_{10}H_{15}S^+$ ([M+H]$^+$) 371.1517, Found 371.1523.

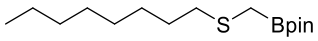
**Borylation at C($sp^2$)-H bond of methyl(3-(4-(methylsulfonyl)phenyl)propyl)sulfane (4y)**



**4y**

**dtbpy**: The mixture of crude product (52.7 mg, 57% yield, ratio of C($sp^3$)–H borylated product **3y** to C($sp^2$)–H borylated product **4y** = 79:21 r.r.); we did not isolate single C($sp^2$)–H borylated product.

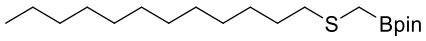
**2-((Octylthio)methyl)- 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6a)**




**6a**

The C($sp^3$)–H borylated product **6a** was obtained by further purification (50.0 mg, 70% yield; colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.53-2.49 (m, 2H), 1.94 (s, 2H), 1.57 (tt, *J* = 7.6, 7.6 Hz, 2H), 1.37-1.32 (m, 2H), 1.29-1.21 (m, 20H), 0.86 (t, *J* = 7.2 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 34.6, 31.8, 29.2, 29.1, 28.8, 24.8, 24.7, 22.6, 14.1; HRMS (ESI$^+$) Calcd for $C_{15}H_{32}BO_2S^+$ ([M+H]$^+$) 287.2211, Found 287.2210.

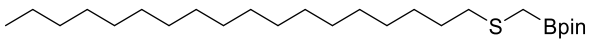
**2-((Dodecylthio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6b)**




**6b**

The C($sp^3$)–H borylated product **6b** was obtained by further purification (54.8 mg, 64% yield, colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.52-2.49 (m, 2H), 1.94 (s, 2H), 1.56 (tt, *J* = 7.5, 7.5 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 2H), 1.27-1.22 (m, 28H), 0.86 (t, *J* = 7.2 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 34.6, 31.9, 29.6, 29.59, 29.57, 29.5, 29.3, 29.2, 29.1, 28.8, 24.7, 22.6, 14.1; HRMS (ESI$^+$) Calcd for $C_{19}H_{40}BO_2S^+$ ([M+H]$^+$) 343.2837, Found 343.2829.

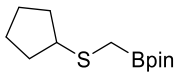
**2-((Octadecylthio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6c)**




**6c**

The C($sp^3$)–H borylated product **6c** was obtained by further purification (76.7 mg, 72% yield, white solid); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.52 (t, *J* = 8.2 Hz, 2H), 1.94 (s, 2H), 1.60-1.55 (m, 2H), 1.38-1.34 (m, 2H), 1.34-1.17 (m, 40H), 0.87 (t, *J* = 7.9 Hz, 3H); $^{13}$CNMR ($CDCl_3$, 201 MHz) δ 83.8, 34.6, 31.9, 29.67, 29.65, 29.64, 29.60, 29.5, 29.33, 29.25, 29.2, 29.14, 29.10, 28.9, 24.8, 24.74, 24.72, 22.7, 14.08, 14.05; HRMS (ESI$^+$) Calcd for $C_{25}H_{52}BO_2S^+$ ([M+H]$^+$) 427.3776, Found 427.3770.

**2-((Cyclopentylthio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6d)**

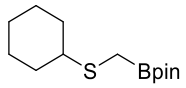



**6d**

The C($sp^3$)–H borylated product **6d** was obtained by further purification (32.7 mg, 54% yield; yellow oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 3.09-3.05 (m, 1H), 2.00 (d, *J* = 2.0 Hz, 2H), 1.98-1.93

(m, 2H), 1.73-1.70 (m, 2H), 1.56-1.50 (m, 4H), 1.26 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 46.0, 33.2, 24.8, 24.7; HRMS (ESI): A target mass was not detected.

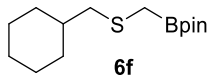
**2-((Cyclohexylthio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6e)**




**6e**

The C(sp$^3$)–H borylated product **6e** was obtained by further purification (42.3 mg, 65% yield; colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.61-2.53 (m, 1H), 2.06-1.93 (m, 4H), 1.77-1.70 (m, 2H), 1.61-1.56 (m, 1H), 1.30-1.18 (m, 17H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 45.1, 32.9, 26.0, 25.8, 24.7; HRMS (ESI$^+$) Calcd for $C_{13}H_{26}BO_2S^+$ ([M+H]$^+$) 257.1741, Found 27.1753.

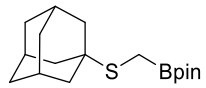
**2-(((Cyclohexylmethyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6f)**




**6f**

The C(sp$^3$)–H borylated product **6f** was obtained by further purification (45.9 mg, 68% yield; colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.42 (d, *J* = 6.9 Hz, 2H), 1.93 (s, 2H), 1.85-1.81 (m, 2H), 1.71-1.67 (m, 2H), 1.66-1.60 (m, 2H), 1.50-1.46 (m, 1H), 1.26 (s, 12H), 1.20-1.09 (m, 2H), 0.95-0.89 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 42.4, 37.4, 32.8, 26.1, 24.8, 24.7; HRMS (ESI$^+$) Calcd for $C_{14}H_{28}BO_2S^+$ ([M+H]$^+$) 271.1898, Found 271.1890.

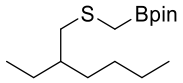
**2-((((3s,5s,7s)-Adamantan1-yl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6g)**




**6g**

The C(sp$^3$)–H borylated product **6g** was obtained by further purification (48.0 mg, 62% yield, white solid); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.03-2.01 (m, 3H), 1.96 (s, 2H), 1.83-1.81 (m, 6H), 1.70-1.66 (m, 3H), 1.65-1.62 (m, 3H), 1.26 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.9, 42.6, 36.4, 29.6, 24.7; HRMS (ESI$^+$) Calcd for $C_{17}H_{30}BO_2S^+$ ([M+H]$^+$) 309.2054, Found 309.2057.

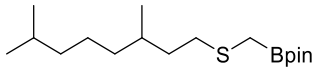
**2-(((2-Ethylhexyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6h)**




**6h**

The C($sp^3$)–H borylated product **6h** was obtained by further purification (51.1 mg, 73% yield; colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.50 (d, *J* = 6.5 Hz, 2H), 1.91 (s, 2H), 1.49-1.45 (m, 1H), 1.43-1.38 (m, 1H), 1.37-1.32 (m, 2H), 1.28-1.20 (m, 17H), 0.87 (t, *J* = 7.2 Hz, 3H), 0.84 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 39.3, 38.8, 32.4, 28.8, 25.5, 24.7, 22.9, 14.1, 10.7; HRMS ($ESI^+$) Calcd for $C_{15}H_{32}BO_2S^+$ ($[M+H]^+$) 281.2211, Found 281.2220.

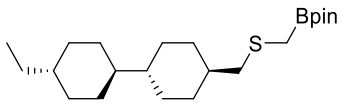
**2-(((3,7-Dimethyloctyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6i)**




**6i**

The C($sp^3$)–H borylated product **6i** was obtained by further purification (52.6 mg, 67% yield; colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.56-2.53 (m, 1H), 2.51-2.47 (m, 1H), 1.95 (s, 2H), 1.62-1.56 (m, 1H), 1.53-1.48 (m, 2H), 1.42-1.36 (m, 2H), 1.26 (s, 12H), 1.25-1.23 (m, 1H), 1.15-1.05 (m, 4H), 0.86-0.84 (m, 9H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 39.2, 37.0, 36.2, 32.3, 32.1, 27.9, 24.74, 24.68, 22.7, 22.6, 19.3; HRMS ($ESI^+$) Calcd for $C_{17}H_{36}BO_2S^+$ ($[M+H]^+$) 315.2524, Found 315.2529.

**2-(((((1*r*,1'*r*,4*R*,4'*R*)-4'-Ethyl-[1,1'-bi(cyclohexan)]-4-yl)methyl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6j)**

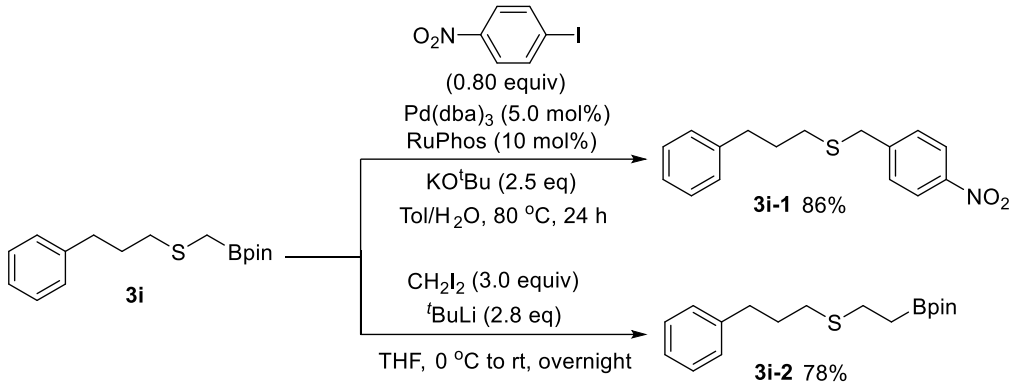



**6j**

The C($sp^3$)–H borylated product **6j** was obtained by further purification (61.8 mg, 65% yield; colorless oil); $^1$H NMR (800 MHz, $CDCl_3$) δ 2.40 (d, *J* = 6.8 Hz, 2H), 1.92 (s, 2H), 1.90-1.85 (m, 2H), 1.76-1.64 (m, 6H), 1.42-1.37 (m, 1H), 1.25 (s, 12H), 1.19-1.13 (m, 2H), 1.04-0.86 (m, 9H), 0.84 (t, *J* = 7.4 Hz, 3H), 0.82-0.77 (m, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 83.8, 43.3, 43.2, 42.4, 39.6, 37.7, 33.1, 33.0, 30.00, 29.99, 29.7, 24.7, 11.5; HRMS ($ESI^+$) Calcd for $C_{22}H_{42}BO_2S^+$ ($[M+H]^+$) 381.2993, Found 381.2990.

**7. Transformation of borylated products**

We investigated transformations of the boryl group of α-Me-C($sp^3$)–H borylated product **3i** (Scheme S1) to give **3i-1** and **3i-2**. In addition, we also used **3i-2** for several further transformations of the boryl group (Scheme S2).




**Scheme S1.** Transformations of the boryl group of borylated product **3i**

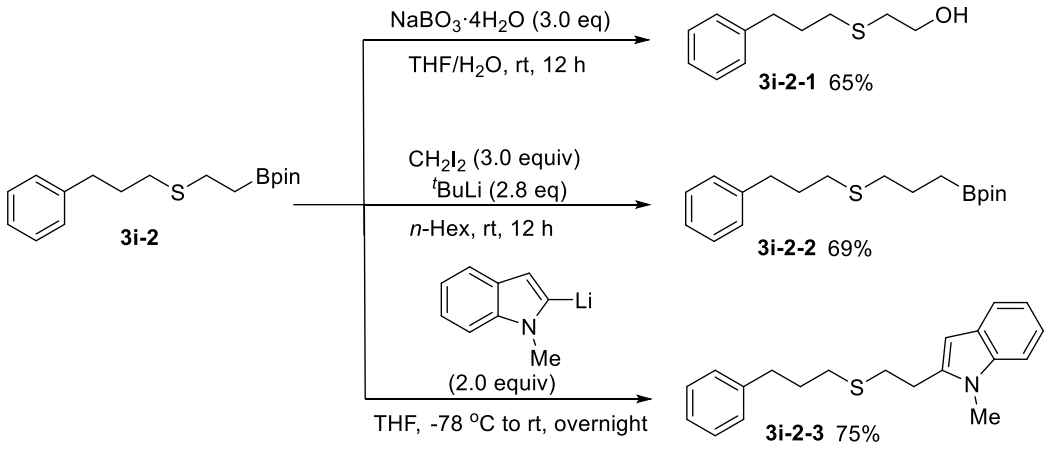
**(4-Nitrobenzyl)(3-phenylpropyl)sulfane (3i-1)**[5]

Into a 50 mL two-necked flask equipped with a reflux condenser, **3i** (87.0 mg, 0.300 mmol), 1-iodo-4-nitrobenzene (62.2 mg, 0.250 mmol), $Pd_2(dba)_3$ (13.7 mg, 0.0150 mmol), RuPhos (14.0 mg, 0.0300 mmol), $^t$BuOK (84.0 mg, 0.750 mmol), toluene (15 mL) and $H_2O$ (10 mL) were added. Then the mixture was heated at 80 °C for 24 h under $N_2$ atmosphere. The reaction mixture was cooled to room temperature and was extracted with EtOAc (2 x 15 mL). Then the organic phase was washed with $H_2O$ and dried over anhydrous $Na_2SO_4$. After filtration, the solvent was removed under vacuum to give a yellow oil crude product, which was further purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to give **3i-1** as a yellow oil. Yield: 74.2 mg, 86%; $^1$H NMR (800 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.26 (dd, *J* = 8.1, 7.5 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 2H), 3.73 (s, 2H), 2.67 (t, *J* = 7.5 Hz, 2H), 2.39 (t, *J* = 7.4 Hz, 2H), 1.87 (tt, *J* = 7.5, 7.4 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 146.8, 146.4, 141.1, 129.6, 128.41, 128.38, 126.0, 123.7, 35.5, 34.6, 30.6, 30.5; HRMS (ESI$^+$) Calcd for $C_{16}H_{17}NNaO_2S^+$ ([M+Na]$^+$) 310.0872, Found 310.0867.

**2-(2-((3-Phenylpropyl)thio)ethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3i-2)**[6]

To a flame-dried 25 mL flask were added **3i** (1.00 g, 3.40 mmol, 1.0 equiv), $CH_2I_2$ (0.82 mL, 10.2 mmol, 3.0 equiv) and hexane (20 mL). After the flask was sealed and flushed with $N_2$ for three times, $^t$BuLi (9.52 mmol, 2.8 equiv) was slowly added dropwise at 0 °C. Then, the mixture

was allowed to warm to room temperature and stirred for overnight. The reaction mixture was diluted with $Et_2O$ (2.0 mL), washed with $H_2O$ (2 x 15 mL) and dried over anhydrous $Na_2SO_4$. After filtration, the solvent was removed under vacuum to give a colorless oil crude product, which was further purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to give **3i-2**. Yield: 811 mg, 78%; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.27 (dd, *J* = 6.7 Hz, 2H), 7.19-7.16 (m, 3H), 2.70 (t, *J* = 7.7 Hz, 2H), 2.63 (t, *J* = 8.0 Hz, 2H), 2.53 (t, *J* = 7.3 Hz, 2H), 1.92-1.87 (tt, *J* = 7.7, 7.3 Hz, 2H), 1.24 (s, 12H), 1.13 (t, *J* = 9.0 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.7, 128.5, 128.3, 125.8, 83.3, 34.8, 31.2, 31.1, 27.1, 24.8; HRMS (ESI$^+$) Calcd for $C_{17}H_{28}BO_2S^+$ ([M+H]$^+$) 307.1898, Found 307.1890.




**Scheme S2.** Transformations of the boryl group of borylated product **3i-2**

**2-((3-Phenylpropyl)thio)ethan-1-ol (3i-2-1)**[7]

A round bottom flask was charged with **3i-2** (1.00 g, 3.20 mmol), $NaBO_3/4H_2O$ (1.48 g, 9.60 mmol), and THF/$H_2O$ (1/1, 20 mL). Then the mixture was stirred at 25 °C for 2 h. The precipitate was filtered, the mixture was extracted with ethyl acetate (2 x 20 mL), and the organic layer was dried with ethyl acetate, filtered, and concentrated in vacuo to give a crude product, which was further purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1) to give **3i-2-1**. Yield: (408 mg, 65%); colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.20-7.16 (m, 3H), 3.69 (t, *J* = 5.9 Hz, 2H), 2.73-2.70 (m, 4H), 2.54-2.51 (m, 2H), 1.91 (tt, *J* = 7.4, 7.4 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.3, 128.5, 128.4, 126.0, 60.1, 35.2, 34.7, 31.2, 30.9; HRMS (ESI$^+$) Calcd for $C_{11}H_{16}NaOS^+$ ([M+Na]$^+$) 219.0814, Found 219.0813.

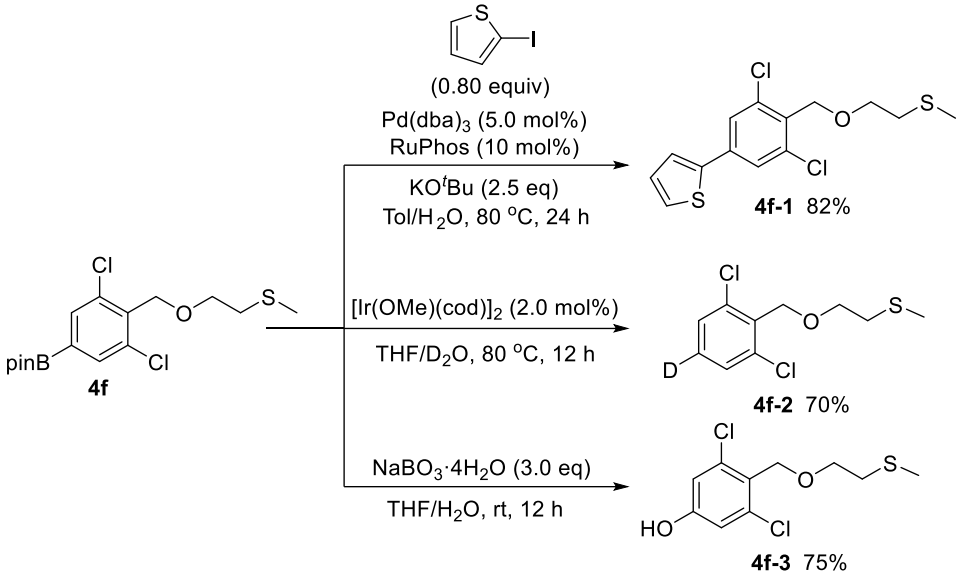
**2-(3-((3-Phenylpropyl)thio)propyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3i-2-2)**[6]

The titled compound **3i-2-2** was prepared according to the synthesis procedure of **3i-2** (0.500 g, 1.56 mmol, 1.0 equiv). Yield: 345 mg, 69%; colorless oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.29-7.26 (m, 2H), 7.19-7.18 (m, 3H), 2.71 (t, *J* = 7.7 Hz, 2H), 2.54-2.48 (m, 4H), 1.91 (t, *J* = 8.7 Hz, 2H), 1.69 (tt, *J* = 7.7, 7.7 Hz, 2H), 1.24 (s, 12H), 0.87 (t, *J* = 7.7 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.7, 128.4, 128.3, 125.8, 83.0, 34.8, 34.3, 31.2, 31.1, 24.8, 24.3; HRMS ($ESI^+$) Calcd for $C_{18}H_{30}BO_2S^+$ ($[M+H]^+$) 321.2054, Found 321.2056.

**1-Methyl-2-(2-((3-phenylpropyl)thio)ethyl)-1H-indole (3i-2-3)**[8]

To a flame-dried 25 mL flask were added *N*-methylindole (0.430 g, 3.27 mmol, 2.0 equiv) and THF (1.0 mL). *n*−BuLi (1.6 M in THF, 0.25 mL, 0.400 mmol) was added at room temperature. The mixture was heated at 70 °C for 3 h. Then the reaction mixture was cooled to -78 °C and a solution of **3i-2-2** (0.500 g, 1.63 mmol, 1.0 equiv) in THF (8.0 mL) was added dropwise. The mixture was stirred at -78 °C for 1 h. A solution of NIS (0.550 g, 2.45 mmol, 1.5 equiv) in THF (8.0 mL) was added dropwise before aq. sat. $Na_2S_2O_3$ (8.0 mL) was added. Then, the mixture was allowed to warm to room temperature. The mixture was diluted with $H_2O$ (30 mL) and extracted with DCM (2 x 30 mL). The combined organic phase was washed with $H_2O$ (30 mL) and brine (30 mL), dried over $Na_2SO_4$, filtered, and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3i-2-3**. Yield: 377 mg, 75%; yellow oil; $^{1}$H NMR (800 MHz, $CDCl_3$) δ 7.58 (t, *J* = 5.9 Hz, 1H), 7.34-7.31 (m, 2H), 7.30-7.28 (m, 1H), 7.25-7.19 (m, 4H), 7.14-7.10 (m, 1H), 6.32 (d, *J* = 3.8 Hz, 1H), 3.67 (s, 3H), 3.06 (t, *J* = 7.7 Hz, 2H), 2.89 (t, *J* = 7.5 Hz, 2H), 2.78-2.75 (m, 2H), 2.64-2.60 (t, *J* = 7.4 Hz, 2H), 1.95 (tt, *J* = 7.7, 7.4 Hz, 2H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.5, 139.2, 137.4, 128.5, 128.4, 127.7, 126.0, 121.0, 120.0, 119.5, 108.9, 99.3, 34.8, 31.7, 31.2, 31.0, 29.5, 27.8; HRMS ($ESI^+$) Calcd for $C_{20}H_{23}NNaS^+$ ($[M+Na]^+$) 332.1443, Found 332.1436.

The boryl group of C($sp^2$)–H borylated product **4f** was converted to a thiophenyl, deuterium atom and hydroxyl group (Scheme S3).




**Scheme S3.** Transformations of the boryl group of borylated product **4f**

**2-(3,5-Dichloro-4-((2-(methylthio)ethoxy)methyl)phenyl)thiophene (4f-1)**

The title compound **4f-1** was prepared according to the synthesis procedure of **3i-1** using **4f** (150 mg, 0.400 mmol) to give **4f-1** as a colorless oil. Yield: 109 mg, 82%; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.54 (s, 2H), 7.34 (d, *J* = 5.1 Hz, 1H), 7.32 (d, *J* = 3.6 Hz, 1H), 7.08 (dd, *J* = 5.1, 3.6 Hz, 1H), 4.79 (s, 2H), 3.74 (t, *J* = 6.9 Hz, 2H), 2.72 (t, *J* = 6.9 Hz, 2H), 2.15 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 140.7, 137.1, 136.4, 131.6, 128.3, 126.5, 125.3, 124.7, 70.0, 66.9, 33.4, 16.0; HRMS (ESI$^+$) Calcd for $C_{14}H_{15}Cl_2OS_2^+$ ([M+H]$^+$) 332.9936, Found 332.9932.

**(2-((2,6-Dichloro-4-deuterium benzyl)oxy)ethyl)(methyl)sulfane (4f-2)**[9]

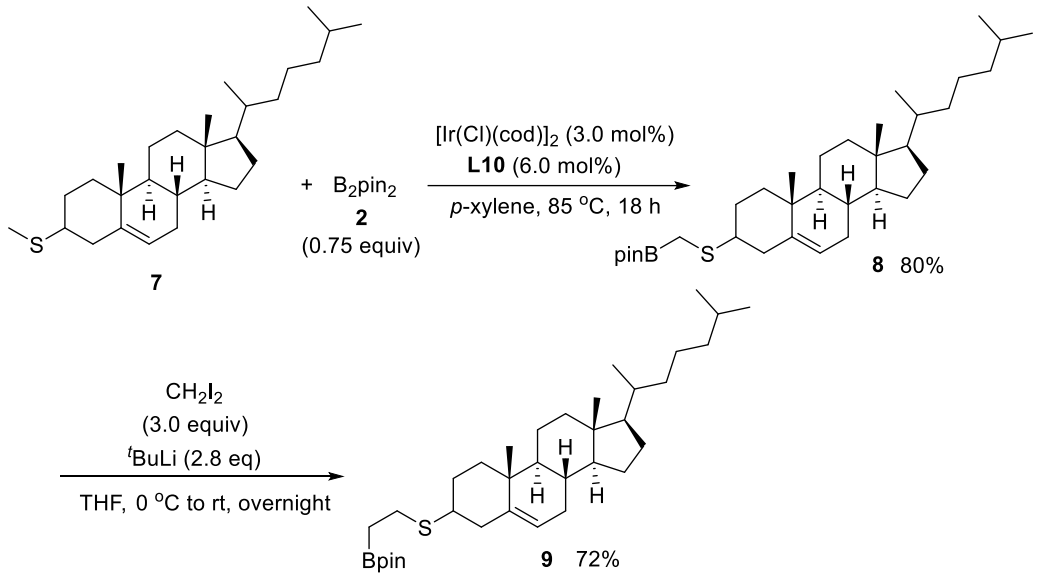
In an argon filled glove box, a flame-dried 10 mL schlenk tube was charged with $[Ir(OMe)(cod)]_2$ (2.65 mg, 2.0 mol%), **4f** (75.4 mg, 0.200 mmol) and dry THF (2.0 mL). The reaction vial was sealed and brought out of the glove box and charged with $D_2O$ (2.0 mL). The reaction vial was resealed and heated at 80 °C for 12 h. The reaction mixture was then cooled to room temperature and extracted with $Et_2O$ (3 x 20 mL). The combine organic layer was washed with brine (20 mL), dried over anhydrous $Na_2SO_4$, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1) to give **4f-2** as colorless oil. Yield: 35.0 mg, 70%; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.31 (s, 2H), 4.80 (s, 2H), 3.73 (t, *J* = 7.0 Hz, 2H), 2.71 (t, *J* = 7.0 Hz, 2H), 2.13 (s, 3H);

$^{13}$C NMR (201 MHz, $CDCl_3$) δ 136.8, 133.2, 128.4, 128.3, 70.0, 67.2, 33.3, 16.0; HRMS ($ESI^+$) Calcd for $C_{10}H_{12}DCl_2OS^+$ ($[M+H]^+$) 252.0121, Found 252.0114.

**3,5-Dichloro-4-((2-(methylthio)ethoxy)methyl)phenol (4f-3)**

The title compound **4f-3** was prepared according to the synthesis procedure of **3i-2-1** using **4f** (0.150 g, 0.400 mmol) to give **4f-3**. Yield: 80.5 mg, 75%, colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.25 (s, 1H), 6.67 (s, 2H), 4.71 (s, 2H), 3.76 (t, *J* = 6.8 Hz, 2H), 2.74 (t, *J* = 6.8 Hz, 2H), 2.13 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 156.8, 136.9, 124.0, 116.0, 69.4, 67.0, 33.2, 15.7; HRMS ($ESI^+$) Calcd for $C_{10}H_{13}Cl_2O_2S^+$ ($[M+H]^+$) 267.0008, Found 267.0004.

**8. Derivatization of methylthiolcholesterol 7 and gram-scale reaction**



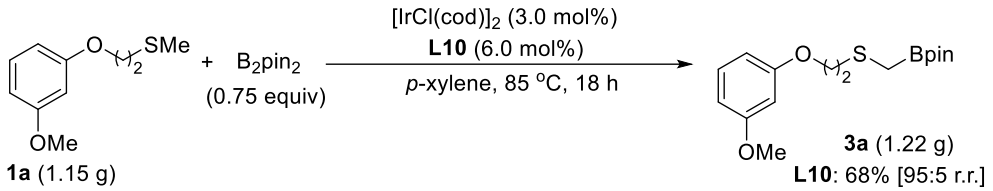

**2-((((8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-(6-methylheptan-2-yl)-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl)thio)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (8)**

The title compound **8** was prepared according to the general procedure for α-C($sp^3$)–H borylation of methyl sulfides using methylthio group-containing thiolcholesterol **7** (104 mg, 0.250 mmol). Yield: 108.5 mg, 80%; white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 5.37-5.29 (m, 1H), 2.59-2.49 (m, 1H), 2.38-2.20 (m, 2H), 2.08-1.93 (m, 4H), 1.92-1.79 (m, 3H), 1.60-1.57 (m, 3H), 1.55-1.41 (m, 6H),1.27-1.21 (m, 16H), 1.20-1.04 (m, 7H), 1.01-0.96 (m, 4H), 0.93-0.83 (m, 9H), 0.72-0.63 (m, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.9, 120.7, 83.9, 56.8, 56.1, 50.3, 46.2, 42.3, 39.8, 39.6, 39.5, 39.3, 36.9, 36.2, 35.8, 31.9, 31.8, 29.1, 28.2, 28.0, 24.7, 23.8, 22.8, 22.5, 20.9, 19.3, 18.9, 11.8; HRMS ($ESI^+$) Calcd for $C_{34}H_{60}BO_2S^+$ ($[M+H]^+$) 543.4402, Found 543.4400.

**2-(2-(((8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-(6-methylheptan-2-yl)-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl)thio)ethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (9)**

The title compound **9** was prepared according to the synthesis procedure of **3i-2** using compound **8** (98.0 mg, 0.180 mmol). Yield: 72.1 mg, 72%; white solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 5.32 (td, *J* = 5.2, 2.2 Hz, 1H), 2.67 (t, *J* = 8.3 Hz, 2H), 2.61-2.54 (m, 1H), 2.31-2.27 (m, 1H), 2.26-2.23 (m, 1H), 2.02-1.99 (m, 1H), 1.98-1.94 (m, 1H), 1.87 (d, *J* = 9.9 Hz, 2H), 1.84-1.79 (m, 1H), 1.53-1.48 (m, 4H), 1.46-1.41 (m, 4H), 1.33 (d, *J* = 4.3 Hz, 2H), 1.30-1.28 (m, 2H), 1.25 (s, 12H), 1.16-1.07 (m, 9H), 0.99 (s, 4H), 0.91 (d, *J* = 6.5 Hz, 3H), 0.86 (dd, *J* = 6.6, 3.9 Hz, 7H), 0.67 (s, 3H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 142.0, 120.7, 83.3, 56.8, 56.1, 50.3, 44.3, 42.3, 40.0, 39.8, 39.7, 39.5, 36.9, 36.2, 35.8, 31.9, 31.8, 29.8, 28.2, 28.0, 25.3, 24.8, 23.8, 22.8, 22.6, 20.9, 19.4, 18.7, 11.8; HRMS (ESI$^+$) Calcd for $C_{35}H_{62}BO_2S^+$ ([M+H]$^+$) 557.4558, Found 557.4553.

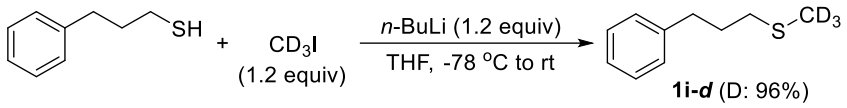
**Gram-scale reaction**:




A mixture of [Ir(Cl)(cod)]$_2$ (117 mg, 0.174 mmol, 3.0 mol%), **L10** (105 mg, 0.348 mmol, 6.0 mol%), and $B_2pin_2$ (1.1g, 4.36 mmol, 0.75 equiv) were added to a solution of methyl sulfides (**1a**, 1.15g, 5.81 mmol) in *p*-xylene (15 mL) under $N_2$ atmosphere in a 25 mL sealed tube. The mixture was stirred at 85 °C for 18 h. Then, the solvent was removed under vacuum and borylation products **3a** and **4**a were separated by column chromatography on silica gel using a mixture of hexane and ethyl acetate as an eluent. The mixture of product (1.22 g, 68% yield, ratio of C($sp^3$)–H borylated product **3a** to C($sp^2$)–H borylated product **4a** =95:5 r.r.); yellow solid; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 8.2, 8.2 Hz, 1H), 6.52-6.49 (m, 2H), 6.47 (s, 1H), 4.14 (t, *J* = 7.2 Hz, 2H), 3.78 (s, 3H), 2.92 (t, *J* = 7.2 Hz, 2H), 2.08 (s, 2H), 1.27 (s, 12H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 160.8, 159.7, 129.8, 106.6, 106.5, 101.0, 84.0, 67.2, 55.2, 33.0, 24.7; HRMS (ESI$^+$) Calcd for $C_{16}H_{26}BO_4S^+$ ([M+H]$^+$) 325.1639, Found 325.1633.

**9. Kinetic isotope effect (KIE) experiment and NMR experiments**

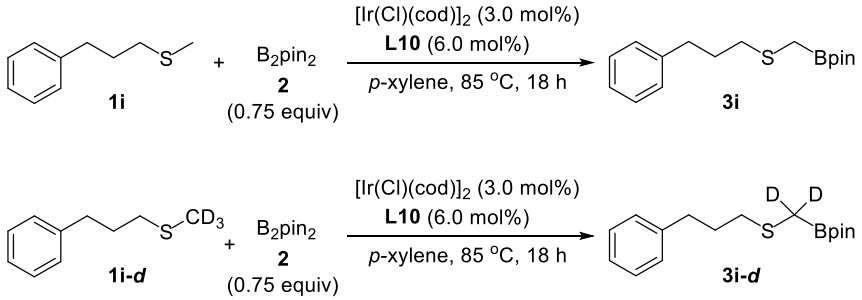
**Synthesis of (methyl-$d_3$)(3-phenylpropyl)sulfane (1i-*d*)**




The titled compound **1i-*d*** was prepared according to "Method-D" using 3-phenylpropane-1-thiol (1.25 g, 8.21 mmol) and $CD_3I$ (1.79 g,12.3 mmol, 1.5 equiv). Yield: 1.18 g, 85%; colorless oil; $^1$H NMR (800 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.23-7.19 (m, 3H), 2.74 (t, *J* = 7.6 Hz, 2H), 2.52 (t, *J* = 7.1 Hz, 2H), 1.96 (tt, *J* = 7.6, 7.1 Hz, 2H), 1.28 (s, 0.13H); $^{13}$C NMR (201 MHz, $CDCl_3$) δ 141.6, 128.5, 128.4, 125.9, 34.8, 33.5, 30.7, 14.9 (tt, *J* = 20.1 Hz); HRMS (ESI$^+$) Calcd for $C_{10}H_{12}D_3S^+$ ([M+H]$^+$) 170.1707, Found 170.1700.

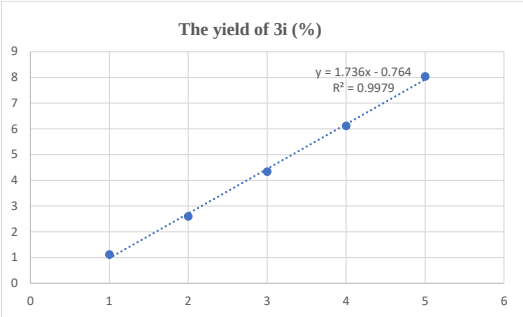
**KIE experiment**

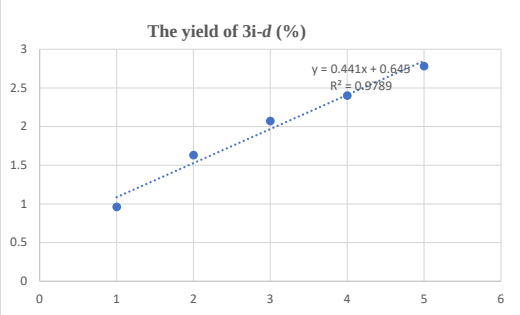
A mixture of $[Ir(Cl)(cod)]_2$ (3.02 mg, 0.00450 mmol, 3.0 mol%), **L10** (2.41 mg, 0.00900 mmol, 6.0 mol%), was divided equally into two NMR tubes under $N_2$ atmosphere. To one tube was added the mixture of methyl(3-phenylpropyl)sulfane (**1i**, 24.9 mg, 0.150 mmol) and $B_2pin_2$ (28.6 mg, 0.113 mmol, 0.75 equiv) in toluene-$d_8$ (0.50 mL), and to the other tube was added the mixture of deuterated (methyl-$d_3$)(3-phenylpropyl)sulfane (**1i-*d***, 25.4 mg, 0.150 mmol) and $B_2pin_2$ (28.6 mg, 0.113 mmol, 0.75 equiv) in toluene-$d_8$ (0.50 mL). These two tubes were placed at 85 °C for several periods to give α-C(sp$^3$)–H borylated products **3i** and **3i-*d***. Because the induction period was observed until 3.5 h, the data were collected after 3.5 h. We collected the yields of **3i** and **3i-*d*** in five entries at different reaction times, respectively. The KIE value was calculated by the ratio of rate constants $k_H$ and $k_D$, and the KIE value was 3.77. This result suggested that the C–H activation step is the rate-determining step in this C(sp$^3$)–H borylation.



| Entry | Time (h) | 3i (%) | 3i-*d* (%) |
|---|---|---|---|
| 1 | 3.5 | 1.12 | 0.96 |
| 2 | 4.0 | 2.60 | 1.63 |
| 3 | 4.5 | 4.43 | 2.07 |
| 4 | 5.0 | 6.12 | 2.40 |
| 5 | 5.5 | 8.04 | 2.78 |

$^1$H NMR yield using 1,1,2,2-tetrachloroethane as an internal standard.

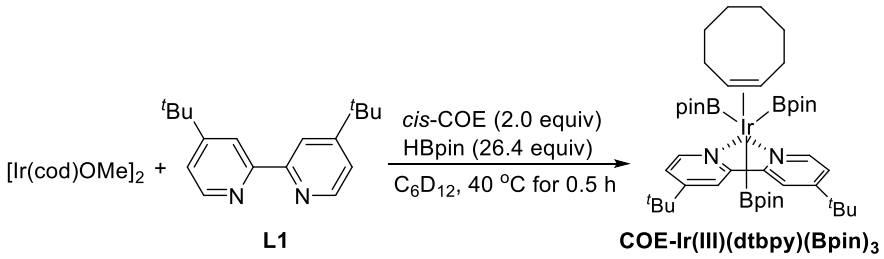



KIE = LINEST (**3i**) / LINEST (**3i-*d***)×0.96 = 3.77

**NMR experiments:**

**Synthesis of COE-Ir(III)(dtbpy)(Bpin)$_3$**




An NMR tube equipped with a screw-cap and septum was charged with [Ir(cod)OMe]$_2$ (0.0091 mmol) and the solid materials were dissolved in $C_6D_{12}$ (0.5 mL). *cis*-Cyclooctene (25 µL, 0.18 mmol) was added to the tube, the sample was mixed, and pinacolborane (25 µL, 0.24 mmol) was added. To the resulting solution was added 4,4'-di-*tert*-butyl-2,2'-bipyridine **L1** (0.019 mmol), and the sample was heated in an oil bath at 40 °C for 0.5 h. At this time, the sample was analyzed by $^1$H NMR spectroscopy at 25 °C. Aromatic resonances for **COE-Ir(III)(dtbpy)(Bpin)$_3$**: $^1$H NMR (800 MHz, $CDCl_3$) δ 9.47 (d, *J* = 6.0 Hz, 2H), 7.94 (s, 2H), 7.12 (d, *J* = 5.5 Hz, 2H) [10].

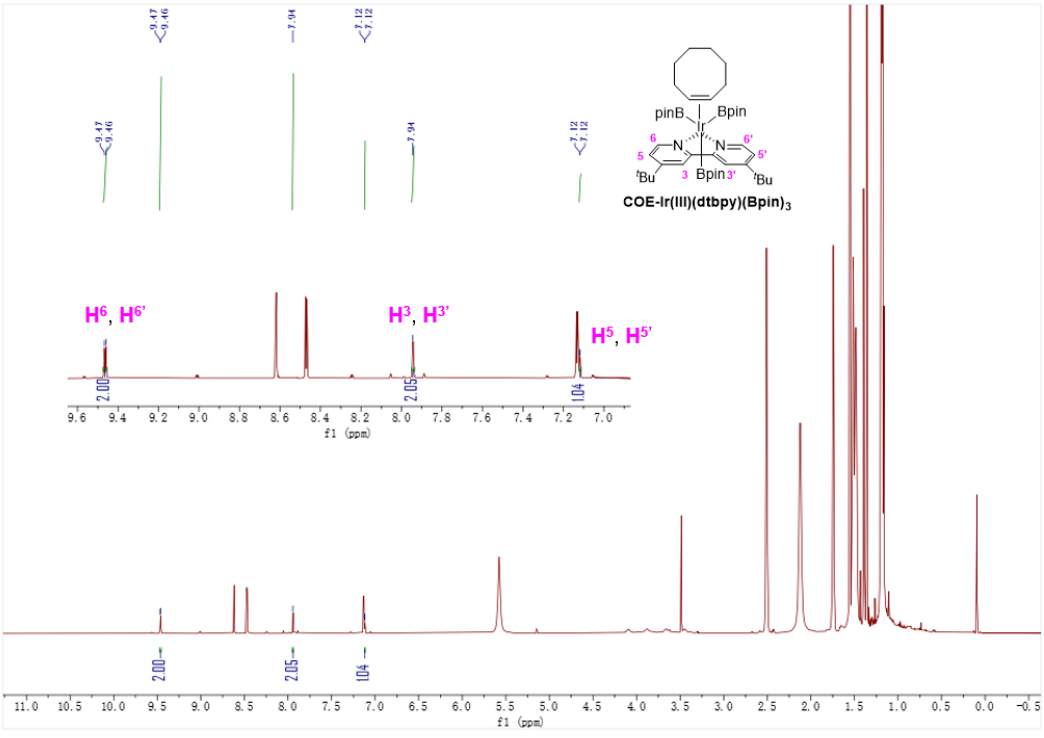
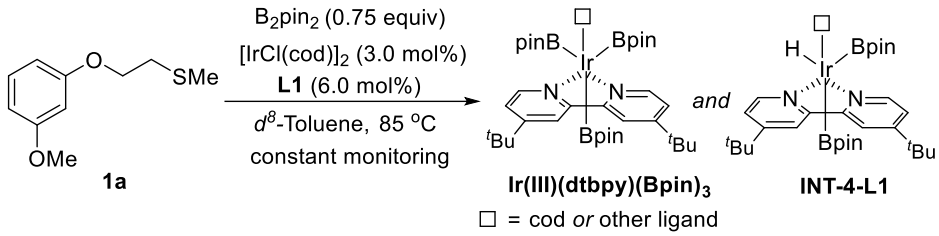



**Figure S9A**. The $^1$HNMR spectrum for the intermediate COE-Ir(III)(dtbpy)(Bpin)$_3$

**Trapping of the intermediate of Ir(III)(dtbpy)(Bpin)$_3$ and INT-4-L1**




An NMR experiment was performed as follows: a mixture of [Ir(Cl)(cod)]$_2$ (2.52 mg, 0.00375 mmol, 3.0 mol%), **L1** (2.01 mg, 0.0075 mmol, 6.0 mol%), and $B_2pin_2$ (23.8 mg, 0.0938 mmol, 0.75 equiv) were added to a solution of methyl sulfides (**1a**, 24.8 mg, 0.1250 mmol) in $d^8$-toluene (1.5 mL) under $N_2$ atmosphere in an NMR tube. The mixture was constant monitoring by $^1$H NMR spectroscopy at 85 °C. After 3 hours, we observed the characteristic peaks of the **Ir(III)(dtbpy)(Bpin)$_3$**: $^1$H NMR (800 MHz, $CDCl_3$) δ 9.47 (d, *J* = 6.0 Hz, 2H), 7.94 (s, 2H), 7.12 (overlapped). Until the experiment had been running for 6 hours, we did not observe Ir-H peak of **INT-4**, which should appear at -4.81 ppm [10].

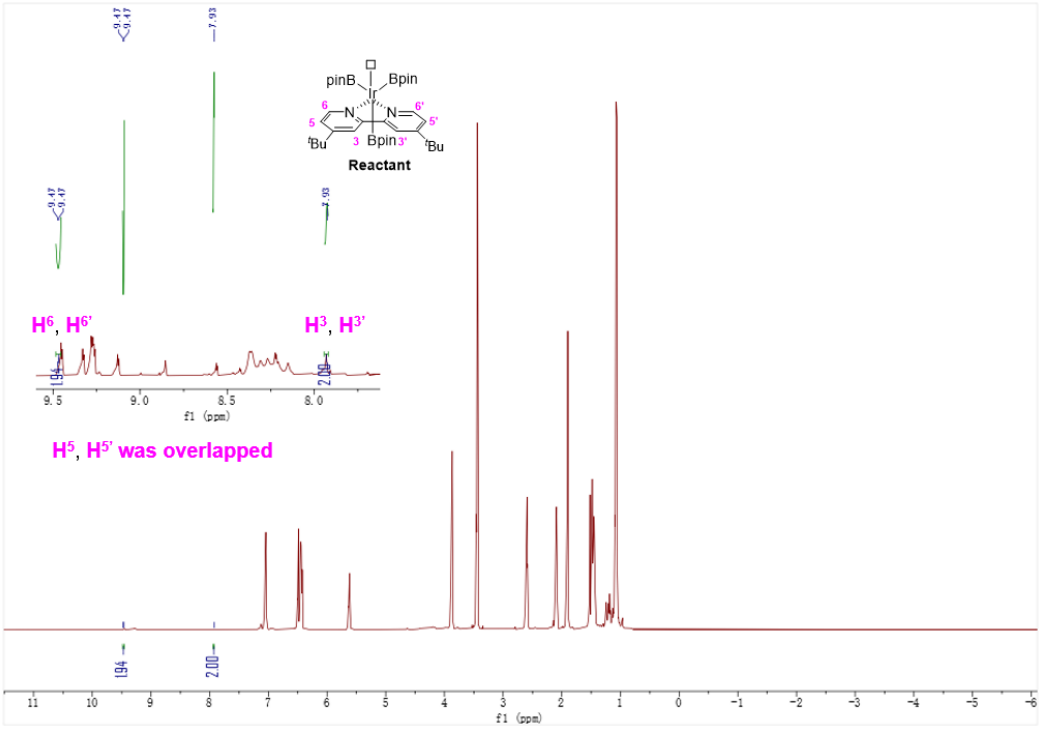
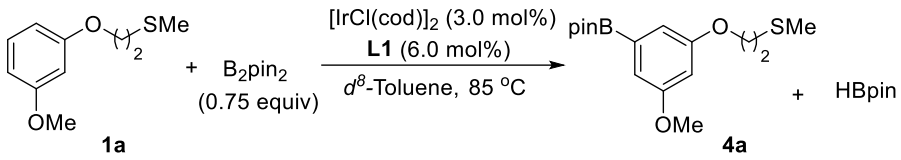



**Figure S9B** $^1$HNMR spectrum for trapping the **Ir(III)(dtbpy)(Bpin)$_3$** and **INT-4-L1**

**$^{11}$B-NMR experiments for observing HBpin**




A mixture of $[Ir(Cl)(cod)]_2$ (2.52 mg, 0.00375 mmol, 3.0 mol%), **L1** (2.01 mg, 0.0075 mmol, 6.0 mol%), and $B_2pin_2$ (23.8 mg, 0.0938 mmol, 0.75 equiv) were added to a solution of methyl sulfides (**1a**, 24.8 mg, 0.1250 mmol) in $d^8$-toluene (1.5 mL) under $N_2$ atmosphere in an NMR tube. The tube was closed and heated at 85 °C (bath temperature). After 5 hours, the mixture was analyzed by $^{11}$B-NMR spectroscopy at 25 °C, the corresponding $^{11}$B peak of HBpin was clearly observed.

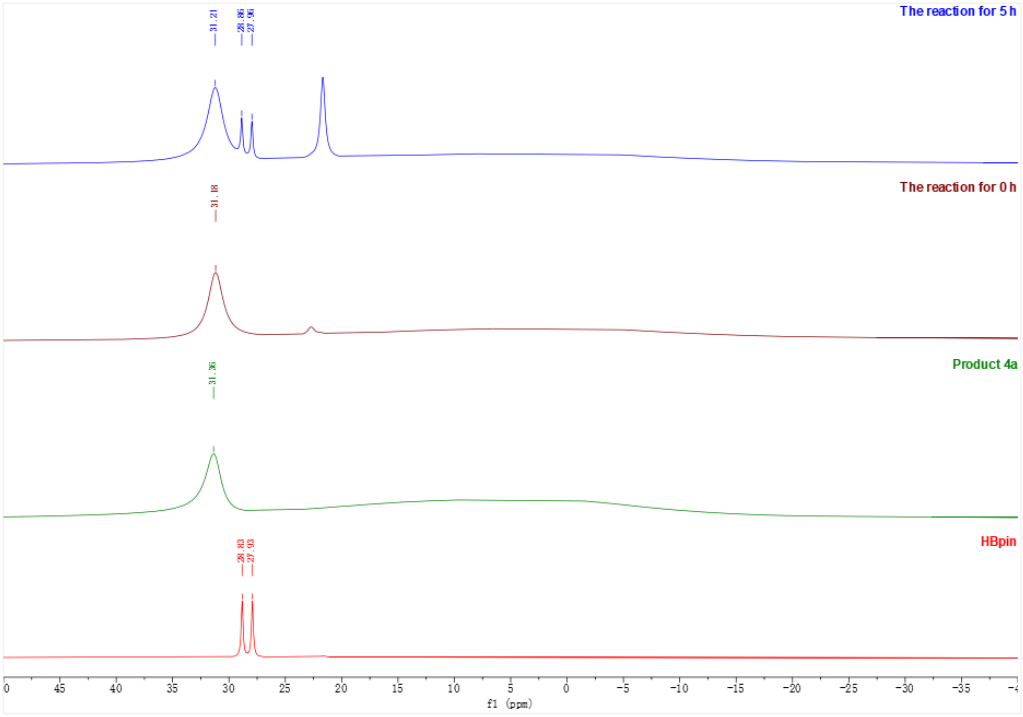



**Figure S9C** Analysis of the C-H borylation using $^{11}$B-NMR spectra

## 10. DFT calculation study

DFT calculations were performed at the B3LYP-D3(BJ)/def2-SVP level using the Gaussian16 program. Fully optimized geometries of all stationary points were characterized by frequency calculations to verify that the transition states (TSs) had one and only one imaginary frequency for the desired reaction coordinate. The intrinsic reaction coordinate (IRC) calculation was performed using the same level of theory to further verify that the TS on the potential energy surface connected to the desired minima on either side of the first-order saddle point. The Gibbs free energies were evaluated at 358.15 K and 1 atm. Then the energies at the optimized geometries were refined at the B3LYP-D3(BJ)/def2-TZVP level.

a) From the dissociation of **3a** or **4a**, the intermediate and transition state is labeled **INT-L10-Bpin** and **TS-L10-Bpin**.

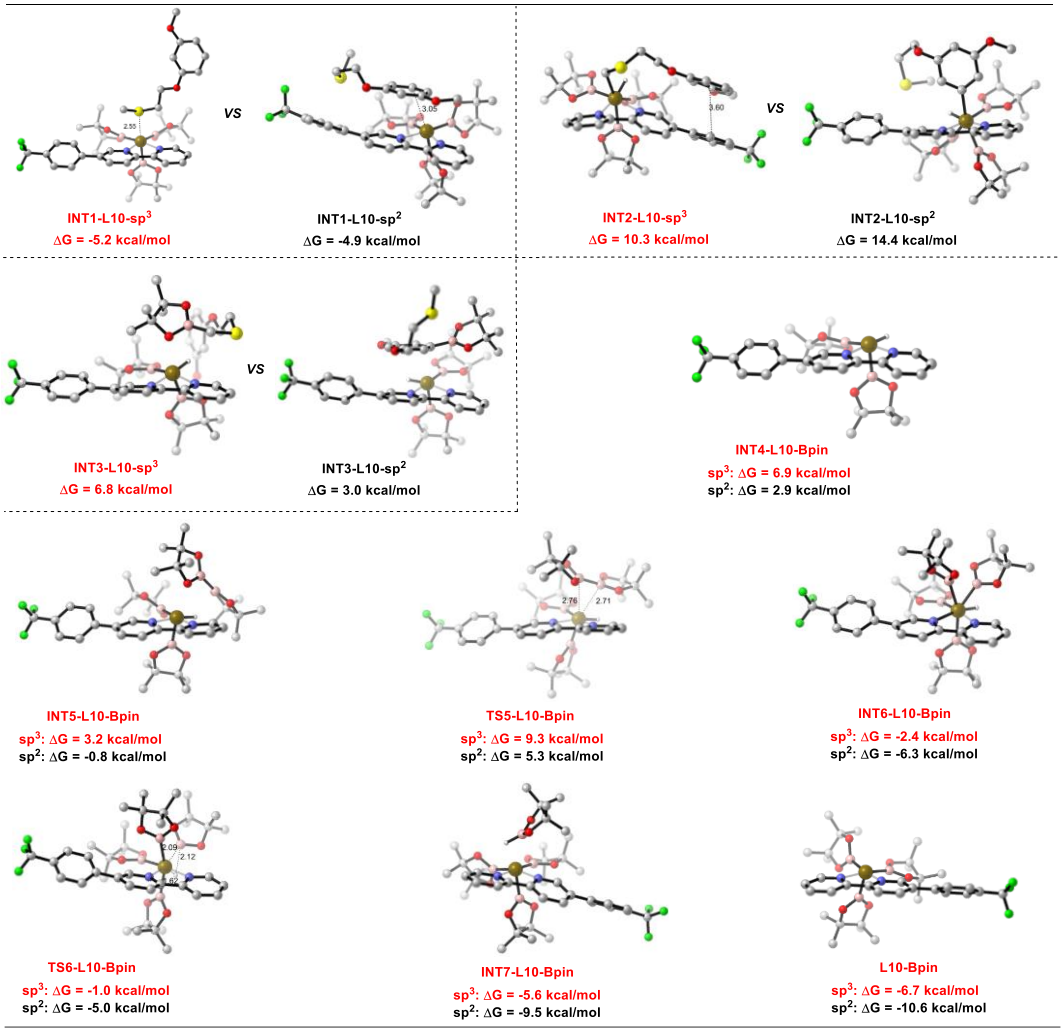



**Figure S10A** The intermediate (**INT1-L10** to **INT7-L10, L10-Bpin**) and transition structures

(**TS5-L10** to **TS6-L10**) of selective borylation of substrate **1a** with ligand **L10**.

b) From the dissociation of **3a** or **4a**, the intermediate and transition state is labeled **INT-L1-Bpin** and **TS-L1-Bpin**.

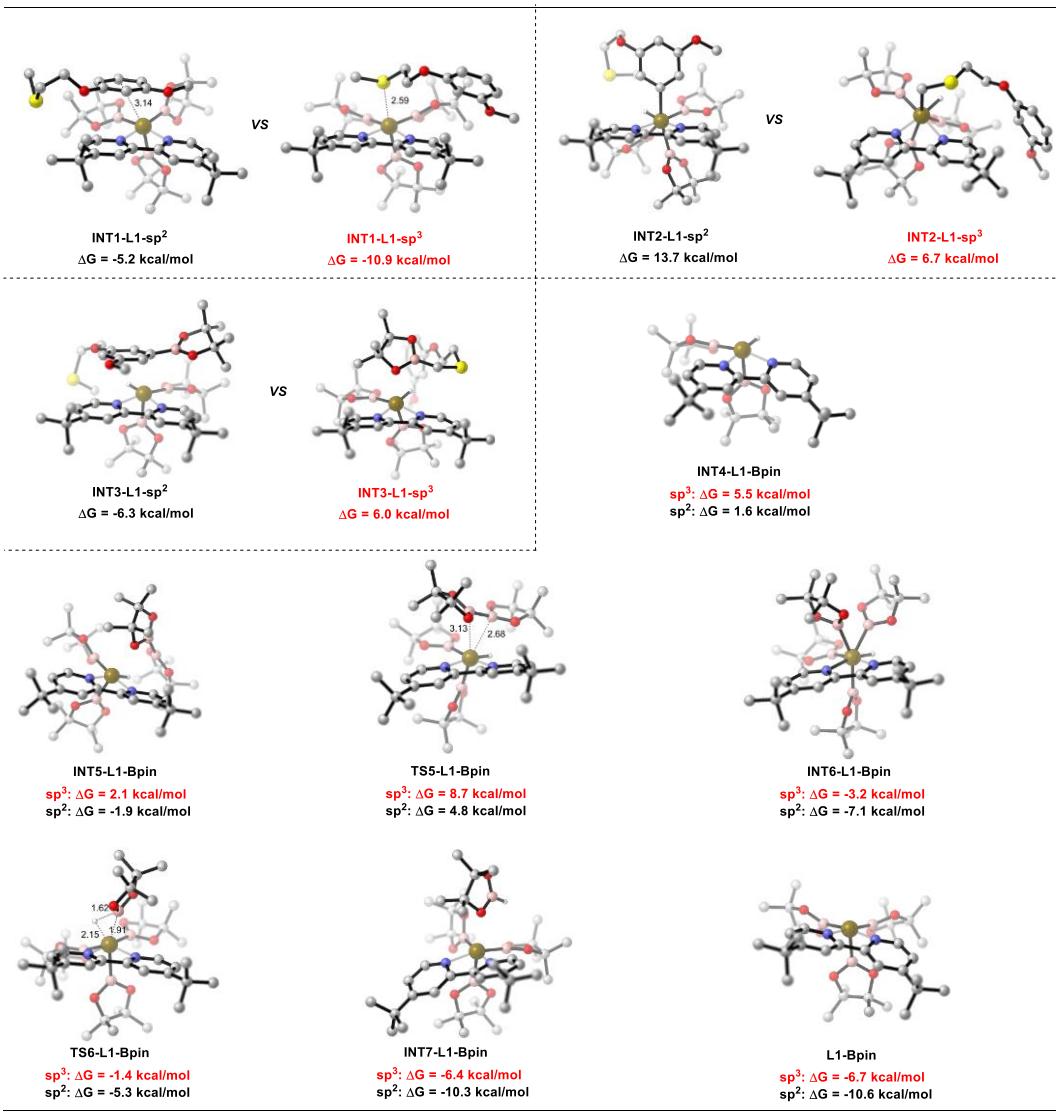
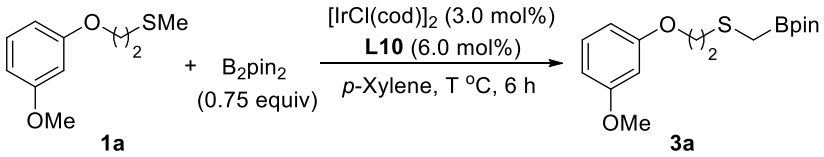



**Figure S10B** The intermediate (**INT1-L1** to **INT7-L1, L1-Bpin**) and transition structures (**TS5-L1** to **TS6-L1**) of selective borylation of substrate **1a** with ligand **L10**.

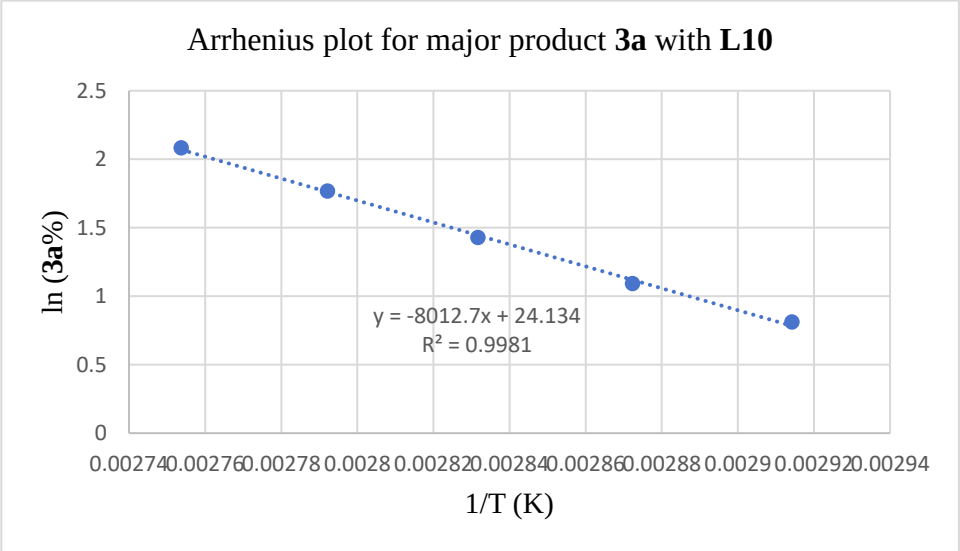
c) Kinetic experiments and Arrhenius plots to determine the activation energy:




A mixture of **1a** (29.7 mg, 0.150 mmol), $B_2pin_2$ (28.6 mg, 0.113 mmol, 0.75 equiv), $[IrCl(cod)]_2$ (3.02 mg, 0.00450 mmol, 3.0 mol%), **L10** (2.71 mg, 0.00900 mmol, 6.0 mol%) was divided equally into five 4 mL tubes, adding *p*-Xylene (2.0 mL) to each tube as solvent. These five tubes were respectively placed at 70 °C, 75 °C, 80 °C, 85 °C, 90 °C for 6 hours. The yield of major C($sp^3$)-H borylation product **3a** was determined by $^1$H-NMR.

| Entry | Temp. (°C) | 3a (%) | 1/T (K) | ln (3a%) |
|---|---|---|---|---|
| 1 | 70 | 2.25 | 0.002914 | 0.810930 |
| 2 | 75 | 2.98 | 0.002872 | 1.091923 |
| 3 | 80 | 4.17 | 0.002832 | 1.427916 |
| 4 | 85 | 5.85 | 0.002792 | 1.766442 |
| 5 | 90 | 8.02 | 0.002754 | 2.081938 |

$^1$H NMR yield using 1,1,2,2-tetrachloroethane as an internal standard



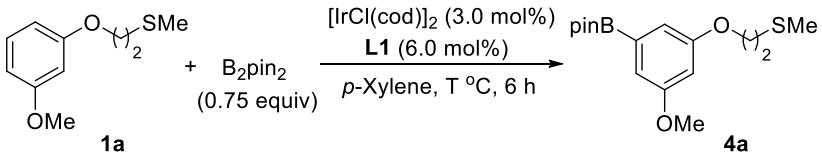

Arrhenius equation: ln k = -Ea/RT + ln A;

Therefore, Ea = 8012.7×*R*/*C*/1000 = 8012.7×8.314/4.184/1000 = 15.9 kcal/mol

1/T (K) = 1/(Temp.+ 273.14); *R* (gas constant) = 8.314 J·mol/K;

*C* (conversion factor) = 4.184 J/cal;

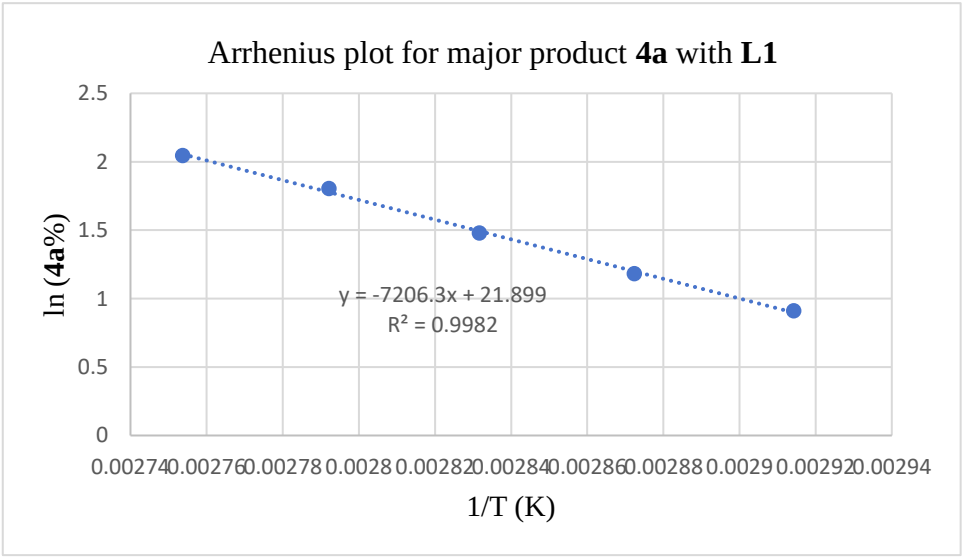
The activation free energy of major C($sp^3$)-H borylation product **3a** with **L10** is 15.9 kcal/mol determined by Arrhenius equation.




A mixture of **1a** (29.7 mg, 0.150 mmol), $B_2pin_2$ (28.6 mg, 0.113 mmol, 0.75 equiv), $[IrCl(cod)]_2$ (3.02 mg, 0.00450 mmol, 3.0 mol%), **L1** (2.71 mg, 0.00900 mmol, 6.0 mol%) was divided equally into five 4 mL tubes, adding *p*-Xylene (2.0 mL) to each tube as solvent. These five tubes were respectively placed at 70 °C, 75 °C, 80 °C, 85 °C, 90 °C for 6 hours. The yield of major C($sp^2$)-H borylation product **4a** was determined by $^1$H-NMR.

| Entry | Temp. (°C) | 4a (%) | 1/T (K) | ln (4a%) |
|---|---|---|---|---|
| 1 | 70 | 2.49 | 0.002914 | 0.912283 |
| 2 | 75 | 3.26 | 0.002872 | 1.181727 |
| 3 | 80 | 4.39 | 0.002832 | 1.479329 |
| 4 | 85 | 6.08 | 0.002792 | 1.805005 |
| 5 | 90 | 7.74 | 0.002754 | 2.046402 |

$^1$H NMR yield using 1,1,2,2-tetrachloroethane as an internal standard




Arrhenius equation: ln k = -Ea/RT + ln A;

Therefore, Ea = 8012.7×*R*/*C*/1000 = 7206.3×8.314/4.184/1000 = 14.3 kcal/mol

1/T (K) = 1/(Temp.+ 273.14); *R* (gas constant) = 8.314 J·mol/K;

*C* (conversion factor) = 4.184 J/cal;

The activation free energy of major C($sp^2$)-H borylation product **4a** with **L1** is 14.3 kcal/mol determined by Arrhenius equation.

d) The Cartesian coordinates (Å) for the optimized structures:

**Ir(Bpin)$_3$ with ligand L10**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C | -2.97498000 | 2.98420900 | -0.76116300 | H | -4.88383400 | 0.22979600 | 3.72605900 |
| Ir | -1.04349100 | 0.47006300 | -0.63867200 | H | -4.89848000 | 1.42426600 | 2.40067200 |
| C | -0.72485300 | 3.57446200 | -0.73184400 | H | -4.40651400 | -0.24619500 | 2.05763100 |
| C | -2.97498000 | 2.98420900 | -0.76116300 | C | -2.86386600 | 2.09137200 | 4.10089300 |
| C | -1.05746300 | 4.93460500 | -0.66215600 | H | -3.52841600 | 2.90564200 | 3.77435500 |
| C | 0.67292600 | 3.08196400 | -0.69743400 | H | -3.20336700 | 1.75024900 | 5.09163800 |
| C | -3.37914500 | 4.31576800 | -0.69165000 | H | -1.85040600 | 2.50192900 | 4.19747500 |
| H | -3.69585100 | 2.16544700 | -0.77295400 | C | -2.69557400 | -1.43653200 | 4.11384100 |
| C | -2.39927000 | 5.30926300 | -0.64754200 | H | -1.97465900 | -2.24497700 | 4.30900000 |
| H | -0.27808100 | 5.69380100 | -0.60505200 | H | -3.12498200 | -1.12129100 | 5.07792500 |
| C | 1.79658500 | 3.91957000 | -0.69063200 | H | -3.49598600 | -1.84272400 | 3.48279700 |
| H | -4.44196800 | 4.56135200 | -0.66780800 | C | -0.72820300 | 0.11692200 | 4.19877300 |
| H | -2.67481000 | 6.36451400 | -0.59137200 | H | -0.95327700 | 0.39496600 | 5.23941800 |
| C | 2.04833000 | 1.20451200 | -0.56574400 | H | -0.03754600 | -0.73874900 | 4.20838400 |
| C | 3.06970600 | 3.36463800 | -0.59804700 | H | -0.21501900 | 0.95907200 | 3.71200300 |
| H | 1.68252900 | 5.00180400 | -0.74268600 | B | -0.26081700 | -1.38334300 | -0.31220200 |
| C | 3.22402900 | 1.97049300 | -0.52552500 | O | 1.07663300 | -1.58806200 | 0.09057400 |
| H | 2.06806500 | 0.11402500 | -0.52464100 | O | -0.88372600 | -2.62159300 | -0.41250300 |
| H | 3.94027800 | 4.02165800 | -0.55852900 | C | 1.23053900 | -2.95047900 | 0.53612600 |
| N | -1.68559600 | 2.62579200 | -0.79579700 | C | 0.07519200 | -3.67583200 | -0.24526600 |
| N | 0.82833600 | 1.74041200 | -0.63700200 | C | 1.01597800 | -2.95623800 | 2.05281100 |
| B | -1.70238400 | 0.35104200 | 1.23014100 | H | 1.16523600 | -3.95748600 | 2.48429600 |
| O | -2.35510900 | 1.41876800 | 1.84238500 | H | 1.74118100 | -2.26878600 | 2.51456900 |
| O | -1.56797900 | -0.70583600 | 2.11739900 | H | 0.00879300 | -2.59359600 | 2.29689800 |
| C | -2.91458100 | 0.95514800 | 3.08665100 | C | 2.63568000 | -3.43441500 | 0.19693200 |
| C | -1.98969000 | -0.27582400 | 3.42338500 | H | 3.37592000 | -2.89535100 | 0.80867600 |
| C | -4.36605800 | 0.55216400 | 2.81010500 | H | 2.74335500 | -4.50863600 | 0.41433200 |

| | | | |
|---|---|---|---|
| H | 2.87969500 | -3.26435100 | -0.85981300 |
| C | -0.58419700 | -4.82468400 | 0.50956600 |
| H | -1.37145300 | -5.27300700 | -0.11521300 |
| H | 0.14741800 | -5.61123500 | 0.75375500 |
| H | -1.05084200 | -4.47132600 | 1.43773500 |
| C | 0.49499600 | -4.13452600 | -1.64573000 |
| H | 1.17293000 | -5.00091800 | -1.61184600 |
| H | -0.40691800 | -4.41785700 | -2.20751200 |
| H | 0.98994800 | -3.31958300 | -2.19360000 |
| B | -2.75206600 | -0.53159700 | -1.03925500 |
| O | -3.02670900 | -0.96770300 | -2.33610900 |
| O | -3.84234900 | -0.81573000 | -0.21469000 |
| C | -4.18104400 | -1.82734300 | -2.30214100 |
| C | -4.92642600 | -1.31963000 | -1.01261200 |
| C | -3.67647100 | -3.26764400 | -2.16705900 |
| H | -4.50225300 | -3.99509200 | -2.18903400 |
| H | -3.00130900 | -3.48059800 | -3.00923200 |
| H | -3.09691200 | -3.38923100 | -1.24273800 |
| C | -4.96185400 | -1.66238800 | -3.60069100 |
| H | -4.35825200 | -2.03455300 | -4.44206300 |
| H | -5.90030400 | -2.23884900 | -3.57207400 |
| H | -5.20073200 | -0.60946800 | -3.79953100 |
| C | -5.86666100 | -0.14136400 | -1.29004500 |
| H | -6.77298300 | -0.45156700 | -1.83159300 |
| H | -6.16934900 | 0.30260700 | -0.32979800 |
| H | -5.35638400 | 0.63358400 | -1.88122200 |
| C | -5.65771700 | -2.40011400 | -0.22453000 |
| H | -6.14717300 | -1.95278000 | 0.65425200 |
| H | -6.43415300 | -2.88178800 | -0.83976200 |
| H | -4.96049100 | -3.16884600 | 0.13167600 |
| C | 4.53747100 | 1.30095900 | -0.40084500 |
| C | 5.71594400 | 1.90374600 | -0.87550200 |
| C | 4.63096900 | 0.02728100 | 0.19314900 |
| C | 6.94694600 | 1.26295200 | -0.75652700 |
| H | 5.67060500 | 2.87540900 | -1.37046800 |
| C | 5.85945600 | -0.61656700 | 0.31120800 |
| H | 3.73347400 | -0.46383200 | 0.57148600 |
| C | 7.02327800 | 0.00041900 | -0.15956300 |
| H | 7.85096900 | 1.73661100 | -1.14229200 |
| H | 5.91437700 | -1.60573600 | 0.76846300 |
| C | 8.36040400 | -0.66954700 | 0.01997400 |
| F | 8.25243900 | -2.00908900 | 0.02255000 |
| F | 9.22290200 | -0.33234800 | -0.95514900 |
| F | 8.93416300 | -0.31965400 | 1.18791300 |

**INT1-L10-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | -0.12063000 | -0.85093200 | -0.23349800 |
| C | -0.42928900 | -0.16606700 | -3.26968400 |
| C | -2.22135100 | -1.47221300 | -2.56455300 |
| C | -0.89301900 | -0.20099700 | -4.59329800 |
| C | 0.80582600 | 0.54117900 | -2.86703200 |
| C | -2.74016000 | -1.54640600 | -3.85556400 |
| H | -2.70774700 | -1.94638800 | -1.71145800 |
| C | -2.06066100 | -0.89958200 | -4.88993900 |
| H | -0.34278000 | 0.30426200 | -5.38640800 |
| C | 1.56618800 | 1.33643000 | -3.73770800 |
| H | -3.65970000 | -2.10446900 | -4.03916400 |
| H | -2.43245800 | -0.93942700 | -5.91602800 |
| C | 2.29348700 | 0.98659100 | -1.13308100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.70930400 | 1.97440200 | -3.27023900 | O | 1.66351800 | 0.40302500 | 1.82050300 |
| H | 1.25643300 | 1.47460900 | -4.77300000 | O | 1.30007100 | -1.76904400 | 2.39959800 |
| C | 3.10204100 | 1.80796100 | -1.93074900 | C | 2.19814100 | 0.25102200 | 3.14949700 |
| H | 2.52492600 | 0.79806800 | -0.08436900 | C | 2.35923800 | -1.30741300 | 3.24574600 |
| H | 3.28005900 | 2.61949700 | -3.94031600 | C | 1.14977000 | 0.80151800 | 4.12140200 |
| N | -1.09694300 | -0.80225400 | -2.28107700 | H | 1.50301700 | 0.78513100 | 5.16342000 |
| N | 1.18470600 | 0.38941900 | -1.57803000 | H | 0.92257500 | 1.84303100 | 3.84796600 |
| B | -1.42653600 | -2.05981000 | 0.74844900 | H | 0.21684400 | 0.22370400 | 4.05444000 |
| O | -2.81938400 | -1.94426200 | 0.53158700 | C | 3.49542100 | 1.04161500 | 3.26997400 |
| O | -1.20013900 | -3.12015700 | 1.61381100 | H | 3.28605100 | 2.12050400 | 3.19257900 |
| C | -3.47089800 | -3.11521200 | 1.06640300 | H | 3.97376300 | 0.86267800 | 4.24571700 |
| C | -2.44276000 | -3.57710000 | 2.15968300 | H | 4.20830100 | 0.77284500 | 2.47982600 |
| C | -3.60125300 | -4.12437700 | -0.08008300 | C | 2.16509600 | -1.88787000 | 4.64168800 |
| H | -4.10748100 | -5.04737700 | 0.23967600 | H | 2.28755400 | -2.98053600 | 4.60358700 |
| H | -4.20069400 | -3.67482800 | -0.88702700 | H | 2.90770300 | -1.48281600 | 5.34763600 |
| H | -2.61147800 | -4.37754800 | -0.48731500 | H | 1.15842100 | -1.67775300 | 5.02550400 |
| C | -4.84513800 | -2.72406800 | 1.59317400 | C | 3.67894800 | -1.80428500 | 2.64478900 |
| H | -5.48676000 | -2.40191700 | 0.75864200 | H | 4.54418200 | -1.54007200 | 3.27170500 |
| H | -5.33405700 | -3.57762000 | 2.08902000 | H | 3.63301600 | -2.89842300 | 2.55483000 |
| H | -4.77972100 | -1.89356800 | 2.30791400 | H | 3.82806200 | -1.40115300 | 1.63306900 |
| C | -2.36474300 | -5.08421000 | 2.37406700 | B | 0.72334800 | -2.65489000 | -0.65716000 |
| H | -1.61587600 | -5.30697700 | 3.14871800 | O | 2.01957600 | -3.07513300 | -0.38706900 |
| H | -3.33396500 | -5.48893300 | 2.70633800 | O | 0.01376500 | -3.68810400 | -1.27921600 |
| H | -2.06179000 | -5.60220300 | 1.45498600 | C | 2.05375200 | -4.51164200 | -0.47972600 |
| C | -2.63469200 | -2.86062600 | 3.50104500 | C | 0.89951800 | -4.79679400 | -1.50943300 |
| H | -3.52609500 | -3.21625900 | 4.04003000 | C | 1.74631300 | -5.05784200 | 0.91926800 |
| H | -1.74670400 | -3.04678100 | 4.12242800 | H | 1.78679000 | -6.15751100 | 0.94862000 |
| H | -2.71900000 | -1.77386300 | 3.35398300 | H | 2.49417000 | -4.66245700 | 1.62076300 |
| B | 1.00039900 | -0.80381000 | 1.45433100 | H | 0.76228400 | -4.71124400 | 1.26499800 |

| | | | |
|---|---|---|---|
| C | 3.44169900 | -4.94850500 | -0.93024200 |
| H | 4.17688000 | -4.69457500 | -0.15181300 |
| H | 3.47868600 | -6.03745600 | -1.09316400 |
| H | 3.74431000 | -4.44261500 | -1.85651900 |
| C | 1.36247300 | -4.71302300 | -2.96717600 |
| H | 1.98783500 | -5.57222700 | -3.25380900 |
| H | 0.47544700 | -4.69447400 | -3.61814900 |
| H | 1.93205200 | -3.78867900 | -3.14253300 |
| C | 0.13526800 | -6.09385200 | -1.27129200 |
| H | -0.65648400 | -6.20343600 | -2.02831200 |
| H | 0.80271200 | -6.96713400 | -1.34481900 |
| H | -0.33864500 | -6.09503800 | -0.28155000 |
| S | -1.38453800 | 1.15992800 | 0.69675200 |
| C | -0.46736500 | 2.66529900 | 0.24692600 |
| H | -0.32260400 | 2.72210500 | -0.84131400 |
| H | -0.96802300 | 3.57152300 | 0.61528400 |
| H | 0.50682900 | 2.55132700 | 0.74081600 |
| C | -2.86943500 | 1.29679700 | -0.34889100 |
| H | -2.57210300 | 1.50775500 | -1.38680400 |
| H | -3.30921900 | 0.28988400 | -0.31197800 |
| C | -3.85905700 | 2.32921400 | 0.15687200 |
| H | -3.41103400 | 3.34002300 | 0.17418300 |
| H | -4.16908500 | 2.08357000 | 1.18832300 |
| O | -4.96947400 | 2.30624900 | -0.72119100 |
| C | -6.01435700 | 3.14111900 | -0.49336200 |
| C | -7.07666200 | 3.07013900 | -1.41525800 |
| C | -6.07549900 | 4.03362400 | 0.57852700 |
| C | -8.17936900 | 3.89561600 | -1.24424600 |
| H | -7.00508400 | 2.36358200 | -2.24305500 |
| C | -7.20114000 | 4.86286500 | 0.73546200 |
| H | -5.28068400 | 4.11968100 | 1.31696100 |
| C | -8.26216300 | 4.80030000 | -0.17531000 |
| H | -9.00527900 | 3.84177000 | -1.95799400 |
| H | -9.14086300 | 5.43420500 | -0.06869800 |
| O | -7.16107800 | 5.69333800 | 1.80886800 |
| C | -8.25071000 | 6.55322700 | 2.04529100 |
| H | -8.01025200 | 7.12301600 | 2.95276000 |
| H | -8.40606200 | 7.25891500 | 1.20924800 |
| H | -9.18795000 | 5.99213600 | 2.21177800 |
| C | 4.29707200 | 2.45976200 | -1.35105100 |
| C | 5.40330300 | 2.80237800 | -2.14856300 |
| C | 4.35648300 | 2.74163900 | 0.02723900 |
| C | 6.52696700 | 3.41057500 | -1.59334300 |
| H | 5.40075500 | 2.56535500 | -3.21388200 |
| C | 5.47893400 | 3.34564700 | 0.58634100 |
| H | 3.51417300 | 2.48857500 | 0.67123700 |
| C | 6.56780600 | 3.68687000 | -0.22301500 |
| H | 7.38351300 | 3.65746800 | -2.22240300 |
| H | 5.51067600 | 3.54909400 | 1.65785900 |
| C | 7.75750700 | 4.39379900 | 0.37135200 |
| F | 7.95948700 | 4.04137400 | 1.65261900 |
| F | 8.88768900 | 4.12857100 | -0.30699900 |
| F | 7.59532700 | 5.73165800 | 0.35408900 |

**INT1-L10-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | 1.45469900 | 0.36832600 | -0.06314500 |
| C | 1.31232500 | 3.35546200 | 0.79186200 |
| C | 3.48616700 | 2.79070800 | 0.19256100 |
| C | 1.72587900 | 4.64173300 | 1.16861800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.07608700 | 2.87378900 | 0.96026500 | C | 4.27798400 | -2.03965800 | -3.95189000 |
| C | 3.96905300 | 4.04690700 | 0.54788400 | H | 3.85893300 | -1.53130000 | -4.83377300 |
| H | 4.14768600 | 2.00181900 | -0.16899400 | H | 5.26543800 | -2.44370700 | -4.22624000 |
| C | 3.06591900 | 4.99417900 | 1.03651600 | H | 3.61270000 | -2.87348700 | -3.69504800 |
| H | 1.01064300 | 5.35427000 | 1.57758900 | C | 5.13138400 | 0.20983900 | -3.24946100 |
| C | -1.14059100 | 3.70390600 | 1.32959000 | H | 6.13545700 | -0.01406100 | -3.64016500 |
| H | 5.03259200 | 4.26969400 | 0.44926500 | H | 4.54945400 | 0.69417800 | -4.04825500 |
| H | 3.40389600 | 5.99117500 | 1.32742600 | H | 5.23165100 | 0.92523700 | -2.41961800 |
| C | -1.50173400 | 1.03475300 | 0.88741600 | B | 0.70085100 | -1.52755500 | -0.07143900 |
| C | -2.41217200 | 3.16345000 | 1.48002500 | O | -0.56049000 | -1.86128500 | 0.45229400 |
| H | -0.98245000 | 4.76932100 | 1.49203800 | O | 1.29237800 | -2.69110800 | -0.56527300 |
| C | -2.62466500 | 1.79541500 | 1.25344500 | C | -0.85946400 | -3.24098600 | 0.17060200 |
| H | -1.56593900 | -0.03348500 | 0.67753400 | C | 0.56920700 | -3.84149500 | -0.09868800 |
| H | -3.23534200 | 3.81218500 | 1.78155700 | C | -1.76295000 | -3.27689300 | -1.06459700 |
| N | 2.19119900 | 2.46363700 | 0.28916900 | H | -2.09532700 | -4.29984900 | -1.29767400 |
| N | -0.28015200 | 1.55351600 | 0.75422600 | H | -2.64918200 | -2.65560500 | -0.87705600 |
| B | 3.02849700 | -0.48881500 | -1.00097400 | H | -1.24463000 | -2.87069700 | -1.94447100 |
| O | 4.24822600 | -0.91318000 | -0.46570000 | C | -1.59336100 | -3.83661100 | 1.36680600 |
| O | 3.07108100 | -0.65187000 | -2.39599300 | H | -2.58317900 | -3.36399900 | 1.46747700 |
| C | 4.96853600 | -1.65723700 | -1.46375400 | H | -1.74903300 | -4.91922200 | 1.23751600 |
| C | 4.39058900 | -1.05333000 | -2.79549300 | H | -1.03821200 | -3.66730100 | 2.29799200 |
| C | 4.60913100 | -3.13514400 | -1.27756800 | C | 0.61808800 | -4.92343800 | -1.17227400 |
| H | 5.15702800 | -3.78237500 | -1.97909900 | H | 1.65288000 | -5.27954400 | -1.28792000 |
| H | 4.87171900 | -3.43373000 | -0.25226000 | H | -0.00908900 | -5.78532300 | -0.89444100 |
| H | 3.52802800 | -3.28399900 | -1.39976300 | H | 0.28349700 | -4.54231400 | -2.14580300 |
| C | 6.46344000 | -1.44466800 | -1.25630800 | C | 1.26179600 | -4.33402700 | 1.17563900 |
| H | 6.77147900 | -1.89792900 | -0.30200000 | H | 0.79580700 | -5.25146800 | 1.56630100 |
| H | 7.04525700 | -1.91953000 | -2.06220500 | H | 2.31370900 | -4.55163100 | 0.93862200 |
| H | 6.71871800 | -0.37740600 | -1.21894600 | H | 1.25260900 | -3.55304300 | 1.94622600 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B | 2.40114800 | -0.18803100 | 1.60974200 | C | -4.43670400 | 1.30131000 | -2.75718600 |
| O | 2.24354800 | -1.36745700 | 2.32810600 | H | -4.97089700 | 2.19326400 | -3.13505100 |
| O | 3.32385800 | 0.63636800 | 2.25238800 | H | -3.93663800 | 0.83280300 | -3.62064400 |
| C | 3.29529100 | -1.45560000 | 3.30787800 | O | -3.47149100 | 1.74963900 | -1.81475400 |
| C | 3.66253500 | 0.05934500 | 3.52353600 | C | -2.14584100 | 1.52963000 | -2.08887600 |
| C | 4.43676700 | -2.25924800 | 2.67762200 | C | -1.64816800 | 0.23554900 | -2.28773100 |
| H | 5.26549300 | -2.41707900 | 3.38442600 | C | -1.29708400 | 2.63873000 | -2.13397300 |
| H | 4.04695500 | -3.24142300 | 2.37339500 | C | -0.28756200 | 0.06947700 | -2.54647400 |
| H | 4.80782300 | -1.75385700 | 1.77616200 | H | -2.31958300 | -0.61453800 | -2.18518300 |
| C | 2.76131100 | -2.16968600 | 4.54366500 | C | 0.06865400 | 2.45852300 | -2.38726500 |
| H | 2.53689200 | -3.21830200 | 4.29671900 | H | -1.69413800 | 3.64072900 | -1.97437100 |
| H | 3.50718700 | -2.16323600 | 5.35423800 | C | 0.58616200 | 1.16752500 | -2.60520800 |
| H | 1.83703600 | -1.70452800 | 4.91019800 | H | 0.12622800 | -0.92325200 | -2.72609100 |
| C | 2.78467900 | 0.74269000 | 4.57716400 | H | 1.62342900 | 0.98809900 | -2.87542600 |
| H | 3.02986400 | 0.41356900 | 5.59828000 | O | 0.83410700 | 3.57911300 | -2.40166400 |
| H | 2.94143800 | 1.82995600 | 4.51386500 | C | 2.14947700 | 3.48138200 | -2.91127200 |
| H | 1.71994300 | 0.54209800 | 4.38848600 | H | 2.59571000 | 4.47967900 | -2.81475100 |
| C | 5.13533900 | 0.32791600 | 3.80831000 | H | 2.75704300 | 2.75909900 | -2.34609900 |
| H | 5.29576100 | 1.40939200 | 3.93672800 | H | 2.14330800 | 3.18150600 | -3.97391900 |
| H | 5.45915300 | -0.17823600 | 4.73150800 | C | -3.95737300 | 1.16439000 | 1.34954200 |
| H | 5.76678900 | -0.01173000 | 2.97760200 | C | -5.13158800 | 1.93573400 | 1.26185300 |
| S | -4.88800400 | -1.31320400 | -1.71059200 | C | -4.08837600 | -0.22761700 | 1.49838100 |
| C | -4.63615800 | -2.01174900 | -3.37162200 | C | -6.38739400 | 1.33998500 | 1.30172800 |
| H | -3.83178200 | -1.49580100 | -3.91810600 | H | -5.06553700 | 3.01435100 | 1.11781200 |
| H | -4.33752100 | -3.05967400 | -3.22779900 | C | -5.34433500 | -0.83001000 | 1.52865400 |
| H | -5.56557100 | -1.98343800 | -3.96097700 | H | -3.20033300 | -0.85457600 | 1.57977600 |
| C | -5.46499700 | 0.36281700 | -2.14223200 | C | -6.49816000 | -0.05085100 | 1.42057900 |
| H | -6.32519900 | 0.27053200 | -2.82611600 | H | -7.28737400 | 1.95196300 | 1.21801300 |
| H | -5.84081500 | 0.78690500 | -1.20195800 | H | -5.42733200 | -1.91298800 | 1.62046300 |

| | | | |
|---|---|---|---|
| C | -7.85472700 | -0.69187300 | 1.32299100 |
| F | -7.85959600 | -1.95232000 | 1.78344000 |
| F | -8.78414800 | -0.00290600 | 2.01236900 |
| F | -8.27945200 | -0.73454400 | 0.04212300 |

**TS1-L10-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | -1.86109500 | 0.54610100 | -0.09758600 |
| C | -0.20682000 | 2.73877300 | 1.35112700 |
| C | 1.22997100 | 1.11982900 | 0.51388800 |
| C | 0.85668500 | 3.37624100 | 2.00331800 |
| C | -1.61669600 | 3.11330800 | 1.57329700 |
| C | 2.33365700 | 1.63643900 | 1.20969300 |
| H | 1.32224800 | 0.24331500 | -0.12426200 |
| C | 2.12742300 | 2.81815800 | 1.93697700 |
| H | 0.68186300 | 4.26069000 | 2.61492800 |
| C | -2.00285700 | 4.33703100 | 2.13927900 |
| H | 2.94539300 | 3.26984600 | 2.50058700 |
| C | -3.82918000 | 2.37241300 | 1.57645400 |
| C | -3.34477700 | 4.56688400 | 2.42296600 |
| H | -1.25642500 | 5.10571600 | 2.33669300 |
| C | -4.27427000 | 3.55798800 | 2.15425300 |
| H | -4.49922000 | 1.54344400 | 1.33648900 |
| H | -3.66165800 | 5.51999300 | 2.85194500 |
| N | 0.00896600 | 1.64277500 | 0.59574700 |
| N | -2.53669800 | 2.16551200 | 1.27406100 |
| B | -1.00699100 | -1.10577900 | -1.00571500 |
| O | 0.18034800 | -1.05556300 | -1.74628600 |
| O | -1.47123100 | -2.41034000 | -0.96809600 |
| C | 0.59774800 | -2.40768300 | -2.06477700 |
| C | -0.75540700 | -3.19493000 | -1.93621000 |
| C | 1.63664100 | -2.82501100 | -1.02216100 |
| H | 1.99810200 | -3.84834400 | -1.20322600 |
| H | 2.49915200 | -2.14913100 | -1.09162600 |
| H | 1.21353900 | -2.76478300 | -0.01089300 |
| C | 1.21736200 | -2.42646900 | -3.45766500 |
| H | 2.18575500 | -1.90711800 | -3.44565200 |
| H | 1.39665800 | -3.46358500 | -3.78308500 |
| H | 0.56526600 | -1.93882700 | -4.19383800 |
| C | -0.62297300 | -4.61927900 | -1.41248800 |
| H | -1.62066900 | -5.07653800 | -1.33544800 |
| H | -0.01427000 | -5.23514300 | -2.09290800 |
| H | -0.16455200 | -4.63980400 | -0.41565300 |
| C | -1.57752200 | -3.18016600 | -3.22891500 |
| H | -1.12544400 | -3.80954500 | -4.00964400 |
| H | -2.58577900 | -3.55826500 | -3.01227100 |
| H | -1.68734300 | -2.15657900 | -3.61356300 |
| B | -3.63738800 | -0.39478000 | -0.41325800 |
| O | -4.70157700 | -0.35791800 | 0.49080300 |
| O | -4.03428100 | -1.06840300 | -1.56288000 |
| C | -5.87810700 | -0.89873500 | -0.13833900 |
| C | -5.25178100 | -1.77862400 | -1.27931400 |
| C | -6.69335000 | 0.28098100 | -0.67763900 |
| H | -7.64512600 | -0.04574500 | -1.12273800 |
| H | -6.92239600 | 0.96784800 | 0.15142300 |
| H | -6.12411200 | 0.83791800 | -1.43623600 |
| C | -6.68268600 | -1.66652500 | 0.90294900 |
| H | -7.07891000 | -0.96820800 | 1.65584900 |
| H | -7.53440500 | -2.18818700 | 0.43832600 |
| H | -6.05619200 | -2.40114400 | 1.42405500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -6.08206900 | -1.87231500 | -2.55287200 | S | -1.56891700 | 3.62883000 | -1.76033700 |
| H | -5.55757800 | -2.50060200 | -3.28842900 | C | -2.54858000 | 2.10142800 | -1.68935400 |
| H | -7.06395000 | -2.32909700 | -2.35122700 | H | -3.49623100 | 2.35778000 | -1.19783700 |
| H | -6.23791300 | -0.88455400 | -3.00572800 | H | -2.81344200 | 1.80493800 | -2.71463100 |
| C | -4.86366300 | -3.17923900 | -0.79241700 | H | -1.72311600 | 0.65845700 | -1.69167900 |
| H | -5.74819500 | -3.80351400 | -0.59583700 | C | -0.47779900 | 3.22544800 | -3.16530000 |
| H | -4.25629400 | -3.66757200 | -1.56647700 | H | -1.11110400 | 2.85111000 | -3.98578300 |
| H | -4.25094200 | -3.12141700 | 0.11788300 | H | -0.03286500 | 4.17685300 | -3.49410900 |
| B | -1.39338100 | -0.81093800 | 1.44920300 | C | 0.63153900 | 2.22487300 | -2.90065400 |
| O | -2.26081400 | -1.31868600 | 2.39402800 | H | 1.04053100 | 1.87583400 | -3.86757600 |
| O | -0.09844400 | -1.28146900 | 1.69051700 | H | 0.26094000 | 1.34058200 | -2.36131400 |
| C | -1.58806400 | -2.35507200 | 3.13869300 | O | 1.66898400 | 2.87144500 | -2.17103600 |
| C | -0.07835600 | -1.95655000 | 2.96370900 | C | 2.86803000 | 2.24459400 | -2.08953400 |
| C | -1.93744700 | -3.68186000 | 2.45729200 | C | 3.98688100 | 3.04299100 | -1.78812500 |
| H | -1.50582100 | -4.54528700 | 2.98568200 | C | 3.02165200 | 0.87170600 | -2.29221200 |
| H | -3.03188900 | -3.79185200 | 2.44836300 | C | 5.24167000 | 2.45016000 | -1.71471600 |
| H | -1.59507600 | -3.68275300 | 1.41314600 | H | 3.84192300 | 4.11319000 | -1.63538200 |
| C | -2.09316600 | -2.34165100 | 4.57510900 | C | 4.29707100 | 0.29195400 | -2.20236800 |
| H | -3.15812300 | -2.61707900 | 4.59336700 | H | 2.16746700 | 0.22636000 | -2.48315400 |
| H | -1.54034200 | -3.06690100 | 5.19310600 | C | 5.42152200 | 1.07612200 | -1.92540200 |
| H | -1.99584800 | -1.34600100 | 5.02688900 | H | 6.11385200 | 3.06777700 | -1.48575500 |
| C | 0.40236200 | -0.93304400 | 3.99733600 | H | 6.41278900 | 0.63579200 | -1.83599600 |
| H | 0.51502300 | -1.37667500 | 4.99786000 | O | 4.33482300 | -1.05590800 | -2.39327700 |
| H | 1.37962800 | -0.54122400 | 3.67767900 | C | 5.58632400 | -1.69904000 | -2.50408900 |
| H | -0.29639400 | -0.08642600 | 4.06313500 | H | 5.37412300 | -2.75812000 | -2.70188800 |
| C | 0.89211500 | -3.12918200 | 2.89634100 | H | 6.17692300 | -1.28497000 | -3.34033000 |
| H | 1.91710600 | -2.75653200 | 2.74827200 | H | 6.17797200 | -1.61586700 | -1.58000200 |
| H | 0.87299900 | -3.70670700 | 3.83388900 | H | -5.33439700 | 3.68527900 | 2.37882300 |
| H | 0.65239300 | -3.80483000 | 2.06595200 | C | 3.62209300 | 0.91654900 | 1.21478600 |

| | | | |
|---|---|---|---|
| C | 3.64579100 | -0.48069400 | 1.05815700 |
| C | 4.84006200 | 1.58854200 | 1.41255200 |
| C | 4.84843900 | -1.18159500 | 1.07769200 |
| H | 2.70869300 | -1.02313300 | 0.94051700 |
| C | 6.04276000 | 0.89136000 | 1.44844000 |
| H | 4.85129100 | 2.67473000 | 1.50753400 |
| C | 6.05198600 | -0.49656600 | 1.27295900 |
| H | 4.84918000 | -2.26507800 | 0.95233900 |
| H | 6.98194800 | 1.42678000 | 1.59687800 |
| C | 7.36436600 | -1.22746100 | 1.23642500 |
| F | 8.25464300 | -0.71567500 | 2.10236600 |
| F | 7.23060200 | -2.53472600 | 1.51152000 |
| F | 7.93910700 | -1.14809500 | 0.00802500 |

**TS1-L10-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | 1.24122100 | 0.06923900 | 0.31205800 |
| C | 0.98144200 | 0.03970000 | 3.37491900 |
| C | 3.19597300 | 0.38322500 | 2.73471400 |
| C | 1.34332000 | 0.10999900 | 4.72775900 |
| C | -0.40492100 | -0.22213900 | 2.92898400 |
| C | 3.62115900 | 0.46332100 | 4.05752500 |
| H | 3.89571700 | 0.44080100 | 1.89972100 |
| C | 2.67294700 | 0.32955500 | 5.07352200 |
| H | 0.59167600 | -0.01389600 | 5.50584200 |
| C | -1.49013800 | -0.33531800 | 3.81043800 |
| H | 4.67768000 | 0.62117400 | 4.27891000 |
| H | 2.96608500 | 0.38582800 | 6.12399500 |
| C | -1.81222200 | -0.57601200 | 1.11199200 |
| C | -2.76790300 | -0.54602000 | 3.30412300 |
| H | -1.34741100 | -0.22868400 | 4.88481000 |
| C | -2.95709000 | -0.66012100 | 1.91823300 |
| H | -1.86167100 | -0.70710400 | 0.02945600 |
| H | -3.62185000 | -0.58764500 | 3.98306100 |
| N | 1.91106700 | 0.19320600 | 2.40667700 |
| N | -0.59361700 | -0.34841500 | 1.60078200 |
| B | 3.02961700 | 0.31063500 | -0.61953600 |
| O | 4.17480000 | -0.43454800 | -0.31499600 |
| O | 3.33194500 | 1.24070700 | -1.60435300 |
| C | 5.11712400 | -0.26109200 | -1.39240100 |
| C | 4.73043300 | 1.16487100 | -1.92963600 |
| C | 4.83707100 | -1.36757900 | -2.41461900 |
| H | 5.53993600 | -1.32995500 | -3.26037200 |
| H | 4.94115000 | -2.34078700 | -1.91665800 |
| H | 3.80625600 | -1.29321000 | -2.78845800 |
| C | 6.53148600 | -0.38786700 | -0.84260600 |
| H | 6.69566100 | -1.41478300 | -0.48273900 |
| H | 7.27790000 | -0.17733600 | -1.62472100 |
| H | 6.70326400 | 0.29660800 | -0.00121700 |
| C | 4.88977100 | 1.34852100 | -3.43444000 |
| H | 4.59884700 | 2.37242700 | -3.71394500 |
| H | 5.93464800 | 1.19084400 | -3.74567100 |
| H | 4.24334500 | 0.65383300 | -3.98494000 |
| C | 5.44310600 | 2.29549400 | -1.18199700 |
| H | 6.51543900 | 2.33771000 | -1.42492000 |
| H | 4.98738100 | 3.25350900 | -1.46916900 |
| H | 5.33396800 | 2.17963000 | -0.09345200 |
| B | 0.58720300 | -0.72360800 | -1.47966700 |
| O | -0.71205100 | -1.20990400 | -1.62895100 |
| O | 1.26477600 | -0.81946500 | -2.68032300 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.97823600 | -1.40434100 | -3.03283800 | H | 2.16951000 | -6.29719700 | -0.06443500 |
| C | 0.47395200 | -1.57670500 | -3.61680600 | H | 0.87058800 | -5.30376800 | -0.78234800 |
| C | -1.67627300 | -0.13701600 | -3.53471700 | C | 0.29842500 | -4.46554800 | 1.64189200 |
| H | -1.98260400 | -0.22485700 | -4.58752200 | H | 0.21661700 | -5.56229900 | 1.60589200 |
| H | -2.57358800 | 0.04812400 | -2.92626900 | H | -0.17550700 | -4.11077900 | 2.56927400 |
| H | -1.01445800 | 0.73486100 | -3.43329600 | H | -0.25884500 | -4.03971300 | 0.79452200 |
| C | -1.89140500 | -2.61206100 | -3.19598300 | C | 2.52592100 | -4.59821000 | 2.79175100 |
| H | -2.87330900 | -2.39768900 | -2.74691800 | H | 1.97643400 | -4.42021800 | 3.72868400 |
| H | -2.04663800 | -2.84690800 | -4.26056100 | H | 2.64502000 | -5.68604500 | 2.66633900 |
| H | -1.47518700 | -3.49641300 | -2.69694800 | H | 3.51961100 | -4.14300200 | 2.89216500 |
| C | 0.67732200 | -0.99027500 | -5.00909400 | S | -3.23956400 | 2.79692500 | -1.57239300 |
| H | 1.71752100 | -1.15504600 | -5.32773900 | C | -1.91892100 | 3.68012000 | -2.45587100 |
| H | 0.01445400 | -1.47654500 | -5.74208000 | H | -1.10213000 | 3.96565600 | -1.77752900 |
| H | 0.48982100 | 0.09084800 | -5.02361300 | H | -1.52500600 | 2.97381400 | -3.19900000 |
| C | 0.96617800 | -3.02486900 | -3.57640400 | H | -2.31192600 | 4.56397800 | -2.98107100 |
| H | 0.44311800 | -3.65175100 | -4.31422500 | C | -3.97493600 | 4.12722400 | -0.55571500 |
| H | 2.04158700 | -3.03889300 | -3.80617600 | H | -4.55787900 | 4.80518400 | -1.20341300 |
| H | 0.84252900 | -3.45093300 | -2.57397100 | H | -4.68533800 | 3.60020100 | 0.09991700 |
| B | 1.74421300 | -1.97991900 | 0.50654400 | C | -3.02041100 | 4.96672900 | 0.29130400 |
| O | 2.03391700 | -2.94292600 | -0.44614900 | H | -3.62666300 | 5.70508800 | 0.84555100 |
| O | 1.73141500 | -2.56210900 | 1.77267200 | H | -2.32840300 | 5.53419100 | -0.35376600 |
| C | 2.43457600 | -4.15830200 | 0.21929300 | O | -2.30185100 | 4.19929300 | 1.23629400 |
| C | 1.75634000 | -3.99353600 | 1.62506900 | C | -0.98384700 | 3.91380800 | 0.94845900 |
| C | 3.96376400 | -4.15241500 | 0.29136900 | C | -0.63318300 | 2.58131800 | 0.72215800 |
| H | 4.35530600 | -5.06299300 | 0.76889100 | C | -0.02627700 | 4.92478900 | 0.88678400 |
| H | 4.36423200 | -4.09939300 | -0.73088200 | C | 0.68353600 | 2.22853600 | 0.40290400 |
| H | 4.32556300 | -3.26982000 | 0.83728200 | H | -1.44094600 | 1.85564000 | 0.74556500 |
| C | 1.94997600 | -5.35454700 | -0.59042000 | C | 1.29588100 | 4.58393500 | 0.55590900 |
| H | 2.46478000 | -5.37767100 | -1.56227300 | H | -0.27875000 | 5.96802400 | 1.08085900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.64569100 | 3.25039200 | 0.29773000 | H | 1.40779000 | 0.18567600 | -0.22928000 |
| H | 0.71448700 | 1.10593900 | -0.80734400 | C | 2.18302000 | 2.98178100 | 1.53576300 |
| H | 2.65201400 | 2.99241600 | -0.02211100 | H | 0.70634100 | 4.42793000 | 2.12955600 |
| O | 2.17349100 | 5.62598100 | 0.50363900 | C | -1.98626600 | 4.30245300 | 1.86508900 |
| C | 3.49694400 | 5.36898100 | 0.10426100 | H | 3.00085400 | 3.50926100 | 2.02976500 |
| H | 4.02553800 | 6.33198700 | 0.12340300 | C | -3.72572000 | 2.21328700 | 1.52240100 |
| H | 4.00764200 | 4.66461400 | 0.78560700 | C | -3.30721800 | 4.45879100 | 2.26762300 |
| H | 3.54168600 | 4.95245200 | -0.91780800 | H | -1.27412300 | 5.11918300 | 1.97487800 |
| C | -4.28745700 | -0.82242800 | 1.29513800 | C | -4.18653700 | 3.38279500 | 2.11778300 |
| C | -5.30407100 | -1.57101100 | 1.91204200 | H | -4.37353600 | 1.35471900 | 1.33906400 |
| C | -4.55808900 | -0.20999900 | 0.05715800 | H | -3.64478300 | 5.40413200 | 2.69786100 |
| C | -6.55461500 | -1.70527700 | 1.31161400 | N | 0.07402800 | 1.63156800 | 0.34837900 |
| H | -5.10770800 | -2.07647300 | 2.85982000 | N | -2.45572000 | 2.07774100 | 1.10007700 |
| C | -5.80752700 | -0.33915900 | -0.54325900 | B | -0.96673600 | -1.35501700 | -0.60963100 |
| H | -3.79518900 | 0.40280600 | -0.42496700 | O | 0.32740200 | -1.50550800 | -1.12478900 |
| C | -6.81061400 | -1.08784500 | 0.08271300 | O | -1.56581500 | -2.59760200 | -0.47477500 |
| H | -7.33231000 | -2.30170100 | 1.79092200 | C | 0.63796600 | -2.91428800 | -1.23326200 |
| H | -6.00119500 | 0.15027900 | -1.49923700 | C | -0.79512200 | -3.56886400 | -1.20569500 |
| C | -8.17849000 | -1.18022000 | -0.54039800 | C | 1.50468800 | -3.28715100 | -0.02893100 |
| F | -8.11784600 | -1.16775200 | -1.88328200 | H | 1.77426600 | -4.35331600 | -0.03604600 |
| F | -8.82273500 | -2.30246900 | -0.17343400 | H | 2.43448900 | -2.70359300 | -0.07861500 |
| F | -8.95904700 | -0.14379300 | -0.17503200 | H | 0.99433400 | -3.04571700 | 0.91276600 |
| **INT2-L10-sp$^3$** | | | | C | 1.41358700 | -3.15338100 | -2.52370400 |
| Ir | -1.85701900 | 0.52012600 | -0.29977300 | H | 2.39787600 | -2.67009200 | -2.46542100 |
| C | -0.15914800 | 2.77329000 | 1.02421500 | H | 1.56603500 | -4.23251100 | -2.68509600 |
| C | 1.30411800 | 1.12824300 | 0.30555100 | H | 0.88234700 | -2.74443200 | -3.39259800 |
| C | 0.89641200 | 3.50135200 | 1.58958300 | C | -0.87626900 | -4.90387100 | -0.47701100 |
| C | -1.57076400 | 3.08645600 | 1.30364100 | H | -1.91607200 | -5.26298000 | -0.48358600 |
| C | 2.40569700 | 1.73858000 | 0.92629000 | H | -0.24770400 | -5.66065400 | -0.97157000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.55752300 | -4.81228000 | 0.56915900 | C | -1.79655900 | -1.63285200 | 3.48865600 |
| C | -1.42457800 | -3.68662700 | -2.59710600 | C | -0.31799700 | -1.10502500 | 3.41831800 |
| H | -0.92306400 | -4.44947100 | -3.21015000 | C | -1.90677700 | -3.13829900 | 3.23607200 |
| H | -2.48090400 | -3.96466700 | -2.48534500 | H | -1.51682900 | -3.72761000 | 4.07940400 |
| H | -1.39421500 | -2.72532300 | -3.12877200 | H | -2.96652700 | -3.39344900 | 3.09065900 |
| B | -3.65284100 | -0.37918200 | -0.62238500 | H | -1.37102300 | -3.41899100 | 2.31898200 |
| O | -4.77298300 | -0.22221200 | 0.19094900 | C | -2.55710500 | -1.24418000 | 4.74911300 |
| O | -3.97232500 | -1.18734300 | -1.70370900 | H | -3.57974500 | -1.64693100 | 4.70184800 |
| C | -5.92046900 | -0.78478100 | -0.47527300 | H | -2.06724100 | -1.65530300 | 5.64590100 |
| C | -5.24339600 | -1.81396100 | -1.44976200 | H | -2.62966000 | -0.15400600 | 4.85432900 |
| C | -6.62448700 | 0.35914800 | -1.21101200 | C | -0.12774000 | 0.24925700 | 4.10935500 |
| H | -7.55451700 | 0.02500500 | -1.69479400 | H | -0.16096000 | 0.16208800 | 5.20550100 |
| H | -6.87657100 | 1.14796300 | -0.48637500 | H | 0.85146400 | 0.65827300 | 3.81937600 |
| H | -5.96689600 | 0.79821700 | -1.97516500 | H | -0.89949200 | 0.96440100 | 3.78911300 |
| C | -6.84502400 | -1.39458500 | 0.57020200 | C | 0.74743900 | -2.08955400 | 3.88048800 |
| H | -7.27191300 | -0.59886000 | 1.19970600 | H | 1.74474700 | -1.64202900 | 3.75213600 |
| H | -7.67782300 | -1.93412000 | 0.09229400 | H | 0.61718500 | -2.33662700 | 4.94570100 |
| H | -6.30152400 | -2.08753500 | 1.22462800 | H | 0.71721700 | -3.02040500 | 3.30026500 |
| C | -5.96821400 | -2.01915700 | -2.77359600 | S | -1.48551200 | 3.46707500 | -2.05497800 |
| H | -5.41512500 | -2.74599600 | -3.38718000 | C | -2.59943800 | 2.06302200 | -1.67583500 |
| H | -6.98400900 | -2.41244800 | -2.60976500 | H | -3.49122400 | 2.53268000 | -1.23157900 |
| H | -6.03880500 | -1.08358700 | -3.34319600 | H | -2.92398100 | 1.63918200 | -2.63792500 |
| C | -4.96760700 | -3.16278100 | -0.77753900 | H | -1.54264800 | -0.25329800 | -1.66297800 |
| H | -5.89736700 | -3.71657800 | -0.57909600 | C | -0.52029600 | 2.73540300 | -3.42146700 |
| H | -4.33915100 | -3.76906700 | -1.44381200 | H | -1.23394400 | 2.23005400 | -4.09181100 |
| H | -4.41522800 | -3.02700600 | 0.16262400 | H | -0.07915700 | 3.57760300 | -3.97633000 |
| B | -1.41646000 | -0.64042000 | 1.45417900 | C | 0.58340400 | 1.75782400 | -3.06044400 |
| O | -2.40317300 | -0.97301000 | 2.35594500 | H | 0.90304900 | 1.21819400 | -3.97191300 |
| O | -0.15948700 | -0.86786900 | 2.00401100 | H | 0.23042000 | 1.01143100 | -2.33409700 |

| | | | |
|---|---|---|---|
| O | 1.69186000 | 2.48855000 | -2.54699500 |
| C | 2.88650200 | 1.86260700 | -2.43212000 |
| C | 4.02079700 | 2.68915200 | -2.32106700 |
| C | 3.02976700 | 0.47251000 | -2.41243800 |
| C | 5.27708100 | 2.10816000 | -2.20522200 |
| H | 3.88204700 | 3.77079600 | -2.34225500 |
| C | 4.30829000 | -0.09286700 | -2.27266300 |
| H | 2.17126100 | -0.19434900 | -2.46073500 |
| C | 5.44486500 | 0.71704400 | -2.18385200 |
| H | 6.15910600 | 2.74843700 | -2.12344300 |
| H | 6.43775800 | 0.28930300 | -2.05908200 |
| O | 4.34198100 | -1.45348900 | -2.21702500 |
| C | 5.58703300 | -2.11340300 | -2.29590300 |
| H | 5.36732100 | -3.18948800 | -2.30024100 |
| H | 6.12332900 | -1.84886500 | -3.22429900 |
| H | 6.23476000 | -1.88144000 | -1.43706200 |
| H | -5.22675900 | 3.44657500 | 2.44033800 |
| C | 3.71132500 | 1.05409000 | 0.98899100 |
| C | 3.76380500 | -0.34978500 | 1.03506800 |
| C | 4.91716200 | 1.77227900 | 1.05276100 |
| C | 4.98189400 | -1.01686400 | 1.12656200 |
| H | 2.83545600 | -0.92001900 | 1.02023600 |
| C | 6.13640800 | 1.11117400 | 1.15603100 |
| H | 4.90370500 | 2.86083700 | 0.98821600 |
| C | 6.17346600 | -0.28702700 | 1.18700900 |
| H | 5.00555700 | -2.10678200 | 1.16197900 |
| H | 7.06640300 | 1.68048900 | 1.19750100 |
| C | 7.50032300 | -0.99098300 | 1.22280500 |
| F | 8.40422200 | -0.33397100 | 1.96822700 |
| F | 7.40380200 | -2.24097600 | 1.70424600 |
| F | 8.03709300 | -1.09729900 | -0.02066600 |

**INT2-L10-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | 1.02989100 | -0.01298700 | 0.26002300 |
| C | 1.06615900 | -0.24497700 | 3.27954500 |
| C | 3.21794300 | 0.16294400 | 2.46764100 |
| C | 1.55449100 | -0.30040200 | 4.59164700 |
| C | -0.36616500 | -0.39899300 | 2.95359700 |
| C | 3.76042400 | 0.12306500 | 3.74933600 |
| H | 3.82499400 | 0.35499800 | 1.57983100 |
| C | 2.91321400 | -0.12036600 | 4.83165500 |
| H | 0.87233500 | -0.49273500 | 5.41861300 |
| C | -1.39427900 | -0.39607100 | 3.90728200 |
| H | 4.83181500 | 0.27756100 | 3.88533600 |
| H | 3.30353000 | -0.16747400 | 5.85047300 |
| C | -1.92370600 | -0.56939300 | 1.23617200 |
| C | -2.71912100 | -0.45029000 | 3.48524200 |
| H | -1.16856700 | -0.30787500 | 4.96947200 |
| C | -3.01494900 | -0.52402300 | 2.11385700 |
| H | -2.06494900 | -0.68597900 | 0.16368500 |
| H | -3.52401700 | -0.39620000 | 4.22057300 |
| N | 1.90893600 | -0.02530900 | 2.23963500 |
| N | -0.65961200 | -0.49393200 | 1.64292200 |
| B | 2.55099900 | 0.73657000 | -0.86641100 |
| O | 3.85452200 | 0.92448900 | -0.39788000 |
| O | 2.43402100 | 1.23793700 | -2.14776900 |
| C | 4.68464500 | 1.34468200 | -1.50153800 |
| C | 3.62438700 | 1.97015100 | -2.48211300 |
| C | 5.34981200 | 0.08544600 | -2.06355600 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 6.02712100 | 0.31677300 | -2.89897700 | H | 0.66290400 | -1.85919800 | -5.20978300 |
| H | 5.93762600 | -0.38970700 | -1.26431600 | H | -0.87063100 | -2.76827100 | -5.15731500 |
| H | 4.59271200 | -0.63801600 | -2.39758900 | H | -0.81487100 | -1.06257400 | -4.63027200 |
| C | 5.73493300 | 2.31974400 | -0.98569600 | C | 1.01845500 | -3.67922500 | -3.28226400 |
| H | 6.42360100 | 1.79944500 | -0.30236400 | H | 0.57364400 | -4.51654700 | -3.84004600 |
| H | 6.32843700 | 2.73375100 | -1.81578500 | H | 1.95233000 | -3.37825800 | -3.77783500 |
| H | 5.27401700 | 3.15122200 | -0.43657200 | H | 1.27983600 | -4.01982900 | -2.27320100 |
| C | 3.92562900 | 1.76685000 | -3.96198200 | B | 1.94901900 | -1.96233100 | 0.19070900 |
| H | 3.13110200 | 2.23156600 | -4.56475300 | O | 2.96368000 | -2.45206500 | -0.60878200 |
| H | 4.88400100 | 2.23374800 | -4.23951400 | O | 1.78006900 | -2.76743600 | 1.30547900 |
| H | 3.96019500 | 0.70025400 | -4.21768000 | C | 3.67226700 | -3.48196100 | 0.11343200 |
| C | 3.33856400 | 3.44770100 | -2.19428400 | C | 2.60344400 | -3.94272800 | 1.17580600 |
| H | 4.18017900 | 4.09580200 | -2.48176300 | C | 4.89925300 | -2.81877900 | 0.74482100 |
| H | 2.45298400 | 3.75147300 | -2.77158900 | H | 5.53682500 | -3.54890800 | 1.26484700 |
| H | 3.10731100 | 3.60598800 | -1.13167500 | H | 5.48826600 | -2.33984600 | -0.04941400 |
| B | 0.41034200 | -1.35660500 | -1.23169200 | H | 4.60339200 | -2.03814100 | 1.45875500 |
| O | -0.67203600 | -2.20953400 | -1.01037300 | C | 4.11291300 | -4.56116900 | -0.86765700 |
| O | 0.79426900 | -1.40993700 | -2.56261800 | H | 4.83492400 | -4.13676300 | -1.58096900 |
| C | -1.16321100 | -2.68837100 | -2.27832400 | H | 4.60212600 | -5.39386400 | -0.33848300 |
| C | 0.08387500 | -2.46846500 | -3.22382800 | H | 3.26786800 | -4.95895700 | -1.44238900 |
| C | -2.37101500 | -1.82680400 | -2.65382500 | C | 1.69899800 | -5.07222700 | 0.67766800 |
| H | -2.83546300 | -2.15629200 | -3.59463500 | H | 2.23612300 | -6.02959100 | 0.60634300 |
| H | -3.12642300 | -1.89872500 | -1.85699900 | H | 0.86146300 | -5.18974800 | 1.38034100 |
| H | -2.09621800 | -0.76920400 | -2.75612600 | H | 1.27433500 | -4.82971300 | -0.30565100 |
| C | -1.59462500 | -4.14108000 | -2.11392800 | C | 3.17143700 | -4.29036300 | 2.54710400 |
| H | -2.45073600 | -4.19546200 | -1.42494800 | H | 2.35308500 | -4.59158300 | 3.21807200 |
| H | -1.90387400 | -4.57052600 | -3.07948600 | H | 3.88460900 | -5.12674600 | 2.47993600 |
| H | -0.78789200 | -4.75651900 | -1.69672900 | H | 3.67820500 | -3.42868500 | 3.00055800 |
| C | -0.26346000 | -2.01142300 | -4.63649900 | S | -2.61794400 | 1.91746400 | -2.40885700 |

| | | | |
|---|---|---|---|
| C | -0.91299200 | 2.11600700 | -3.01725100 |
| H | -0.25772200 | 2.54735600 | -2.24889400 |
| H | -0.53024900 | 1.11084300 | -3.24209400 |
| H | -0.89188900 | 2.72239000 | -3.93543000 |
| C | -3.16253000 | 3.65476800 | -2.20553900 |
| H | -3.31181800 | 4.09318900 | -3.20751400 |
| H | -4.15230100 | 3.57454300 | -1.72981600 |
| C | -2.28997700 | 4.61516800 | -1.39916000 |
| H | -2.74259400 | 5.61876700 | -1.50453100 |
| H | -1.27589300 | 4.67354000 | -1.82968300 |
| O | -2.22081900 | 4.31581700 | -0.01639000 |
| C | -0.98870400 | 3.87700400 | 0.43504800 |
| C | -0.68270000 | 2.51725700 | 0.35776200 |
| C | -0.05983600 | 4.79463400 | 0.92214700 |
| C | 0.59157200 | 2.03922500 | 0.68528900 |
| H | -1.45573300 | 1.86202600 | -0.03950800 |
| C | 1.20577100 | 4.32408500 | 1.30797100 |
| H | -0.29409900 | 5.85731300 | 0.99185500 |
| C | 1.53077000 | 2.96518400 | 1.17719200 |
| H | 0.21454400 | 0.27802500 | -1.08464000 |
| H | 2.53790200 | 2.62846200 | 1.42107600 |
| O | 2.07505700 | 5.27062500 | 1.77206600 |
| C | 3.36768900 | 4.86916500 | 2.14707200 |
| H | 3.89103000 | 5.77053800 | 2.49509100 |
| H | 3.35078700 | 4.12502400 | 2.96475100 |
| H | 3.92999100 | 4.43460700 | 1.29991000 |
| C | -4.39125100 | -0.53348300 | 1.57457200 |
| C | -5.45194600 | -1.12327900 | 2.28350300 |
| C | -4.66072800 | 0.04918700 | 0.32095900 |
| C | -6.74279000 | -1.13439400 | 1.75940000 |
| H | -5.26169700 | -1.60526200 | 3.24446700 |
| C | -5.94952700 | 0.03601900 | -0.20579600 |
| H | -3.86359600 | 0.53727200 | -0.24316600 |
| C | -6.99553000 | -0.55408000 | 0.51201700 |
| H | -7.55531200 | -1.60870000 | 2.31177900 |
| H | -6.14078300 | 0.48743900 | -1.18064800 |
| C | -8.39850800 | -0.51765300 | -0.03439900 |
| F | -8.41289100 | -0.55785400 | -1.37801900 |
| F | -9.13649500 | -1.55065600 | 0.41057800 |
| F | -9.04228300 | 0.60853200 | 0.33028600 |

**TS2-L10-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | 1.79533900 | 0.03199400 | 0.28358900 |
| C | 0.11111800 | 1.34035400 | 2.48395800 |
| C | -1.25819300 | 0.83811500 | 0.66681000 |
| C | -0.95259800 | 1.98543400 | 3.13139800 |
| C | 1.48714600 | 1.29568500 | 3.01725700 |
| C | -2.36871300 | 1.47321800 | 1.23862600 |
| H | -1.32488100 | 0.33742200 | -0.29958000 |
| C | -2.19410900 | 2.04404800 | 2.51012800 |
| H | -0.80856200 | 2.45821700 | 4.10197500 |
| C | 1.81379000 | 1.72357000 | 4.31146900 |
| H | -3.02419000 | 2.56041200 | 2.99554700 |
| C | 3.73075200 | 0.81551200 | 2.57702800 |
| C | 3.13727500 | 1.68430800 | 4.73470600 |
| H | 1.03174800 | 2.06487600 | 4.98819400 |
| C | 4.11533600 | 1.22139000 | 3.85088300 |
| H | 4.44534700 | 0.42560500 | 1.84927400 |
| H | 3.40199800 | 2.00480700 | 5.74455500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -0.07421100 | 0.77043200 | 1.27494000 | H | 0.79288500 | -5.77795200 | -1.36893900 |
| N | 2.45067800 | 0.85392200 | 2.17059500 | H | 2.39135500 | -5.12078900 | -0.92305800 |
| B | 1.79758500 | 1.91018100 | -0.60506700 | H | 0.95883700 | -4.72098000 | 0.05481700 |
| O | 0.77441200 | 2.36373200 | -1.42922500 | C | 1.53419100 | -3.97040400 | -3.28686100 |
| O | 2.69898400 | 2.92849300 | -0.34723700 | H | 2.54542200 | -4.40485200 | -3.28572500 |
| C | 0.86061100 | 3.79971000 | -1.51134800 | H | 0.85114200 | -4.69578200 | -3.75621400 |
| C | 2.37999700 | 4.05230600 | -1.19724800 | H | 1.56074700 | -3.05886400 | -3.89697200 |
| C | -0.07458700 | 4.36233000 | -0.43436200 | C | -1.43684800 | -4.06404400 | -1.45078500 |
| H | -0.12816300 | 5.46080200 | -0.46486000 | H | -2.40607700 | -3.55196200 | -1.40327600 |
| H | -1.08601700 | 3.96125600 | -0.59725400 | H | -1.47778400 | -4.80669800 | -2.26316300 |
| H | 0.25083800 | 4.05348700 | 0.57000600 | H | -1.28176400 | -4.59321500 | -0.50175400 |
| C | 0.40456400 | 4.24908800 | -2.89321800 | C | -0.71015000 | -2.14694800 | -2.89523600 |
| H | -0.66644300 | 4.02913700 | -3.02006000 | H | -0.93678600 | -2.73110900 | -3.79986300 |
| H | 0.54751000 | 5.33356200 | -3.02231300 | H | -1.60235300 | -1.57450500 | -2.61012900 |
| H | 0.95249500 | 3.72296700 | -3.68507900 | H | 0.09861000 | -1.43948400 | -3.12832700 |
| C | 2.67502500 | 5.34169000 | -0.44217800 | B | 3.58950600 | -0.27438300 | -0.62338700 |
| H | 3.75718100 | 5.42457200 | -0.26112500 | O | 3.87843200 | -0.09857900 | -1.96646500 |
| H | 2.35745200 | 6.22054500 | -1.02536800 | O | 4.73408300 | -0.70025900 | 0.05809200 |
| H | 2.16858000 | 5.36293200 | 0.53154300 | C | 5.29030700 | -0.27276800 | -2.17653100 |
| C | 3.26965800 | 3.94448200 | -2.43805800 | C | 5.71292300 | -1.11666100 | -0.91786200 |
| H | 3.12929400 | 4.79683800 | -3.11959400 | C | 5.92116200 | 1.12258700 | -2.19986800 |
| H | 4.32103400 | 3.92402500 | -2.11742800 | H | 7.00069800 | 1.08435200 | -2.40991400 |
| H | 3.06762800 | 3.01116400 | -2.98272300 | H | 5.43463100 | 1.71562300 | -2.98729300 |
| B | 1.17112900 | -1.78937300 | -0.51089100 | H | 5.76003700 | 1.64160300 | -1.24383500 |
| O | 1.93369000 | -2.60166000 | -1.35119200 | C | 5.50400000 | -0.97304500 | -3.51323600 |
| O | -0.17574200 | -2.19254300 | -0.55966000 | H | 5.17975900 | -0.31218300 | -4.33119400 |
| C | 1.10702800 | -3.66396100 | -1.85635400 | H | 6.56744300 | -1.21489500 | -3.66864300 |
| C | -0.33280400 | -3.04940900 | -1.71635800 | H | 4.91571800 | -1.89738900 | -3.57406700 |
| C | 1.31559300 | -4.89608200 | -0.97006100 | C | 5.51984700 | -2.62311000 | -1.11940600 |

| | | | |
|---|---|---|---|
| H | 6.25734300 | -3.04156100 | -1.82068200 |
| H | 5.64043000 | -3.12570800 | -0.14799600 |
| H | 4.50475600 | -2.83516000 | -1.48419900 |
| C | 7.10744300 | -0.82235600 | -0.38167300 |
| H | 7.30406000 | -1.44788500 | 0.50234500 |
| H | 7.87457200 | -1.05152900 | -1.13801900 |
| H | 7.21228200 | 0.22939300 | -0.08449900 |
| S | 1.03808500 | -2.00658700 | 3.03762100 |
| C | 1.92275100 | -2.02024000 | 1.44178200 |
| H | 2.97989700 | -1.87041200 | 1.69912000 |
| H | 1.88948300 | -3.04737000 | 1.05817800 |
| H | 1.22406900 | -0.20717000 | -1.18398600 |
| C | -0.61725500 | -2.68095100 | 2.61847400 |
| H | -0.67562000 | -2.77661600 | 1.52788100 |
| H | -0.73141100 | -3.67785700 | 3.07182400 |
| C | -1.69209300 | -1.74736000 | 3.16516800 |
| H | -1.68806400 | -0.79718900 | 2.61676600 |
| H | -1.48051700 | -1.52446700 | 4.22224500 |
| O | -3.00217500 | -2.30423000 | 3.16221600 |
| C | -3.80818400 | -2.16258200 | 2.07941800 |
| C | -5.18548800 | -2.33981900 | 2.31389400 |
| C | -3.35032700 | -1.87441800 | 0.79019700 |
| C | -6.08038200 | -2.22836600 | 1.25677700 |
| H | -5.51587700 | -2.56482800 | 3.32881700 |
| C | -4.27478000 | -1.75874600 | -0.26145700 |
| H | -2.29317900 | -1.77153600 | 0.55298300 |
| C | -5.64452100 | -1.93695400 | -0.04199200 |
| H | -7.14931100 | -2.36319700 | 1.44070700 |
| H | -6.36796100 | -1.82487100 | -0.84686000 |
| O | -3.73877100 | -1.47476200 | -1.48242200 |
| C | -4.56275000 | -1.55918400 | -2.62539000 |
| H | -3.91353100 | -1.36434900 | -3.48936600 |
| H | -5.00676000 | -2.56512000 | -2.72528900 |
| H | -5.37314700 | -0.81455200 | -2.60523400 |
| H | 5.16594600 | 1.16733400 | 4.13938500 |
| C | -3.66141400 | 1.51196500 | 0.52777000 |
| C | -3.70261500 | 1.71325600 | -0.86260300 |
| C | -4.86734000 | 1.33477700 | 1.22473400 |
| C | -4.91991900 | 1.73952100 | -1.53638100 |
| H | -2.77216100 | 1.86239900 | -1.41363100 |
| C | -6.08503500 | 1.34501700 | 0.55135300 |
| H | -4.84928300 | 1.13291900 | 2.29678800 |
| C | -6.11352000 | 1.54649600 | -0.83161600 |
| H | -4.94539300 | 1.90980700 | -2.61395200 |
| H | -7.01387400 | 1.17502100 | 1.09606300 |
| C | -7.41417900 | 1.47782000 | -1.58255800 |
| F | -8.47391100 | 1.71380600 | -0.79462100 |
| F | -7.45677500 | 2.35379500 | -2.60055400 |
| F | -7.60249000 | 0.24874300 | -2.12880900 |

**TS2-L10-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | -0.60841000 | 0.42464000 | -0.17801600 |
| C | -0.50139500 | -0.74602300 | 2.65523400 |
| C | -2.62599000 | 0.10863400 | 2.22863700 |
| C | -0.89403700 | -1.15908700 | 3.93563300 |
| C | 0.87978100 | -0.89209400 | 2.15024200 |
| C | -3.07533600 | -0.26357400 | 3.49366600 |
| H | -3.26296700 | 0.62413600 | 1.51113500 |
| C | -2.19785600 | -0.91901600 | 4.35787900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.18676100 | -1.65855200 | 4.59675400 | C | -3.53574000 | -2.23287100 | -3.33335600 |
| C | 1.93880800 | -1.41754800 | 2.90521200 | H | -4.39981300 | -2.86036700 | -3.59751200 |
| H | -4.10312000 | -0.04309000 | 3.78614200 | H | -2.99035900 | -1.98403100 | -4.25565800 |
| H | -2.52237200 | -1.23713800 | 5.35094400 | H | -2.85939400 | -2.81463000 | -2.69403500 |
| C | 2.34508700 | -0.41478200 | 0.39717100 | B | 0.22809300 | 2.18769700 | 0.61190300 |
| C | 3.22844000 | -1.40081800 | 2.38642200 | O | 1.52984900 | 2.54550100 | 0.28718800 |
| H | 1.76363800 | -1.80494300 | 3.90795500 | O | -0.24944000 | 2.99502300 | 1.63242400 |
| C | 3.46382700 | -0.86495700 | 1.10885600 | C | 1.85608400 | 3.77813700 | 0.96032500 |
| H | 2.43136600 | -0.02437500 | -0.61620700 | C | 0.85109000 | 3.75988300 | 2.16807900 |
| H | 4.06147000 | -1.76615800 | 2.99006000 | C | 1.58425900 | 4.91435100 | -0.02807200 |
| N | -1.37461200 | -0.13859800 | 1.81852400 | H | 1.85348600 | 5.89680000 | 0.38792800 |
| N | 1.11273800 | -0.42407900 | 0.90411200 | H | 2.18187000 | 4.74257800 | -0.93505500 |
| B | -2.32413500 | -0.37408100 | -1.15429300 | H | 0.52759000 | 4.92338900 | -0.32754400 |
| O | -3.32595700 | -0.96852600 | -0.38766200 | C | 3.32874000 | 3.75129400 | 1.35154500 |
| O | -2.78578500 | -0.13521200 | -2.44593500 | H | 3.95335000 | 3.77456400 | 0.44564100 |
| C | -4.50745600 | -1.15083900 | -1.18048300 | H | 3.59053700 | 4.62779300 | 1.96483500 |
| C | -3.96949300 | -0.92933600 | -2.65394600 | H | 3.58124700 | 2.84161300 | 1.91212200 |
| C | -5.52477700 | -0.09934100 | -0.73565900 | C | 0.34471100 | 5.12721200 | 2.60704000 |
| H | -6.47901600 | -0.19242100 | -1.27562600 | H | -0.37245900 | 5.00921200 | 3.43309500 |
| H | -5.72325400 | -0.23664200 | 0.33835000 | H | 1.17576700 | 5.75750600 | 2.96081900 |
| H | -5.12038100 | 0.90852600 | -0.87057400 | H | -0.16657300 | 5.64978500 | 1.78896000 |
| C | -5.05801000 | -2.54953600 | -0.91510900 | C | 1.38202700 | 2.97647500 | 3.37327300 |
| H | -5.40080000 | -2.61734800 | 0.12793900 | H | 2.18414600 | 3.51703000 | 3.89748900 |
| H | -5.91349600 | -2.76713200 | -1.57396900 | H | 0.55367700 | 2.80977900 | 4.07748100 |
| H | -4.29028400 | -3.31986300 | -1.05353700 | H | 1.76539700 | 1.99271700 | 3.06399200 |
| C | -4.91882800 | -0.16261400 | -3.56716100 | B | -1.85101800 | 1.99608100 | -0.68589600 |
| H | -4.44741700 | -0.02019300 | -4.55106900 | O | -1.47804700 | 3.05843700 | -1.49853400 |
| H | -5.85767900 | -0.71926900 | -3.71274600 | O | -3.12808100 | 2.22346900 | -0.17057600 |
| H | -5.15979400 | 0.82766800 | -3.16148900 | C | -2.61405100 | 3.91326100 | -1.71374200 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.52508500 | 3.57778900 | -0.47498300 | C | -0.43750000 | -3.95209700 | -0.57291000 |
| C | -3.23252300 | 3.49623800 | -3.05113400 | C | -0.88459500 | -2.67448300 | -0.22276300 |
| H | -4.09485600 | 4.12306100 | -3.32379600 | C | 0.10782500 | -4.18218000 | -1.83833000 |
| H | -2.46755300 | 3.59587200 | -3.83499400 | C | -0.75878500 | -1.59834300 | -1.11297100 |
| H | -3.53856300 | 2.44193700 | -3.02332000 | H | -1.37402900 | -2.50904000 | 0.73258000 |
| C | -2.14013800 | 5.36017400 | -1.77854300 | C | 0.21401000 | -3.11902600 | -2.74691600 |
| H | -1.47532800 | 5.49082400 | -2.64521800 | H | 0.44706000 | -5.17871100 | -2.12140200 |
| H | -2.99278400 | 6.04804500 | -1.89217700 | C | -0.20220600 | -1.83003800 | -2.38309200 |
| H | -1.58140800 | 5.64317100 | -0.87752100 | H | 0.07977300 | 0.84356700 | -1.53644300 |
| C | -3.20976700 | 4.42374500 | 0.76162500 | H | -0.14066000 | -1.00035300 | -3.08363700 |
| H | -3.51469700 | 5.47264900 | 0.62941700 | O | 0.74441000 | -3.43180600 | -3.96188300 |
| H | -3.76079700 | 4.00925700 | 1.61926400 | C | 0.86335800 | -2.41290700 | -4.92586500 |
| H | -2.14144000 | 4.37640800 | 1.00574700 | H | 1.29834700 | -2.87705700 | -5.82157600 |
| C | -5.02102800 | 3.62211200 | -0.76286900 | H | -0.11713700 | -1.97567400 | -5.18673100 |
| H | -5.58255700 | 3.32269000 | 0.13463400 | H | 1.52707300 | -1.59751300 | -4.58557800 |
| H | -5.32905600 | 4.64452600 | -1.03260800 | C | 4.81676100 | -0.73032400 | 0.52998400 |
| H | -5.30433900 | 2.94952600 | -1.58084500 | C | 5.81231500 | -1.69491800 | 0.76024500 |
| S | -3.04206300 | -3.72897500 | 2.07136300 | C | 5.13352600 | 0.39336400 | -0.25605000 |
| C | -4.19868700 | -4.12830200 | 3.41403200 | C | 7.08696400 | -1.54653100 | 0.21824500 |
| H | -3.72047800 | -4.02956000 | 4.40201900 | H | 5.58101800 | -2.58298900 | 1.35175900 |
| H | -5.02295200 | -3.40416800 | 3.34581700 | C | 6.40734500 | 0.54387400 | -0.79867600 |
| H | -4.61150400 | -5.14307700 | 3.30527600 | H | 4.38109700 | 1.16835000 | -0.41532900 |
| C | -1.81306100 | -5.05707200 | 2.36603300 | C | 7.38731400 | -0.42670700 | -0.56445400 |
| H | -1.62109600 | -5.10631600 | 3.45156600 | H | 7.85248400 | -2.30214200 | 0.40094300 |
| H | -2.23310500 | -6.02619400 | 2.05086300 | H | 6.64750700 | 1.42578700 | -1.39441800 |
| C | -0.47499200 | -4.84090300 | 1.66637100 | C | 8.74914100 | -0.29119400 | -1.19480300 |
| H | -0.05958200 | -3.85012100 | 1.91587800 | F | 9.09863400 | 0.99688300 | -1.35588300 |
| H | 0.22206900 | -5.60251900 | 2.05860300 | F | 9.70329700 | -0.88141500 | -0.45315800 |
| O | -0.52042500 | -5.03276100 | 0.26694200 | F | 8.78875900 | -0.86413900 | -2.41272300 |

**INT3-L10-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | 0.60513200 | 0.62472500 | 0.49157700 |
| C | 0.07269300 | 3.29607600 | 1.93834800 |
| C | 2.36399400 | 2.86052800 | 1.93331600 |
| C | 0.27397600 | 4.49909400 | 2.62727100 |
| C | -1.26487900 | 2.74960800 | 1.61917000 |
| C | 2.63679500 | 4.03798400 | 2.62924700 |
| H | 3.14874400 | 2.16610800 | 1.63492600 |
| C | 1.57348700 | 4.87818500 | 2.96527700 |
| H | -0.57320500 | 5.12101900 | 2.91614900 |
| C | -2.45897100 | 3.47302800 | 1.73484600 |
| H | 3.66688700 | 4.28979500 | 2.88466500 |
| H | 1.74995400 | 5.81342500 | 3.50103600 |
| C | -2.45204000 | 0.84908400 | 0.98149800 |
| C | -3.67054600 | 2.85592600 | 1.43684400 |
| H | -2.44089600 | 4.52300100 | 2.02677300 |
| C | -3.68942900 | 1.50394600 | 1.05208800 |
| H | -2.36814100 | -0.19805600 | 0.68854100 |
| H | -4.59514500 | 3.43421000 | 1.47964600 |
| N | 1.11998200 | 2.52034900 | 1.57586700 |
| N | -1.28665600 | 1.45555400 | 1.21912500 |
| B | 1.37175400 | -0.47699200 | 1.95826500 |
| O | 2.71602200 | -0.40202500 | 2.31127300 |
| O | 0.69125800 | -1.32790000 | 2.82003500 |
| C | 2.91121800 | -1.07864200 | 3.56559300 |
| C | 1.65245900 | -2.02702600 | 3.63726100 |
| C | 2.91498500 | -0.00435600 | 4.65782200 |
| H | 3.12541200 | -0.42598200 | 5.65216300 |
| H | 3.69489600 | 0.73510300 | 4.42242800 |
| H | 1.94996300 | 0.52221100 | 4.69563000 |
| C | 4.25360900 | -1.80005300 | 3.52190500 |
| H | 5.06816300 | -1.06003100 | 3.49639200 |
| H | 4.39459400 | -2.43038100 | 4.41430500 |
| H | 4.33461800 | -2.41926800 | 2.61974900 |
| C | 1.06746800 | -2.21058800 | 5.03255400 |
| H | 0.19274000 | -2.87608900 | 4.97962900 |
| H | 1.80486700 | -2.66828200 | 5.71085100 |
| H | 0.73763200 | -1.25598200 | 5.46227500 |
| C | 1.89832200 | -3.38727200 | 2.98219700 |
| H | 2.60268600 | -3.99747500 | 3.56756500 |
| H | 0.94354000 | -3.93046600 | 2.92690800 |
| H | 2.28672900 | -3.26269800 | 1.96343000 |
| B | 1.25214800 | 2.94588800 | -1.96412100 |
| O | 0.02428200 | 2.49909900 | -1.50582300 |
| O | 1.49855100 | 2.56131800 | -3.24743300 |
| C | -0.73008000 | 2.11362500 | -2.70602100 |
| C | 0.42384000 | 1.68123000 | -3.67562300 |
| C | -1.45817500 | 3.38018000 | -3.16480500 |
| H | -2.11528200 | 3.17517000 | -4.02208200 |
| H | -2.07720900 | 3.74940300 | -2.33421300 |
| H | -0.75360600 | 4.17562000 | -3.44945300 |
| C | -1.73460900 | 1.02539600 | -2.38412600 |
| H | -2.52958300 | 1.42491900 | -1.73846500 |
| H | -2.20461800 | 0.66973800 | -3.31422300 |
| H | -1.28048100 | 0.17387800 | -1.87007100 |
| C | 0.14757900 | 1.94352400 | -5.14926400 |
| H | 1.00601900 | 1.60700100 | -5.74875900 |
| H | -0.73995500 | 1.38274300 | -5.48063800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.01140100 | 3.01062300 | -5.35185900 | H | 2.06898800 | 4.91764900 | -1.83229700 |
| C | 0.89229000 | 0.24439700 | -3.45990300 | H | 1.97659800 | 0.20651100 | -0.15887800 |
| H | 0.17214500 | -0.47106600 | -3.88038900 | C | 4.37901500 | 2.40325300 | -2.22378900 |
| H | 1.86077900 | 0.10398000 | -3.95911100 | H | 3.76016100 | 2.53908900 | -3.11880400 |
| H | 1.02990800 | 0.01473000 | -2.39401400 | H | 5.42865900 | 2.58449300 | -2.49975700 |
| B | 0.02870900 | -1.20427500 | -0.18485700 | C | 4.18936100 | 1.00887900 | -1.65351600 |
| O | 0.84571900 | -2.30592100 | -0.42228700 | H | 3.20840900 | 0.92099400 | -1.16175900 |
| O | -1.31462900 | -1.59988600 | -0.40085300 | H | 4.95590100 | 0.80448400 | -0.88472100 |
| C | 0.07620200 | -3.38895700 | -0.96653700 | O | 4.28293900 | 0.06709900 | -2.71249300 |
| C | -1.37425100 | -3.03793100 | -0.47971400 | C | 4.22154600 | -1.25670000 | -2.41707700 |
| C | 0.62244000 | -4.71064900 | -0.44079200 | C | 4.29430000 | -2.13189400 | -3.51934800 |
| H | -0.02252800 | -5.55015100 | -0.74515800 | C | 4.10594700 | -1.76544000 | -1.12082900 |
| H | 1.62338200 | -4.87837200 | -0.86162500 | C | 4.27631400 | -3.50267100 | -3.30403300 |
| H | 0.70646400 | -4.70415100 | 0.65201800 | H | 4.37746400 | -1.70595700 | -4.52019600 |
| C | 0.23141800 | -3.33862800 | -2.48978300 | C | 4.11661100 | -3.15604000 | -0.92443800 |
| H | 1.30403100 | -3.33242300 | -2.73157400 | H | 3.98854900 | -1.13037900 | -0.24482100 |
| H | -0.23737800 | -4.20595300 | -2.97924700 | C | 4.19788900 | -4.03633300 | -2.00924100 |
| H | -0.21327300 | -2.42254300 | -2.90061900 | H | 4.33477500 | -4.18292700 | -4.15752500 |
| C | -2.48934900 | -3.44144400 | -1.43675800 | H | 4.20004600 | -5.11571000 | -1.86676600 |
| H | -2.48990900 | -4.53030800 | -1.60147500 | O | 4.04995400 | -3.56848400 | 0.37330200 |
| H | -3.46671200 | -3.16662500 | -1.01026600 | C | 4.26164400 | -4.92853200 | 0.66865200 |
| H | -2.38717400 | -2.94126200 | -2.40861000 | H | 4.25576400 | -5.01467400 | 1.76314700 |
| C | -1.67093200 | -3.54847100 | 0.93383500 | H | 3.46207900 | -5.57047500 | 0.26071400 |
| H | -2.62570500 | -3.11899500 | 1.27400400 | H | 5.23413500 | -5.28098200 | 0.28134900 |
| H | -1.75674700 | -4.64493100 | 0.96708200 | C | -4.92488800 | 0.77532800 | 0.68880900 |
| H | -0.88954200 | -3.22130500 | 1.63355900 | C | -6.17846000 | 1.15559400 | 1.19950300 |
| S | 3.95763900 | 3.68121300 | -0.98150900 | C | -4.86684800 | -0.32806800 | -0.18642600 |
| C | 2.16103100 | 3.99732600 | -1.22719900 | C | -7.33653900 | 0.46659400 | 0.84608000 |
| H | 1.75523800 | 4.22778500 | -0.23539500 | H | -6.25001800 | 1.98561800 | 1.90459600 |

| | | | |
|---|---|---|---|
| C | -6.02260200 | -1.01889500 | -0.53982000 |
| H | -3.90944500 | -0.64798300 | -0.60025900 |
| C | -7.26299700 | -0.62229600 | -0.02835900 |
| H | -8.30029500 | 0.76492600 | 1.26149700 |
| H | -5.96040200 | -1.87351400 | -1.21553300 |
| C | -8.51905300 | -1.33317500 | -0.45834400 |
| F | -8.29074700 | -2.62866100 | -0.73508800 |
| F | -9.47285800 | -1.28117400 | 0.48812100 |
| F | -9.04188800 | -0.78141600 | -1.57138000 |

**INT3-L10-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | 0.79104300 | 0.95232700 | 0.08416100 |
| C | 0.47826800 | -0.15966700 | -2.73988600 |
| C | 2.73344200 | 0.02577700 | -2.18703900 |
| C | 0.80295400 | -0.57644000 | -4.03722700 |
| C | -0.91340300 | 0.08140100 | -2.30423800 |
| C | 3.12200700 | -0.36129300 | -3.46736700 |
| H | 3.45272700 | 0.28307000 | -1.40864400 |
| C | 2.14134300 | -0.68294800 | -4.40684300 |
| H | 0.01515100 | -0.78423800 | -4.76083300 |
| C | -2.03973300 | -0.33834600 | -3.02467400 |
| H | 4.18362200 | -0.41080900 | -3.71502500 |
| H | 2.41182300 | -0.99528300 | -5.41778200 |
| C | -2.27313300 | 1.04818100 | -0.68212600 |
| C | -3.30882800 | -0.07192900 | -2.52424400 |
| H | -1.92518700 | -0.89512600 | -3.95426400 |
| C | -3.44954000 | 0.64033600 | -1.32414200 |
| H | -2.30310800 | 1.57849600 | 0.27085200 |
| H | -4.19483600 | -0.41351900 | -3.06269500 |
| N | 1.44398800 | 0.11296400 | -1.82759400 |
| N | -1.05450900 | 0.76551500 | -1.14641000 |
| B | 1.64770900 | -2.46230600 | 0.40329900 |
| O | 2.08328100 | -2.94071800 | -0.80266100 |
| O | 2.46472200 | -2.82560900 | 1.44688900 |
| C | 3.34044400 | -3.62792200 | -0.58134900 |
| C | 3.28337100 | -3.91947900 | 0.96512300 |
| C | 4.46952600 | -2.67035200 | -0.95912700 |
| H | 5.45358600 | -3.14740400 | -0.84062900 |
| H | 4.35162900 | -2.38282200 | -2.01222300 |
| H | 4.43449700 | -1.75688400 | -0.34942700 |
| C | 3.36363200 | -4.86779200 | -1.46580100 |
| H | 3.40531800 | -4.56338300 | -2.52226800 |
| H | 4.24908700 | -5.48641400 | -1.25197700 |
| H | 2.46011600 | -5.47512800 | -1.32572800 |
| C | 4.62684600 | -3.90120700 | 1.67698900 |
| H | 4.47909700 | -4.08080600 | 2.75201900 |
| H | 5.28370000 | -4.69211300 | 1.28315300 |
| H | 5.13227100 | -2.93660900 | 1.55955100 |
| C | 2.52417100 | -5.20845600 | 1.29955700 |
| H | 3.10293700 | -6.10320100 | 1.02710600 |
| H | 2.33102300 | -5.23266400 | 2.38175600 |
| H | 1.55388100 | -5.24304100 | 0.78213900 |
| B | 1.48927900 | 2.74793500 | -0.46821800 |
| O | 0.83136900 | 3.96211500 | -0.31194500 |
| O | 2.68741200 | 2.94389700 | -1.15958300 |
| C | 1.70530900 | 5.02351400 | -0.73429800 |
| C | 2.68755800 | 4.27215900 | -1.70651100 |
| C | 2.40433600 | 5.56257400 | 0.51776200 |
| H | 3.04293400 | 6.43049300 | 0.29412700 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.63815600 | 5.86802500 | 1.24491800 | H | 5.57811600 | 2.31670700 | 0.19175000 |
| H | 3.01943000 | 4.78244600 | 0.98803100 | H | 4.40775900 | 3.07532400 | 1.28216000 |
| C | 0.87400700 | 6.12277400 | -1.38495800 | C | 5.94145900 | -0.00894200 | 1.63429400 |
| H | 0.21794200 | 6.58445100 | -0.63180500 | H | 6.43610600 | 0.02420600 | 0.65160800 |
| H | 1.52050700 | 6.90975300 | -1.80481900 | H | 6.68522200 | 0.26083500 | 2.40039500 |
| H | 0.23760600 | 5.72395000 | -2.18548900 | H | 5.61364200 | -1.03814500 | 1.81806200 |
| C | 4.11433400 | 4.80692800 | -1.72255700 | S | -1.38082600 | -5.43902200 | -0.28050600 |
| H | 4.72531700 | 4.20894600 | -2.41582900 | C | -1.73503500 | -7.21741400 | -0.13020800 |
| H | 4.13835800 | 5.85468500 | -2.06161000 | H | -1.84333600 | -7.69456200 | -1.11720500 |
| H | 4.57764200 | 4.74681800 | -0.73010900 | H | -0.87934300 | -7.66961100 | 0.39088000 |
| C | 2.14742800 | 4.16799100 | -3.13733300 | H | -2.64409500 | -7.39454200 | 0.46539200 |
| H | 2.17825600 | 5.13347000 | -3.66448500 | C | -2.92933800 | -4.95298600 | -1.13950500 |
| H | 2.76352800 | 3.44567900 | -3.69338200 | H | -3.04512600 | -5.60583200 | -2.02140200 |
| H | 1.11131700 | 3.79894700 | -3.13834100 | H | -3.78368900 | -5.13693400 | -0.46741500 |
| B | 2.50611500 | 0.93590700 | 1.17265200 | C | -2.99111800 | -3.50675300 | -1.62307600 |
| O | 2.62206400 | 1.28598900 | 2.51981100 | H | -2.11739500 | -3.25121300 | -2.24421300 |
| O | 3.77386900 | 0.54048500 | 0.70418500 | H | -3.88183100 | -3.41136400 | -2.26364300 |
| C | 3.94263200 | 0.96969300 | 2.99210800 | O | -3.18663600 | -2.56166300 | -0.58941400 |
| C | 4.76810100 | 0.96040800 | 1.65673700 | C | -2.11854200 | -2.07928900 | 0.11612200 |
| C | 3.87201800 | -0.40743000 | 3.66051000 | C | -0.78706300 | -2.32134000 | -0.22162100 |
| H | 4.83377100 | -0.69654800 | 4.11182400 | C | -2.43650100 | -1.28172000 | 1.22499600 |
| H | 3.11700100 | -0.36863900 | 4.46027900 | C | 0.24225000 | -1.83321600 | 0.60827000 |
| H | 3.56290900 | -1.18151600 | 2.94443600 | H | -0.51017400 | -2.93851400 | -1.07251900 |
| C | 4.37376500 | 2.02702900 | 4.00181100 | C | -1.41933700 | -0.73580200 | 2.01143900 |
| H | 3.73674700 | 1.96446900 | 4.89694600 | H | -3.47858000 | -1.07464100 | 1.46777700 |
| H | 5.41881000 | 1.87187700 | 4.31429000 | C | -0.06711100 | -1.03316100 | 1.72468200 |
| H | 4.27453900 | 3.03961200 | 3.59012100 | H | 0.18867100 | 1.74941800 | 1.32368900 |
| C | 5.23677500 | 2.35718800 | 1.23583300 | H | 0.71961500 | -0.75029100 | 2.41876600 |
| H | 6.06137300 | 2.72202700 | 1.86641400 | O | -1.80411800 | 0.07060300 | 3.02102200 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.81122800 | 0.59503500 | 3.89227300 | H | -6.16077000 | -3.01165400 | -1.02871700 |
| H | -1.33551600 | 1.27585200 | 4.57528900 | H | -4.94392800 | -4.98054200 | -0.02013300 |
| H | -0.33726000 | -0.21055600 | 4.48039800 | C | 0.88526100 | -1.16525200 | -0.50777900 |
| H | -0.03513500 | 1.14468800 | 3.33748600 | C | 1.35173300 | -3.43144700 | 0.09919200 |
| C | -4.76377200 | 0.87890100 | -0.69386600 | H | -0.36999000 | -4.72202400 | 0.08493400 |
| C | -5.72182900 | -0.14926100 | -0.65122600 | C | 1.82707600 | -2.12707400 | -0.11534200 |
| C | -5.06925700 | 2.11329200 | -0.09591600 | H | 1.15794800 | -0.12315900 | -0.68251300 |
| C | -6.95684700 | 0.05544700 | -0.04044800 | H | 2.03617000 | -4.23487300 | 0.37651300 |
| H | -5.47030900 | -1.12884600 | -1.06021300 | N | -3.00459600 | -1.83516500 | -1.18191800 |
| C | -6.30376600 | 2.32059700 | 0.51569500 | N | -0.41163800 | -1.43509800 | -0.68578500 |
| H | -4.33880200 | 2.92408500 | -0.12816400 | B | -2.36364000 | 0.54096900 | 0.52958200 |
| C | -7.25196100 | 1.29241400 | 0.54291400 | O | -3.67540100 | 0.59997000 | 0.97355900 |
| H | -7.69356400 | -0.74884800 | -0.00879300 | O | -1.47598000 | 0.66537900 | 1.59426600 |
| H | -6.53780600 | 3.28707100 | 0.96453400 | C | -3.66690700 | 0.52221200 | 2.41086200 |
| C | -8.56593000 | 1.49530600 | 1.25039300 | C | -2.22746100 | 1.05412400 | 2.76208800 |
| F | -8.95496400 | 2.78222200 | 1.22561800 | C | -3.86123700 | -0.95389000 | 2.77721300 |
| F | -9.54981400 | 0.76378700 | 0.69579700 | H | -3.94564700 | -1.10450800 | 3.86391800 |
| F | -8.49317400 | 1.13279200 | 2.54568100 | H | -4.78444700 | -1.31547800 | 2.30073000 |
| **INT4-L10-Bpin** | | | | H | -3.02642100 | -1.56401400 | 2.40134800 |
| Ir | -1.83833500 | 0.10159300 | -1.32761000 | C | -4.81389100 | 1.35985200 | 2.96028500 |
| C | -2.33613700 | -2.87578500 | -0.63307600 | H | -5.77450800 | 0.91407700 | 2.66112000 |
| C | -4.33582200 | -1.89545000 | -1.30949700 | H | -4.78163200 | 1.39953500 | 4.06063000 |
| C | -3.01472400 | -4.02689700 | -0.20988300 | H | -4.78132800 | 2.38374400 | 2.56700000 |
| C | -0.87747300 | -2.68767300 | -0.46174100 | C | -1.59135200 | 0.41841200 | 3.99174100 |
| C | -5.07623400 | -3.00686300 | -0.90882900 | H | -0.58980400 | 0.84486400 | 4.15252300 |
| H | -4.80983500 | -1.00922300 | -1.73492800 | H | -2.19468000 | 0.61432100 | 4.89222200 |
| C | -4.39958300 | -4.09385400 | -0.35195500 | H | -1.47912800 | -0.66690800 | 3.87142000 |
| H | -2.47075600 | -4.85338200 | 0.24673500 | C | -2.16395800 | 2.58039100 | 2.85845100 |
| C | -0.00140500 | -3.70833100 | -0.07020900 | H | -2.69812300 | 2.95771000 | 3.74311100 |

| | | | |
|---|---|---|---|
| H | -1.11053100 | 2.88548900 | 2.93797100 |
| H | -2.58028800 | 3.04835100 | 1.95551700 |
| B | -0.67907400 | 1.75938500 | -1.14657500 |
| O | -1.06401500 | 3.02361500 | -0.71119000 |
| O | 0.72570000 | 1.74877600 | -1.30662400 |
| C | 0.06343500 | 3.91332800 | -0.73580800 |
| C | 1.27228900 | 2.91505100 | -0.65770900 |
| C | -0.04106600 | 4.88444300 | 0.43415100 |
| H | 0.85222100 | 5.52623700 | 0.49548200 |
| H | -0.91973400 | 5.53259700 | 0.29767400 |
| H | -0.16098500 | 4.35290600 | 1.38570900 |
| C | 0.01159300 | 4.68138500 | -2.06086500 |
| H | -0.96651800 | 5.17786800 | -2.13993200 |
| H | 0.79904900 | 5.44776800 | -2.12507300 |
| H | 0.11266500 | 3.99741300 | -2.91583400 |
| C | 2.52740400 | 3.36000600 | -1.39792800 |
| H | 2.90838300 | 4.30929900 | -0.98946800 |
| H | 3.31834100 | 2.60295700 | -1.28030600 |
| H | 2.33792900 | 3.48898200 | -2.47121600 |
| C | 1.61711000 | 2.50848000 | 0.78035200 |
| H | 2.35395300 | 1.69093400 | 0.75535600 |
| H | 2.05703800 | 3.34134100 | 1.34906100 |
| H | 0.72297100 | 2.14057000 | 1.30360600 |
| H | -2.95956100 | 1.11394500 | -1.84603100 |
| C | 3.24512100 | -1.73918000 | 0.05495300 |
| C | 4.09354000 | -2.44149000 | 0.92913900 |
| C | 3.77386700 | -0.63686700 | -0.64492400 |
| C | 5.42384100 | -2.06376800 | 1.09659400 |
| H | 3.70359000 | -3.27835900 | 1.51102900 |
| C | 5.10232500 | -0.25544900 | -0.47807600 |
| H | 3.14178800 | -0.07261400 | -1.33192600 |
| C | 5.93397600 | -0.96937600 | 0.39122200 |
| H | 6.06546100 | -2.60972900 | 1.78986200 |
| H | 5.49488200 | 0.60414100 | -1.02359700 |
| C | 7.38553100 | -0.59158400 | 0.52900500 |
| F | 7.58019400 | 0.72406900 | 0.33547100 |
| F | 7.86891300 | -0.90009600 | 1.74539200 |
| F | 8.15108500 | -1.23817600 | -0.37183700 |

**INT5-L10-Bpin**

| | | | |
|---|---|---|---|
| Ir | 0.99563900 | -0.04798900 | -0.51611600 |
| C | 0.73377700 | -0.85996400 | -3.47928900 |
| C | 2.99202200 | -0.76647700 | -2.89906300 |
| C | 1.05759600 | -1.27400000 | -4.77948700 |
| C | -0.65631800 | -0.70978400 | -2.99294200 |
| C | 3.38375700 | -1.17876600 | -4.17288300 |
| H | 3.71303900 | -0.57234100 | -2.10010600 |
| C | 2.39764600 | -1.42941500 | -5.12988900 |
| H | 0.27335800 | -1.48798900 | -5.50524200 |
| C | -1.78323800 | -0.79847000 | -3.82076100 |
| H | 4.44358700 | -1.30093400 | -4.40211000 |
| H | 2.66693200 | -1.75332000 | -6.13765600 |
| C | -2.02095200 | -0.38776300 | -1.13190700 |
| C | -3.05521200 | -0.68810700 | -3.27001100 |
| H | -1.66836200 | -0.95797400 | -4.89254200 |
| C | -3.19621900 | -0.49077600 | -1.88583200 |
| H | -2.04332300 | -0.21537700 | -0.05628500 |
| H | -3.93548300 | -0.78137000 | -3.90846100 |
| N | 1.70342900 | -0.60281600 | -2.57365600 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -0.79773100 | -0.49009500 | -1.66242900 | H | 0.66150700 | 2.68528900 | 4.54910000 |
| B | 0.66343900 | 1.91243700 | -0.65702000 | H | -0.89471500 | 2.87817500 | 3.71449800 |
| O | 1.65389700 | 2.89222600 | -0.60347300 | C | 1.02201500 | 0.04503900 | 4.30455300 |
| O | -0.58457600 | 2.51677700 | -0.83415300 | H | 1.97010500 | 0.59684300 | 4.36605400 |
| C | 1.08042200 | 4.16470400 | -0.93906300 | H | 0.67951600 | -0.18868700 | 5.32412500 |
| C | -0.44401500 | 3.93355600 | -0.62157400 | H | 1.23388400 | -0.89432100 | 3.77512000 |
| C | 1.34940800 | 4.40568900 | -2.42824800 | C | -1.69795700 | -1.00913200 | 4.06209400 |
| H | 1.00583100 | 5.39869500 | -2.75559300 | H | -1.98948600 | -0.58054800 | 5.03392400 |
| H | 2.43256900 | 4.33477100 | -2.60661100 | H | -2.56918500 | -1.54338800 | 3.65215500 |
| H | 0.85435600 | 3.64088700 | -3.04453000 | H | -0.89995500 | -1.74242200 | 4.23078400 |
| C | 1.75707300 | 5.24364500 | -0.10143000 | C | -2.45478400 | 0.99132000 | 2.75752000 |
| H | 2.81554100 | 5.32539000 | -0.39167300 | H | -3.24383200 | 0.39038300 | 2.28240600 |
| H | 1.28172000 | 6.22488700 | -0.25859400 | H | -2.88258400 | 1.46400200 | 3.65409900 |
| H | 1.72048000 | 4.99784300 | 0.96735800 | H | -2.15603900 | 1.77739700 | 2.05041400 |
| C | -1.41269300 | 4.67033500 | -1.53848500 | H | 2.34530700 | 0.41653700 | 0.15902500 |
| H | -2.44723600 | 4.43673600 | -1.24433900 | C | -4.51336600 | -0.39520900 | -1.22023600 |
| H | -1.27420000 | 5.76066700 | -1.46525300 | C | -5.61614400 | 0.18799400 | -1.86810900 |
| H | -1.28433700 | 4.36807800 | -2.58598100 | C | -4.68691600 | -0.88117800 | 0.08914000 |
| C | -0.78621100 | 4.21035300 | 0.84567500 | C | -6.85205900 | 0.28292800 | -1.23216200 |
| H | -0.74272900 | 5.28366900 | 1.08376500 | H | -5.49858400 | 0.60086700 | -2.87174400 |
| H | -1.80974100 | 3.85694900 | 1.04122600 | C | -5.92019000 | -0.78700200 | 0.72857200 |
| H | -0.10513500 | 3.66139700 | 1.51029800 | H | -3.84838700 | -1.34915600 | 0.60708400 |
| B | 0.23215800 | 0.27481700 | 1.32526600 | C | -7.00841100 | -0.20588400 | 0.06884000 |
| O | 0.59721900 | 1.22891800 | 2.27293000 | H | -7.69556400 | 0.75292500 | -1.74008300 |
| O | -0.81594300 | -0.51087900 | 1.86275800 | H | -6.03892300 | -1.16384400 | 1.74562700 |
| C | 0.00488400 | 0.89813800 | 3.53798700 | C | -8.35628100 | -0.15451800 | 0.73887900 |
| C | -1.26545000 | 0.08766200 | 3.09747300 | F | -8.24687500 | -0.04790600 | 2.07444800 |
| C | -0.28621700 | 2.18215800 | 4.30545300 | F | -9.09100500 | 0.88510100 | 0.30636400 |
| H | -0.81161900 | 1.96685000 | 5.24940900 | F | -9.07265500 | -1.26938900 | 0.49275300 |

| | | | |
|---|---|---|---|
| B | 3.87288100 | -0.99570800 | 0.95377500 |
| B | 2.80564500 | -2.31933900 | 0.82918100 |
| O | 4.03229800 | -0.29165800 | 2.11160000 |
| O | 4.69454300 | -0.55632800 | -0.05754000 |
| O | 2.78407000 | -3.43423400 | 1.61366900 |
| O | 1.77000400 | -2.34129100 | -0.09758600 |
| C | 1.54735600 | -4.15573300 | 1.37794000 |
| C | 1.10983300 | -3.63849400 | -0.04243800 |
| C | 4.85378900 | 0.87297000 | 1.86320700 |
| C | 5.38910300 | 0.64134600 | 0.37391600 |
| C | 6.88422000 | 0.33664900 | 0.28239400 |
| H | 7.13501600 | 0.08961200 | -0.76006200 |
| H | 7.49199900 | 1.20157500 | 0.58640000 |
| H | 7.16013900 | -0.52340800 | 0.90717200 |
| C | 5.02685000 | 1.76516700 | -0.59702700 |
| H | 5.52562900 | 2.70322700 | -0.30955200 |
| H | 5.37542100 | 1.49631900 | -1.60651000 |
| H | 3.94520400 | 1.94424000 | -0.63809800 |
| C | 5.94740800 | 0.88931500 | 2.92985800 |
| H | 6.62592800 | 1.74453500 | 2.79194000 |
| H | 5.47771700 | 0.98038900 | 3.92016900 |
| H | 6.53920000 | -0.03526500 | 2.92279700 |
| C | 0.57757900 | -3.73620200 | 2.48410400 |
| H | -0.35278700 | -4.32179900 | 2.44901000 |
| H | 1.05956100 | -3.90644900 | 3.45775400 |
| H | 0.31752100 | -2.67279000 | 2.40178300 |
| C | 1.83333800 | -5.64921400 | 1.45139500 |
| H | 2.13219800 | -5.91596400 | 2.47575700 |
| H | 0.93398600 | -6.23024400 | 1.19466700 |
| H | 2.64723800 | -5.94063400 | 0.77514100 |
| C | -0.39182300 | -3.45164700 | -0.20631500 |
| H | -0.62230300 | -3.15034100 | -1.23708800 |
| H | -0.91428500 | -4.39960400 | -0.00498600 |
| H | -0.77199300 | -2.67603200 | 0.46939500 |
| C | 1.68279400 | -4.45397000 | -1.20180100 |
| H | 1.19736200 | -5.43764600 | -1.28301700 |
| H | 1.51204300 | -3.90262900 | -2.13826300 |
| H | 2.76609900 | -4.60438000 | -1.08897600 |
| C | 3.96117100 | 2.10501800 | 2.02198600 |
| H | 3.57187700 | 2.12939400 | 3.05000600 |
| H | 4.53138000 | 3.02981300 | 1.84743600 |
| H | 3.10000800 | 2.08282000 | 1.34504400 |

**TS5-L10-Bpin**

| | | | |
|---|---|---|---|
| Ir | 1.29620200 | 0.35641900 | -0.61920400 |
| C | 1.24901800 | -1.66457700 | -2.95132300 |
| C | 3.38572100 | -0.75870200 | -2.79308700 |
| C | 1.67138200 | -2.54970400 | -3.95212900 |
| C | -0.14225100 | -1.61271200 | -2.45866200 |
| C | 3.87285400 | -1.60148800 | -3.79106200 |
| H | 4.02805300 | -0.04804800 | -2.27616500 |
| C | 2.99800800 | -2.51797900 | -4.37610300 |
| H | 0.97407100 | -3.26565800 | -4.38609600 |
| C | -1.21345000 | -2.25460300 | -3.09456200 |
| H | 4.92024200 | -1.54107800 | -4.09065800 |
| H | 3.34412100 | -3.20499300 | -5.15150800 |
| C | -1.59294100 | -0.72429100 | -0.87363900 |
| C | -2.49972600 | -2.12938600 | -2.58129600 |
| H | -1.04447300 | -2.84784500 | -3.99253100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.71557600 | -1.34096100 | -1.43850700 | C | 0.41160700 | 1.94455900 | 3.25076900 |
| H | -1.67543900 | -0.07330900 | -0.00357600 | C | -1.04529300 | 1.64372500 | 2.74315800 |
| H | -3.32817100 | -2.65080500 | -3.06367300 | C | 0.59023300 | 3.31139200 | 3.90209400 |
| N | 2.11211800 | -0.79023200 | -2.38550700 | H | -0.05442100 | 3.41488600 | 4.78949000 |
| N | -0.35349000 | -0.86795300 | -1.35034400 | H | 1.63551100 | 3.42796000 | 4.22538000 |
| B | 0.30753500 | 1.96905100 | -1.27864900 | H | 0.36319900 | 4.12375200 | 3.19986900 |
| O | 0.33981100 | 3.28603100 | -0.84660700 | C | 0.96829200 | 0.84582000 | 4.16237100 |
| O | -0.60736900 | 1.83046100 | -2.32518800 | H | 2.04772100 | 1.00876600 | 4.28572300 |
| C | -0.41537500 | 4.09406500 | -1.76995500 | H | 0.48913300 | 0.85578600 | 5.15374500 |
| C | -1.38488200 | 3.03754100 | -2.41756700 | H | 0.85182900 | -0.14669200 | 3.70669000 |
| C | 0.58062900 | 4.68210200 | -2.77385700 | C | -1.91264100 | 0.84820300 | 3.71031400 |
| H | 0.09532700 | 5.37451000 | -3.47810000 | H | -2.06094200 | 1.40263900 | 4.65008500 |
| H | 1.35465600 | 5.23253900 | -2.21947500 | H | -2.90418700 | 0.67027100 | 3.26451300 |
| H | 1.07700400 | 3.88560700 | -3.34702200 | H | -1.46244900 | -0.12359900 | 3.94646200 |
| C | -1.10827500 | 5.21319500 | -1.00285800 | C | -1.78478100 | 2.90185100 | 2.28138800 |
| H | -0.35329300 | 5.88105100 | -0.56187000 | H | -2.71013200 | 2.60399600 | 1.76541300 |
| H | -1.74537300 | 5.81036800 | -1.67423200 | H | -2.05794300 | 3.55203100 | 3.12564300 |
| H | -1.72937000 | 4.82158000 | -0.18799700 | H | -1.16419500 | 3.47099200 | 1.57626700 |
| C | -1.73577600 | 3.29323400 | -3.87766900 | H | 2.48664000 | 1.35813800 | -0.31515800 |
| H | -2.40474400 | 2.49824400 | -4.24071600 | C | -4.04537600 | -1.13381700 | -0.82514100 |
| H | -2.25543900 | 4.25731800 | -3.99447500 | C | -5.22468300 | -1.22892800 | -1.58502400 |
| H | -0.84009300 | 3.29574200 | -4.51192600 | C | -4.15757000 | -0.81296900 | 0.54223600 |
| C | -2.65952200 | 2.80972100 | -1.59805600 | C | -6.47272200 | -1.01852700 | -1.00299400 |
| H | -3.35250400 | 3.66182400 | -1.66277100 | H | -5.16715700 | -1.44240700 | -2.65372300 |
| H | -3.17177600 | 1.91483300 | -1.98186400 | C | -5.40304300 | -0.60119400 | 1.12641900 |
| H | -2.41648000 | 2.63075400 | -0.54217700 | H | -3.26189600 | -0.73199100 | 1.15875300 |
| B | 0.51690300 | 1.11681900 | 1.10352300 | C | -6.56674200 | -0.70622700 | 0.35696100 |
| O | 1.16385600 | 1.91294100 | 2.03028100 | H | -7.37770600 | -1.08116600 | -1.60925700 |
| O | -0.78816500 | 0.84512400 | 1.57004100 | H | -5.47176500 | -0.34929700 | 2.18592700 |

| | | | |
|---|---|---|---|
| C | -7.91695200 | -0.53355800 | 1.00074700 |
| F | -7.86933900 | 0.31173000 | 2.04488700 |
| F | -8.82780400 | -0.05758800 | 0.13324100 |
| F | -8.39559500 | -1.70440600 | 1.46647400 |
| B | 3.29970100 | -0.58895800 | 0.94927800 |
| B | 2.02593000 | -1.75906300 | 0.99724100 |
| O | 3.61535100 | 0.07155600 | 2.10663600 |
| O | 4.35703200 | -0.60558300 | 0.06042800 |
| O | 1.45135800 | -2.05550000 | 2.20862000 |
| O | 1.71438500 | -2.69863600 | 0.04109100 |
| C | 0.56551500 | -3.18622800 | 2.05650500 |
| C | 1.03347000 | -3.80602000 | 0.67847300 |
| C | 4.83555200 | 0.81210000 | 1.90886800 |
| C | 5.47979300 | 0.08226300 | 0.65589100 |
| C | 6.49838600 | -0.99726200 | 1.02922000 |
| H | 6.75479100 | -1.57033400 | 0.12575400 |
| H | 7.42186900 | -0.56439300 | 1.44142900 |
| H | 6.07997200 | -1.69794300 | 1.76543100 |
| C | 6.07382500 | 1.02484400 | -0.38584900 |
| H | 6.89566900 | 1.61847000 | 0.04299500 |
| H | 6.48108000 | 0.43985900 | -1.22506000 |
| H | 5.31449100 | 1.71232300 | -0.77898900 |
| C | 5.66049900 | 0.71771700 | 3.18923400 |
| H | 6.64048600 | 1.20366600 | 3.06355600 |
| H | 5.12629500 | 1.23230400 | 4.00137500 |
| H | 5.81843500 | -0.32377300 | 3.49720200 |
| C | -0.86204700 | -2.64102400 | 2.03177700 |
| H | -1.60436900 | -3.44591300 | 1.92931100 |
| H | -1.05554900 | -2.10729400 | 2.97183000 |
| H | -0.99167000 | -1.92139400 | 1.21733300 |
| C | 0.74816000 | -4.10385600 | 3.26083100 |
| H | 0.42087100 | -3.57990100 | 4.17071300 |
| H | 0.14175300 | -5.01663200 | 3.15385800 |
| H | 1.79816200 | -4.39092300 | 3.39801200 |
| C | -0.09941200 | -4.27918100 | -0.22330600 |
| H | 0.31391900 | -4.62016300 | -1.18394000 |
| H | -0.63423100 | -5.12283700 | 0.23947200 |
| H | -0.82130600 | -3.48215000 | -0.42885700 |
| C | 2.07766900 | -4.91523700 | 0.82912000 |
| H | 1.64445800 | -5.82867500 | 1.26228000 |
| H | 2.48156900 | -5.15677500 | -0.16494200 |
| H | 2.91480400 | -4.58829800 | 1.46194300 |
| C | 4.45381000 | 2.27139800 | 1.64985500 |
| H | 3.85596000 | 2.63360400 | 2.49660400 |
| H | 5.34680500 | 2.90543500 | 1.54269600 |
| H | 3.82214200 | 2.36825200 | 0.75839600 |

**INT6-L10-Bpin**

| | | | |
|---|---|---|---|
| Ir | 1.35637500 | 0.46671300 | -0.04540100 |
| C | 1.36526800 | 1.30542700 | -3.01589300 |
| C | 3.56645300 | 1.19089100 | -2.26620100 |
| C | 1.79237800 | 1.72794800 | -4.28444800 |
| C | -0.05222400 | 1.11465800 | -2.66367400 |
| C | 4.05893800 | 1.60795600 | -3.50019600 |
| H | 4.22347800 | 0.93072400 | -1.43634100 |
| C | 3.15313800 | 1.88408800 | -4.52805100 |
| H | 1.06832500 | 1.93624500 | -5.07128700 |
| C | -1.10825900 | 1.25907500 | -3.57535700 |
| H | 5.13520600 | 1.71046500 | -3.64769600 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.50257300 | 2.21520400 | -5.50833300 | H | 0.05511800 | 3.71469100 | 2.96675200 |
| C | -1.57067300 | 0.56040300 | -0.97998000 | B | 0.38636500 | 0.09856700 | 1.71477600 |
| C | -2.41388800 | 1.01055600 | -3.17308900 | O | 0.97114600 | -0.06036600 | 2.96242100 |
| H | -0.90410100 | 1.53521400 | -4.60876500 | O | -0.99494500 | -0.08831600 | 1.82798100 |
| C | -2.66883300 | 0.63875200 | -1.84184700 | C | 0.03541600 | -0.73169700 | 3.82253400 |
| H | -1.68497500 | 0.31891800 | 0.07637300 | C | -1.34561800 | -0.29611700 | 3.20779900 |
| H | -3.22596900 | 1.07537300 | -3.89917800 | C | 0.26827400 | -0.28154500 | 5.25895900 |
| N | 2.25503800 | 1.05130900 | -2.03031100 | H | -0.49011400 | -0.70867100 | 5.93416600 |
| N | -0.30993000 | 0.76375800 | -1.37983500 | H | 1.25810700 | -0.62486300 | 5.59510000 |
| B | 1.08404700 | 2.51031100 | 0.49726900 | H | 0.24424300 | 0.81232200 | 5.34699300 |
| O | 2.06180600 | 3.36812400 | 0.97072400 | C | 0.29390400 | -2.23643000 | 3.68338300 |
| O | -0.11814500 | 3.18888500 | 0.34377700 | H | 1.34629400 | -2.43494300 | 3.92924800 |
| C | 1.56439600 | 4.71990700 | 0.89911300 | H | -0.34559600 | -2.82585100 | 4.35816000 |
| C | 0.00928500 | 4.49856500 | 0.93543300 | H | 0.13592300 | -2.56272500 | 2.64614700 |
| C | 2.05169600 | 5.30637700 | -0.43030300 | C | -2.44241700 | -1.35318600 | 3.27623100 |
| H | 1.77944000 | 6.36717700 | -0.53842900 | H | -2.65443500 | -1.63660700 | 4.31902000 |
| H | 3.14743200 | 5.22068400 | -0.47200700 | H | -3.37093900 | -0.95399100 | 2.83932100 |
| H | 1.63689900 | 4.74721500 | -1.28191200 | H | -2.15743300 | -2.25207800 | 2.71466600 |
| C | 2.13002000 | 5.52082600 | 2.06510600 | C | -1.85598500 | 1.03681300 | 3.75803200 |
| H | 3.22068600 | 5.61486400 | 1.95406200 | H | -2.68828900 | 1.38683000 | 3.12913000 |
| H | 1.69912200 | 6.53432900 | 2.09278600 | H | -2.21680300 | 0.94275900 | 4.79330200 |
| H | 1.93256200 | 5.02620200 | 3.02446700 | H | -1.06649300 | 1.79896000 | 3.72583000 |
| C | -0.80589400 | 5.49081400 | 0.11572300 | H | 2.60458900 | 0.60984600 | 0.95055600 |
| H | -1.87597600 | 5.24797700 | 0.20020100 | C | -4.01461800 | 0.29897600 | -1.33101400 |
| H | -0.65846800 | 6.51958300 | 0.48075200 | C | -5.17796600 | 0.84234000 | -1.90285500 |
| H | -0.53500100 | 5.45174400 | -0.94731500 | C | -4.15361400 | -0.58951100 | -0.24605100 |
| C | -0.54399400 | 4.40824100 | 2.35988200 | C | -6.43949800 | 0.50833900 | -1.41478200 |
| H | -0.56061500 | 5.38935200 | 2.85777500 | H | -5.09801300 | 1.55749100 | -2.72350000 |
| H | -1.57144500 | 4.01919900 | 2.31665500 | C | -5.41280200 | -0.92358300 | 0.24420300 |

| | | | |
|---|---|---|---|
| H | -3.26745900 | -1.02815300 | 0.21451400 |
| C | -6.56139600 | -0.37877100 | -0.34050500 |
| H | -7.33346900 | 0.94888300 | -1.85878100 |
| H | -5.50392500 | -1.61007400 | 1.08746700 |
| C | -7.92452200 | -0.78717800 | 0.15190500 |
| F | -7.91583900 | -1.07933500 | 1.46406200 |
| F | -8.83845500 | 0.17995100 | -0.04323400 |
| F | -8.37337200 | -1.88429000 | -0.48997400 |
| B | 2.76557000 | -1.04535400 | 0.36779400 |
| B | 0.95485800 | -1.59743100 | -0.65621700 |
| O | 2.74292800 | -2.04438400 | 1.33297200 |
| O | 4.01927000 | -1.01913700 | -0.25261700 |
| O | -0.07335500 | -2.31355200 | -0.07491700 |
| O | 1.30574100 | -2.15220100 | -1.87399700 |
| C | -0.28181000 | -3.52944500 | -0.81977300 |
| C | 0.33789500 | -3.16821200 | -2.22213000 |
| C | 4.09277400 | -2.48131300 | 1.57202900 |
| C | 4.78609700 | -2.15064500 | 0.19908100 |
| C | 4.61808300 | -3.26117500 | -0.84195400 |
| H | 4.93282500 | -2.87515000 | -1.82249100 |
| H | 5.22532200 | -4.14654600 | -0.60127100 |
| H | 3.56494700 | -3.55826200 | -0.93035900 |
| C | 6.25083900 | -1.74435300 | 0.30496100 |
| H | 6.85236400 | -2.55694200 | 0.74190300 |
| H | 6.64962000 | -1.52754700 | -0.69777100 |
| H | 6.37398400 | -0.84460700 | 0.92120500 |
| C | 4.07583500 | -3.95754200 | 1.94621200 |
| H | 5.10043400 | -4.34458400 | 2.06141000 |
| H | 3.54969600 | -4.08920400 | 2.90343000 |
| H | 3.55588900 | -4.56043300 | 1.19111100 |
| C | -1.77394400 | -3.83876000 | -0.83822200 |
| H | -1.98720900 | -4.72107200 | -1.46167000 |
| H | -2.11674200 | -4.05250400 | 0.18525400 |
| H | -2.35824800 | -2.99097200 | -1.21782100 |
| C | 0.48064100 | -4.63685200 | -0.08885100 |
| H | 0.11593800 | -4.69310600 | 0.94692800 |
| H | 0.33890300 | -5.61840400 | -0.56487000 |
| H | 1.55375500 | -4.40882900 | -0.04619600 |
| C | -0.66867200 | -2.51548600 | -3.17284500 |
| H | -0.12229300 | -2.08463800 | -4.02448800 |
| H | -1.39921700 | -3.24238000 | -3.55772900 |
| H | -1.21595500 | -1.70344300 | -2.67657400 |
| C | 1.05688400 | -4.31310600 | -2.92368700 |
| H | 0.36095500 | -5.13849300 | -3.14096100 |
| H | 1.47544200 | -3.95717400 | -3.87697300 |
| H | 1.88442100 | -4.70261100 | -2.31778900 |
| C | 4.63535100 | -1.64470900 | 2.73484100 |
| H | 3.95698500 | -1.75466800 | 3.59281200 |
| H | 5.64355500 | -1.96564200 | 3.03715600 |
| H | 4.66510400 | -0.57726000 | 2.47384700 |

**TS6-L10-Bpin**

| | | | |
|---|---|---|---|
| Ir | 1.38372000 | 0.44697100 | -0.06682200 |
| C | 1.32311700 | 1.55779800 | -2.94102900 |
| C | 3.53693400 | 1.19627900 | -2.31488600 |
| C | 1.73269000 | 2.13005700 | -4.15575400 |
| C | -0.09053500 | 1.36940700 | -2.57378000 |
| C | 4.01218700 | 1.74830700 | -3.50146900 |
| H | 4.20012000 | 0.78577000 | -1.54995100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.09097800 | 2.23149500 | -4.43593600 | H | -1.41796100 | 4.24803400 | 2.36480100 |
| H | 0.99629600 | 2.50048700 | -4.86837000 | C | 1.97937300 | 4.94306600 | 2.38523300 |
| C | -1.15774700 | 1.54753100 | -3.46806100 | H | 1.94054800 | 6.04007900 | 2.46271900 |
| H | 5.08677600 | 1.79808300 | -3.68470900 | H | 2.13018200 | 4.52687400 | 3.39187400 |
| H | 3.42792500 | 2.68049700 | -5.37279500 | H | 2.84601300 | 4.66253000 | 1.76952700 |
| C | -1.58600700 | 0.67103700 | -0.92045000 | B | 0.46384900 | -0.02737400 | 1.69284400 |
| C | -2.45451100 | 1.24072500 | -3.07546500 | O | 1.07524100 | -0.29218900 | 2.90751900 |
| H | -0.96516500 | 1.88202500 | -4.48659300 | O | -0.92465500 | -0.10838900 | 1.84683800 |
| C | -2.68999300 | 0.77193800 | -1.77046100 | C | 0.10186900 | -0.85359500 | 3.80201300 |
| H | -1.68493200 | 0.35425300 | 0.11809200 | C | -1.23816000 | -0.25115600 | 3.24437500 |
| H | -3.27349500 | 1.32819400 | -3.79168600 | C | 0.44426500 | -0.44577400 | 5.22890000 |
| N | 2.22774000 | 1.11575500 | -2.04035400 | H | -0.33270000 | -0.78270000 | 5.93353100 |
| N | -0.33274100 | 0.93434700 | -1.31224700 | H | 1.39842000 | -0.90761000 | 5.52428400 |
| B | 1.21619200 | 2.47547100 | 0.61136300 | H | 0.55534200 | 0.64260500 | 5.31655200 |
| O | 1.25243200 | 3.51778500 | -0.30198000 | C | 0.17312400 | -2.37680800 | 3.64587800 |
| O | 0.80290100 | 2.92797300 | 1.84792300 | H | 1.20484300 | -2.70142900 | 3.84067600 |
| C | 0.53022800 | 4.63277800 | 0.26419400 | H | -0.49920900 | -2.89570600 | 4.34606500 |
| C | 0.68536600 | 4.36734600 | 1.80538100 | H | -0.07510500 | -2.67157600 | 2.61669500 |
| C | -0.91922500 | 4.50727800 | -0.21745500 | C | -2.46027400 | -1.15136000 | 3.38122000 |
| H | -1.53593300 | 5.36043600 | 0.10189800 | H | -2.67428100 | -1.36856200 | 4.43956800 |
| H | -0.92324700 | 4.46515700 | -1.31679500 | H | -3.34149400 | -0.64894900 | 2.95281000 |
| H | -1.37886900 | 3.58093200 | 0.15657500 | H | -2.31694800 | -2.10031300 | 2.84819000 |
| C | 1.14636300 | 5.93187600 | -0.23548900 | C | -1.53516200 | 1.14866000 | 3.78909200 |
| H | 0.99655700 | 6.01786600 | -1.32234600 | H | -2.35940600 | 1.58706600 | 3.20574700 |
| H | 0.67255600 | 6.80203600 | 0.24560300 | H | -1.83720700 | 1.12242400 | 4.84702100 |
| H | 2.22583000 | 5.96530200 | -0.04065500 | H | -0.65815000 | 1.79947500 | 3.67294300 |
| C | -0.50836900 | 4.79025600 | 2.65218100 | H | 2.52719800 | 1.14059600 | 0.84762000 |
| H | -0.30864700 | 4.57204100 | 3.71182800 | C | -4.01747100 | 0.34854200 | -1.27530500 |
| H | -0.69330300 | 5.87171500 | 2.55501900 | C | -5.20521200 | 0.91123300 | -1.77233800 |

| | | | |
|---|---|---|---|
| C | -4.10803900 | -0.64486600 | -0.27948800 |
| C | -6.44714900 | 0.49758300 | -1.29437300 |
| H | -5.15957400 | 1.70194000 | -2.52371000 |
| C | -5.34762600 | -1.05676000 | 0.20128800 |
| H | -3.19864200 | -1.10508000 | 0.11049600 |
| C | -6.52207300 | -0.48919000 | -0.30627700 |
| H | -7.36195500 | 0.95202800 | -1.67760000 |
| H | -5.40343700 | -1.82304700 | 0.97616400 |
| C | -7.86219300 | -0.97963600 | 0.17437200 |
| F | -7.82299000 | -1.35738600 | 1.46406000 |
| F | -8.81388000 | -0.03670800 | 0.05600600 |
| F | -8.28017900 | -2.04830000 | -0.53292300 |
| B | 2.87050700 | -0.91415400 | 0.46754800 |
| B | 0.82766700 | -1.50637300 | -0.80283100 |
| O | 2.73174500 | -2.11677600 | 1.14176100 |
| O | 4.19956800 | -0.73701400 | 0.08716500 |
| O | -0.34301800 | -2.13849300 | -0.42110000 |
| O | 1.42657000 | -2.19276600 | -1.84788000 |
| C | -0.41700100 | -3.42217700 | -1.07533300 |
| C | 0.50887700 | -3.20066900 | -2.32567600 |
| C | 4.03797600 | -2.65753200 | 1.41219700 |
| C | 4.90823000 | -1.97742300 | 0.29380600 |
| C | 4.87636400 | -2.73839100 | -1.03527000 |
| H | 5.33951200 | -2.11116200 | -1.81185700 |
| H | 5.43473600 | -3.68498800 | -0.97964100 |
| H | 3.84147500 | -2.94041800 | -1.34495800 |
| C | 6.34306500 | -1.66576900 | 0.69811600 |
| H | 6.88590200 | -2.58851600 | 0.95709500 |
| H | 6.86985900 | -1.18562100 | -0.14053100 |
| H | 6.37956300 | -0.98255400 | 1.55619300 |
| C | 3.96882400 | -4.17733100 | 1.33331200 |
| H | 4.96692900 | -4.62358700 | 1.46629200 |
| H | 3.31357800 | -4.55830900 | 2.13077200 |
| H | 3.56110100 | -4.51237300 | 0.37116000 |
| C | -1.87475400 | -3.72387600 | -1.40018400 |
| H | -1.96466100 | -4.65226100 | -1.98591300 |
| H | -2.44130200 | -3.85545000 | -0.46606800 |
| H | -2.34216000 | -2.90552800 | -1.96296800 |
| C | 0.13869400 | -4.45455400 | -0.09153800 |
| H | -0.45867900 | -4.41920300 | 0.83127100 |
| H | 0.09255800 | -5.47686500 | -0.49569100 |
| H | 1.17574700 | -4.21351800 | 0.17759700 |
| C | -0.23438700 | -2.58676800 | -3.51639300 |
| H | 0.50515100 | -2.25254900 | -4.25890100 |
| H | -0.91168400 | -3.30822700 | -3.99735000 |
| H | -0.82028500 | -1.70938400 | -3.20487800 |
| C | 1.30168500 | -4.42369000 | -2.76645100 |
| H | 0.62847800 | -5.24298900 | -3.06423400 |
| H | 1.93123300 | -4.16555400 | -3.63122600 |
| H | 1.95974500 | -4.78416200 | -1.96549900 |
| C | 4.42286400 | -2.21573300 | 2.82683700 |
| H | 3.64552900 | -2.55642800 | 3.52550600 |
| H | 5.38844100 | -2.63948000 | 3.14156200 |
| H | 4.47183800 | -1.11999400 | 2.89662700 |

**TNT7-L10-Bpin**

| | | | |
|---|---|---|---|
| Ir | 1.40423300 | 0.30097200 | -0.30145300 |
| C | 1.21228200 | 1.05334800 | -3.31857200 |
| C | 3.43174800 | 0.67947000 | -2.72355900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.59589300 | 1.40499500 | -4.62113900 | H | 1.33361600 | 6.07100700 | -0.79460900 |
| C | -0.19689600 | 1.01589200 | -2.87198400 | C | -0.00595900 | 4.77624300 | 2.73179700 |
| C | 3.88389600 | 1.00918800 | -3.99937800 | H | 0.55201700 | 4.73222600 | 3.67877200 |
| H | 4.11521800 | 0.39269800 | -1.92091400 | H | -0.42102300 | 5.79074000 | 2.62599400 |
| C | 2.94489000 | 1.38151400 | -4.96477700 | H | -0.83304700 | 4.06175900 | 2.79359000 |
| H | 0.84731400 | 1.70778000 | -5.35307400 | C | 2.15653600 | 5.37418300 | 1.62482900 |
| C | -1.28699400 | 1.00227700 | -3.75493700 | H | 1.87529900 | 6.43765900 | 1.62232000 |
| H | 4.95106000 | 0.97668700 | -4.22440500 | H | 2.71138500 | 5.16204800 | 2.55011500 |
| H | 3.26044300 | 1.65610700 | -5.97369400 | H | 2.82840400 | 5.18579700 | 0.77496700 |
| C | -1.62934100 | 0.75331100 | -1.05969500 | B | 0.56475900 | 0.00681100 | 1.53750300 |
| C | -2.57252900 | 0.81241400 | -3.25809300 | O | 1.16033200 | -0.47325500 | 2.69543200 |
| H | -1.12657100 | 1.07717800 | -4.83014600 | O | -0.79057200 | 0.27135400 | 1.80190800 |
| C | -2.76307600 | 0.65081200 | -1.87589200 | C | 0.14575300 | -0.83428000 | 3.64558300 |
| H | -1.69521800 | 0.66859200 | 0.02631000 | C | -1.06257800 | 0.07184100 | 3.20157000 |
| H | -3.41575900 | 0.73374400 | -3.94702200 | C | 0.66899300 | -0.56553900 | 5.05152500 |
| N | 2.13370900 | 0.70108500 | -2.39688100 | H | -0.11268200 | -0.74637900 | 5.80634100 |
| N | -0.39521000 | 0.91369100 | -1.54079900 | H | 1.51123700 | -1.24116400 | 5.26326800 |
| B | 1.55729000 | 2.61746000 | 0.40497700 | H | 1.03057500 | 0.46560200 | 5.15475600 |
| O | 1.03264500 | 3.46217200 | -0.54329200 | C | -0.13541600 | -2.32863100 | 3.45865000 |
| O | 1.40857700 | 3.10016600 | 1.68121500 | H | 0.80762800 | -2.88025600 | 3.58111300 |
| C | 0.23612500 | 4.44813700 | 0.15867600 | H | -0.86038400 | -2.70655000 | 4.19561800 |
| C | 0.92607900 | 4.46477200 | 1.57070000 | H | -0.50566500 | -2.52205400 | 2.44347300 |
| C | -1.19879900 | 3.91790500 | 0.21138200 | C | -2.43679800 | -0.57374400 | 3.34565200 |
| H | -1.88419200 | 4.65199100 | 0.65973200 | H | -2.65127100 | -0.81506100 | 4.39859600 |
| H | -1.53787200 | 3.70644800 | -0.81271700 | H | -3.21316000 | 0.12160500 | 2.99099700 |
| H | -1.25183100 | 2.98341500 | 0.78704000 | H | -2.50851300 | -1.49530100 | 2.75364900 |
| C | 0.29748500 | 5.76177800 | -0.60673100 | C | -1.05131800 | 1.44751300 | 3.86921600 |
| H | -0.20379000 | 5.64631900 | -1.57939300 | H | -1.81234600 | 2.07990500 | 3.38754200 |
| H | -0.21571200 | 6.56130300 | -0.05010800 | H | -1.28655200 | 1.38689900 | 4.94229000 |

| | | | |
|---|---|---|---|
| H | -0.07372900 | 1.93034500 | 3.73903200 |
| H | 2.45527100 | 1.78534100 | 0.12903100 |
| C | -4.06689100 | 0.32545700 | -1.26075400 |
| C | -5.27823800 | 0.79371400 | -1.79687600 |
| C | -4.10652000 | -0.48135600 | -0.10639900 |
| C | -6.49502300 | 0.46926000 | -1.20034400 |
| H | -5.26879000 | 1.44121800 | -2.67597000 |
| C | -5.32114800 | -0.80441200 | 0.49227600 |
| H | -3.17713800 | -0.86887300 | 0.31458400 |
| C | -6.51982500 | -0.33177600 | -0.05374900 |
| H | -7.42909400 | 0.85055800 | -1.61573800 |
| H | -5.33746400 | -1.42567200 | 1.38910800 |
| C | -7.83581100 | -0.72920600 | 0.56106600 |
| F | -7.73250100 | -0.91358700 | 1.88867100 |
| F | -8.78685700 | 0.19899600 | 0.35273500 |
| F | -8.29628200 | -1.88396300 | 0.04042800 |
| B | 2.98889400 | -0.71569600 | 0.47183200 |
| B | 0.62773900 | -1.54796900 | -0.71872800 |
| O | 3.02077300 | -2.07577300 | 0.77079000 |
| O | 4.26401300 | -0.17166300 | 0.64354200 |
| O | -0.34879100 | -2.24857800 | -0.02130700 |
| O | 0.94780100 | -2.21679600 | -1.89296900 |
| C | -0.46627300 | -3.56487700 | -0.60088900 |
| C | 0.02791300 | -3.31100300 | -2.07092000 |
| C | 4.25740100 | -2.38376700 | 1.43333100 |
| C | 5.19936600 | -1.23297900 | 0.91684400 |
| C | 5.88865700 | -1.57933000 | -0.40725900 |
| H | 6.36161900 | -0.67012700 | -0.80896400 |
| H | 6.66921200 | -2.34437600 | -0.27987000 |
| H | 5.15858000 | -1.94297400 | -1.14524800 |
| C | 6.22513800 | -0.73897600 | 1.92941700 |
| H | 6.90896200 | -1.54990100 | 2.22671200 |
| H | 6.82481900 | 0.06980100 | 1.48479100 |
| H | 5.73659400 | -0.34111100 | 2.82772500 |
| C | 4.69040900 | -3.79218200 | 1.04123500 |
| H | 5.68435300 | -4.02969200 | 1.45253900 |
| H | 3.97238500 | -4.52261400 | 1.44369700 |
| H | 4.72001900 | -3.91616400 | -0.04911100 |
| C | -1.91261000 | -4.02707000 | -0.47694100 |
| H | -2.06414500 | -4.98990000 | -0.98982300 |
| H | -2.16616100 | -4.16458700 | 0.58516500 |
| H | -2.61063900 | -3.29117300 | -0.89731200 |
| C | 0.46615500 | -4.49054100 | 0.18628800 |
| H | 0.16726800 | -4.48077900 | 1.24413600 |
| H | 0.41561900 | -5.52747200 | -0.17831400 |
| H | 1.50275700 | -4.12981000 | 0.13316600 |
| C | -1.08820700 | -2.81183100 | -2.99445900 |
| H | -0.63562200 | -2.43476100 | -3.92346500 |
| H | -1.80016500 | -3.61042300 | -3.25173200 |
| H | -1.64298200 | -1.98467800 | -2.52960900 |
| C | 0.76619500 | -4.47820900 | -2.71282800 |
| H | 0.11921700 | -5.36734600 | -2.77803100 |
| H | 1.07594500 | -4.20419000 | -3.73278800 |
| H | 1.66813400 | -4.73723800 | -2.14405400 |
| C | 3.99795000 | -2.31332000 | 2.94147800 |
| H | 3.19515000 | -3.02250100 | 3.19001900 |
| H | 4.89256500 | -2.57997000 | 3.52435300 |
| H | 3.65083400 | -1.31297900 | 3.23215500 |

**$Ir(Bpin)_3$ with ligand L1**

| | | | |
|---|---|---|---|
| Ir | -0.49992400 | 0.31584600 | -0.84597500 |
| C | 2.43357800 | -0.69243900 | -0.71655700 |
| C | 1.04512500 | -2.46098000 | -1.26491000 |
| C | 3.45683200 | -1.57521300 | -0.36648000 |
| C | 2.57251600 | 0.78466700 | -0.61960500 |
| C | 2.03124700 | -3.39480200 | -0.94629000 |
| H | 0.05482600 | -2.75755600 | -1.61598200 |
| C | 3.27161600 | -2.96338800 | -0.46246300 |
| H | 4.39759200 | -1.17907800 | 0.01267000 |
| C | 3.80358700 | 1.41980100 | -0.44300900 |
| H | 1.79972700 | -4.45220100 | -1.06207300 |
| C | 1.48538000 | 2.83285500 | -0.64510700 |
| C | 3.88902800 | 2.81759200 | -0.35667000 |
| H | 4.70865200 | 0.81719800 | -0.38588200 |
| C | 2.68451400 | 3.52326600 | -0.46667900 |
| H | 0.52373900 | 3.34753400 | -0.73011900 |
| N | 1.23343400 | -1.14547300 | -1.13873000 |
| N | 1.42777800 | 1.49834300 | -0.71687300 |
| B | -2.07299800 | -0.95300000 | -1.07049800 |
| O | -2.03419300 | -2.00896300 | -2.00026700 |
| O | -3.24410900 | -1.05237700 | -0.32683800 |
| C | -3.06495800 | -2.96059100 | -1.67108600 |
| C | -4.08872900 | -2.06932500 | -0.87658200 |
| C | -2.42004200 | -4.04201900 | -0.79572500 |
| H | -3.14067400 | -4.82189300 | -0.50707200 |
| H | -1.61059200 | -4.52606500 | -1.36430200 |
| H | -1.98211900 | -3.59700800 | 0.10868200 |
| C | -3.60607000 | -3.57487900 | -2.95624800 |
| H | -2.81618000 | -4.16417700 | -3.44658200 |
| H | -4.45298900 | -4.24725000 | -2.74542400 |
| H | -3.93655900 | -2.80300400 | -3.66293300 |
| C | -4.80931200 | -2.78024200 | 0.26413300 |
| H | -5.48829600 | -2.07454500 | 0.76576000 |
| H | -5.40715200 | -3.62703100 | -0.10892600 |
| H | -4.09875600 | -3.15296000 | 1.01308100 |
| C | -5.10680500 | -1.37012000 | -1.78409000 |
| H | -5.85420900 | -2.07034900 | -2.18750700 |
| H | -5.62628000 | -0.60055200 | -1.19454900 |
| H | -4.60323600 | -0.86842100 | -2.62307100 |
| B | -1.81333000 | 1.77483400 | -0.36146000 |
| O | -1.62533100 | 3.08558000 | -0.85619800 |
| O | -2.90614700 | 1.77185700 | 0.49279100 |
| C | -2.74150800 | 3.90184500 | -0.45358300 |
| C | -3.26786300 | 3.12138600 | 0.80476100 |
| C | -3.74354000 | 3.90723800 | -1.61206600 |
| H | -4.59771600 | 4.57301100 | -1.41576000 |
| H | -3.23150200 | 4.25502800 | -2.52166200 |
| H | -4.12303400 | 2.89297200 | -1.80221300 |
| C | -2.24896000 | 5.31739400 | -0.17738900 |
| H | -1.89166600 | 5.77679100 | -1.11201700 |
| H | -3.06063700 | 5.94594600 | 0.22217900 |
| H | -1.41957300 | 5.32051900 | 0.54220300 |
| C | -4.77518200 | 3.19311100 | 1.02169200 |
| H | -5.04445300 | 2.61118900 | 1.91591700 |
| H | -5.10567000 | 4.23292500 | 1.17528700 |
| H | -5.32229900 | 2.76853100 | 0.17024100 |
| C | -2.53162800 | 3.50672300 | 2.09350900 |

| | | | |
|---|---|---|---|
| H | -2.80332800 | 4.51578300 | 2.43956300 |
| H | -2.79538200 | 2.78328700 | 2.87767600 |
| H | -1.44260900 | 3.45294800 | 1.95450200 |
| B | -0.66865300 | -0.38420900 | 0.99815300 |
| O | -0.74581100 | 0.36178300 | 2.16302100 |
| O | -0.61297500 | -1.74813400 | 1.30055300 |
| C | -1.11334400 | -0.53183000 | 3.23148400 |
| C | -0.51303700 | -1.89489300 | 2.72716900 |
| C | -2.64441500 | -0.54812500 | 3.29384800 |
| H | -3.01554900 | -1.17995200 | 4.11517900 |
| H | -2.99855100 | 0.47975800 | 3.45413200 |
| H | -3.06900500 | -0.89097500 | 2.33962900 |
| C | -0.52516300 | -0.01429900 | 4.53686000 |
| H | -0.99623500 | 0.94516200 | 4.79789500 |
| H | -0.71187800 | -0.72242300 | 5.35983100 |
| H | 0.55678400 | 0.15335700 | 4.45350700 |
| C | 0.97492000 | -2.05575800 | 3.05713900 |
| H | 1.14474500 | -2.26044200 | 4.12505100 |
| H | 1.37415800 | -2.89654400 | 2.46995200 |
| H | 1.53694000 | -1.15286700 | 2.77687900 |
| C | -1.28866000 | -3.13470100 | 3.15340800 |
| H | -0.80459400 | -4.03574500 | 2.74657100 |
| H | -1.31500600 | -3.22559800 | 4.25081700 |
| H | -2.31928100 | -3.10471400 | 2.77807400 |
| H | 2.65297400 | 4.61020800 | -0.41496300 |
| C | 5.24974300 | 3.49378000 | -0.15712000 |
| C | 5.12541600 | 5.02273700 | -0.08010000 |
| H | 6.12081400 | 5.46880100 | 0.06610700 |
| H | 4.70449400 | 5.44536000 | -1.00514200 |
| H | 4.49206800 | 5.33874800 | 0.76282400 |
| C | 5.87534600 | 2.98429800 | 1.15879200 |
| H | 6.03186800 | 1.89526500 | 1.14347100 |
| H | 6.85464000 | 3.46093400 | 1.32359200 |
| H | 5.22950700 | 3.22014900 | 2.01866300 |
| C | 6.16982100 | 3.13355200 | -1.34283600 |
| H | 5.73801300 | 3.47870100 | -2.29496400 |
| H | 7.15413900 | 3.61222700 | -1.21881900 |
| H | 6.33318300 | 2.04820900 | -1.42056300 |
| C | 4.38635400 | -3.91866200 | -0.02327800 |
| C | 5.66309900 | -3.62454900 | -0.83818200 |
| H | 6.01692300 | -2.59331100 | -0.68961600 |
| H | 6.47486800 | -4.30301100 | -0.53142800 |
| H | 5.48453200 | -3.76838800 | -1.91511200 |
| C | 4.66451800 | -3.69523300 | 1.47889100 |
| H | 3.76000800 | -3.88295800 | 2.07757600 |
| H | 5.45610700 | -4.37833300 | 1.82584300 |
| H | 4.99436900 | -2.66597800 | 1.68523900 |
| C | 3.99838400 | -5.38950100 | -0.23571600 |
| H | 3.10937100 | -5.66571000 | 0.35132400 |
| H | 3.79361900 | -5.60849500 | -1.29487600 |
| H | 4.82462000 | -6.04153000 | 0.08597900 |

**INT1-L1-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | -0.97803300 | 0.08897000 | -0.14319700 |
| C | 1.59661500 | 1.56750500 | 0.84319300 |
| C | 1.86481000 | -0.71983900 | 1.06666300 |
| C | 2.91283800 | 1.77952300 | 1.26342200 |
| C | 0.66051800 | 2.66846700 | 0.51014800 |
| C | 3.17940500 | -0.57331400 | 1.50037400 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.41318400 | -1.70169600 | 0.95706600 | C | -2.01069200 | -4.21479100 | -2.25645000 |
| C | 3.75392500 | 0.69958800 | 1.57147700 | H | -1.77665400 | -5.17580000 | -2.73962800 |
| H | 3.29504600 | 2.79622100 | 1.33486800 | H | -3.10330500 | -4.09754500 | -2.21260300 |
| C | 1.02843800 | 4.01684500 | 0.55877500 | H | -1.61042200 | -3.39908900 | -2.87633000 |
| H | 3.74484000 | -1.47399800 | 1.72500500 | B | -2.93224800 | 0.12911900 | -0.69865200 |
| C | -1.49308200 | 3.25468200 | -0.11216700 | O | -3.44430400 | 1.23354400 | -1.43193200 |
| C | 0.10673100 | 5.03095900 | 0.26675100 | O | -3.96827500 | -0.76324600 | -0.47656600 |
| H | 2.04973100 | 4.27896500 | 0.82876700 | C | -4.78159800 | 0.92832100 | -1.86639800 |
| C | -1.18807100 | 4.61388700 | -0.06941200 | C | -5.21766100 | -0.14984900 | -0.81057200 |
| H | -2.48245300 | 2.89626600 | -0.40464100 | C | -4.67725000 | 0.36153100 | -3.28619500 |
| N | 1.10394500 | 0.31569800 | 0.70313400 | H | -5.66617400 | 0.14981800 | -3.72007300 |
| N | -0.59537500 | 2.30065100 | 0.16225700 | H | -4.16840300 | 1.09624600 | -3.92854700 |
| B | -0.96167400 | -1.91265100 | -0.46406900 | H | -4.08129600 | -0.56225000 | -3.29302300 |
| O | 0.22256300 | -2.52091300 | -0.94627900 | C | -5.61035000 | 2.20696800 | -1.86839800 |
| O | -1.91686400 | -2.89905000 | -0.26633500 | H | -5.22129500 | 2.90300800 | -2.62799300 |
| C | 0.09996100 | -3.95078200 | -0.79110400 | H | -6.66348400 | 1.99409300 | -2.11146400 |
| C | -1.45665500 | -4.13484800 | -0.82971400 | H | -5.57240500 | 2.71098300 | -0.89374200 |
| C | 0.70029000 | -4.31454600 | 0.57198000 | C | -6.16645900 | -1.21971300 | -1.33922400 |
| H | 0.67855400 | -5.40024500 | 0.75144900 | H | -6.40158500 | -1.93022900 | -0.53277000 |
| H | 1.74622800 | -3.97991700 | 0.58790700 | H | -7.11061500 | -0.77505900 | -1.69273600 |
| H | 0.15790100 | -3.80614800 | 1.38185500 | H | -5.71080300 | -1.78680600 | -2.16116800 |
| C | 0.87263400 | -4.63883000 | -1.90883500 | C | -5.78483100 | 0.47144600 | 0.47095200 |
| H | 1.94739400 | -4.43699900 | -1.78749600 | H | -6.77474000 | 0.92418100 | 0.30708700 |
| H | 0.72129800 | -5.72975100 | -1.87706400 | H | -5.88233300 | -0.31683700 | 1.23013200 |
| H | 0.56341500 | -4.27234000 | -2.89668600 | H | -5.10023800 | 1.22934800 | 0.87673300 |
| C | -1.99024400 | -5.28954600 | 0.00952400 | B | -1.60794400 | -0.53724100 | 1.68090300 |
| H | -3.08637100 | -5.33146000 | -0.07618900 | O | -2.78492600 | -0.22175800 | 2.34978300 |
| H | -1.58071100 | -6.25252900 | -0.33507500 | O | -0.86805200 | -1.45008900 | 2.44769700 |
| H | -1.74115700 | -5.15927200 | 1.07059600 | C | -3.00307500 | -1.21409800 | 3.36888100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.53349500 | -1.66185900 | 3.70286200 | C | 4.23717500 | -0.55168000 | -2.40882800 |
| C | -3.83106700 | -2.33815300 | 2.73521700 | C | 5.62423000 | -0.50391500 | -2.65076700 |
| H | -4.07659100 | -3.12626100 | 3.46363900 | C | 3.70029900 | -1.55301000 | -1.59559400 |
| H | -4.76858700 | -1.91056300 | 2.35408200 | C | 6.45432500 | -1.44588000 | -2.05817400 |
| H | -3.30327600 | -2.77565600 | 1.87608200 | H | 6.01410600 | 0.28689200 | -3.29272300 |
| C | -3.76225400 | -0.57951300 | 4.52701600 | C | 4.56094400 | -2.48602400 | -0.99353400 |
| H | -4.76976000 | -0.29115300 | 4.19121200 | H | 2.63286300 | -1.65108500 | -1.40193800 |
| H | -3.87042300 | -1.28873200 | 5.36320000 | C | 5.94199800 | -2.44325600 | -1.21579600 |
| H | -3.25826300 | 0.32447600 | 4.89346500 | H | 7.53093400 | -1.40527900 | -2.24091600 |
| C | -0.85253100 | -0.76082500 | 4.73784200 | H | 6.61559200 | -3.16405800 | -0.75554400 |
| H | -1.25084900 | -0.91899100 | 5.75176400 | O | 3.95276100 | -3.40068500 | -0.18673500 |
| H | 0.22462800 | -0.98603800 | 4.74671600 | C | 4.72758700 | -4.41501600 | 0.41107300 |
| H | -0.97544400 | 0.29911500 | 4.47189900 | H | 4.02871600 | -5.04435700 | 0.97768900 |
| C | -1.38366500 | -3.12649700 | 4.09801700 | H | 5.24137200 | -5.03419600 | -0.34481300 |
| H | -0.32467800 | -3.35094300 | 4.29876300 | H | 5.48134700 | -3.99934800 | 1.10340500 |
| H | -1.96026800 | -3.35272100 | 5.00905700 | H | -1.97445900 | 5.32788100 | -0.30811300 |
| H | -1.72417700 | -3.78921900 | 3.29236900 | C | 0.53515800 | 6.50139200 | 0.32266500 |
| S | -0.57740300 | 0.30358500 | -2.69256600 | C | 1.68348500 | 6.72908700 | -0.68318700 |
| C | -0.75350400 | 2.03467000 | -3.22233600 | H | 2.00598100 | 7.78217200 | -0.66129900 |
| H | -0.06007600 | 2.70444600 | -2.69565900 | H | 2.56051700 | 6.10601600 | -0.45228000 |
| H | -0.61959000 | 2.12083800 | -4.31057900 | H | 1.36096500 | 6.49071700 | -1.70868100 |
| H | -1.78337700 | 2.29316800 | -2.94410600 | C | 1.02249700 | 6.83099100 | 1.74952400 |
| C | 1.11806800 | -0.09822600 | -3.24249800 | H | 1.33351700 | 7.88594800 | 1.81143300 |
| H | 1.20733000 | -1.17103800 | -3.02147700 | H | 0.22164100 | 6.66520800 | 2.48655100 |
| H | 1.18752000 | 0.04347000 | -4.33258900 | H | 1.88296700 | 6.21079300 | 2.04208400 |
| C | 2.19112500 | 0.70293100 | -2.52291500 | C | -0.62047100 | 7.44931900 | -0.03108500 |
| H | 2.13047100 | 0.52278200 | -1.44371100 | H | -0.99581900 | 7.27279900 | -1.05069900 |
| H | 2.04423000 | 1.77905500 | -2.69584800 | H | -1.46320700 | 7.34454600 | 0.66911800 |
| O | 3.50117100 | 0.42312200 | -3.00104100 | H | -0.27369100 | 8.49260500 | 0.01963500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 5.22716300 | 0.93516400 | 1.91634700 | H | -0.46540300 | 3.15813200 | 0.94171800 |
| C | 5.33147200 | 1.87513100 | 3.13413900 | N | 1.12306200 | -1.08248800 | 0.44031400 |
| H | 6.38857100 | 2.05369900 | 3.38735800 | N | 0.79849900 | 1.53950600 | 0.84599800 |
| H | 4.86700100 | 2.85367100 | 2.93952300 | B | -1.88723800 | -1.26961800 | -0.93410200 |
| H | 4.83695300 | 1.43602800 | 4.01461800 | O | -2.56883100 | -2.37743900 | -0.41845900 |
| C | 5.95275300 | -0.37975400 | 2.24083900 | O | -2.04298700 | -1.25716600 | -2.32870900 |
| H | 5.94104400 | -1.06794200 | 1.38238100 | C | -3.44764700 | -2.90268500 | -1.42926800 |
| H | 7.00534500 | -0.17052700 | 2.48554000 | C | -2.73485100 | -2.44073000 | -2.75382100 |
| H | 5.50363200 | -0.89065000 | 3.10659500 | C | -4.81669700 | -2.24312400 | -1.23152700 |
| C | 5.91357300 | 1.57982000 | 0.69210400 | H | -5.56081400 | -2.62003100 | -1.94948800 |
| H | 6.98101800 | 1.75380800 | 0.90311500 | H | -5.17218000 | -2.46644500 | -0.21530000 |
| H | 5.83866400 | 0.92551800 | -0.18940400 | H | -4.73199000 | -1.15193700 | -1.32069600 |
| H | 5.45983900 | 2.54916200 | 0.43507200 | C | -3.55794000 | -4.41256300 | -1.25095700 |

**INT1-L1-sp$^2$**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ir | -0.74155800 | 0.08527100 | 0.03437800 | H | -4.06111600 | -4.63464900 | -0.29780000 |
| C | 2.20886500 | -0.40326200 | 0.86582500 | H | -4.15074300 | -4.86381100 | -2.06238700 |
| C | 1.14933300 | -2.41908100 | 0.44919300 | H | -2.57003400 | -4.89116900 | -1.22839900 |
| C | 3.36286000 | -1.07515200 | 1.27989500 | C | -3.67661100 | -2.07570000 | -3.89561300 |
| C | 2.06282900 | 1.07235700 | 0.93107400 | H | -3.09060900 | -1.76174100 | -4.77299000 |
| C | 2.26939500 | -3.14648000 | 0.84181500 | H | -4.29827500 | -2.93661700 | -4.18869700 |
| H | 0.22502900 | -2.91233200 | 0.14454900 | H | -4.33335300 | -1.24350400 | -3.61274000 |
| C | 3.42375600 | -2.47603700 | 1.26640400 | C | -1.67719300 | -3.43663300 | -3.24118400 |
| H | 4.21373100 | -0.49660200 | 1.63676900 | H | -2.12651000 | -4.34876400 | -3.66199700 |
| C | 3.14534300 | 1.94035300 | 1.09801400 | H | -1.07139000 | -2.95418300 | -4.02296700 |
| H | 2.22250000 | -4.23247400 | 0.80792100 | H | -1.00561100 | -3.72451400 | -2.41992400 |
| C | 0.58019700 | 2.84805000 | 1.01318000 | B | -2.39854800 | 1.26228200 | -0.12517700 |
| C | 2.94265300 | 3.31969800 | 1.23893700 | O | -2.40493200 | 2.63980200 | 0.17572400 |
| H | 4.15518900 | 1.53393300 | 1.08908500 | O | -3.68320200 | 0.90234400 | -0.53503900 |
| C | 1.61234400 | 3.75703300 | 1.22923500 | C | -3.67459600 | 3.21384500 | -0.18129700 |
| | | | | C | -4.61107200 | 1.95004600 | -0.22001900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.51181500 | 3.87356700 | -1.55505000 | C | -0.86320900 | -1.21601500 | 4.67735600 |
| H | -4.42906300 | 4.38900900 | -1.87648700 | H | -1.27420000 | -1.35121000 | 5.68932200 |
| H | -2.70369000 | 4.61826500 | -1.50151400 | H | 0.14948900 | -1.64564500 | 4.65148700 |
| H | -3.24294500 | 3.12991100 | -2.31878600 | H | -0.77954800 | -0.13888000 | 4.47173100 |
| C | -4.05305000 | 4.26165400 | 0.85904300 | C | -1.84382200 | -3.39625400 | 3.91948600 |
| H | -3.34318200 | 5.10251600 | 0.81658900 | H | -0.84429600 | -3.82532500 | 4.08902600 |
| H | -5.06266400 | 4.65973900 | 0.67071000 | H | -2.44608100 | -3.56243000 | 4.82672400 |
| H | -4.02237300 | 3.84340800 | 1.87301200 | H | -2.30584900 | -3.93558000 | 3.08295200 |
| C | -5.69660400 | 1.98806800 | -1.29084300 | S | 3.74800900 | -3.62950300 | -2.45555300 |
| H | -6.29618400 | 1.06686700 | -1.23841500 | C | 2.00721000 | -3.96835100 | -2.86765900 |
| H | -6.37397500 | 2.84344100 | -1.13872600 | H | 1.68675600 | -3.43050700 | -3.77137400 |
| H | -5.26742900 | 2.05142700 | -2.29926500 | H | 1.92100800 | -5.04793900 | -3.05364800 |
| C | -5.22913300 | 1.62115300 | 1.14281700 | H | 1.35102100 | -3.69384000 | -2.02967800 |
| H | -5.99285100 | 2.35767900 | 1.43566200 | C | 3.63469000 | -1.84443700 | -2.11091400 |
| H | -5.70589500 | 0.63205100 | 1.07813100 | H | 2.72017400 | -1.65556600 | -1.53577500 |
| H | -4.45376100 | 1.55897900 | 1.91722200 | H | 4.48342600 | -1.59260800 | -1.46132500 |
| B | -1.57453100 | -0.65990600 | 1.68015300 | C | 3.67662300 | -0.96633500 | -3.35392300 |
| O | -2.69134500 | -0.18764400 | 2.35976300 | H | 2.86753100 | -1.22234400 | -4.05806300 |
| O | -1.03536500 | -1.75435300 | 2.35534600 | H | 4.63064000 | -1.10622200 | -3.88221300 |
| C | -3.07880100 | -1.16987200 | 3.33866900 | O | 3.62508700 | 0.40377900 | -2.99609100 |
| C | -1.71647200 | -1.90939200 | 3.61020700 | C | 2.42617000 | 1.00077500 | -2.74080900 |
| C | -4.12215700 | -2.07780600 | 2.68077000 | C | 1.17618000 | 0.36314200 | -2.81574600 |
| H | -4.51556800 | -2.82754700 | 3.38391500 | C | 2.49789500 | 2.35693400 | -2.40960900 |
| H | -4.95791700 | -1.45438500 | 2.33136300 | C | 0.01769500 | 1.11776600 | -2.60159400 |
| H | -3.69148200 | -2.58134300 | 1.80486300 | H | 1.07295200 | -0.69480200 | -3.04846300 |
| C | -3.67675300 | -0.45756200 | 4.54545700 | C | 1.33216000 | 3.09379400 | -2.17616200 |
| H | -4.62267400 | 0.02558100 | 4.25775600 | H | 3.47184600 | 2.83987700 | -2.34909300 |
| H | -3.89142800 | -1.17129400 | 5.35660900 | C | 0.07732100 | 2.47799700 | -2.28244700 |
| H | -3.00357800 | 0.32044600 | 4.92845800 | H | -0.94804400 | 0.62266600 | -2.71376000 |

| | | | |
|---|---|---|---|
| H | -0.84271900 | 3.01870600 | -2.08215000 |
| O | 1.51160600 | 4.40467500 | -1.85051900 |
| C | 0.36917400 | 5.21439600 | -1.68277100 |
| H | 0.73209900 | 6.21895900 | -1.42742500 |
| H | -0.22776400 | 5.26997900 | -2.61015200 |
| H | -0.28072300 | 4.84539200 | -0.87173600 |
| H | 1.35995100 | 4.80846900 | 1.34984700 |
| C | 4.13199800 | 4.28139400 | 1.31920200 |
| C | 4.77111400 | 4.34944900 | -0.08570500 |
| H | 5.62228800 | 5.04932600 | -0.08464800 |
| H | 5.14103300 | 3.36331100 | -0.40579700 |
| H | 4.03288400 | 4.69095900 | -0.82634600 |
| C | 5.16608800 | 3.77547800 | 2.34370800 |
| H | 6.01180400 | 4.47818200 | 2.40437400 |
| H | 4.72043800 | 3.68854900 | 3.34708400 |
| H | 5.57739000 | 2.79313700 | 2.06844100 |
| C | 3.69444900 | 5.69681500 | 1.72747300 |
| H | 3.02488900 | 6.14788300 | 0.98019700 |
| H | 3.17923200 | 5.69882500 | 2.70069700 |
| H | 4.57761300 | 6.34808600 | 1.81189800 |
| C | 4.69283500 | -3.20315600 | 1.72427600 |
| C | 4.94372200 | -2.86981400 | 3.21019900 |
| H | 5.84366100 | -3.39298700 | 3.57084800 |
| H | 5.09648500 | -1.79121200 | 3.36720200 |
| H | 4.09106100 | -3.18320100 | 3.83229000 |
| C | 5.89300200 | -2.73233900 | 0.87647100 |
| H | 6.81758700 | -3.21473500 | 1.23057700 |
| H | 5.75213200 | -3.00507900 | -0.17971600 |
| H | 6.04118100 | -1.64363000 | 0.93680500 |
| C | 4.56358700 | -4.72577600 | 1.56761900 |
| H | 3.75532800 | -5.13417400 | 2.19337600 |
| H | 4.37057100 | -5.00108600 | 0.51992200 |
| H | 5.50085800 | -5.21129100 | 1.87942000 |

**TS1-L1-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | -0.99229300 | -0.14128300 | -0.47825600 |
| C | 0.96451600 | 2.15108700 | 0.27630600 |
| C | 2.11078000 | 0.14739700 | 0.31463100 |
| C | 2.08064800 | 2.82227700 | 0.78266600 |
| C | -0.34049500 | 2.81835900 | 0.06694100 |
| C | 3.25631400 | 0.75312800 | 0.82536700 |
| H | 2.07612000 | -0.92241200 | 0.11677000 |
| C | 3.26389000 | 2.12936800 | 1.07509400 |
| H | 2.01525100 | 3.89072100 | 0.97954600 |
| C | -0.49127600 | 4.20740100 | 0.06294500 |
| C | -2.63540200 | 2.54618700 | -0.16170800 |
| C | -1.75501900 | 4.79886500 | -0.05710200 |
| H | 0.39703800 | 4.83218600 | 0.13726900 |
| C | -2.84525200 | 3.92315300 | -0.15226500 |
| H | -3.45800900 | 1.83068800 | -0.23822800 |
| N | 0.99440100 | 0.82335300 | 0.04260200 |
| N | -1.41336900 | 2.00407500 | -0.07444700 |
| B | -0.41855400 | -2.11630500 | -0.30719100 |
| O | 0.83109800 | -2.59235600 | -0.73212200 |
| O | -1.11754100 | -3.14869000 | 0.30010500 |
| C | 1.04672800 | -3.90616200 | -0.16409800 |
| C | -0.42793400 | -4.38875600 | 0.07555900 |
| C | 1.83545800 | -3.71263200 | 1.13481900 |
| H | 2.04778900 | -4.67440800 | 1.62610500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.79802600 | -3.23918500 | 0.89540200 | H | -6.33521300 | -3.11690900 | -2.22410300 |
| H | 1.28794900 | -3.06068700 | 1.82879500 | H | -5.09952400 | -2.38778200 | -3.29133400 |
| C | 1.84521400 | -4.75680400 | -1.14502000 | C | -4.65741200 | -3.20931100 | 0.05298200 |
| H | 2.88049600 | -4.39212500 | -1.20510500 | H | -5.68118500 | -3.52466500 | 0.30522800 |
| H | 1.87955300 | -5.80434900 | -0.80549000 | H | -4.05835700 | -4.10266300 | -0.17125200 |
| H | 1.40367900 | -4.73112200 | -2.14985800 | H | -4.20303300 | -2.72057200 | 0.92584500 |
| C | -0.61706300 | -5.28650600 | 1.29182300 | B | -1.13650700 | -0.58668000 | 1.57700800 |
| H | -1.68008800 | -5.55165700 | 1.39293800 | O | -2.27270600 | -0.47710600 | 2.35748000 |
| H | -0.03913700 | -6.21828200 | 1.18727900 | O | -0.05301200 | -0.97162700 | 2.36558900 |
| H | -0.30501200 | -4.78201000 | 2.21490700 | C | -2.00488000 | -1.04234200 | 3.65589200 |
| C | -1.05392000 | -5.03608600 | -1.16378100 | C | -0.44048200 | -0.91929800 | 3.75034900 |
| H | -0.62513900 | -6.02781200 | -1.37159100 | C | -2.48853900 | -2.49513200 | 3.61316600 |
| H | -2.13413100 | -5.14864600 | -0.99519900 | H | -2.35601100 | -3.00504600 | 4.57935500 |
| H | -0.92351400 | -4.39702500 | -2.04834500 | H | -3.55982100 | -2.50018000 | 3.36361500 |
| B | -2.87891800 | -0.85249200 | -0.74653900 | H | -1.96217600 | -3.05365500 | 2.82743300 |
| O | -4.03028200 | -0.19021900 | -0.31025700 | C | -2.77600400 | -0.25559900 | 4.70793100 |
| O | -3.24811200 | -1.99568900 | -1.44866000 | H | -3.85630900 | -0.39136500 | 4.54968200 |
| C | -5.19165200 | -0.84848600 | -0.84665000 | H | -2.53063900 | -0.60882200 | 5.72220700 |
| C | -4.62728000 | -2.27997300 | -1.16579400 | H | -2.56042800 | 0.81890500 | 4.64617900 |
| C | -5.61306900 | -0.08181800 | -2.10414500 | C | 0.02564200 | 0.43820400 | 4.28750300 |
| H | -6.53830200 | -0.48534300 | -2.54253800 | H | -0.16120400 | 0.54426000 | 5.36681300 |
| H | -5.79004700 | 0.97152000 | -1.83834500 | H | 1.10671300 | 0.53441000 | 4.10655100 |
| H | -4.82018900 | -0.11271400 | -2.86563900 | H | -0.47809600 | 1.26082100 | 3.75928800 |
| C | -6.30290100 | -0.81112200 | 0.19524700 | C | 0.24901000 | -2.04885600 | 4.50552000 |
| H | -6.63445500 | 0.22726200 | 0.34908000 | H | 1.33804400 | -1.89028100 | 4.49683400 |
| H | -7.17248400 | -1.40255100 | -0.13279300 | H | -0.08460800 | -2.08193900 | 5.55475600 |
| H | -5.95222300 | -1.19776900 | 1.16031300 | H | 0.04600500 | -3.02287800 | 4.04298500 |
| C | -5.25382700 | -2.96764300 | -2.37203700 | S | 0.24449600 | 1.60132900 | -3.30629600 |
| H | -4.78881700 | -3.95474600 | -2.51477100 | C | -1.10267100 | 0.54840400 | -2.68805300 |

| | | | |
|---|---|---|---|
| H | -1.96245500 | 1.21351300 | -2.53073800 |
| H | -1.40396800 | -0.14232400 | -3.48907900 |
| H | -0.62333800 | -0.81501200 | -1.89250300 |
| C | 1.24347100 | 0.33966300 | -4.16626600 |
| H | 0.55735200 | -0.31725700 | -4.72423500 |
| H | 1.86291200 | 0.87727300 | -4.90030500 |
| C | 2.14386900 | -0.50419700 | -3.28510500 |
| H | 2.53430200 | -1.36182400 | -3.86623600 |
| H | 1.59845700 | -0.90821000 | -2.41838500 |
| O | 3.23400200 | 0.30966900 | -2.86898800 |
| C | 4.22588700 | -0.24542800 | -2.14391700 |
| C | 5.36250300 | 0.55662900 | -1.91965800 |
| C | 4.16220600 | -1.53376600 | -1.60866600 |
| C | 6.40353800 | 0.06060600 | -1.14750200 |
| H | 5.39033100 | 1.55468700 | -2.35822500 |
| C | 5.22049100 | -2.01282900 | -0.81968800 |
| H | 3.28542000 | -2.16406000 | -1.73586100 |
| C | 6.35129400 | -1.22225100 | -0.57942900 |
| H | 7.28678100 | 0.68076100 | -0.97541900 |
| H | 7.18196400 | -1.58316100 | 0.02459300 |
| O | 5.04629300 | -3.26708100 | -0.31978300 |
| C | 6.03934400 | -3.81885900 | 0.51252000 |
| H | 5.68087300 | -4.81332800 | 0.80911100 |
| H | 7.00302000 | -3.92546500 | -0.01656000 |
| H | 6.19770800 | -3.20825800 | 1.41936900 |
| H | -3.86724900 | 4.28953500 | -0.23089600 |
| H | 4.13072700 | 0.13151500 | 1.00552400 |
| C | 4.48565500 | 2.87481400 | 1.62235000 |
| C | 5.58627500 | 1.90456600 | 2.07845300 |
| H | 6.43868300 | 2.47337200 | 2.48078400 |
| H | 5.22592400 | 1.23153200 | 2.87201400 |
| H | 5.95622400 | 1.28762700 | 1.24804300 |
| C | 5.04680400 | 3.77233100 | 0.49861500 |
| H | 5.34516500 | 3.16506200 | -0.36873300 |
| H | 4.29941300 | 4.50472000 | 0.15676900 |
| H | 5.92963600 | 4.32733400 | 0.85510300 |
| C | 4.07463900 | 3.74491100 | 2.82743100 |
| H | 3.63471400 | 3.12825500 | 3.62676800 |
| H | 4.95639800 | 4.26132200 | 3.23855700 |
| H | 3.34033400 | 4.51683100 | 2.55320300 |
| C | -1.89108800 | 6.32488600 | -0.08436300 |
| C | -1.10902400 | 6.87307500 | -1.29700700 |
| H | -1.19562900 | 7.97045000 | -1.34090300 |
| H | -0.03919300 | 6.62246400 | -1.24151800 |
| H | -1.50199100 | 6.45861700 | -2.23812000 |
| C | -1.30590300 | 6.90928400 | 1.21865200 |
| H | -1.39629900 | 8.00716200 | 1.21731300 |
| H | -1.84154000 | 6.52186500 | 2.09920700 |
| H | -0.24024500 | 6.66210200 | 1.33634800 |
| C | -3.35666100 | 6.76848700 | -0.20440600 |
| H | -3.81962500 | 6.39981300 | -1.13239800 |
| H | -3.96087800 | 6.41664900 | 0.64582200 |
| H | -3.41156700 | 7.86761000 | -0.21955800 |

**TS1-L1-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | -0.76912700 | 0.15815000 | -0.19544700 |
| C | 1.95783900 | 0.05594600 | 1.22047100 |
| C | 1.08880800 | -2.08480100 | 1.05205700 |
| C | 3.12282000 | -0.44490300 | 1.80731000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.70947100 | 1.50703000 | 1.04357600 | H | -3.75173000 | -4.15575400 | -3.72162300 |
| C | 2.22107100 | -2.64183400 | 1.64104000 | H | -4.34667600 | -2.59962000 | -3.06449700 |
| H | 0.23988900 | -2.69560800 | 0.73674200 | C | -1.01218200 | -3.46087800 | -3.44374300 |
| C | 3.28753100 | -1.81965700 | 2.02542200 | H | -1.12226400 | -4.49286800 | -3.81005200 |
| H | 3.89776800 | 0.25310200 | 2.12008000 | H | -0.86302600 | -2.79486000 | -4.30578100 |
| C | 2.73095800 | 2.45615800 | 1.06107200 | H | -0.11173100 | -3.40406400 | -2.81669200 |
| H | 2.25739800 | -3.71972800 | 1.77957700 | B | -2.57984100 | 1.10547800 | -0.43966000 |
| C | 0.11789800 | 3.15835400 | 0.77092100 | O | -2.83409300 | 2.33359400 | 0.17943200 |
| C | 2.44241000 | 3.81969400 | 0.90219400 | O | -3.66602300 | 0.72619500 | -1.20046800 |
| H | 3.76420200 | 2.12408600 | 1.14863000 | C | -4.04950200 | 2.88585000 | -0.36363400 |
| C | 1.08822700 | 4.16214200 | 0.80749400 | C | -4.77143900 | 1.60558400 | -0.93447500 |
| H | -0.94449300 | 3.37776700 | 0.63686100 | C | -3.63943000 | 3.88029600 | -1.45463900 |
| N | 0.96765300 | -0.77213700 | 0.82852800 | H | -4.50804700 | 4.39206900 | -1.89493900 |
| N | 0.42370100 | 1.86370300 | 0.84417600 | H | -2.97894100 | 4.64214900 | -1.01308100 |
| B | -1.54077800 | -1.50859400 | -1.04735000 | H | -3.08546400 | 3.37392000 | -2.25855100 |
| O | -1.54661500 | -2.77470900 | -0.44288700 | C | -4.80202600 | 3.60362300 | 0.74982200 |
| O | -2.03451000 | -1.60856600 | -2.33550900 | H | -4.21870800 | 4.47086100 | 1.09531500 |
| C | -2.36585900 | -3.65073300 | -1.24565700 | H | -5.77840600 | 3.96835700 | 0.39427400 |
| C | -2.24501000 | -2.98829100 | -2.66618800 | H | -4.96601000 | 2.94160500 | 1.60963000 |
| C | -3.78625300 | -3.57669700 | -0.67872800 | C | -5.53843600 | 1.83160200 | -2.23275100 |
| H | -4.47780800 | -4.24158200 | -1.21716100 | H | -5.99366400 | 0.88404300 | -2.55689500 |
| H | -3.76024100 | -3.88058400 | 0.37673100 | H | -6.34462700 | 2.56886400 | -2.09160300 |
| H | -4.16638200 | -2.54588500 | -0.71998700 | H | -4.87773300 | 2.17696600 | -3.03809900 |
| C | -1.82552400 | -5.07104800 | -1.14633500 | C | -5.66918300 | 0.91207800 | 0.09295800 |
| H | -1.93567500 | -5.43901300 | -0.11485400 | H | -6.57148900 | 1.50172600 | 0.31481700 |
| H | -2.38303800 | -5.74933400 | -1.81111200 | H | -5.98010500 | -0.06060400 | -0.31587400 |
| H | -0.76178700 | -5.11945800 | -1.41235600 | H | -5.11755200 | 0.71424300 | 1.01929700 |
| C | -3.49198400 | -3.10152700 | -3.53504700 | B | -1.84606300 | -0.34929700 | 1.55100500 |
| H | -3.30965500 | -2.61541400 | -4.50508200 | O | -3.18281900 | -0.68385500 | 1.72433400 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -1.20076000 | -0.34141100 | 2.78394700 | H | 4.15855500 | -2.74602400 | -3.77163700 |
| C | -3.39019900 | -1.09667900 | 3.09090700 | O | 3.59006700 | -0.83874700 | -3.45493500 |
| C | -2.19394100 | -0.39470100 | 3.82455500 | C | 2.65696900 | 0.05916300 | -3.01272300 |
| C | -3.29604100 | -2.62439800 | 3.12151800 | C | 1.49270600 | -0.29452000 | -2.31108600 |
| H | -3.47783200 | -3.02680400 | 4.12927400 | C | 2.93320300 | 1.39993100 | -3.29780700 |
| H | -4.05385200 | -3.03737600 | 2.44101700 | C | 0.61936400 | 0.69946300 | -1.84828300 |
| H | -2.31063600 | -2.96286700 | 2.77105100 | H | 1.27986200 | -1.33662100 | -2.08281100 |
| C | -4.77365100 | -0.64906200 | 3.54661800 | C | 2.02894100 | 2.38631500 | -2.89321100 |
| H | -5.54447900 | -1.17008200 | 2.95958700 | H | 3.83660400 | 1.66957400 | -3.84457500 |
| H | -4.93117000 | -0.89043800 | 4.60980600 | C | 0.87183800 | 2.03864700 | -2.18322100 |
| H | -4.91731500 | 0.42996000 | 3.40890200 | H | -1.04782200 | 0.63091300 | -1.70524300 |
| C | -2.50523300 | 1.05446500 | 4.21443400 | H | 0.17743200 | 2.80987000 | -1.85393400 |
| H | -3.21264800 | 1.11499500 | 5.05526700 | O | 2.36450300 | 3.67369200 | -3.21331700 |
| H | -1.56746600 | 1.54710800 | 4.51082300 | C | 1.41056100 | 4.68695300 | -2.99984000 |
| H | -2.91787000 | 1.60726500 | 3.35752200 | H | 1.84691700 | 5.61756400 | -3.38826500 |
| C | -1.62552200 | -1.15729700 | 5.01400200 | H | 0.46757100 | 4.47849700 | -3.53588600 |
| H | -0.79005900 | -0.58966200 | 5.45096300 | H | 1.18011700 | 4.81925700 | -1.92839100 |
| H | -2.38916000 | -1.29872700 | 5.79521100 | H | 0.76801900 | 5.19911000 | 0.72001300 |
| H | -1.24273600 | -2.14079300 | 4.71192600 | C | 3.58361200 | 4.83586100 | 0.80154000 |
| S | 3.90802700 | -4.21394200 | -1.18617600 | C | 4.48202800 | 4.44442000 | -0.39343600 |
| C | 2.14828100 | -4.65738000 | -1.36074200 | H | 5.28775400 | 5.18553400 | -0.51693400 |
| H | 1.85350300 | -4.76619600 | -2.41358600 | H | 4.95382200 | 3.46201600 | -0.24296400 |
| H | 2.01093600 | -5.62443800 | -0.85691400 | H | 3.90661100 | 4.39183500 | -1.32978600 |
| H | 1.50385900 | -3.91187500 | -0.87525700 | C | 4.40654500 | 4.81064200 | 2.10621200 |
| C | 3.86674900 | -2.45138300 | -1.65279000 | H | 5.24188800 | 5.52587100 | 2.04255300 |
| H | 3.20832700 | -1.90705000 | -0.96151600 | H | 3.78400600 | 5.08599900 | 2.97191600 |
| H | 4.89035100 | -2.08188200 | -1.49000500 | H | 4.83356000 | 3.81517200 | 2.30010900 |
| C | 3.47101800 | -2.20352500 | -3.10679900 | C | 3.06207000 | 6.26274100 | 0.57611200 |
| H | 2.45155700 | -2.57280100 | -3.31023300 | H | 2.48769100 | 6.34116800 | -0.35935700 |

| | | | |
|---|---|---|---|
| H | 2.42234700 | 6.60249700 | 1.40522500 |
| H | 3.91026500 | 6.96008600 | 0.50358800 |
| C | 4.57410100 | -2.35446500 | 2.66202200 |
| C | 4.75842100 | -1.70478800 | 4.04940000 |
| H | 5.67371900 | -2.08804400 | 4.52751200 |
| H | 4.84975000 | -0.61010200 | 3.98352800 |
| H | 3.90578400 | -1.93341800 | 4.70751100 |
| C | 5.76802500 | -1.99219000 | 1.75339300 |
| H | 6.70849100 | -2.34473800 | 2.20554400 |
| H | 5.66219100 | -2.46977900 | 0.76865600 |
| H | 5.85430900 | -0.90565000 | 1.60138100 |
| C | 4.53630400 | -3.88101200 | 2.82827800 |
| H | 3.71765800 | -4.19769700 | 3.49302800 |
| H | 4.41759400 | -4.38330800 | 1.85689200 |
| H | 5.48015800 | -4.22738400 | 3.27617900 |

**INT2-L1-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | -0.70898700 | -0.32641500 | -0.68455900 |
| C | 0.80233900 | 2.31072400 | -0.13716400 |
| C | 2.29906900 | 0.57059500 | 0.09357900 |
| C | 1.84477700 | 3.24711900 | -0.10481600 |
| C | -0.62411500 | 2.69119800 | -0.23177200 |
| C | 3.38003900 | 1.44143600 | 0.13977500 |
| H | 2.42892400 | -0.50279200 | 0.20667600 |
| C | 3.17244200 | 2.82278200 | 0.01360300 |
| H | 1.61289300 | 4.30486800 | -0.19846100 |
| C | -1.07099300 | 4.00080300 | -0.04100400 |
| C | -2.81412200 | 1.96888900 | -0.53463900 |
| C | -2.43368600 | 4.31868700 | -0.08851100 |
| H | -0.33911000 | 4.77587400 | 0.17738600 |
| C | -3.30863600 | 3.25764800 | -0.35558700 |
| H | -3.46832200 | 1.11980100 | -0.73773600 |
| N | 1.04323600 | 0.99076500 | -0.07276200 |
| N | -1.50466300 | 1.68597600 | -0.46509600 |
| B | -0.19615500 | -1.95550500 | 0.52253700 |
| O | 1.13995400 | -2.22330500 | 0.85697400 |
| O | -1.00875400 | -2.96803300 | 1.01709400 |
| C | 1.17266500 | -3.33413400 | 1.78009100 |
| C | -0.17849500 | -4.06149300 | 1.44491000 |
| C | 1.21608700 | -2.74156700 | 3.19098300 |
| H | 1.28753100 | -3.52313400 | 3.96225700 |
| H | 2.10321600 | -2.09557300 | 3.26492600 |
| H | 0.33383900 | -2.11674800 | 3.38316600 |
| C | 2.41642800 | -4.17782400 | 1.53041700 |
| H | 3.31891100 | -3.61711900 | 1.80887700 |
| H | 2.38166300 | -5.09557300 | 2.13871900 |
| H | 2.50245100 | -4.46841500 | 0.47526300 |
| C | -0.84074400 | -4.75734700 | 2.62613700 |
| H | -1.79582400 | -5.20029300 | 2.30661900 |
| H | -0.19957400 | -5.56433700 | 3.01388600 |
| H | -1.05023300 | -4.05520000 | 3.44279700 |
| C | -0.06367600 | -5.02235000 | 0.25704200 |
| H | 0.49318700 | -5.93497300 | 0.51614500 |
| H | -1.07588700 | -5.30422500 | -0.06558600 |
| H | 0.42943000 | -4.53570800 | -0.59662500 |
| B | -2.35200200 | -1.31684800 | -1.35148100 |
| O | -3.60038900 | -0.72839500 | -1.55226700 |
| O | -2.41581800 | -2.66386000 | -1.68265200 |
| C | -4.49496300 | -1.69752500 | -2.13263000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.80021700 | -3.04876400 | -1.73159600 | H | -4.41808900 | 1.43729100 | 2.45922800 |
| C | -4.50828800 | -1.45755000 | -3.64428200 | C | -1.97875900 | 2.03976800 | 3.24596200 |
| H | -5.22743400 | -2.11314000 | -4.15825100 | H | -2.66178100 | 2.47152900 | 3.99281500 |
| H | -4.79211600 | -0.41195000 | -3.83573500 | H | -0.98506800 | 2.49209200 | 3.37832700 |
| H | -3.50992500 | -1.62151800 | -4.07476000 | H | -2.34122700 | 2.31010500 | 2.24529400 |
| C | -5.88636500 | -1.49161000 | -1.54679400 | C | -1.37241100 | 0.17629700 | 4.80457800 |
| H | -6.29496100 | -0.52702900 | -1.88567400 | H | -0.45913300 | 0.74594400 | 5.03273100 |
| H | -6.57419600 | -2.28657000 | -1.87564200 | H | -2.13619800 | 0.43627100 | 5.55420800 |
| H | -5.85511000 | -1.48088800 | -0.44982000 | H | -1.13662500 | -0.89087200 | 4.90112100 |
| C | -3.96879400 | -4.18250700 | -2.73424200 | S | 1.38524900 | 0.24670500 | -3.37304600 |
| H | -3.44303400 | -5.07747400 | -2.36876900 | C | -0.34172400 | 0.29216100 | -2.75575300 |
| H | -5.03214000 | -4.43957100 | -2.86349800 | H | -0.60875400 | 1.35808500 | -2.85044000 |
| H | -3.54693400 | -3.92064300 | -3.71324500 | H | -0.96360400 | -0.24214300 | -3.49153300 |
| C | -4.18675800 | -3.51437600 | -0.32276000 | H | -0.05761100 | -1.72076700 | -1.13444100 |
| H | -5.22184300 | -3.88657100 | -0.28274400 | C | 1.67584600 | -1.55822200 | -3.48804400 |
| H | -3.50745300 | -4.32439000 | -0.02260500 | H | 0.70727000 | -2.07118700 | -3.39665400 |
| H | -4.06130400 | -2.69792700 | 0.40228800 | H | 2.08486100 | -1.77383900 | -4.48705600 |
| B | -1.49888300 | -0.36802200 | 1.30553100 | C | 2.62887900 | -2.07278500 | -2.42724800 |
| O | -2.86041200 | -0.46810800 | 1.52462200 | H | 2.75434500 | -3.17053800 | -2.50470800 |
| O | -0.85795000 | 0.08660600 | 2.44703200 | H | 2.23430600 | -1.84764500 | -1.42796600 |
| C | -3.13363600 | -0.26091100 | 2.92332700 | O | 3.88995900 | -1.44171300 | -2.63833200 |
| C | -1.85112300 | 0.52056200 | 3.39980100 | C | 4.74313900 | -1.25032900 | -1.61510400 |
| C | -3.26995000 | -1.64418300 | 3.56274700 | C | 5.84690900 | -0.40937200 | -1.86891200 |
| H | -3.52494400 | -1.58161300 | 4.63115700 | C | 4.58039000 | -1.81805800 | -0.34907900 |
| H | -4.06716000 | -2.19637500 | 3.04430200 | C | 6.74126600 | -0.13031800 | -0.84465600 |
| H | -2.34304700 | -2.21972000 | 3.44407200 | H | 5.95562300 | 0.01958700 | -2.86549500 |
| C | -4.43969600 | 0.51394900 | 3.05250100 | C | 5.48251200 | -1.50690900 | 0.68114200 |
| H | -5.27135300 | -0.10433600 | 2.68289300 | H | 3.74235100 | -2.46888500 | -0.11821000 |
| H | -4.64455000 | 0.77183100 | 4.10345300 | C | 6.57205900 | -0.65806500 | 0.44579400 |

| | | | |
|---|---|---|---|
| H | 7.59140800 | 0.52818700 | -1.03958600 |
| H | 7.28417500 | -0.41134900 | 1.23135800 |
| O | 5.20450400 | -2.07369800 | 1.88730100 |
| C | 6.03166100 | -1.78054600 | 2.98830400 |
| H | 5.61351600 | -2.32258100 | 3.84682700 |
| H | 7.07094900 | -2.11617800 | 2.82227400 |
| H | 6.04049000 | -0.69941100 | 3.21554800 |
| H | -4.38498900 | 3.40556300 | -0.41905100 |
| H | 4.37929400 | 1.02373300 | 0.24750500 |
| C | 4.36625500 | 3.77989500 | -0.03455900 |
| C | 5.29351500 | 3.51420800 | 1.16927800 |
| H | 6.15409600 | 4.20131400 | 1.14147700 |
| H | 4.76107300 | 3.67002000 | 2.12086800 |
| H | 5.68715500 | 2.48741700 | 1.16227600 |
| C | 5.13543700 | 3.51019400 | -1.34662000 |
| H | 5.48916500 | 2.47049100 | -1.39513400 |
| H | 4.49066400 | 3.68487700 | -2.22166400 |
| H | 6.00952800 | 4.17749100 | -1.42044700 |
| C | 3.92997000 | 5.25202400 | -0.00448500 |
| H | 3.35302300 | 5.48760900 | 0.90383900 |
| H | 4.81711700 | 5.90330900 | -0.01566200 |
| H | 3.31887500 | 5.51646300 | -0.88108000 |
| C | -2.90015400 | 5.75338000 | 0.17564500 |
| C | -2.22040100 | 6.70597400 | -0.82983700 |
| H | -2.54584400 | 7.74276100 | -0.64987600 |
| H | -1.12392900 | 6.68108200 | -0.74316200 |
| H | -2.48323500 | 6.43857100 | -1.86498200 |
| C | -2.49937200 | 6.14244700 | 1.61516900 |
| H | -2.83311500 | 7.16800800 | 1.83965100 |
| H | -2.95982400 | 5.46201200 | 2.34827000 |
| H | -1.40933400 | 6.10410100 | 1.76001700 |
| C | -4.42279800 | 5.89640300 | 0.03423700 |
| H | -4.76487200 | 5.63127200 | -0.97785400 |
| H | -4.96149000 | 5.26460000 | 0.75679800 |
| H | -4.71651900 | 6.94008800 | 0.22296300 |

**INT2-L1-sp$^2$**

| | | | |
|---|---|---|---|
| Ir | 0.34297500 | -0.05187600 | -0.04354300 |
| C | -2.60012600 | 0.15914800 | 0.63887100 |
| C | -1.72684200 | -1.82956100 | 1.46219300 |
| C | -3.87442000 | -0.21259200 | 1.07092700 |
| C | -2.33549300 | 1.44578400 | -0.04491600 |
| C | -2.97542600 | -2.24282500 | 1.91944200 |
| H | -0.83510800 | -2.44913700 | 1.57873000 |
| C | -4.10004900 | -1.43499700 | 1.71566300 |
| H | -4.70938800 | 0.45876600 | 0.88269400 |
| C | -3.29702000 | 2.45085500 | -0.17883800 |
| H | -3.04565900 | -3.20869000 | 2.41622600 |
| C | -0.77010000 | 2.75334600 | -1.13635800 |
| C | -2.98883400 | 3.66006600 | -0.81706900 |
| H | -4.29352300 | 2.29813400 | 0.23102100 |
| C | -1.68189700 | 3.79427100 | -1.30217600 |
| H | 0.24948000 | 2.82438500 | -1.51520500 |
| N | -1.54026000 | -0.66550500 | 0.82644300 |
| N | -1.08741400 | 1.61210200 | -0.52497400 |
| B | 1.57825600 | -1.52147300 | 0.63799100 |
| O | 1.13614900 | -2.67923400 | 1.28934300 |
| O | 2.95952700 | -1.49820300 | 0.62466900 |
| C | 2.26071600 | -3.56183900 | 1.47842500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.46564600 | -2.55157900 | 1.45852500 | H | 0.67120800 | 0.27229200 | -5.48402900 |
| C | 2.27128500 | -4.52913400 | 0.29130800 | C | 4.31401500 | -0.12524400 | -3.75263800 |
| H | 3.08526300 | -5.26541100 | 0.36768700 | H | 4.81803500 | -1.07971000 | -3.54004000 |
| H | 1.31456000 | -5.07187100 | 0.27063500 | H | 4.59361800 | 0.19298500 | -4.76928400 |
| H | 2.36335300 | -3.97960700 | -0.65615500 | H | 4.68486400 | 0.61840400 | -3.03568600 |
| C | 2.07986700 | -4.32080000 | 2.78656700 | C | 2.35239000 | -1.49417700 | -4.49356000 |
| H | 1.21211200 | -4.99413200 | 2.71080700 | H | 2.61941700 | -1.36013400 | -5.55239500 |
| H | 2.96672400 | -4.93390300 | 3.01114400 | H | 2.83691700 | -2.40688400 | -4.11839700 |
| H | 1.90675800 | -3.63524000 | 3.62651200 | H | 1.26871700 | -1.64374300 | -4.41246300 |
| C | 4.74605000 | -3.09560100 | 0.83650400 | B | -0.38286000 | -1.35256800 | -1.60465600 |
| H | 5.52521700 | -2.31915500 | 0.86367300 | O | 0.07569200 | -2.58188500 | -2.03821000 |
| H | 5.11599700 | -3.97224400 | 1.39173700 | O | -1.69031100 | -1.15312700 | -2.02019700 |
| H | 4.58901100 | -3.37650500 | -0.21263000 | C | -1.03926400 | -3.34811100 | -2.53964500 |
| C | 3.75789900 | -1.93962700 | 2.83270700 | C | -2.08612800 | -2.22430700 | -2.89590100 |
| H | 4.20485300 | -2.66970300 | 3.52429800 | C | -1.50136800 | -4.25896600 | -1.39879900 |
| H | 4.46453200 | -1.10696700 | 2.70318100 | H | -2.31248400 | -4.93178100 | -1.71466500 |
| H | 2.84442800 | -1.52685900 | 3.28328500 | H | -0.64844400 | -4.86720500 | -1.06691400 |
| B | 1.30733400 | -0.00600200 | -1.90745900 | H | -1.84650300 | -3.67016800 | -0.53836100 |
| O | 0.89512000 | 0.86380300 | -2.91947800 | C | -0.57035500 | -4.19042400 | -3.71954300 |
| O | 2.49292200 | -0.62931900 | -2.26928300 | H | 0.17450900 | -4.92278800 | -3.37447700 |
| C | 1.95936100 | 0.99977400 | -3.88142900 | H | -1.41278600 | -4.74151900 | -4.16615000 |
| C | 2.80505600 | -0.31149800 | -3.63304000 | H | -0.10100300 | -3.57605100 | -4.49741400 |
| C | 2.71950100 | 2.28324400 | -3.53962400 | C | -1.95471600 | -1.70449800 | -4.32933500 |
| H | 3.52973400 | 2.48557100 | -4.25544400 | H | -2.29309000 | -2.44434300 | -5.06989200 |
| H | 2.01812900 | 3.13084400 | -3.56864800 | H | -2.56673700 | -0.79679400 | -4.43304500 |
| H | 3.14876900 | 2.24263200 | -2.52980500 | H | -0.91472400 | -1.42926800 | -4.55139600 |
| C | 1.34557800 | 1.11151700 | -5.27225600 | C | -3.53807000 | -2.58119100 | -2.59472900 |
| H | 0.75982500 | 2.04034600 | -5.34337300 | H | -4.18734000 | -1.73436200 | -2.86326700 |
| H | 2.12843700 | 1.13979400 | -6.04613900 | H | -3.86055300 | -3.45875100 | -3.17660900 |

| | | | |
|---|---|---|---|
| H | -3.68411600 | -2.79032500 | -1.52682900 |
| S | 4.08492800 | 3.06300700 | -0.05590700 |
| C | 4.45358400 | 1.37294900 | 0.50243400 |
| H | 3.80697000 | 1.07912300 | 1.33908000 |
| H | 4.21531200 | 0.69883000 | -0.33150200 |
| H | 5.51579700 | 1.26050900 | 0.77058500 |
| C | 4.58910600 | 4.06705500 | 1.39039200 |
| H | 5.69128300 | 4.06256800 | 1.46113500 |
| H | 4.28025100 | 5.09145700 | 1.13012200 |
| C | 4.03223900 | 3.70455800 | 2.76657700 |
| H | 4.51990200 | 4.37706700 | 3.49671900 |
| H | 4.31575700 | 2.67384500 | 3.03984000 |
| O | 2.63141100 | 3.87615000 | 2.88991600 |
| C | 1.89642200 | 2.70725300 | 2.97897200 |
| C | 1.36939200 | 2.14784100 | 1.81362300 |
| C | 1.73331500 | 2.08192200 | 4.21493900 |
| C | 0.74769700 | 0.89205600 | 1.83154000 |
| H | 1.55304200 | 2.68286700 | 0.88297800 |
| C | 1.05341000 | 0.85498700 | 4.25936800 |
| H | 2.13642200 | 2.51769100 | 5.12981700 |
| C | 0.57937300 | 0.26248000 | 3.07974000 |
| H | 1.72947800 | 0.63510700 | -0.46512300 |
| H | 0.11960100 | -0.72415300 | 3.12414300 |
| O | 0.93112700 | 0.28625800 | 5.49748000 |
| C | 0.29364800 | -0.96007200 | 5.60210500 |
| H | 0.29339100 | -1.22802200 | 6.66798900 |
| H | -0.75083600 | -0.92510200 | 5.24033100 |
| H | 0.82484700 | -1.74808800 | 5.03631000 |
| H | -1.35009100 | 4.69893400 | -1.80824100 |
| C | -4.05448700 | 4.75404700 | -0.94717100 |
| C | -3.51856400 | 5.99205400 | -1.68149900 |
| H | -4.31192200 | 6.75114200 | -1.75652200 |
| H | -2.67147100 | 6.44842000 | -1.14719600 |
| H | -3.19159100 | 5.75013000 | -2.70437400 |
| C | -5.25615500 | 4.19518600 | -1.73805100 |
| H | -4.94925900 | 3.87476500 | -2.74572400 |
| H | -5.71215200 | 3.32985800 | -1.23386100 |
| H | -6.03384600 | 4.96801200 | -1.84492900 |
| C | -4.51287300 | 5.17917600 | 0.46399200 |
| H | -3.66724600 | 5.56835800 | 1.05154600 |
| H | -5.27637400 | 5.97015000 | 0.39351900 |
| H | -4.95203700 | 4.33917000 | 1.02287400 |
| C | -5.51723700 | -1.83510800 | 2.13640000 |
| C | -6.39799400 | -1.92983900 | 0.87184200 |
| H | -7.42315000 | -2.22818200 | 1.14286600 |
| H | -6.45696400 | -0.96751800 | 0.34166200 |
| H | -5.99671800 | -2.67602200 | 0.16853000 |
| C | -5.53967600 | -3.19327100 | 2.85320600 |
| H | -4.92936800 | -3.18104100 | 3.76920700 |
| H | -6.57138500 | -3.44269600 | 3.14376700 |
| H | -5.17258000 | -4.00346100 | 2.20486900 |
| C | -6.08769700 | -0.76499900 | 3.09041700 |
| H | -7.10785300 | -1.03933800 | 3.40216000 |
| H | -5.46586400 | -0.67139400 | 3.99409400 |
| H | -6.13980300 | 0.22511700 | 2.61355300 |

**TS2-L1-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | -1.09672000 | -0.32455100 | 0.01034800 |
| C | 1.01322900 | 1.88840500 | 0.22714100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.82853300 | -0.02982300 | 1.24228300 | H | -4.10904300 | 2.88231900 | 3.71490000 |
| C | 2.19604800 | 2.57131900 | 0.52998300 | H | -3.27897200 | 2.52716100 | 5.25191000 |
| C | -0.15009400 | 2.51246700 | -0.44275000 | H | -2.36467200 | 3.18413700 | 3.86331500 |
| C | 3.02370500 | 0.59710100 | 1.57979000 | C | -4.15428100 | 0.21154300 | 3.88167300 |
| H | 1.65058600 | -1.07724800 | 1.48389800 | H | -4.45029600 | 0.17474300 | 4.94090000 |
| C | 3.25169900 | 1.92117700 | 1.18501100 | H | -4.98847900 | 0.63058600 | 3.30101400 |
| H | 2.30757800 | 3.61066900 | 0.22656600 | H | -3.97674300 | -0.81173500 | 3.52160300 |
| C | -0.13916400 | 3.83002900 | -0.90502300 | B | -0.36854400 | -2.11895500 | -0.73857800 |
| C | -2.34839500 | 2.26209600 | -1.15809600 | O | -1.11442400 | -3.23947000 | -1.10521500 |
| C | -1.25922800 | 4.39076700 | -1.52772600 | O | 0.99169200 | -2.46987200 | -0.64401200 |
| H | 0.76916200 | 4.41871300 | -0.79442200 | C | -0.21972100 | -4.32313800 | -1.40685500 |
| C | -2.38550000 | 3.56443700 | -1.64554500 | C | 1.07455200 | -3.91157300 | -0.61346900 |
| H | -3.19972800 | 1.58675900 | -1.25811100 | C | 0.00002200 | -4.35494700 | -2.92292900 |
| N | 0.86492900 | 0.58803000 | 0.55784200 | H | 0.59196800 | -5.22955300 | -3.23095800 |
| N | -1.26209900 | 1.74396300 | -0.56894800 | H | -0.97929200 | -4.40442100 | -3.42138700 |
| B | -1.72915200 | 0.14319100 | 1.93496100 | H | 0.51515100 | -3.45005500 | -3.27491500 |
| O | -1.19260100 | -0.39538000 | 3.09522400 | C | -0.86372200 | -5.62494300 | -0.94493100 |
| O | -2.66485600 | 1.12035100 | 2.24302700 | H | -1.75312100 | -5.83521000 | -1.55802100 |
| C | -1.59933000 | 0.42204800 | 4.20886100 | H | -0.16615700 | -6.47056700 | -1.05242400 |
| C | -2.91611200 | 1.08479500 | 3.66374600 | H | -1.18564800 | -5.55887000 | 0.10198400 |
| C | -0.47588100 | 1.43725100 | 4.44892700 | C | 2.38506800 | -4.35862900 | -1.24909200 |
| H | -0.66398500 | 2.06188600 | 5.33519500 | H | 3.22772000 | -4.05641700 | -0.61294400 |
| H | 0.46641400 | 0.89007400 | 4.59990400 | H | 2.40799000 | -5.45496000 | -1.35227700 |
| H | -0.34687100 | 2.09351700 | 3.57561800 | H | 2.52978000 | -3.91177100 | -2.24104400 |
| C | -1.78245400 | -0.46234400 | 5.43556900 | C | 1.03543600 | -4.33382200 | 0.85875300 |
| H | -0.81109700 | -0.88339800 | 5.73616000 | H | 1.16358200 | -5.42027000 | 0.97690900 |
| H | -2.18240300 | 0.11639900 | 6.28327700 | H | 1.85829400 | -3.82421800 | 1.37906000 |
| H | -2.46114900 | -1.29889100 | 5.22637800 | H | 0.08844400 | -4.03771600 | 1.33260400 |
| C | -3.17461700 | 2.50323400 | 4.15553000 | B | -3.00073200 | -0.96714100 | -0.31731800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -3.71783500 | -1.88401800 | 0.43544500 | H | 3.02583000 | 0.79631200 | -1.32654400 |
| O | -3.77844700 | -0.53366100 | -1.39838800 | H | 3.23228500 | 1.46039000 | -2.95903900 |
| C | -5.05680500 | -1.98265400 | -0.07979600 | O | 4.56812100 | 0.02896100 | -2.48536400 |
| C | -4.88742900 | -1.44337100 | -1.54693100 | C | 5.10388500 | -0.68379400 | -1.46332300 |
| C | -5.94791400 | -1.08613100 | 0.78448100 | C | 6.50949000 | -0.68268900 | -1.37094500 |
| H | -7.00556800 | -1.14641700 | 0.48635600 | C | 4.34289700 | -1.37901300 | -0.52191600 |
| H | -5.86358600 | -1.40838700 | 1.83196900 | C | 7.12588500 | -1.35773400 | -0.32524900 |
| H | -5.61978800 | -0.03802100 | 0.72929700 | H | 7.08178100 | -0.13635600 | -2.12173200 |
| C | -5.51358300 | -3.43350400 | 0.01744800 | C | 4.98391100 | -2.03585700 | 0.54008900 |
| H | -5.60228300 | -3.72169400 | 1.07577600 | H | 3.25885100 | -1.43878600 | -0.57675200 |
| H | -6.49684800 | -3.57226600 | -0.45973100 | C | 6.37875600 | -2.03391600 | 0.65097100 |
| H | -4.78926900 | -4.10881700 | -0.45521700 | H | 8.21607300 | -1.35197000 | -0.24991500 |
| C | -4.43690200 | -2.52991800 | -2.52979000 | H | 6.88705600 | -2.54126200 | 1.46919900 |
| H | -5.24057300 | -3.25083400 | -2.74278000 | O | 4.14868500 | -2.64272100 | 1.43274000 |
| H | -4.14249100 | -2.04886200 | -3.47459600 | C | 4.70406400 | -3.36571900 | 2.50776100 |
| H | -3.56056100 | -3.06619700 | -2.13748600 | H | 3.85999400 | -3.78960700 | 3.06756400 |
| C | -6.08566800 | -0.68440900 | -2.10087500 | H | 5.35176000 | -4.18746300 | 2.15516600 |
| H | -5.86349500 | -0.33628800 | -3.12111400 | H | 5.29104900 | -2.71356200 | 3.17880500 |
| H | -6.97404600 | -1.33382200 | -2.14823700 | H | -3.30180900 | 3.91036100 | -2.11990500 |
| H | -6.32597600 | 0.19371800 | -1.48719300 | H | 3.77781700 | 0.01551700 | 2.10219600 |
| S | 0.58253700 | 0.51674600 | -2.97740100 | C | 4.59595900 | 2.62764600 | 1.38602300 |
| C | -0.62742700 | -0.65247000 | -2.27448200 | C | 5.61576900 | 1.71926700 | 2.09034200 |
| H | -1.60633800 | -0.26514700 | -2.58578800 | H | 6.56867100 | 2.25719100 | 2.20899700 |
| H | -0.52885700 | -1.59542000 | -2.82626600 | H | 5.27372000 | 1.42421100 | 3.09451100 |
| H | -0.96758900 | -1.69685400 | 0.81333100 | H | 5.81808200 | 0.80727000 | 1.50927200 |
| C | 2.16223900 | -0.41120100 | -2.89902100 | C | 5.16103300 | 3.00236400 | -0.00231900 |
| H | 2.01079200 | -1.27206600 | -2.23737900 | H | 4.49210800 | 3.68727700 | -0.54509700 |
| H | 2.43964600 | -0.77350400 | -3.90152500 | H | 6.13578200 | 3.50339500 | 0.10896400 |
| C | 3.23660500 | 0.52963300 | -2.37069800 | H | 5.30714800 | 2.10663100 | -0.62405300 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.38905700 | 3.90150700 | 2.22938300 | C | 1.28642200 | 1.88919800 | -2.35982900 |
| H | 3.98052200 | 3.65446200 | 3.22172900 | C | 3.55025100 | 2.39953300 | -1.68598400 |
| H | 5.34844800 | 4.42336100 | 2.37328500 | H | 3.91549500 | 1.95489500 | 0.39450600 |
| H | 3.69567300 | 4.60598200 | 1.74519800 | C | 2.55441200 | 2.37376500 | -2.67137400 |
| C | -1.20706700 | 5.82791000 | -2.05603700 | H | 0.49009300 | 1.83878400 | -3.10319200 |
| C | -0.09953600 | 5.92303400 | -3.12731300 | N | 0.25327600 | 0.34278300 | 1.18440600 |
| H | -0.04932200 | 6.94602600 | -3.53300300 | N | 0.97448400 | 1.43057500 | -1.14675400 |
| H | 0.89036700 | 5.67648500 | -2.71505600 | B | -1.25258000 | -1.79118600 | -0.49923500 |
| H | -0.29771600 | 5.23052400 | -3.95973000 | O | -0.76957800 | -2.46576800 | 0.62376500 |
| C | -2.53970700 | 6.25551000 | -2.68868100 | O | -2.17613500 | -2.58653100 | -1.17431100 |
| H | -3.36682800 | 6.21618700 | -1.96337800 | C | -1.38406700 | -3.75806100 | 0.71954600 |
| H | -2.46283200 | 7.29205000 | -3.05052500 | C | -2.01839700 | -3.94336900 | -0.71936000 |
| H | -2.80475100 | 5.62229600 | -3.54898500 | C | -2.42143100 | -3.69038500 | 1.84082700 |
| C | -0.88652100 | 6.78573700 | -0.88938000 | H | -2.91693700 | -4.65905800 | 2.00587200 |
| H | -0.84433000 | 7.82518500 | -1.25163200 | H | -1.91134300 | -3.40058500 | 2.77220300 |
| H | -1.65909400 | 6.72570700 | -0.10718500 | H | -3.17074800 | -2.92336400 | 1.62397700 |
| H | 0.08327100 | 6.55491500 | -0.42365000 | C | -0.31036700 | -4.78510800 | 1.06951200 |
| **TS2-L1-sp$^2$** | | | | H | 0.06581300 | -4.58783500 | 2.08473800 |
| Ir | -0.86485600 | 0.28335700 | -0.71257000 | H | -0.72229600 | -5.80655500 | 1.04995300 |
| C | 1.47229900 | 0.92597600 | 1.15244800 | H | 0.54532000 | -4.72566000 | 0.38688600 |
| C | -0.20183400 | -0.15401500 | 2.33799300 | C | -3.38148400 | -4.62535600 | -0.72878500 |
| C | 2.27357200 | 0.98468300 | 2.29378000 | H | -3.76062600 | -4.67479800 | -1.76051800 |
| C | 1.89695600 | 1.46730300 | -0.16060400 | H | -3.30882800 | -5.65283000 | -0.33923100 |
| C | 0.55850800 | -0.13578200 | 3.50553600 | H | -4.11391400 | -4.07442100 | -0.12589900 |
| H | -1.20189800 | -0.58622900 | 2.30424900 | C | -1.07623300 | -4.65007000 | -1.70055600 |
| C | 1.84019200 | 0.42583900 | 3.50285500 | H | -0.96757000 | -5.71879400 | -1.46298100 |
| H | 3.25107600 | 1.45990200 | 2.23658400 | H | -1.49284200 | -4.55839900 | -2.71447900 |
| C | 3.18201400 | 1.95478600 | -0.40934700 | H | -0.08152000 | -4.18577800 | -1.70689000 |
| H | 0.13369700 | -0.58187000 | 4.40273700 | B | -1.63450500 | 2.18270800 | -0.24291800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -1.62395300 | 3.20906300 | -1.17215300 | C | -6.19052900 | 1.16484300 | -0.24944800 |
| O | -1.97945300 | 2.67142600 | 1.01057600 | H | -6.44569000 | 1.30797600 | -1.30994000 |
| C | -2.18654600 | 4.38997600 | -0.56662200 | H | -7.10739900 | 0.87854300 | 0.28966000 |
| C | -1.94932600 | 4.11220300 | 0.96140000 | H | -5.83843400 | 2.12599600 | 0.14587300 |
| C | -3.66950800 | 4.42508600 | -0.94446400 | C | -4.68008000 | 1.06411700 | 2.23758500 |
| H | -4.17131400 | 5.32878500 | -0.56691100 | H | -5.71451400 | 1.35223200 | 2.47772900 |
| H | -3.75357800 | 4.40919500 | -2.04071400 | H | -4.15422000 | 0.84370900 | 3.17874400 |
| H | -4.18819500 | 3.53548700 | -0.56212400 | H | -4.16075500 | 1.90584100 | 1.76464600 |
| C | -1.46807500 | 5.61635600 | -1.11511300 | C | -5.31472300 | -1.34433500 | 2.04614800 |
| H | -1.68776200 | 5.72334800 | -2.18793900 | H | -4.87160900 | -1.49564800 | 3.04177300 |
| H | -1.80514700 | 6.53207500 | -0.60392500 | H | -6.38713300 | -1.13113900 | 2.17873300 |
| H | -0.37962100 | 5.52881500 | -1.00166800 | H | -5.21652000 | -2.28066100 | 1.48468900 |
| C | -3.01605200 | 4.67216800 | 1.89298100 | S | 2.81953600 | -2.96524800 | 1.88530000 |
| H | -2.78357900 | 4.39429600 | 2.93202300 | C | 3.37044600 | -4.13229700 | 3.16536600 |
| H | -3.05127100 | 5.77130800 | 1.83055100 | H | 4.05716800 | -3.65773300 | 3.88437600 |
| H | -4.01108000 | 4.27716300 | 1.65354400 | H | 2.47001200 | -4.46449800 | 3.70119700 |
| C | -0.55502100 | 4.53586500 | 1.43650800 | H | 3.85823400 | -5.01082400 | 2.71606300 |
| H | -0.45373000 | 5.62952100 | 1.50218500 | C | 4.44544200 | -2.59780000 | 1.13035300 |
| H | -0.37796200 | 4.10648200 | 2.43372300 | H | 5.07902500 | -2.08813900 | 1.87677200 |
| H | 0.22214400 | 4.14967300 | 0.76045200 | H | 4.93503000 | -3.54550400 | 0.85411100 |
| B | -2.82103300 | 0.05404800 | -0.08370100 | C | 4.35128800 | -1.71651600 | -0.10987600 |
| O | -3.92657200 | 0.52684300 | -0.77921400 | H | 3.73874000 | -0.82199000 | 0.08511500 |
| O | -3.23242300 | -0.48884900 | 1.13623100 | H | 5.37290800 | -1.36838800 | -0.34445700 |
| C | -5.12539400 | 0.08216100 | -0.12375900 | O | 3.89275500 | -2.41130900 | -1.25077500 |
| C | -4.62627000 | -0.17880500 | 1.34552700 | C | 2.65707300 | -2.13761400 | -1.78104400 |
| C | -5.57580700 | -1.19203600 | -0.84477800 | C | 1.57939300 | -1.66084800 | -1.02762500 |
| H | -6.51582600 | -1.59170300 | -0.4352680 | C | 2.50526300 | -2.37847800 | -3.14894800 |
| H | -5.73184600 | -0.95401900 | -1.90713300 | C | 0.35285300 | -1.36063000 | -1.63917200 |
| H | -4.79459700 | -1.96226200 | -0.79257300 | H | 1.66979100 | -1.54847600 | 0.04956200 |

| | | | |
|---|---|---|---|
| C | 1.26727300 | -2.13247300 | -3.75983300 |
| H | 3.33900600 | -2.76173500 | -3.73750600 |
| C | 0.19974300 | -1.61303300 | -3.01325100 |
| H | -1.59519600 | 0.38381700 | -2.11188900 |
| H | -0.76604400 | -1.41566200 | -3.47311500 |
| O | 1.19995600 | -2.41215200 | -5.09210800 |
| C | -0.02324600 | -2.21017200 | -5.75855800 |
| H | 0.13454200 | -2.51072200 | -6.80354600 |
| H | -0.83454400 | -2.82274700 | -5.32601200 |
| H | -0.33869500 | -1.15129500 | -5.73299800 |
| H | 2.74841800 | 2.70644700 | -3.68912400 |
| C | 4.99146500 | 2.84376300 | -1.95486500 |
| C | 5.92656000 | 1.64201300 | -1.69503800 |
| H | 6.97145400 | 1.92011700 | -1.90520000 |
| H | 5.87362700 | 1.30315100 | -0.64944300 |
| H | 5.65907700 | 0.78917100 | -2.33784300 |
| C | 5.18704300 | 3.31266900 | -3.40418500 |
| H | 4.54286900 | 4.17224700 | -3.64508700 |
| H | 6.23106900 | 3.62638600 | -3.55474400 |
| H | 4.97486800 | 2.50878400 | -4.12520100 |
| C | 5.35683300 | 4.00464000 | -1.00693900 |
| H | 6.39399600 | 4.32915500 | -1.18617400 |
| H | 4.69434600 | 4.86897800 | -1.16930000 |
| H | 5.27735900 | 3.71287700 | 0.05102000 |
| C | 2.76177300 | 0.43827100 | 4.72625100 |
| C | 2.14697600 | -0.32125200 | 5.91104000 |
| H | 2.84265800 | -0.30651600 | 6.76383300 |
| H | 1.20317400 | 0.13555400 | 6.24537200 |
| H | 1.94958100 | -1.37371800 | 5.65610600 |
| C | 3.02074800 | 1.89863300 | 5.15031000 |
| H | 3.48931900 | 2.48011700 | 4.34178700 |
| H | 2.08003500 | 2.40103800 | 5.42420700 |
| H | 3.69423300 | 1.93069000 | 6.02175900 |
| C | 4.09514600 | -0.24385800 | 4.35115400 |
| H | 3.90951800 | -1.25936500 | 3.97214500 |
| H | 4.63354300 | 0.31199000 | 3.56857800 |
| H | 4.75503000 | -0.30263300 | 5.23108600 |

**INT3-L1-sp$^3$**

| | | | |
|---|---|---|---|
| Ir | 0.01023800 | 0.18027100 | -0.24632400 |
| C | -2.91059800 | -0.73246700 | -0.55122000 |
| C | -1.53731000 | -2.59530400 | -0.38597200 |
| C | -4.04174200 | -1.54728000 | -0.62358100 |
| C | -2.95217800 | 0.74446000 | -0.69401500 |
| C | -2.62660700 | -3.46255000 | -0.46296400 |
| H | -0.51484200 | -2.96207300 | -0.30223600 |
| C | -3.92420300 | -2.94562700 | -0.55806100 |
| H | -5.02317600 | -1.09154900 | -0.74447200 |
| C | -4.14219800 | 1.47402900 | -0.71133600 |
| H | -2.43751000 | -4.53311100 | -0.42006200 |
| C | -1.72484000 | 2.67924900 | -1.05906000 |
| C | -4.13579100 | 2.86169500 | -0.91287700 |
| H | -5.08531300 | 0.95339000 | -0.55286900 |
| C | -2.88203300 | 3.45569200 | -1.10822000 |
| H | -0.72704500 | 3.11497600 | -1.15685000 |
| N | -1.67915600 | -1.26798300 | -0.39448800 |
| N | -1.75223400 | 1.35880400 | -0.84083000 |
| B | 0.86313700 | -0.56366900 | -1.87615900 |
| O | 1.25157700 | -1.89980800 | -1.96541600 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | 1.07925600 | 0.08073500 | -3.08931800 | H | -1.39108800 | 3.34760100 | 1.60520600 |
| C | 1.56082300 | -2.20986700 | -3.33427200 | H | -0.13709900 | 3.75798800 | 2.79837600 |
| C | 1.85024500 | -0.78456500 | -3.94538100 | H | 0.23100400 | 2.65716800 | 1.44245200 |
| C | 0.31941500 | -2.87789500 | -3.93463500 | C | 0.23374100 | 1.78180200 | 5.34475200 |
| H | 0.48859300 | -3.21286300 | -4.96913700 | H | 1.04856600 | 1.29617500 | 5.90143500 |
| H | 0.06095000 | -3.75543200 | -3.32328200 | H | 0.45439800 | 2.85894200 | 5.28884300 |
| H | -0.54069100 | -2.19232700 | -3.92210800 | H | -0.69664000 | 1.63931500 | 5.90985300 |
| C | 2.74648700 | -3.16816200 | -3.35724400 | C | 1.51825000 | 1.16602400 | 3.27890900 |
| H | 2.44340000 | -4.13892400 | -2.93565400 | H | 1.96560800 | 2.16960000 | 3.27334600 |
| H | 3.09916100 | -3.33961600 | -4.38678600 | H | 2.18022400 | 0.48807500 | 3.83445500 |
| H | 3.57181800 | -2.78072400 | -2.74686500 | H | 1.46370100 | 0.80602400 | 2.24160300 |
| C | 1.38052800 | -0.59735400 | -5.38331600 | B | 1.52187800 | 1.52617000 | -0.41999800 |
| H | 1.61474000 | 0.42504900 | -5.71612000 | O | 2.88672300 | 1.24110500 | -0.46884500 |
| H | 1.89059100 | -1.30240700 | -6.05879900 | O | 1.35385300 | 2.91571600 | -0.60423600 |
| H | 0.29630800 | -0.74075600 | -5.47668000 | C | 3.64379300 | 2.45838500 | -0.49762300 |
| C | 3.31570000 | -0.36768400 | -3.80774200 | C | 2.59578500 | 3.48414000 | -1.05991700 |
| H | 3.97153700 | -0.96705900 | -4.45730600 | C | 4.87895600 | 2.26323400 | -1.36915400 |
| H | 3.41242900 | 0.68635200 | -4.10665300 | H | 5.41854400 | 3.21390800 | -1.50577000 |
| H | 3.64847200 | -0.46448000 | -2.76659700 | H | 5.55721200 | 1.55240900 | -0.87660800 |
| B | -1.10637600 | -0.47724200 | 3.00615300 | H | 4.61518200 | 1.85885600 | -2.35341300 |
| O | -1.35807700 | 0.63482000 | 2.22483200 | C | 4.07458600 | 2.76024500 | 0.94181400 |
| O | -0.30124200 | -0.19537400 | 4.06898200 | H | 4.58802300 | 1.87495300 | 1.34425900 |
| C | -0.97925300 | 1.79298900 | 3.04247100 | H | 4.75687100 | 3.62248400 | 0.99596200 |
| C | 0.14618000 | 1.18299700 | 3.94813400 | H | 3.20256200 | 2.96350200 | 1.57797700 |
| C | -2.23816600 | 2.18043200 | 3.82406000 | C | 2.72681200 | 4.90098800 | -0.51527300 |
| H | -2.07698100 | 3.09310500 | 4.41566000 | H | 3.70682500 | 5.33234500 | -0.77405500 |
| H | -3.05066500 | 2.36992500 | 3.10721600 | H | 1.94673500 | 5.54246700 | -0.95348000 |
| H | -2.55957400 | 1.37765000 | 4.50420800 | H | 2.61108400 | 4.92526700 | 0.57608800 |
| C | -0.53509400 | 2.94810700 | 2.16718000 | C | 2.54247200 | 3.50134500 | -2.59117700 |

| | | | |
|---|---|---|---|
| H | 1.67630500 | 4.10121400 | -2.90965600 |
| H | 3.44852200 | 3.94395500 | -3.03199300 |
| H | 2.40409300 | 2.48402900 | -2.98238800 |
| S | -0.90753900 | -3.43712700 | 2.83242700 |
| C | -1.85121600 | -1.85712200 | 2.87026400 |
| H | -2.49103500 | -1.86201200 | 1.98012300 |
| H | -2.52276600 | -1.89807600 | 3.74722600 |
| H | 1.15152500 | -0.70622600 | 0.37644700 |
| C | 0.73331100 | -3.01654300 | 3.52515900 |
| H | 0.62246900 | -2.24709700 | 4.29847200 |
| H | 1.10187100 | -3.93592100 | 4.00456800 |
| C | 1.68528100 | -2.54229300 | 2.44075700 |
| H | 1.21069100 | -1.77771900 | 1.80582500 |
| H | 1.96092700 | -3.38432000 | 1.78073200 |
| O | 2.83931300 | -2.00081300 | 3.06723300 |
| C | 3.87756600 | -1.58587000 | 2.29705700 |
| C | 4.96293400 | -1.01893500 | 2.99483200 |
| C | 3.91876900 | -1.70244600 | 0.90553500 |
| C | 6.08255900 | -0.59973400 | 2.29043100 |
| H | 4.89933700 | -0.93498700 | 4.08062800 |
| C | 5.07330700 | -1.29706700 | 0.21596800 |
| H | 3.08283600 | -2.07869900 | 0.31886000 |
| C | 6.16128500 | -0.73963100 | 0.89720800 |
| H | 6.92551300 | -0.16042700 | 2.82999700 |
| H | 7.05649300 | -0.41491500 | 0.36956100 |
| O | 5.05386600 | -1.49304800 | -1.13279000 |
| C | 6.23723400 | -1.29274800 | -1.86801900 |
| H | 6.01717200 | -1.59180700 | -2.90119900 |
| H | 6.55110700 | -0.23486700 | -1.86678800 |
| H | 7.06588600 | -1.91124700 | -1.47941300 |
| H | -2.77829000 | 4.52524200 | -1.28291900 |
| C | -5.45084800 | 3.64801700 | -0.89558200 |
| C | -6.10662900 | 3.48673800 | 0.49270100 |
| H | -7.05236200 | 4.05006800 | 0.53614600 |
| H | -6.33241300 | 2.43376800 | 0.71869600 |
| H | -5.44406300 | 3.86645000 | 1.28613100 |
| C | -5.22878900 | 5.14431100 | -1.16172800 |
| H | -4.77017300 | 5.31953700 | -2.14688800 |
| H | -6.19460100 | 5.67181700 | -1.14508300 |
| H | -4.58593300 | 5.60431100 | -0.39582500 |
| C | -6.39308700 | 3.09031900 | -1.98296900 |
| H | -7.34446800 | 3.64558100 | -1.98356300 |
| H | -5.93997300 | 3.18473500 | -2.98195000 |
| H | -6.62717400 | 2.02791700 | -1.81814500 |
| C | -5.17910500 | -3.82424700 | -0.59273800 |
| C | -4.83436400 | -5.31916100 | -0.51754300 |
| H | -4.29886900 | -5.56776600 | 0.41128600 |
| H | -5.75972900 | -5.91463200 | -0.53854300 |
| H | -4.21404000 | -5.63805800 | -1.36903300 |
| C | -6.06834900 | -3.46414100 | 0.61669100 |
| H | -5.53034700 | -3.63272000 | 1.56246800 |
| H | -6.38527500 | -2.41056900 | 0.59226400 |
| H | -6.97631000 | -4.08794500 | 0.62181400 |
| C | -5.95058000 | -3.56158300 | -1.90293800 |
| H | -6.26777800 | -2.51155200 | -1.99045100 |
| H | -5.32885600 | -3.80022600 | -2.77971600 |
| H | -6.85569200 | -4.18814100 | -1.94317800 |

**INT3-L1-sp$^2$**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ir | 0.37679300 | -0.73555400 | -0.16035700 | H | 3.42400700 | 6.04742300 | -1.39887300 |
| C | -1.55723300 | 1.20333600 | 1.18478800 | H | 1.80675700 | 5.87176800 | -2.13869900 |
| C | 0.63135600 | 1.79578600 | 1.67198000 | C | 4.67686900 | 3.04344500 | -2.29502400 |
| C | -2.02884100 | 2.32572000 | 1.86910400 | H | 5.02302200 | 2.52648000 | -3.20210400 |
| C | -2.45733600 | 0.20571900 | 0.55661500 | H | 5.26085700 | 3.96988900 | -2.18200400 |
| C | 0.21769300 | 2.93237800 | 2.36197000 | H | 4.87428000 | 2.39435300 | -1.43651600 |
| H | 1.68450200 | 1.53190600 | 1.56632500 | C | 2.91339900 | 4.08682900 | -3.73102200 |
| C | -1.14499000 | 3.23743400 | 2.46060500 | H | 3.49385800 | 5.01780400 | -3.80933600 |
| H | -3.10207200 | 2.49507900 | 1.93380200 | H | 3.19250000 | 3.43024400 | -4.56776600 |
| C | -3.85010000 | 0.29024600 | 0.60490000 | H | 1.84542900 | 4.32917800 | -3.83312400 |
| H | 0.97915300 | 3.57258000 | 2.80331800 | B | 0.56335100 | -2.01031900 | 1.36464700 |
| C | -2.58879200 | -1.78668900 | -0.62250200 | O | 1.07091600 | -1.69816300 | 2.62768300 |
| C | -4.65154500 | -0.68752100 | 0.00036800 | O | 0.11820500 | -3.32910300 | 1.34952500 |
| H | -4.31839900 | 1.13722500 | 1.10237200 | C | 0.73951400 | -2.76777500 | 3.53112100 |
| C | -3.98212600 | -1.75747600 | -0.60546400 | C | 0.57678300 | -3.98080700 | 2.54636200 |
| H | -2.04721900 | -2.59316100 | -1.12336600 | C | -0.57345300 | -2.38164300 | 4.22073400 |
| N | -0.22789000 | 0.96203100 | 1.07446800 | H | -0.87060400 | -3.11395800 | 4.98653100 |
| N | -1.84674300 | -0.82140800 | -0.07360500 | H | -0.44095700 | -1.40294800 | 4.70536700 |
| B | 1.24824800 | 2.33367800 | -1.85326900 | H | -1.38711900 | -2.28866000 | 3.48650700 |
| O | 1.22458600 | 3.50060000 | -1.13385600 | C | 1.84995600 | -2.91976000 | 4.56307700 |
| O | 2.45155600 | 2.11109100 | -2.47022300 | H | 1.90885800 | -2.01081600 | 5.18069300 |
| C | 2.55772700 | 4.06898800 | -1.16196100 | H | 1.65105000 | -3.77475400 | 5.22853800 |
| C | 3.19343700 | 3.35247800 | -2.41619300 | H | 2.82763600 | -3.06700300 | 4.08769800 |
| C | 3.24605400 | 3.69413200 | 0.14937900 | C | -0.45113300 | -5.02124700 | 2.97273700 |
| H | 4.25074000 | 4.13729300 | 0.21489200 | H | -0.49478900 | -5.82815800 | 2.22557000 |
| H | 2.64598200 | 4.08137600 | 0.98538400 | H | -0.18014600 | -5.46922000 | 3.94197100 |
| H | 3.32434600 | 2.60433700 | 0.25549900 | H | -1.45462800 | -4.58373800 | 3.05336100 |
| C | 2.43257500 | 5.58229700 | -1.28485600 | C | 1.91199900 | -4.65369400 | 2.20946800 |
| H | 1.96922600 | 5.98669100 | -0.37238800 | H | 2.32038900 | -5.21580700 | 3.06285300 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.75550600 | -5.35366100 | 1.37593600 | H | 0.55974800 | -4.43722600 | -4.34907200 |
| H | 2.64856500 | -3.90815800 | 1.87835300 | H | -1.07595200 | -3.94823700 | -4.84886500 |
| B | 2.40310100 | -0.71117100 | 0.03619700 | C | 0.04997000 | -2.40381900 | -3.85347700 |
| O | 3.24314500 | -1.80960000 | -0.18499300 | H | 0.61118600 | -2.03969500 | -4.73566100 |
| O | 3.19096800 | 0.33301900 | 0.57992000 | H | 0.68190300 | -2.28313600 | -2.96055600 |
| C | 4.60762700 | -1.44011300 | 0.05199800 | O | -1.14972800 | -1.65537200 | -3.71230100 |
| C | 4.45099900 | -0.21599100 | 1.01847100 | C | -1.12001800 | -0.42244000 | -3.16277300 |
| C | 5.21448600 | -1.05185300 | -1.30180600 | C | 0.06161800 | 0.22218200 | -2.73043400 |
| H | 6.28972600 | -0.82732600 | -1.22819600 | C | -2.35490300 | 0.20734700 | -3.00968300 |
| H | 5.08262600 | -1.89352500 | -1.99770400 | C | -0.02713400 | 1.48590800 | -2.11660000 |
| H | 4.69481900 | -0.17968600 | -1.72472600 | H | 1.04241900 | -0.18670800 | -2.96081400 |
| C | 5.35096900 | -2.63155200 | 0.64402500 | C | -2.44031600 | 1.45192900 | -2.37072900 |
| H | 5.39156100 | -3.44613300 | -0.09477600 | H | -3.26089200 | -0.29373300 | -3.34816900 |
| H | 6.38424600 | -2.36049300 | 0.91360500 | C | -1.28469400 | 2.08911900 | -1.91048000 |
| H | 4.84341800 | -3.01436400 | 1.53872900 | H | 0.67384900 | -2.01750400 | -1.04247100 |
| C | 4.28186800 | -0.62458000 | 2.48524800 | H | -1.32275400 | 3.05860300 | -1.41824700 |
| H | 5.21268300 | -1.03124100 | 2.90871900 | O | -3.69728000 | 1.96022800 | -2.23359600 |
| H | 3.99768500 | 0.26440500 | 3.06860000 | C | -3.84895200 | 3.20876100 | -1.60097600 |
| H | 3.47255400 | -1.35599300 | 2.59621300 | H | -4.92535900 | 3.42435200 | -1.58444800 |
| C | 5.55391400 | 0.82862200 | 0.90581300 | H | -3.46751500 | 3.19141400 | -0.56515100 |
| H | 5.34839900 | 1.67036300 | 1.58402000 | H | -3.32733300 | 4.01230900 | -2.15018800 |
| H | 6.52379600 | 0.39233700 | 1.19243400 | H | -4.51787300 | -2.56960700 | -1.09329300 |
| H | 5.64494400 | 1.22352600 | -0.11185400 | C | -6.17662000 | -0.54311000 | 0.01101300 |
| S | -1.07797400 | -4.65853500 | -2.57984200 | C | -6.86286300 | -1.66921400 | -0.77629500 |
| C | 0.40157300 | -4.90026200 | -1.54600700 | H | -7.95405200 | -1.52712700 | -0.75286300 |
| H | 0.88232400 | -3.94329700 | -1.30036500 | H | -6.54896900 | -1.67609500 | -1.83124300 |
| H | 0.04868200 | -5.33446100 | -0.60192200 | H | -6.64759900 | -2.65933600 | -0.34661700 |
| H | 1.10946500 | -5.58930300 | -2.03210800 | C | -6.67852100 | -0.58154200 | 1.46946500 |
| C | -0.32898600 | -3.86105600 | -4.04482200 | H | -6.23716100 | 0.22568700 | 2.07355500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -7.77364300 | -0.46411700 | 1.49995000 | C | 2.12122600 | 2.52502900 | 0.01048200 |
| H | -6.42240900 | -1.53917400 | 1.94875400 | H | 3.68189700 | -3.22857500 | -1.82728600 |
| C | -6.55345000 | 0.80749200 | -0.63531400 | C | -0.58843900 | 2.48656300 | -0.30178300 |
| H | -6.12788600 | 0.89193900 | -1.64604800 | C | 1.41455500 | 3.67375800 | 0.37862300 |
| H | -7.64882700 | 0.90529200 | -0.69895700 | H | 3.20407900 | 2.49474800 | 0.09813900 |
| H | -6.17788500 | 1.65721300 | -0.04567500 | C | 0.02078000 | 3.62677100 | 0.20814300 |
| C | -1.68354800 | 4.49659000 | 3.14731600 | H | -1.67025800 | 2.40915900 | -0.43946200 |
| C | -2.64562100 | 4.09209400 | 4.28332200 | N | 1.43984500 | -0.73784900 | -1.59044500 |
| H | -3.04342900 | 4.98897600 | 4.78436400 | N | 0.10972800 | 1.39223100 | -0.64839600 |
| H | -3.50214100 | 3.51187500 | 3.90853600 | B | -0.71781400 | -1.39385000 | 0.29222000 |
| H | -2.12763300 | 3.47895400 | 5.03690100 | O | -0.20209000 | -2.67215000 | 0.45899200 |
| C | -2.44048900 | 5.34150500 | 2.09979900 | O | -0.99314800 | -0.81376000 | 1.52862600 |
| H | -2.83011500 | 6.26382100 | 2.55952900 | C | 0.09424000 | -2.86282200 | 1.85275800 |
| H | -1.77410600 | 5.62384600 | 1.26996500 | C | -0.87518400 | -1.83117200 | 2.54138000 |
| H | -3.29461700 | 4.79312200 | 1.67416800 | C | 1.57444200 | -2.51089500 | 2.04634100 |
| C | -0.55500400 | 5.35223700 | 3.74166900 | H | 1.91804200 | -2.70521800 | 3.07353300 |
| H | 0.01481200 | 4.80100300 | 4.50523100 | H | 2.17204500 | -3.12171800 | 1.35388300 |
| H | 0.14851200 | 5.69336000 | 2.96695800 | H | 1.76259100 | -1.45442400 | 1.80603700 |
| H | -0.97971200 | 6.24628100 | 4.22314300 | C | -0.15290200 | -4.32072900 | 2.21816300 |
| **INT4-L1-Bpin** | | | | H | 0.56646600 | -4.96230200 | 1.68702600 |
| Ir | -0.80619600 | -0.44537100 | -1.44000800 | H | -0.02533500 | -4.48405600 | 3.30011100 |
| C | 2.15858400 | 0.15154700 | -0.86729900 | H | -1.16284500 | -4.63664200 | 1.92788100 |
| C | 2.00252700 | -1.90510100 | -1.91462000 | C | -0.33408100 | -1.19690700 | 3.81679700 |
| C | 3.45918600 | -0.13772200 | -0.44977500 | H | -1.07300600 | -0.48787500 | 4.21945800 |
| C | 1.45217400 | 1.40177400 | -0.49227500 | H | -0.13985600 | -1.96175100 | 4.58539200 |
| C | 3.29839400 | -2.25285500 | -1.53423800 | H | 0.59450600 | -0.64281800 | 3.62738200 |
| H | 1.37283500 | -2.59470000 | -2.47957900 | C | -2.27571000 | -2.40027000 | 2.78254800 |
| C | 4.06316800 | -1.36267300 | -0.77052600 | H | -2.27613400 | -3.17219500 | 3.56660100 |
| H | 3.99283600 | 0.58499000 | 0.16553900 | H | -2.93731800 | -1.58305600 | 3.10456700 |

| | | | |
|---|---|---|---|
| H | -2.69207200 | -2.82112400 | 1.85678500 |
| B | -2.73783800 | -0.13862700 | -0.91331500 |
| O | -3.64688600 | -1.08158000 | -0.43517300 |
| O | -3.32758100 | 1.13941900 | -0.82757500 |
| C | -4.91147200 | -0.45088600 | -0.18385000 |
| C | -4.49610900 | 1.05069800 | 0.00960300 |
| C | -5.56083100 | -1.09735000 | 1.03437300 |
| H | -6.49382500 | -0.57831100 | 1.30632300 |
| H | -5.80565400 | -2.14627700 | 0.80888300 |
| H | -4.88636900 | -1.08904500 | 1.89890900 |
| C | -5.78773500 | -0.67062000 | -1.42195500 |
| H | -5.84517400 | -1.75039400 | -1.62297000 |
| H | -6.80927600 | -0.28611100 | -1.27911000 |
| H | -5.34732400 | -0.18613600 | -2.30527300 |
| C | -5.52669600 | 2.07167400 | -0.45503400 |
| H | -6.46800800 | 1.96413800 | 0.10718700 |
| H | -5.14456100 | 3.09027400 | -0.28629600 |
| H | -5.74214400 | 1.96605500 | -1.52603000 |
| C | -4.04389100 | 1.35880100 | 1.44247300 |
| H | -3.59901700 | 2.36562200 | 1.46679300 |
| H | -4.88324600 | 1.34015100 | 2.15398100 |
| H | -3.27401200 | 0.64389100 | 1.76700800 |
| H | -1.34417700 | -1.80003100 | -2.09154000 |
| C | 2.09141700 | 4.92915700 | 0.93775900 |
| C | 1.78567700 | 6.12196100 | 0.00729800 |
| H | 2.17113800 | 5.93816900 | -1.00760200 |
| H | 0.70509100 | 6.31163500 | -0.07184100 |
| H | 2.26015500 | 7.03774200 | 0.39431400 |
| C | 1.52999700 | 5.21324600 | 2.34724200 |
| H | 0.44288000 | 5.37949300 | 2.32811400 |
| H | 1.72988300 | 4.37089200 | 3.02755600 |
| H | 2.00069100 | 6.11541000 | 2.76927700 |
| C | 3.61536800 | 4.76715100 | 1.04148600 |
| H | 3.89367000 | 3.94014700 | 1.71291200 |
| H | 4.07537900 | 4.58456900 | 0.05804300 |
| H | 4.05961200 | 5.68787900 | 1.44881100 |
| C | 5.47068900 | -1.68294600 | -0.25679700 |
| C | 6.45455500 | -0.60513400 | -0.75771100 |
| H | 6.17887200 | 0.39927300 | -0.40298200 |
| H | 7.47157600 | -0.82001200 | -0.39335400 |
| H | 6.48301600 | -0.57874900 | -1.85810100 |
| C | 5.95962900 | -3.05596900 | -0.74109500 |
| H | 6.97427200 | -3.24459100 | -0.35888100 |
| H | 5.31288200 | -3.87014600 | -0.38025500 |
| H | 6.00183300 | -3.10992500 | -1.83979700 |
| C | 5.44398800 | -1.68662600 | 1.28711500 |
| H | 5.14461800 | -0.70880600 | 1.69329900 |
| H | 4.73450500 | -2.43797300 | 1.66587800 |
| H | 6.44368300 | -1.92393800 | 1.68437200 |
| H | -0.60873700 | 4.47776900 | 0.47160500 |

**INT5-L1-Bpin**

| | | | |
|---|---|---|---|
| Ir | -0.28467400 | -0.06902400 | -0.11702100 |
| C | 2.66634100 | 0.67913400 | -0.57698300 |
| C | 1.31990100 | 2.42244900 | -1.30093900 |
| C | 3.81058700 | 1.46229900 | -0.75002200 |
| C | 2.70028300 | -0.69745100 | -0.02625700 |
| C | 2.42410100 | 3.25254900 | -1.49683300 |
| H | 0.29963600 | 2.77530900 | -1.47224800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.71386400 | 2.78088600 | -1.21929400 | H | -2.88689900 | -4.60969300 | -2.65628300 |
| H | 4.78314100 | 1.04859300 | -0.48743300 | H | -1.87823700 | -4.71032700 | -1.18908900 |
| C | 3.87951200 | -1.44759400 | 0.07177700 | H | -2.89417900 | -3.27542700 | -1.45482700 |
| H | 2.25183600 | 4.26605700 | -1.85475700 | B | -1.71315300 | -1.11486600 | 0.84756500 |
| C | 1.48459000 | -2.41628700 | 0.94025500 | O | -2.97279300 | -1.52892800 | 0.41091500 |
| C | 3.86713600 | -2.73089700 | 0.62483300 | O | -1.54183000 | -1.54301200 | 2.18437200 |
| H | 4.80480900 | -1.02078000 | -0.30654900 | C | -3.74187100 | -1.98303200 | 1.53480400 |
| C | 2.62081900 | -3.20149000 | 1.07383100 | C | -2.61799400 | -2.43580000 | 2.53217800 |
| H | 0.50783100 | -2.75289700 | 1.28529900 | C | -4.68439600 | -3.09263200 | 1.08345800 |
| N | 1.43835600 | 1.16777400 | -0.85710100 | H | -5.23577000 | -3.51305000 | 1.93958200 |
| N | 1.51327000 | -1.19058100 | 0.39322500 | H | -5.41802000 | -2.68394900 | 0.37240600 |
| B | -0.74873200 | -1.34978100 | -1.56740700 | H | -4.14428200 | -3.90415900 | 0.57977700 |
| O | -1.56311500 | -1.05958200 | -2.66310600 | C | -4.54713000 | -0.78493800 | 2.05006300 |
| O | -0.31620600 | -2.67888300 | -1.64899800 | H | -5.15225100 | -0.38568600 | 1.22454400 |
| C | -1.53272700 | -2.15855600 | -3.58405000 | H | -5.21831700 | -1.06430200 | 2.87648400 |
| C | -1.08553600 | -3.35232700 | -2.65985900 | H | -3.88548800 | 0.02709700 | 2.38270500 |
| C | -0.49864800 | -1.82048300 | -4.66329200 | C | -2.96001200 | -2.27126600 | 4.00751800 |
| H | -0.46425000 | -2.58195600 | -5.45735300 | H | -3.81595200 | -2.90776100 | 4.28266100 |
| H | -0.76628300 | -0.85472800 | -5.11700100 | H | -2.09926500 | -2.57159000 | 4.62469000 |
| H | 0.50552600 | -1.72164500 | -4.22571200 | H | -3.20676500 | -1.23155800 | 4.25434600 |
| C | -2.91435400 | -2.31195800 | -4.21017900 | C | -2.12411900 | -3.86123900 | 2.26064000 |
| H | -3.13794300 | -1.42985200 | -4.82927800 | H | -1.20953900 | -4.03730300 | 2.84742600 |
| H | -2.96213000 | -3.20435000 | -4.85444900 | H | -2.86723300 | -4.62004100 | 2.54828800 |
| H | -3.69238900 | -2.38693700 | -3.44006000 | H | -1.88019000 | -3.99079100 | 1.19640600 |
| C | -0.20734400 | -4.39772200 | -3.33706500 | H | -1.50907000 | 0.74795700 | -0.68936700 |
| H | 0.05892900 | -5.18087300 | -2.61081500 | B | -2.24799600 | 2.65437300 | 0.24257400 |
| H | -0.73702800 | -4.87575100 | -4.17638000 | B | -1.25926100 | 2.47342700 | 1.62012600 |
| H | 0.72512300 | -3.95715100 | -3.71326100 | O | -3.54333800 | 2.22643300 | 0.20800500 |
| C | -2.26911400 | -4.02581100 | -1.95739300 | O | -1.86073900 | 3.28357300 | -0.91648500 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -1.48197400 | 2.97560500 | 2.86896300 | H | 0.42943500 | -0.31925900 | 3.16216400 |
| O | -0.10444600 | 1.70440000 | 1.59139600 | C | 1.69482100 | 2.86113600 | 2.64930500 |
| C | -0.57563600 | 2.33095300 | 3.80190400 | H | 2.31607700 | 2.98022400 | 3.54929500 |
| C | 0.58582300 | 1.83001300 | 2.86619700 | H | 2.33853500 | 2.52080500 | 1.82481200 |
| C | -4.06729900 | 2.36552400 | -1.13339700 | H | 1.28148900 | 3.84222800 | 2.37426100 |
| C | -2.90950800 | 3.15211700 | -1.90874600 | C | -4.33522000 | 0.95918700 | -1.67157400 |
| C | -3.28822800 | 4.56933300 | -2.33820800 | H | -5.09206500 | 0.47530700 | -1.03753600 |
| H | -2.40425100 | 5.05892900 | -2.77360500 | H | -4.72476100 | 0.99950000 | -2.69994400 |
| H | -4.08470200 | 4.56099000 | -3.09691500 | H | -3.43825300 | 0.32995300 | -1.65338800 |
| H | -3.62195800 | 5.17518100 | -1.48527000 | C | 4.97682300 | 3.63508000 | -1.37521700 |
| C | -2.32904400 | 2.38767600 | -3.09905800 | C | 5.94926800 | 2.93257400 | -2.34575200 |
| H | -3.08501900 | 2.26458700 | -3.88937100 | H | 6.86435400 | 3.53334500 | -2.46861300 |
| H | -1.49165200 | 2.96432400 | -3.52218700 | H | 6.24880300 | 1.93923900 | -1.97940600 |
| H | -1.95909000 | 1.39527700 | -2.81343400 | H | 5.48906900 | 2.80175800 | -3.33737400 |
| C | -5.38364500 | 3.13368200 | -1.02157600 | C | 5.64509900 | 3.79137700 | 0.00767400 |
| H | -5.84201000 | 3.28773100 | -2.00999000 | H | 6.55236100 | 4.41076700 | -0.07499100 |
| H | -6.08371100 | 2.55076800 | -0.40532200 | H | 4.96127600 | 4.27693000 | 0.72114800 |
| H | -5.24658800 | 4.11089800 | -0.54026100 | H | 5.93997700 | 2.81978200 | 0.43182400 |
| C | -1.35439400 | 1.17968800 | 4.44064600 | C | 4.66012800 | 5.03314300 | -1.92676400 |
| H | -0.77875800 | 0.69935700 | 5.24544800 | H | 4.18541700 | 4.98211400 | -2.91855000 |
| H | -2.28514500 | 1.57946000 | 4.86898400 | H | 3.99463200 | 5.59642300 | -1.25507200 |
| H | -1.60875400 | 0.41457300 | 3.69520000 | H | 5.59133300 | 5.61027100 | -2.03198200 |
| C | -0.15370300 | 3.34779600 | 4.85310600 | C | 5.11978300 | -3.60427200 | 0.74471800 |
| H | -1.02732500 | 3.63898200 | 5.45470500 | C | 4.90059900 | -4.90535100 | -0.05632300 |
| H | 0.60001600 | 2.91644400 | 5.53008800 | H | 4.72118900 | -4.68588300 | -1.12016500 |
| H | 0.26024900 | 4.25600100 | 4.39625100 | H | 5.78910000 | -5.55263500 | 0.01716300 |
| C | 1.17237600 | 0.48166500 | 3.26041700 | H | 4.03756900 | -5.47479700 | 0.31898200 |
| H | 2.02279200 | 0.23801500 | 2.60980800 | C | 5.35589500 | -3.94392800 | 2.23159300 |
| H | 1.53871900 | 0.51813100 | 4.29814900 | H | 5.50830200 | -3.02870000 | 2.82472000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 4.50517200 | -4.48922800 | 2.66621000 | C | -2.01940900 | -2.83807400 | -3.30358100 |
| H | 6.25103800 | -4.57680300 | 2.34048100 | C | -0.73182700 | -3.52893900 | -2.71886700 |
| C | 6.37058000 | -2.89878200 | 0.19967900 | C | -1.78473500 | -2.21043300 | -4.68117300 |
| H | 6.26861700 | -2.65376400 | -0.86873200 | H | -1.68284300 | -2.97150900 | -5.46955100 |
| H | 6.58743100 | -1.96932000 | 0.74870800 | H | -2.64294800 | -1.56719000 | -4.92451900 |
| H | 7.24521300 | -3.55816700 | 0.30622100 | H | -0.88208200 | -1.58234100 | -4.67743500 |
| H | 2.51984700 | -4.18897800 | 1.52577400 | C | -3.26207500 | -3.71960000 | -3.33548700 |

**TS5-L1-Bpin**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ir | -0.53606700 | 0.07123300 | -0.56164700 | H | -4.11170700 | -3.14461400 | -3.7330970 |
| C | 2.51623100 | 0.40781900 | -0.72070400 | H | -3.10519800 | -4.59524200 | -3.98516400 |
| C | 1.53332700 | 2.08910700 | -1.96866800 | H | -3.53405500 | -4.07114400 | -2.33245900 |
| C | 3.77061300 | 1.00084600 | -0.87504800 | C | 0.20697400 | -4.12867900 | -3.75836200 |
| C | 2.31060500 | -0.85081500 | 0.03120900 | H | 1.07779700 | -4.57523400 | -3.25462500 |
| C | 2.75854200 | 2.72264500 | -2.17241300 | H | -0.29765600 | -4.91961900 | -4.33555000 |
| H | 0.60760200 | 2.50572300 | -2.36136400 | H | 0.57625300 | -3.36463600 | -4.45438600 |
| C | 3.92160700 | 2.18786500 | -1.60576800 | C | -1.04708000 | -4.56188000 | -1.63220200 |
| H | 4.63681000 | 0.54336200 | -0.40020600 | H | -1.49745700 | -5.47647200 | -2.04641000 |
| C | 3.37325700 | -1.68934000 | 0.39286800 | H | -0.10935000 | -4.83273700 | -1.12419500 |
| H | 2.77716200 | 3.63908900 | -2.75946100 | H | -1.72790900 | -4.13947800 | -0.88109600 |
| C | 0.78982800 | -2.31162800 | 0.98820000 | B | -2.20946500 | -0.65883500 | 0.34062200 |
| C | 3.14418100 | -2.87590400 | 1.09246600 | O | -3.50440700 | -0.19117600 | 0.19503500 |
| H | 4.38305400 | -1.40792400 | 0.10788100 | O | -2.20671100 | -1.70953200 | 1.28004300 |
| C | 1.80267200 | -3.17420800 | 1.38478100 | C | -4.32589600 | -0.71629400 | 1.24478300 |
| H | -0.26221500 | -2.51555200 | 1.19744000 | C | -3.56769200 | -2.04176800 | 1.61842600 |
| N | 1.40838200 | 0.96695500 | -1.25684600 | C | -5.73919000 | -0.91821500 | 0.70871200 |
| N | 1.03361600 | -1.16378800 | 0.33475700 | H | -6.37824000 | -1.41950600 | 1.45322400 |
| B | -1.02743800 | -1.45585000 | -1.75814800 | H | -6.18640200 | 0.06099500 | 0.48052200 |
| O | -2.23254400 | -1.75937200 | -2.37608300 | H | -5.73747700 | -1.50982500 | -0.21579100 |
| O | -0.07300000 | -2.42743400 | -2.07112800 | C | -4.33419500 | 0.31226800 | 2.38116700 |
| | | | | H | -4.66965600 | 1.27658600 | 1.97555900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -5.00847000 | 0.01295200 | 3.19876700 | C | -4.15380200 | 4.52132800 | 0.18623400 |
| H | -3.32336600 | 0.47507800 | 2.77881400 | H | -4.51200100 | 5.25638300 | -0.55127900 |
| C | -3.63707500 | -2.42982200 | 3.08963800 | H | -5.02194500 | 3.95243800 | 0.55035600 |
| H | -4.67718600 | -2.62624000 | 3.39429400 | H | -3.72097500 | 5.05786000 | 1.04026800 |
| H | -3.05208300 | -3.34655400 | 3.26262000 | C | -0.21319000 | -0.47991300 | 3.93726700 |
| H | -3.22942000 | -1.63901700 | 3.73113700 | H | 0.49443400 | -0.90897300 | 4.66197500 |
| C | -3.97744000 | -3.22483700 | 0.73664900 | H | -1.23424300 | -0.68115200 | 4.28867800 |
| H | -3.28240700 | -4.05983000 | 0.91237300 | H | -0.09886500 | -0.98605500 | 2.97313600 |
| H | -4.99631700 | -3.57377500 | 0.96158000 | C | -0.30455600 | 1.71447100 | 5.13021800 |
| H | -3.92059300 | -2.94596500 | -0.32447600 | H | -1.28262800 | 1.38671400 | 5.51163100 |
| H | -1.57209100 | 0.89845900 | -1.42820800 | H | 0.46137900 | 1.44558200 | 5.87427400 |
| B | -1.31102500 | 2.46394000 | 0.36609700 | H | -0.33208800 | 2.80676500 | 5.03009600 |
| B | -0.39640100 | 1.71191800 | 1.62946300 | C | 2.44726200 | 0.40684700 | 3.23165200 |
| O | -2.64365400 | 2.69817800 | 0.59233300 | H | 3.32709500 | 0.74463900 | 2.66430800 |
| O | -0.78909300 | 3.34697700 | -0.56364700 | H | 2.74491000 | 0.27917700 | 4.28402500 |
| O | -1.00838300 | 1.49013300 | 2.83867300 | H | 2.14277200 | -0.56750800 | 2.83589900 |
| O | 0.97179800 | 1.59088100 | 1.72176900 | C | 1.85664200 | 2.81399100 | 3.56009500 |
| C | -0.02876600 | 1.03055100 | 3.79511400 | H | 2.21253700 | 2.79822000 | 4.60073600 |
| C | 1.33746400 | 1.44457900 | 3.11378100 | H | 2.69425700 | 3.10208200 | 2.90783200 |
| C | -3.15243500 | 3.55758000 | -0.44426600 | H | 1.07717300 | 3.58321000 | 3.46583600 |
| C | -1.83338300 | 4.24564000 | -0.99376100 | C | -3.86635100 | 2.67509500 | -1.47133600 |
| C | -1.53260200 | 5.59978800 | -0.34638300 | H | -4.64340700 | 2.09562400 | -0.95569600 |
| H | -0.52051500 | 5.91578100 | -0.64036700 | H | -4.33242200 | 3.27988900 | -2.26392400 |
| H | -2.24628000 | 6.37456200 | -0.66378000 | H | -3.18028800 | 1.94541000 | -1.91863100 |
| H | -1.55803800 | 5.52672100 | 0.75006300 | C | 4.26692500 | -3.82051000 | 1.53060500 |
| C | -1.77040700 | 4.36630500 | -2.51306300 | C | 5.65118100 | -3.31181600 | 1.10142000 |
| H | -2.58984900 | 4.99564900 | -2.89312600 | H | 5.73317900 | -3.22497300 | 0.00704000 |
| H | -0.81834800 | 4.83431200 | -2.80807300 | H | 5.88085500 | -2.33034900 | 1.54436300 |
| H | -1.83470300 | 3.38168100 | -2.99292700 | H | 6.42684100 | -4.01657500 | 1.43734100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.24219200 | -3.93931400 | 3.06940200 | H | 0.54751000 | 2.32095200 | -2.55947100 |
| H | 4.39524400 | -2.95597300 | 3.54103600 | C | 3.86500000 | 2.20754300 | -1.73637300 |
| H | 3.28436700 | -4.34077900 | 3.43193300 | H | 4.58570100 | 0.87915500 | -0.19904200 |
| H | 5.04200600 | -4.61432900 | 3.41352400 | C | 3.28733800 | -0.86161400 | 1.35592500 |
| C | 4.03446100 | -5.20844500 | 0.89736700 | H | 2.71384200 | 3.36875400 | -3.17728800 |
| H | 4.83045700 | -5.90577900 | 1.20372700 | C | 0.73155600 | -1.74151500 | 1.65721500 |
| H | 3.07161700 | -5.64172800 | 1.20570500 | C | 3.05123900 | -1.82201900 | 2.34473400 |
| H | 4.03783200 | -5.14347800 | -0.20174300 | H | 4.29502900 | -0.48057800 | 1.20584700 |
| C | 5.30207400 | 2.84052300 | -1.73375900 | C | 1.72748700 | -2.26274900 | 2.47627500 |
| C | 6.27789400 | 1.84228800 | -2.39148100 | H | -0.30717700 | -2.06808100 | 1.72838100 |
| H | 6.38624700 | 0.92260100 | -1.79730700 | N | 1.36029300 | 1.06104900 | -1.15082200 |
| H | 5.92970000 | 1.55565600 | -3.39589800 | N | 0.98197100 | -0.81197800 | 0.72350900 |
| H | 7.27686600 | 2.29585900 | -2.49076400 | B | -0.10266700 | -1.71991500 | -1.77702200 |
| C | 5.80913600 | 3.20978900 | -0.32311700 | O | -0.95067400 | -2.44824800 | -2.59568900 |
| H | 5.11907800 | 3.91147300 | 0.17047000 | O | 1.13627000 | -2.35342500 | -1.69941000 |
| H | 5.90554400 | 2.32328600 | 0.32155000 | C | -0.20683800 | -3.51554200 | -3.21776600 |
| H | 6.79957000 | 3.68801300 | -0.38707200 | C | 1.00550400 | -3.68406600 | -2.23382400 |
| C | 5.25748400 | 4.11634900 | -2.58767800 | C | 0.21464000 | -3.02465400 | -4.60599300 |
| H | 6.26588600 | 4.55173200 | -2.65798500 | H | 0.72551700 | -3.81029800 | -5.18325300 |
| H | 4.91173900 | 3.90937800 | -3.61205800 | H | -0.68516700 | -2.71512200 | -5.15746500 |
| H | 4.59618900 | 4.87846800 | -2.14810500 | H | 0.88042800 | -2.15289200 | -4.52871200 |
| H | 1.52930000 | -4.08300000 | 1.92242000 | C | -1.10469100 | -4.74001500 | -3.34455800 |

**INT6-L1-Bpin**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ir | -0.54241800 | -0.00486800 | -0.58473500 | H | -1.93483700 | -4.51992800 | -4.03245000 |
| C | 2.46178900 | 0.66428400 | -0.47860300 | H | -0.54307700 | -5.59777200 | -3.74785700 |
| C | 1.47790400 | 2.01166800 | -2.08264700 | H | -1.53613700 | -5.02464700 | -2.37725500 |
| C | 3.71506300 | 1.22007700 | -0.75567100 | C | 2.31924100 | -4.09280700 | -2.88676500 |
| C | 2.25135900 | -0.36806100 | 0.55845800 | H | 3.10471400 | -4.16897300 | -2.11937600 |
| C | 2.69799600 | 2.60152900 | -2.40513600 | H | 2.22638400 | -5.07341600 | -3.38002600 |
| | | | | H | 2.64540600 | -3.35385900 | -3.62997100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.68920900 | -4.60235700 | -1.04783900 | O | -1.36862200 | 2.81968500 | -1.42519600 |
| H | 0.62389900 | -5.65969700 | -1.34574300 | O | -1.45644300 | 0.70395600 | 2.30208500 |
| H | 1.49048100 | -4.49824300 | -0.30073500 | O | 0.02088700 | 2.27752900 | 1.58777100 |
| H | -0.25455900 | -4.30487200 | -0.56887400 | C | -1.25972000 | 1.57762400 | 3.43069000 |
| B | -2.14608100 | -1.15111600 | -0.06745600 | C | 0.05741000 | 2.34393500 | 3.03027100 |
| O | -3.44790500 | -0.98197000 | -0.51168600 | C | -3.61552300 | 3.05487700 | -0.82405000 |
| O | -2.09835400 | -2.23191800 | 0.82456000 | C | -2.35040300 | 3.86340700 | -1.29188100 |
| C | -4.32579900 | -1.70541600 | 0.36096600 | C | -1.83573900 | 4.84086700 | -0.23080100 |
| C | -3.39281700 | -2.86411700 | 0.86543400 | H | -0.84344200 | 5.20278600 | -0.53762400 |
| C | -5.54796500 | -2.16006500 | -0.42651100 | H | -2.50351700 | 5.70694600 | -0.10928800 |
| H | -6.19865400 | -2.80223200 | 0.18842300 | H | -1.71515900 | 4.33799400 | 0.73779200 |
| H | -6.13120200 | -1.28030000 | -0.73775800 | C | -2.50477600 | 4.57204400 | -2.63194900 |
| H | -5.25904300 | -2.70935700 | -1.33180000 | H | -3.31914300 | 5.31264800 | -2.59238800 |
| C | -4.73601700 | -0.74421800 | 1.48373100 | H | -1.57357700 | 5.10358200 | -2.88104900 |
| H | -5.17599800 | 0.15406500 | 1.02812300 | H | -2.71556800 | 3.85973600 | -3.43984000 |
| H | -5.47228300 | -1.19646000 | 2.16611200 | C | -4.55050400 | 3.80749600 | 0.11363600 |
| H | -3.85484500 | -0.41919300 | 2.05486300 | H | -4.96758300 | 4.69897200 | -0.38071300 |
| C | -3.66513700 | -3.33750800 | 2.28743200 | H | -5.38630600 | 3.15333600 | 0.40358900 |
| H | -4.68932300 | -3.73205700 | 2.38138200 | H | -4.03644200 | 4.12297200 | 1.03039800 |
| H | -2.96437600 | -4.14438300 | 2.55295700 | C | -1.14806900 | 0.72713200 | 4.69012700 |
| H | -3.53374800 | -2.52117100 | 3.00930700 | H | -0.90502400 | 1.34828000 | 5.56657000 |
| C | -3.35064300 | -4.05131600 | -0.10016600 | H | -2.10856500 | 0.22576500 | 4.88123500 |
| H | -2.53912200 | -4.72984100 | 0.20398800 | H | -0.37974500 | -0.04930300 | 4.58186500 |
| H | -4.29313800 | -4.61930000 | -0.09517900 | C | -2.48774400 | 2.48764700 | 3.50948600 |
| H | -3.14178400 | -3.70631900 | -1.12223200 | H | -3.38720700 | 1.86055000 | 3.59004800 |
| H | -1.51184500 | 0.35990700 | -1.80653600 | H | -2.44760400 | 3.16016400 | 4.37932000 |
| B | -1.74671800 | 1.73606200 | -0.62299400 | H | -2.58830100 | 3.08638900 | 2.59471500 |
| B | -0.79123000 | 1.22247000 | 1.20757800 | C | 1.33274300 | 1.62364100 | 3.47839600 |
| O | -3.01648200 | 1.96136900 | -0.10842000 | H | 2.19360600 | 2.07995700 | 2.96820600 |

| | | | |
|---|---|---|---|
| H | 1.48722800 | 1.70443500 | 4.56484300 |
| H | 1.30608700 | 0.55985600 | 3.20884200 |
| C | 0.10593300 | 3.80651300 | 3.45363800 |
| H | 0.06194700 | 3.89975900 | 4.55014800 |
| H | 1.04727000 | 4.25950000 | 3.10795400 |
| H | -0.72250100 | 4.38002400 | 3.01947200 |
| C | -4.40562700 | 2.44740500 | -1.98743900 |
| H | -5.11082500 | 1.70812300 | -1.58205400 |
| H | -4.96940000 | 3.21016100 | -2.54563900 |
| H | -3.73922800 | 1.91666600 | -2.68203600 |
| H | 1.44383700 | -3.01160500 | 3.21341900 |
| C | 4.20116000 | -2.32220600 | 3.22437400 |
| C | 3.73299500 | -3.38427300 | 4.23029600 |
| H | 4.58566200 | -3.72027800 | 4.83970800 |
| H | 2.96955100 | -2.98778600 | 4.91691200 |
| H | 3.31543600 | -4.26836100 | 3.72473800 |
| C | 5.29457600 | -2.94104700 | 2.32865800 |
| H | 4.89555000 | -3.78917200 | 1.75102900 |
| H | 5.70225400 | -2.21010900 | 1.61447800 |
| H | 6.13014900 | -3.30775200 | 2.94581900 |
| C | 4.78330400 | -1.12538000 | 4.00667900 |
| H | 4.01223600 | -0.65720600 | 4.63811300 |
| H | 5.60690300 | -1.45871200 | 4.65802800 |
| H | 5.18021800 | -0.35120900 | 3.33296200 |
| C | 5.24797800 | 2.80280600 | -2.02464400 |
| C | 6.19994600 | 1.67363500 | -2.47242600 |
| H | 7.20075800 | 2.08121300 | -2.68690600 |
| H | 6.31230500 | 0.90103000 | -1.69702300 |
| H | 5.82604000 | 1.18284900 | -3.38426100 |
| C | 5.19550400 | 3.86604400 | -3.13185400 |
| H | 4.54639400 | 4.71100900 | -2.85570300 |
| H | 6.20502700 | 4.26653200 | -3.31050500 |
| H | 4.83046200 | 3.44745400 | -4.08216900 |
| C | 5.79141700 | 3.45987100 | -0.73815900 |
| H | 5.12071500 | 4.26197600 | -0.39323200 |
| H | 5.89466600 | 2.73227500 | 0.08088400 |
| H | 6.78496700 | 3.89812000 | -0.92404200 |

**TS6-L1-Bpin**

| | | | |
|---|---|---|---|
| Ir | -0.51378700 | -0.02408600 | -0.45225000 |
| C | 2.35397400 | 1.05945900 | -0.15515300 |
| C | 1.16390200 | 2.48553700 | -1.53863600 |
| C | 3.52333500 | 1.79625900 | -0.37058300 |
| C | 2.29667400 | -0.12180400 | 0.73249000 |
| C | 2.29439600 | 3.25955200 | -1.79100500 |
| H | 0.18810400 | 2.72282700 | -1.96900900 |
| C | 3.52213400 | 2.91940900 | -1.20569700 |
| H | 4.44777500 | 1.48651200 | 0.11317800 |
| C | 3.39297200 | -0.56317500 | 1.47921300 |
| H | 2.19541800 | 4.12130500 | -2.44883800 |
| C | 0.98321000 | -1.82048000 | 1.63276100 |
| C | 3.30049400 | -1.67547600 | 2.32249000 |
| H | 4.33557100 | -0.02600500 | 1.39755100 |
| C | 2.04684400 | -2.29937500 | 2.39037300 |
| H | -0.00573400 | -2.28380700 | 1.65298200 |
| N | 1.19383000 | 1.40809700 | -0.74883800 |
| N | 1.10502300 | -0.76583300 | 0.81086800 |
| B | 0.37380200 | -1.38413900 | -1.85566100 |
| O | 1.66802700 | -1.18566400 | -2.31512800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -0.07300500 | -2.64241500 | -2.20755900 | H | -5.40829700 | -1.06227100 | 0.11741500 |
| C | 2.20723300 | -2.45993700 | -2.72181900 | H | -5.57156400 | -2.44253400 | 1.24172600 |
| C | 0.90313600 | -3.26898800 | -3.06640000 | H | -4.26847100 | -1.22908600 | 1.46302700 |
| C | 2.96206500 | -3.02729200 | -1.51416400 | C | -3.34549600 | -3.97395000 | 1.92964400 |
| H | 3.47232200 | -3.97216200 | -1.75369900 | H | -4.21812100 | -4.63430400 | 1.80268900 |
| H | 3.71647100 | -2.29407300 | -1.19335000 | H | -2.54327100 | -4.55882800 | 2.40579900 |
| H | 2.28230400 | -3.19932300 | -0.66758500 | H | -3.61520100 | -3.15533300 | 2.60903900 |
| C | 3.16362600 | -2.24571500 | -3.88735200 | C | -2.25786300 | -4.56414900 | -0.25752600 |
| H | 4.03157600 | -1.65978400 | -3.54884800 | H | -1.39010300 | -4.97800000 | 0.27886700 |
| H | 3.53064900 | -3.20801600 | -4.27789500 | H | -2.97558700 | -5.37977200 | -0.43423700 |
| H | 2.68305300 | -1.69330300 | -4.70472300 | H | -1.89968600 | -4.17287000 | -1.21933900 |
| C | 0.96404600 | -4.75540000 | -2.73706100 | H | -0.99247300 | -0.06180600 | -1.99639700 |
| H | 0.01412300 | -5.23633700 | -3.01409100 | B | -2.09221800 | 1.28495200 | -0.83323000 |
| H | 1.77394500 | -5.24919100 | -3.29702300 | B | -1.10767600 | 0.92387000 | 1.39641700 |
| H | 1.12200400 | -4.92178600 | -1.66383800 | O | -3.35183700 | 1.31278200 | -0.25367800 |
| C | 0.43333900 | -3.06297200 | -4.50849800 | O | -1.96943800 | 2.34193800 | -1.73624200 |
| H | 1.08523200 | -3.57839100 | -5.22998400 | O | -1.54336800 | 0.21269600 | 2.49800300 |
| H | -0.58527200 | -3.46524700 | -4.60806000 | O | -0.95428300 | 2.26632300 | 1.72056900 |
| H | 0.40030400 | -1.99376600 | -4.76241400 | C | -1.93532400 | 1.14013200 | 3.52899300 |
| B | -1.92285600 | -1.46437200 | -0.15388300 | C | -1.10685800 | 2.42023900 | 3.14688600 |
| O | -3.09002600 | -1.63919800 | -0.88583000 | C | -4.17038800 | 2.26757300 | -0.95168100 |
| O | -1.82980500 | -2.46786400 | 0.81503900 | C | -3.09253300 | 3.23068500 | -1.56936900 |
| C | -3.92354400 | -2.58741400 | -0.20471900 | C | -2.65223400 | 4.33604600 | -0.60470600 |
| C | -2.86609900 | -3.43924900 | 0.58587600 | H | -1.77485700 | 4.84652600 | -1.02998800 |
| C | -4.73554900 | -3.36481700 | -1.23288700 | H | -3.44338400 | 5.08494300 | -0.44887400 |
| H | -5.32031900 | -4.16555200 | -0.75246200 | H | -2.35150700 | 3.91098200 | 0.36250000 |
| H | -5.43725700 | -2.68405000 | -1.73821300 | C | -3.46135700 | 3.82039900 | -2.92462400 |
| H | -4.08722100 | -3.80941000 | -1.99887600 | H | -4.37576600 | 4.43013600 | -2.85092700 |
| C | -4.85166300 | -1.79256300 | 0.72127200 | H | -2.64742300 | 4.46992700 | -3.28116600 |

| | | | |
|---|---|---|---|
| H | -3.62038400 | 3.03519500 | -3.67467000 |
| C | -5.12104800 | 2.92465000 | 0.04120900 |
| H | -5.71804300 | 3.71058600 | -0.44779000 |
| H | -5.81204800 | 2.16957400 | 0.44473000 |
| H | -4.57834200 | 3.37111700 | 0.88396900 |
| C | -1.59853800 | 0.53722700 | 4.88689600 |
| H | -1.80479500 | 1.25245700 | 5.69898100 |
| H | -2.21584200 | -0.35812200 | 5.05367100 |
| H | -0.54511500 | 0.23336800 | 4.94218900 |
| C | -3.44720000 | 1.33995500 | 3.39201600 |
| H | -3.94076600 | 0.36225200 | 3.49366100 |
| H | -3.84805300 | 2.01374300 | 4.16423100 |
| H | -3.69582200 | 1.73187400 | 2.39682000 |
| C | 0.30491400 | 2.41985300 | 3.74210500 |
| H | 0.89019100 | 3.21686600 | 3.25999400 |
| H | 0.29693600 | 2.59922200 | 4.82780300 |
| H | 0.81154200 | 1.46320600 | 3.54616900 |
| C | -1.80085700 | 3.74569900 | 3.43293900 |
| H | -1.99737000 | 3.86243100 | 4.51050700 |
| H | -1.15853300 | 4.57849000 | 3.10906000 |
| H | -2.75315200 | 3.82453200 | 2.89337200 |
| C | -4.96157000 | 1.49252400 | -2.00949400 |
| H | -5.53238400 | 0.69770600 | -1.50884400 |
| H | -5.66452000 | 2.14035500 | 2.55469800 |
| H | -4.28604600 | 1.00901400 | -2.72902000 |
| H | 1.87315700 | -3.16617800 | 3.02541700 |
| C | 4.52837200 | -2.15461400 | 3.10349300 |
| C | 5.63854900 | -2.53443200 | 2.10032600 |
| H | 5.94068700 | -1.67646300 | 1.48112600 |
| H | 6.53181400 | -2.89256300 | 2.63651100 |
| H | 5.29928400 | -3.33404100 | 1.42369400 |
| C | 5.02310000 | -1.01670600 | 4.02087400 |
| H | 4.24102800 | -0.72178400 | 4.73756700 |
| H | 5.90653200 | -1.34414800 | 4.59176200 |
| H | 5.30860900 | -0.12212100 | 3.44741100 |
| C | 4.21242300 | -3.38141000 | 3.97192700 |
| H | 3.43368300 | -3.16302500 | 4.71851500 |
| H | 3.87684400 | -4.23567000 | 3.36440800 |
| H | 5.11666800 | -3.69457600 | 4.51563100 |
| C | 4.81788500 | 3.70439400 | -1.44113200 |
| C | 4.60322100 | 4.89666200 | -2.38536900 |
| H | 3.87555700 | 5.61455000 | -1.97706700 |
| H | 5.55396100 | 5.43214600 | -2.52977500 |
| H | 4.24924800 | 4.57347300 | -3.37618100 |
| C | 5.33998700 | 4.23632500 | -0.08982500 |
| H | 4.60126300 | 4.90256700 | 0.38200800 |
| H | 5.55583700 | 3.42003100 | 0.61579800 |
| H | 6.27138800 | 4.80583800 | -0.23795900 |
| C | 5.86796600 | 2.76358300 | -2.06908900 |
| H | 6.09801400 | 1.91100100 | -1.41255400 |
| H | 5.51011500 | 2.36132000 | -3.02941200 |
| H | 6.80770400 | 3.30862200 | -2.25253100 |

**INT7-L1-Bpin**

| | | | |
|---|---|---|---|
| Ir | 0.40253100 | -0.14970900 | 0.04759200 |
| C | -2.65425500 | -0.65627100 | -0.33268000 |
| C | -1.46480100 | -2.17984900 | -1.60689700 |
| C | -3.85859400 | -1.28040800 | -0.66450200 |
| C | -2.58041700 | 0.52470800 | 0.56167400 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.63347800 | -2.84917600 | -1.97398600 | H | 3.00170200 | -3.77661200 | -3.06562900 |
| H | -0.47936800 | -2.47611400 | -1.97677300 | C | 1.94975300 | -0.74717400 | -4.39838000 |
| C | -3.87550100 | -2.40862300 | -1.49815100 | H | 2.63444900 | -0.66175000 | -5.25595500 |
| H | -4.78697700 | -0.89474600 | -0.24446900 | H | 0.99845500 | -1.16904400 | -4.75726700 |
| C | -3.66068700 | 1.39623700 | 0.74759300 | H | 1.74168900 | 0.25136800 | -3.99005000 |
| H | -2.54977500 | -3.71158000 | -2.63325800 | B | 0.39422300 | 1.55310300 | -1.00031000 |
| C | -1.25395000 | 1.80341000 | 1.95200000 | O | 0.93282300 | 1.78770800 | -2.26716500 |
| C | -3.53075300 | 2.52354700 | 1.56511500 | O | -0.23983800 | 2.71872800 | -0.55394800 |
| H | -4.58696100 | 1.20491600 | 0.21135600 | C | 0.94428200 | 3.20470000 | -2.50565700 |
| C | -2.28670900 | 2.69970900 | 2.19137200 | C | -0.25376400 | 3.68648300 | -1.61012900 |
| H | -0.26237400 | 1.95529100 | 2.38141700 | C | 0.77869800 | 3.46176500 | -3.99801200 |
| N | -1.47237800 | -1.11536800 | -0.79811400 | H | 0.68105900 | 4.53977700 | -4.20321200 |
| N | -1.38775900 | 0.73913700 | 1.15026200 | H | 1.66325400 | 3.09143900 | -4.53819600 |
| B | 1.78854000 | -0.76304000 | -1.29811800 | H | -0.10191700 | 2.94403800 | -4.40047700 |
| O | 3.08882100 | -0.30377400 | -1.48577000 | C | 2.29690800 | 3.73088400 | -2.01405500 |
| O | 1.51304100 | -1.74098400 | -2.27010300 | H | 3.09446600 | 3.17744500 | -2.53119700 |
| C | 3.73187200 | -1.03229100 | -2.53954200 | H | 2.42232900 | 4.80508700 | -2.21963900 |
| C | 2.50945500 | -1.66526100 | -3.30620600 | H | 2.41046400 | 3.54467300 | -0.93703400 |
| C | 4.64121600 | -2.07823900 | -1.88728300 | C | -0.09162400 | 5.07683800 | -1.00703200 |
| H | 5.23239700 | -2.63347500 | -2.63131400 | H | -0.00122200 | 5.84338300 | -1.79308800 |
| H | 5.33540300 | -1.56655000 | -1.20406400 | H | -0.97354900 | 5.31784800 | -0.39318200 |
| H | 4.05606700 | -2.79448800 | -1.29437700 | H | 0.79324800 | 5.12506700 | -0.35987000 |
| C | 4.56415800 | -0.05616200 | -3.36542200 | C | -1.61119500 | 3.56887100 | -2.31294900 |
| H | 5.38985400 | 0.33546900 | -2.75213300 | H | -2.40436900 | 3.68426400 | -1.55854700 |
| H | 4.99837400 | -0.55046400 | -4.24900900 | H | -1.74842500 | 4.33811600 | -3.08813700 |
| H | 3.95694400 | 0.79605900 | -3.69564900 | H | -1.72675000 | 2.57738200 | -2.77459200 |
| C | 2.75561300 | -3.06273400 | -3.86240600 | H | 2.66443800 | -2.68278500 | 0.50003800 |
| H | 1.84932500 | -3.42308900 | -4.37322400 | B | 1.83712500 | -2.84819300 | 1.33673100 |
| H | 3.57761500 | -3.05559600 | -4.59564600 | B | 2.01940500 | 0.58988600 | 1.00710800 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | 1.96343400 | -3.74005800 | 2.35762000 | H | 3.18574100 | -0.13589600 | 4.42565300 |
| O | 0.59944500 | -2.23543500 | 1.33141100 | H | 4.05893800 | 1.41395700 | 4.50989900 |
| O | 2.51616300 | 1.89526400 | 1.03664200 | H | 2.36998400 | 1.36599100 | 3.92855400 |
| O | 2.82337900 | -0.21648900 | 1.83079500 | C | 5.12727900 | -0.19202100 | 2.51291600 |
| C | 3.83351000 | 1.89349000 | 1.61101800 | H | 5.94311700 | 0.41469300 | 2.93701100 |
| C | 3.81453100 | 0.58425000 | 2.49066000 | H | 5.01076500 | -1.09420200 | 3.13266300 |
| C | 0.66979500 | -3.89016000 | 2.99142600 | H | 5.41132600 | -0.51339400 | 1.50302300 |
| C | -0.06274700 | -2.55669300 | 2.59164600 | C | 0.01991100 | -5.13427400 | 2.38015000 |
| C | 0.21251000 | -1.40951100 | 3.56040000 | H | 0.69904800 | -5.98925300 | 2.51022400 |
| H | -0.14838500 | -0.47729400 | 3.11015200 | H | -0.93789000 | -5.37233500 | 2.86547900 |
| H | -0.30742900 | -1.56604800 | 4.51664000 | H | -0.15659000 | -4.99983900 | 1.30311500 |
| H | 1.28733400 | -1.29275400 | 3.73934900 | C | -4.64733800 | 3.55570100 | 1.74911200 |
| C | -1.55789700 | -2.69813300 | 2.34255800 | C | -5.93499400 | 3.15190100 | 1.01543000 |
| H | -2.05571200 | -3.11070100 | 3.23357000 | H | -5.77913400 | 3.07339900 | -0.07139000 |
| H | -1.99193400 | -1.71177000 | 2.13807100 | H | -6.32718200 | 2.18940200 | 1.37920900 |
| H | -1.76834000 | -3.34873700 | 1.48453100 | H | -6.71232300 | 3.91266600 | 1.18328500 |
| C | 0.87618800 | -4.07951100 | 4.48780300 | C | -4.96431100 | 3.70569200 | 3.25128700 |
| H | -0.09016100 | -4.10892200 | 5.01466500 | H | -4.08594500 | 4.03647600 | 3.82468200 |
| H | 1.39615200 | -5.03152500 | 4.67048500 | H | -5.76053700 | 4.45240500 | 3.39925200 |
| H | 1.48590300 | -3.27268900 | 4.91296100 | H | -5.30669000 | 2.75023100 | 3.67868800 |
| C | 4.02907800 | 3.18893400 | 2.39174900 | C | -4.16039000 | 4.90688100 | 1.18142300 |
| H | 4.99741200 | 3.19306600 | 2.91695800 | H | -4.94408800 | 5.67318000 | 1.29277400 |
| H | 4.01570000 | 4.04088700 | 1.69531900 | H | -3.25957900 | 5.26552300 | 1.70095100 |
| H | 3.22833400 | 3.34397000 | 3.12676000 | H | -3.91508800 | 4.81672200 | 0.11198700 |
| C | 4.83555700 | 1.82164900 | 0.45405300 | C | -5.20298200 | -3.09701300 | -1.83411100 |
| H | 4.67626800 | 2.68801400 | -0.20431800 | C | -5.00719200 | -4.29472100 | -2.77544000 |
| H | 5.87659400 | 1.84357000 | 0.81048300 | H | -4.36606100 | -5.06772600 | -2.32495300 |
| H | 4.66323700 | 0.91913000 | -0.14599600 | H | -5.98129200 | -4.75758400 | -2.99503300 |
| C | 3.33160400 | 0.83233400 | 3.92386900 | H | -4.55888600 | -3.99124200 | -3.73379500 |

| | | | |
|---|---|---|---|
| C | -6.14071300 | -2.08108000 | -2.51987900 |
| H | -6.35551200 | -1.21866000 | -1.87121500 |
| H | -5.69370500 | -1.69988000 | -3.45102700 |
| H | -7.10131900 | -2.55852100 | -2.77044600 |
| C | -5.85060200 | -3.59963800 | -0.52621000 |
| H | -5.19358500 | -4.31977000 | -0.01414800 |
| H | -6.05532800 | -2.77462200 | 0.17246200 |
| H | -6.80712400 | -4.10149000 | -0.74269700 |
| H | -2.09659300 | 3.55478600 | 2.84084000 |

**3a**

| | | | |
|---|---|---|---|
| B | 2.31801000 | -0.03856100 | -0.86481200 |
| O | 1.17500200 | -0.68892200 | -1.23890800 |
| O | 2.94407600 | -0.62574700 | 0.19562300 |
| C | 1.11120900 | -1.94712700 | -0.51845100 |
| C | 2.09161200 | -1.69135600 | 0.69717500 |
| C | 1.61047600 | -3.02403800 | -1.48389800 |
| H | 1.54578000 | -4.02779200 | -1.03966900 |
| H | 0.98701000 | -3.00377500 | -2.38946600 |
| H | 2.65230400 | -2.84158300 | -1.78508000 |
| C | -0.33594700 | -2.21963900 | -0.12924700 |
| H | -0.94306700 | -2.34473200 | -1.03763000 |
| H | -0.40784000 | -3.14517700 | 0.46244600 |
| H | -0.77086800 | -1.39741500 | 0.44980400 |
| C | 2.97370100 | -2.87737200 | 1.06632100 |
| H | 3.62504500 | -2.60206300 | 1.90873500 |
| H | 2.35932600 | -3.73699200 | 1.37502100 |
| H | 3.61474700 | -3.18408600 | 0.23031700 |
| C | 1.38220000 | -1.15919800 | 1.94325200 |
| H | 0.77233400 | -1.94106100 | 2.41839200 |
| H | 2.13994300 | -0.82430000 | 2.66680500 |
| H | 0.73064900 | -0.30691600 | 1.71402400 |
| S | 2.87003200 | 2.80568000 | -0.63299900 |
| C | 2.82749000 | 1.24701100 | -1.61914600 |
| H | 2.22727300 | 1.40636200 | -2.52733700 |
| H | 3.87066400 | 1.07869000 | -1.93289100 |
| C | 1.66468200 | 2.46921300 | 0.69225200 |
| H | 1.98796800 | 1.59332400 | 1.27176200 |
| H | 1.71388500 | 3.34172800 | 1.36083500 |
| C | 0.24879900 | 2.25706100 | 0.17973700 |
| H | 0.24295000 | 1.50233100 | -0.62060200 |
| H | -0.16915700 | 3.19309200 | -0.23100200 |
| O | -0.53462400 | 1.79206300 | 1.27300400 |
| C | -1.68838100 | 1.12059100 | 1.02783600 |
| C | -2.27204700 | 0.47052800 | 2.13236400 |
| C | -2.27965100 | 1.02943500 | -0.23294100 |
| C | -3.42969600 | -0.27340600 | 1.94675200 |
| H | -1.79266700 | 0.56004900 | 3.10788100 |
| C | -3.45006100 | 0.26873300 | -0.40262200 |
| H | -1.86298200 | 1.51850300 | -1.11111100 |
| C | -4.03268300 | -0.39176100 | 0.68609500 |
| H | -3.88165600 | -0.78423800 | 2.80066600 |
| H | -4.93724200 | -0.98674200 | 0.57197800 |
| O | -3.93781500 | 0.23334800 | -1.66862600 |
| C | -5.10858100 | -0.50476900 | -1.92760500 |
| H | -5.31930900 | -0.39351800 | -2.99954900 |
| H | -4.97697700 | -1.57755300 | -1.69738100 |
| H | -5.97052300 | -0.12357500 | -1.35088500 |

**4a**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| S | -6.59369600 | -1.24777600 | -0.35617100 | C | 3.99084200 | -1.60477000 | -0.12281500 |
| C | -6.87579300 | -0.79160800 | 1.38486300 | C | 4.80381900 | -0.03480000 | 1.77534300 |
| H | -6.31208300 | 0.10638200 | 1.67801500 | H | 3.95762400 | -0.39935100 | 2.37559500 |
| H | -7.94925900 | -0.57626300 | 1.48361100 | H | 5.70731700 | -0.58785100 | 2.07111200 |
| C | -4.81520300 | -1.64634500 | -0.30575400 | H | 4.95376200 | 1.02890400 | 2.01088600 |
| H | -4.60037700 | -2.29785100 | 0.55619600 | C | 5.71245100 | 0.31982300 | -0.53211600 |
| H | -4.60510100 | -2.22743100 | -1.21637400 | H | 6.00512300 | 1.32254100 | -0.18689600 |
| C | -3.92899900 | -0.41204400 | -0.26870500 | H | 6.57516200 | -0.35194100 | -0.40303100 |
| H | -4.15368500 | 0.20440800 | 0.62107300 | H | 5.47457300 | 0.38714300 | -1.60117600 |
| H | -4.11478400 | 0.21356000 | -1.16020700 | C | 4.49428300 | -2.74286200 | 0.75504600 |
| O | -2.58588200 | -0.85339900 | -0.23072000 | H | 4.06967700 | -3.69513400 | 0.40438100 |
| C | -1.58569400 | 0.06483400 | -0.17734900 | H | 5.59161800 | -2.81786800 | 0.70485600 |
| C | -0.27615900 | -0.44323800 | -0.12205700 | H | 4.19710600 | -2.60684900 | 1.80251400 |
| C | -1.80028100 | 1.44472300 | -0.17702100 | C | 4.21597900 | -1.93601400 | -1.60014400 |
| C | 0.81320300 | 0.42843700 | -0.06458300 | H | 3.87011400 | -1.11800700 | -2.24863000 |
| H | -0.13238000 | -1.52457700 | -0.12546900 | H | 5.27659300 | -2.13073500 | -1.81672800 |
| C | -0.70210900 | 2.32336300 | -0.11924600 | H | 3.63740300 | -2.83639100 | -1.85272300 |
| H | -2.79485200 | 1.88488500 | -0.22284200 | H | -6.61877000 | -1.62472700 | 2.05716300 |
| C | 0.60066100 | 1.82348500 | -0.06225400 | **1a** | | | |
| H | 1.46367400 | 2.48582600 | -0.01622200 | C | 4.32895500 | 1.20222700 | -1.16253900 |
| O | -1.01952500 | 3.64478100 | -0.12370300 | H | 5.13100500 | 1.95394500 | -1.15405500 |
| C | 0.02323000 | 4.58984600 | -0.07269500 | H | 3.38783800 | 1.70052000 | -1.43838100 |
| H | -0.44973600 | 5.58093700 | -0.08929100 | H | 4.57306700 | 0.43297100 | -1.91135400 |
| H | 0.62136800 | 4.49204400 | 0.85117000 | S | 4.26829700 | 0.48692600 | 0.51179800 |
| H | 0.70156000 | 4.50011000 | -0.94017700 | C | 2.96826600 | -0.77100900 | 0.28318300 |
| B | 2.26119700 | -0.13048300 | -0.00396200 | H | 3.06427900 | -1.46872200 | 1.12876400 |
| O | 3.37723600 | 0.66626100 | -0.01288000 | H | 3.15760100 | -1.34383200 | -0.63854700 |
| O | 2.56301300 | -1.46480500 | 0.06399500 | C | 1.56786700 | -0.18085900 | 0.26046000 |
| C | 4.52022900 | -0.17243300 | 0.27751900 | H | 1.46511600 | 0.55240300 | -0.56015900 |

| | | | |
|---|---|---|---|
| H | 1.36570100 | 0.35055900 | 1.20749600 |
| O | 0.65794400 | -1.24924900 | 0.07638900 |
| C | -0.67139300 | -0.98480000 | 0.00394400 |
| C | -1.51421800 | -2.09414200 | -0.20104300 |
| C | -1.21456800 | 0.29604600 | 0.12088000 |
| C | -2.88566200 | -1.89717400 | -0.28517000 |
| H | -1.06526500 | -3.08424400 | -0.28875700 |
| C | -2.60707800 | 0.47631400 | 0.03223100 |
| H | -0.60244500 | 1.18113900 | 0.28335200 |
| C | -3.45362200 | -0.61953200 | -0.17158300 |
| H | -3.54182300 | -2.75658000 | -0.44415500 |
| H | -4.53326500 | -0.49832200 | -0.24234500 |
| O | -3.03221000 | 1.75969600 | 0.15817900 |
| C | -4.41215000 | 2.02986600 | 0.08467100 |
| H | -4.97484700 | 1.51387800 | 0.88349200 |
| H | -4.52715400 | 3.11464800 | 0.21125800 |
| H | -4.83681300 | 1.73562800 | -0.89213000 |

**$B_2pin_2$**

| | | | |
|---|---|---|---|
| B | 0.85255700 | 0.00000900 | -0.00004100 |
| B | -0.85256200 | 0.00001700 | -0.00001900 |
| O | 1.61611500 | -0.49153500 | 1.02701300 |
| O | 1.61615300 | 0.49151800 | -1.02707000 |
| O | -1.61614900 | 1.02733900 | 0.49090500 |
| O | -1.61613300 | -1.02732800 | -0.49092900 |
| C | 2.99773900 | -0.52349600 | 0.58845100 |
| C | 2.99775600 | 0.52350800 | -0.58842500 |
| C | -2.99774300 | 0.58872600 | 0.52317600 |
| C | -2.99774800 | -0.58873900 | -0.52316000 |
| C | 3.89519500 | -0.16675200 | 1.76642300 |
| H | 3.82080600 | -0.94821300 | 2.53708300 |
| H | 4.94721900 | -0.09805100 | 1.44848400 |
| H | 3.60207700 | 0.78659400 | 2.22378600 |
| C | 3.28020800 | -1.95409200 | 0.12321300 |
| H | 4.33398300 | -2.08862700 | -0.16215900 |
| H | 3.05099100 | -2.64573900 | 0.94685700 |
| H | 2.64664300 | -2.22604500 | -0.73330200 |
| C | 3.28018500 | 1.95413200 | -0.12324600 |
| H | 4.33394600 | 2.08870000 | 0.16216200 |
| H | 3.05099500 | 2.64572700 | -0.94694200 |
| H | 2.64657800 | 2.22613000 | 0.73322100 |
| C | 3.89526300 | 0.16672600 | -1.76633600 |
| H | 3.82085700 | 0.94812800 | -2.53705400 |
| H | 4.94727900 | 0.09810100 | -1.44835600 |
| H | 3.60220500 | -0.78667200 | -2.22363300 |
| C | -3.89520900 | -1.76650700 | -0.16577600 |
| H | -4.94722500 | -1.44851100 | -0.09720600 |
| H | -3.82085200 | -2.53755500 | -0.94685500 |
| H | -3.60207000 | -2.22339900 | 0.78779000 |
| C | -3.28019200 | -0.12428900 | -1.95401400 |
| H | -3.05108000 | -0.94836300 | -2.64518300 |
| H | -4.33394000 | 0.16111800 | -2.08869600 |
| H | -2.64653800 | 0.73200000 | -2.22647900 |
| C | -3.28016600 | 0.12433700 | 1.95405900 |
| H | -3.05097000 | 0.94842100 | 2.64519000 |
| H | -4.33392800 | -0.16098800 | 2.08879000 |
| H | -2.64656400 | -0.73197900 | 2.22654500 |
| C | -3.89527100 | 1.76643600 | 0.16575500 |
| H | -4.94727000 | 1.44837900 | 0.09721700 |

| | | | |
|---|---|---|---|
| H | -3.82094100 | 2.53751900 | 0.94680300 |
| H | -3.60217700 | 2.22330400 | -0.78783800 |

**H**Bpin

| | | | |
|---|---|---|---|
| B | -0.00000100 | 1.94464600 | -0.00000200 |
| O | -1.07839100 | 1.19860000 | -0.37036500 |
| O | 1.07839200 | 1.19860200 | 0.37035800 |
| C | -0.78826700 | -0.18662200 | -0.04902800 |
| C | 0.78826700 | -0.18662200 | 0.04902800 |
| C | 1.36272400 | -1.07543600 | 1.14431900 |
| H | 1.08738600 | -2.12796400 | 0.97560700 |
| H | 2.46032900 | -1.00361200 | 1.14009400 |
| H | 1.00895200 | -0.77353600 | 2.13810700 |
| C | 1.47656700 | -0.48239700 | -1.28547400 |
| H | 2.54829000 | -0.25612000 | -1.18885900 |
| H | 1.36750200 | -1.53833500 | -1.57290300 |
| H | 1.06935800 | 0.14386000 | -2.09232800 |
| C | -1.47656500 | -0.48238900 | 1.28547600 |
| H | -2.54828800 | -0.25611100 | 1.18886200 |
| H | -1.36750000 | -1.53832500 | 1.57291000 |
| H | -1.06935300 | 0.14387300 | 2.09232600 |
| C | -1.36272700 | -1.07544300 | -1.14431300 |
| H | -1.08738700 | -2.12797000 | -0.97559600 |
| H | -2.46033100 | -1.00362000 | -1.14008500 |
| H | -1.00895800 | -0.77354700 | -2.13810400 |
| H | 0.00000100 | 3.14401800 | -0.00000900 |

**11. References**

1. J. H. Seo, D. J. Kim, S. H. Kim, Y. J. Kim, S. D. Moon, W. S. Cho, H. S. Lee, D. U. Jung, KR2014121343 A. 2014.10.15.

2. X. Sheng, Y. Wang, Y. Qin, X. Wang, F. Wang, *RSC Adv.* 2014, **4**, 54043-54050.

3. T. Moriya, S. Yoneda, K. Kawana, R. Ikeda, T. Konakahara, N. Sakai, *Org. Lett.* 2012, **14**, 4842-4845.

4. S. Murphy, F. Ivol, A. R. Neale, P. Goodrich, F. Ghamouss, C. Hardacre, J. Jacquemin, *Chem. Phys. Chem.* 2018, **19**, 3226-3236.

5. Y. Fang, T. Rogge, L. Ackermann, S. Y. Wang, S. J. Ji, *Nat. Commun.* 2018, **9**, 2240-2248.

6. Q. Xie, G. Dong, *J. Am. Chem. Soc.* 2022, **144**, 8498-8503.

7. S. Z. Sun, Y. Duan, R. S. Mega, R. J. Somerville, R. S. Martin, *Angew. Chem. Int. Ed.* 2020, **59**, 4370-4374.

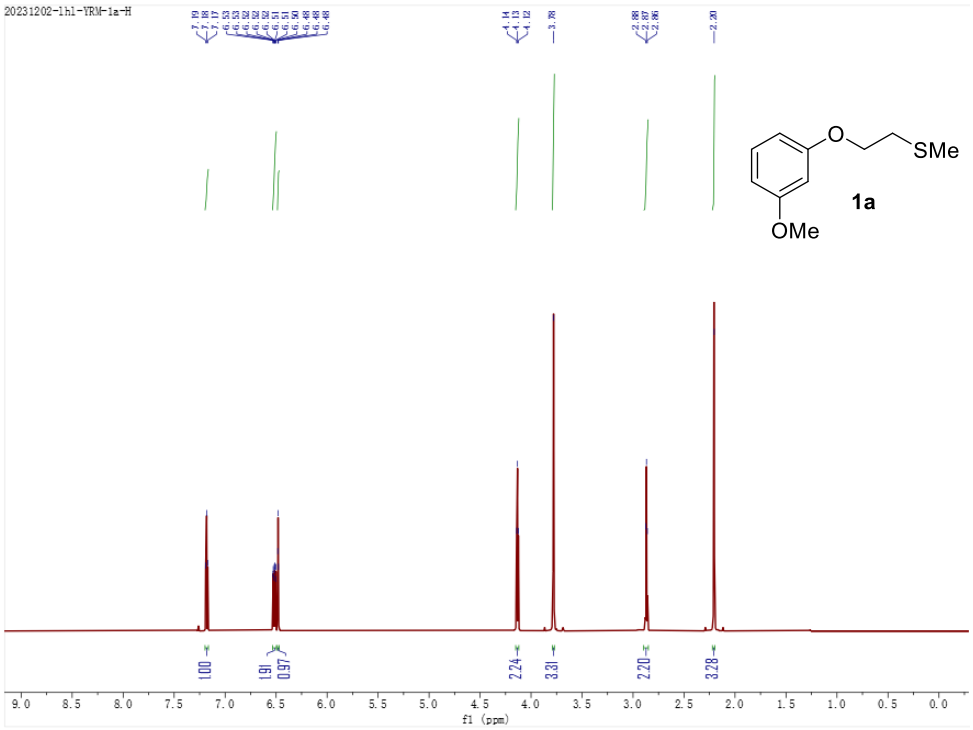
8. A. Bonet, M. Odachowski, D. Leonori, S. Essafi, V. K. Aggarwal, *Nat. Chem.* 2014, **6**, 584-589.

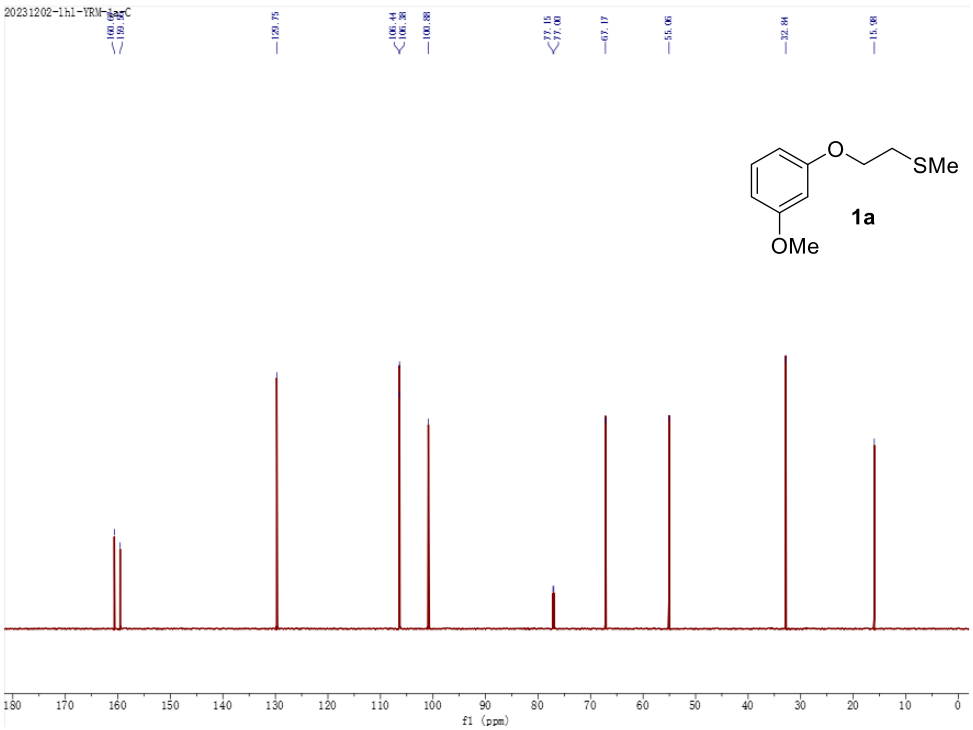
9. V. A. Kallepalli, K. A. Gore, F. Shi, L. Sanchez, G. A. Chotana, S. L. Miller, Jr. R. E. Maleczka, M. Smith III, *J. Org. Chem.* 2015, **80**, 8341-8353.

10. T. M. Boller, J. M. Murphy, M. Hapke, T. Ishiyama, N. Miyaura, J. F. Hartwig, J *J. Am. Chem. Soc.* **2005**, *127*, 14263-14278.

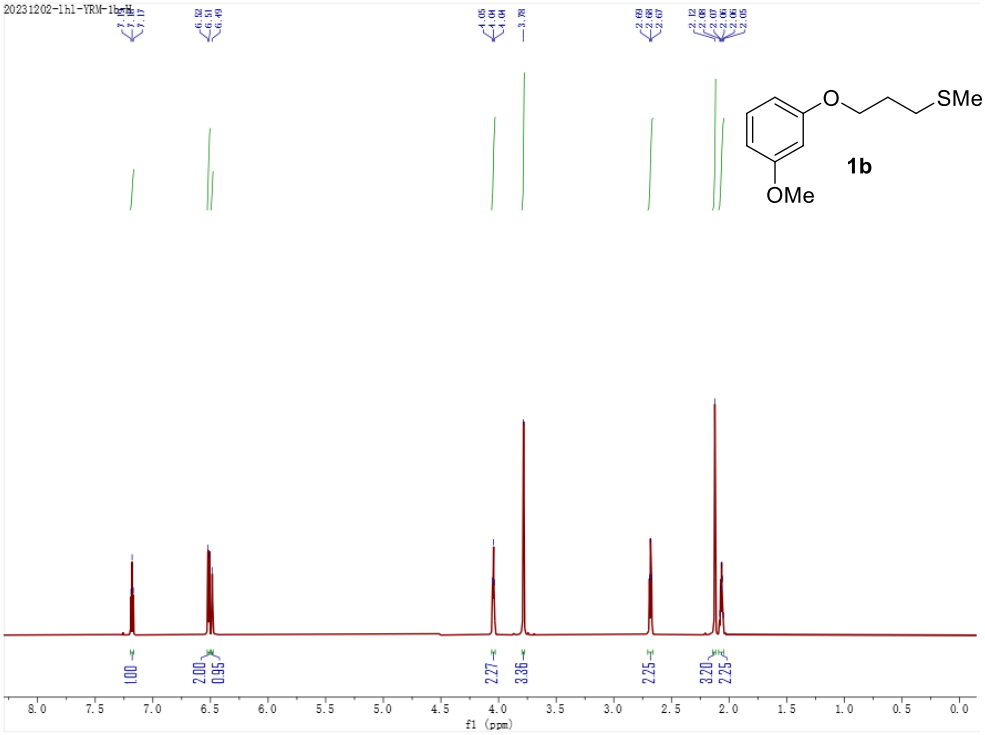
## 12 NMR-Chart

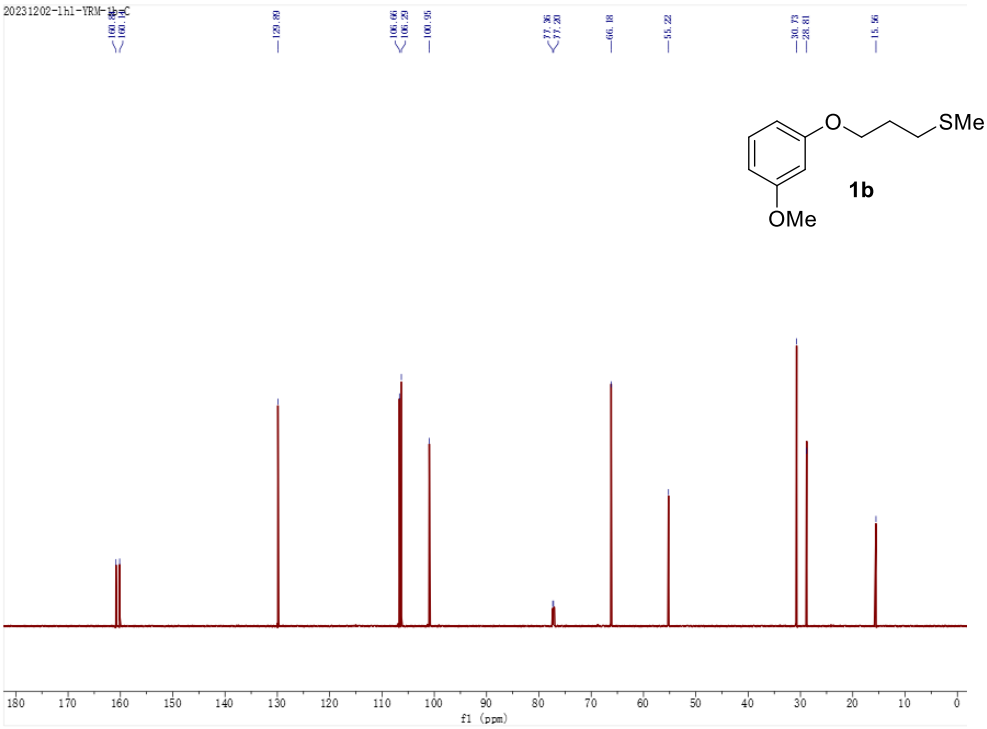
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1a**



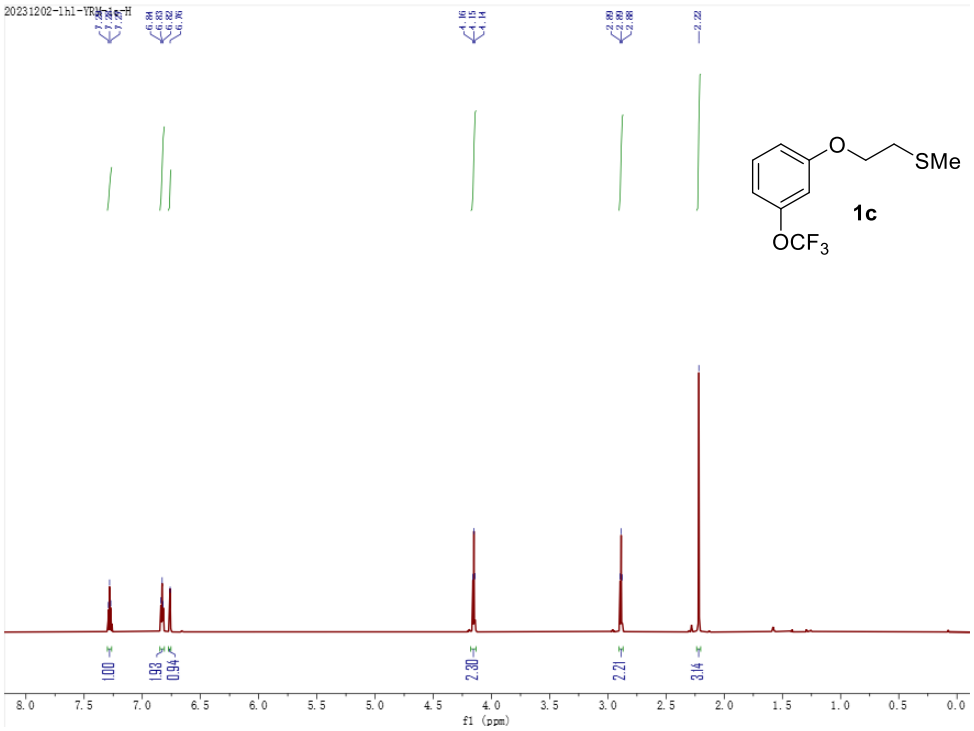



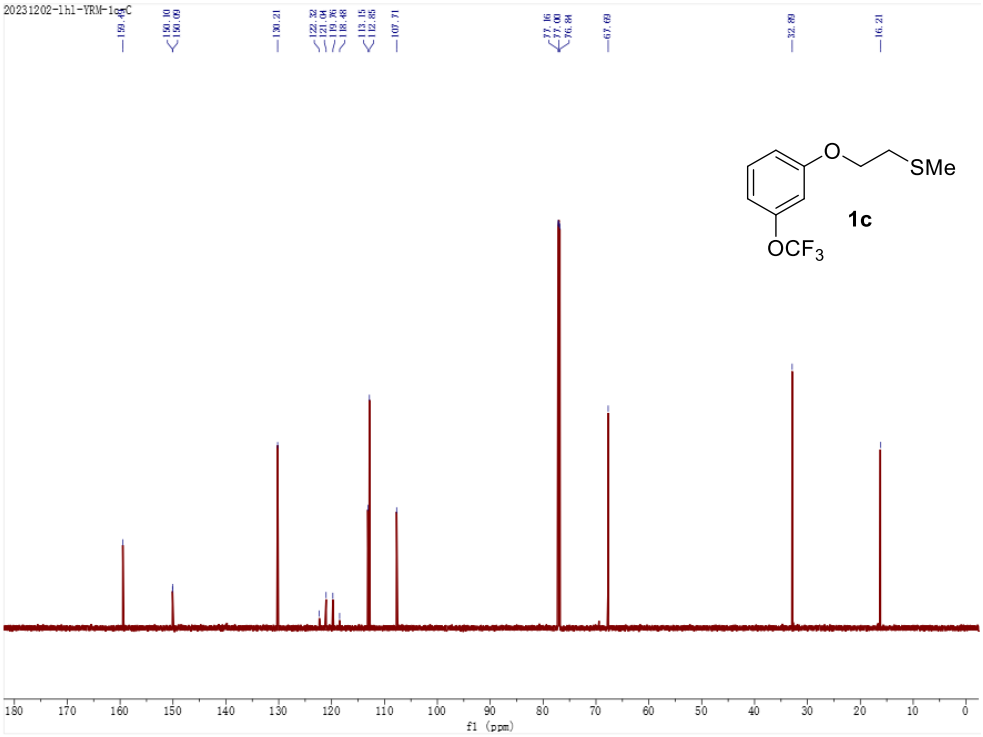
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1b**



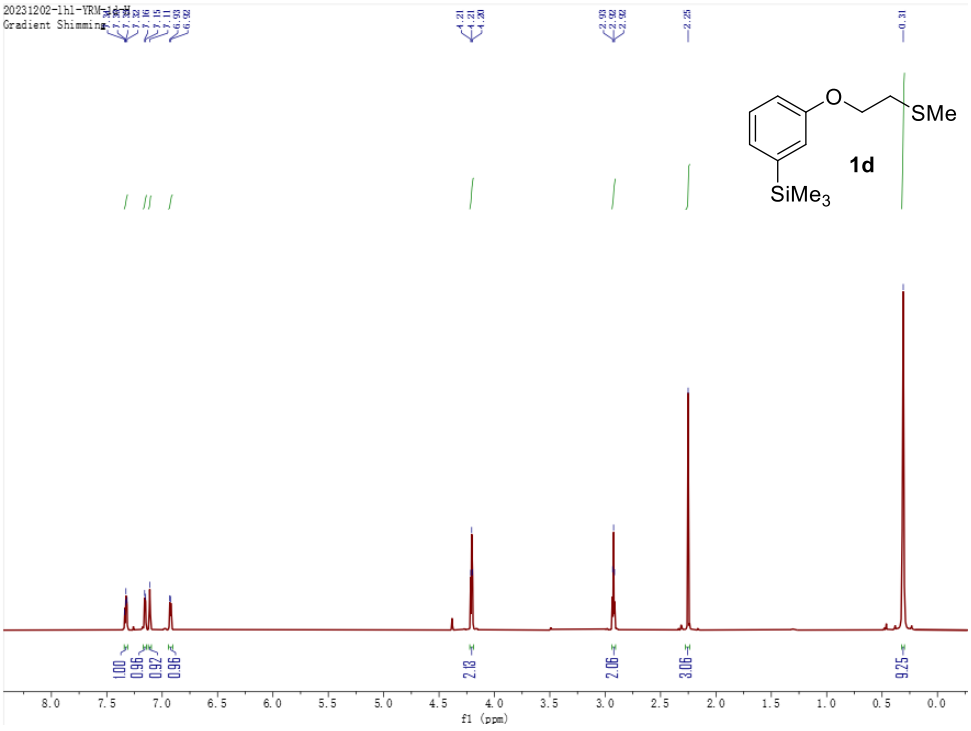



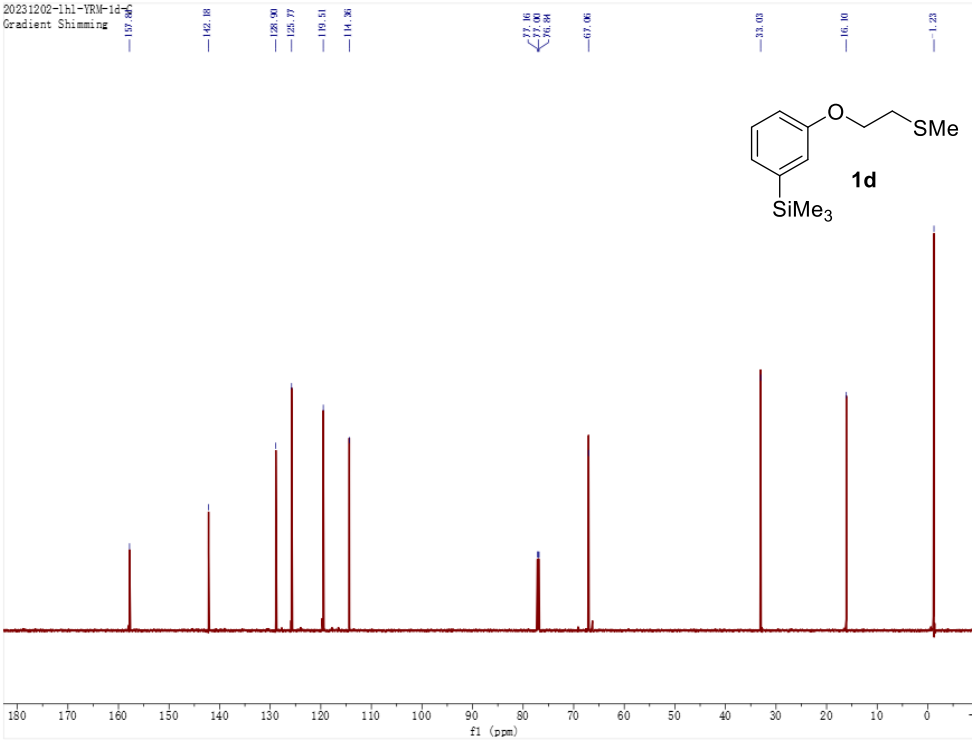
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1c**



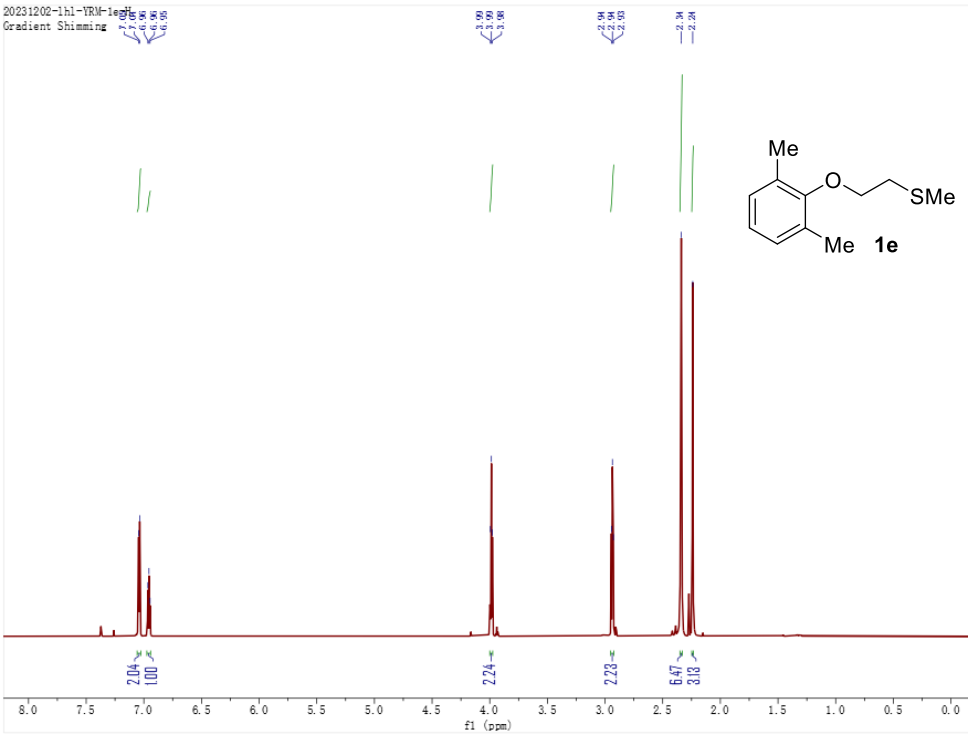



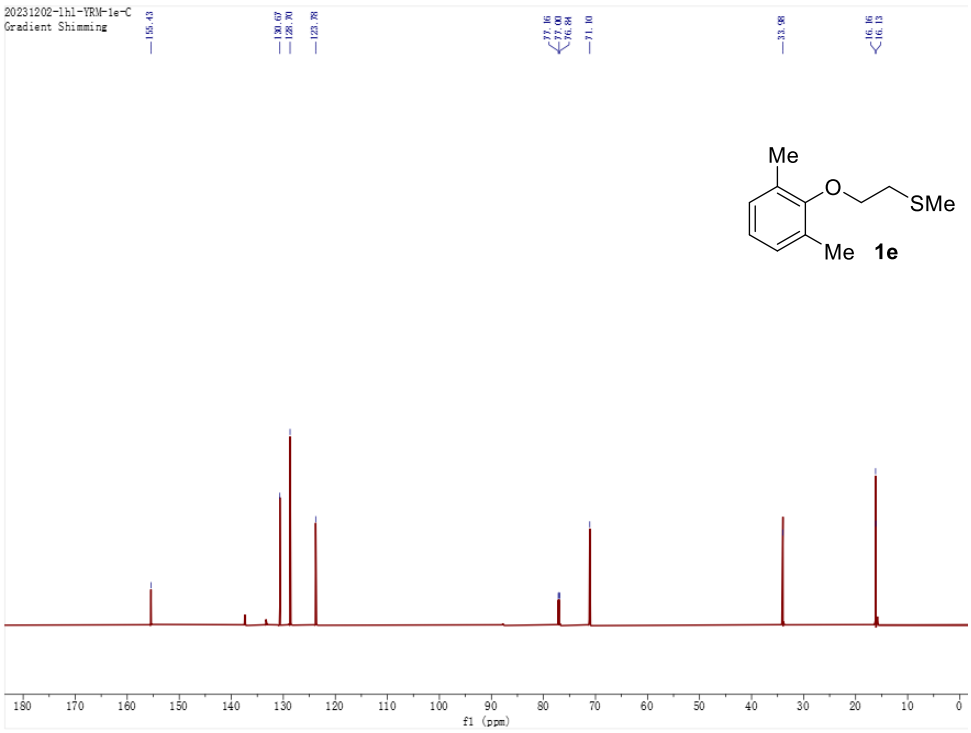
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1d**



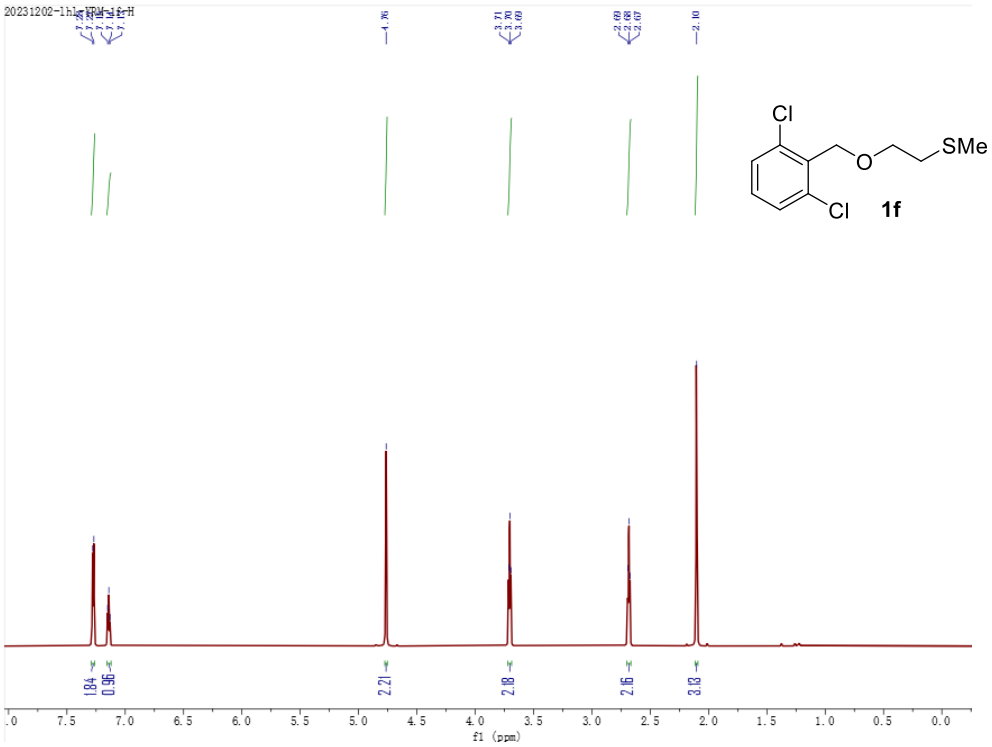



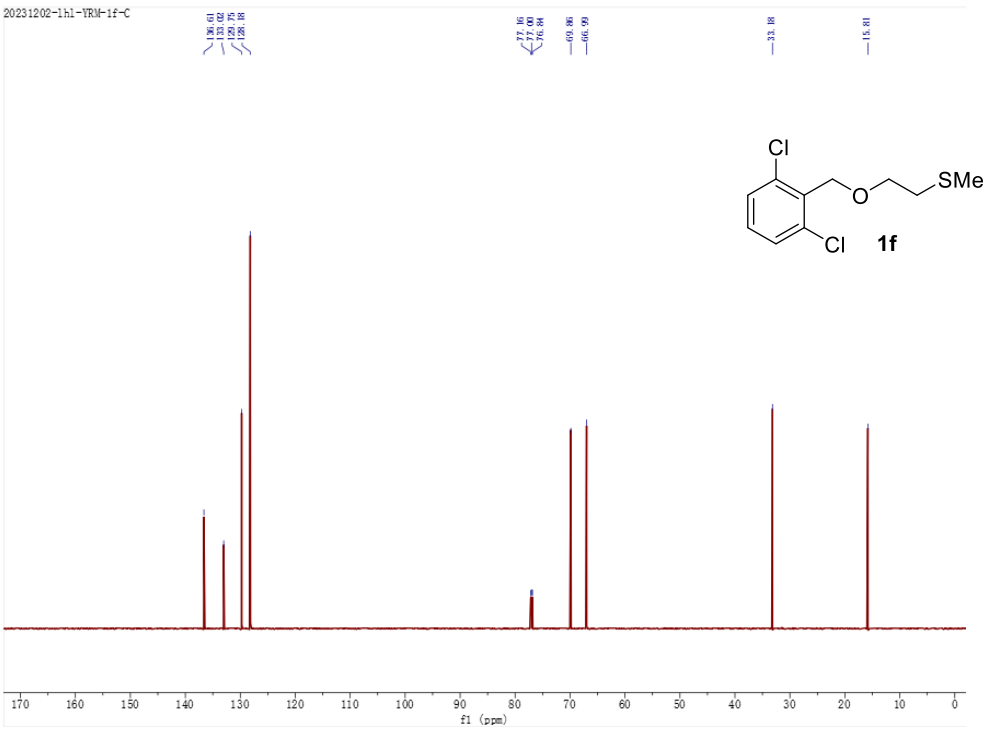
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1e**



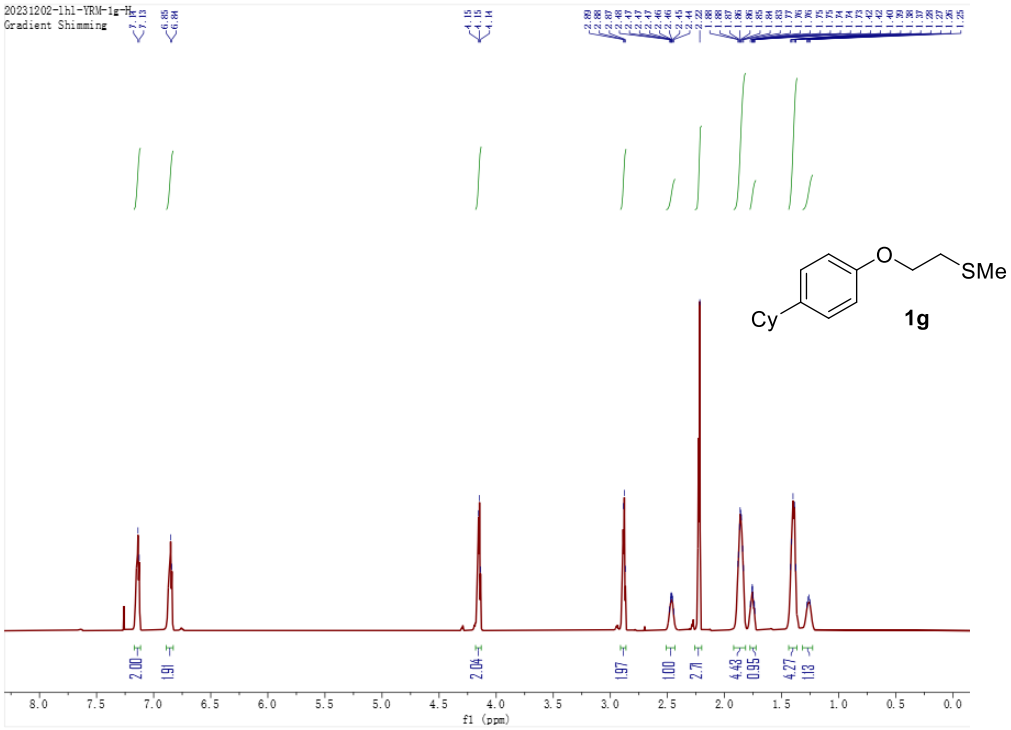



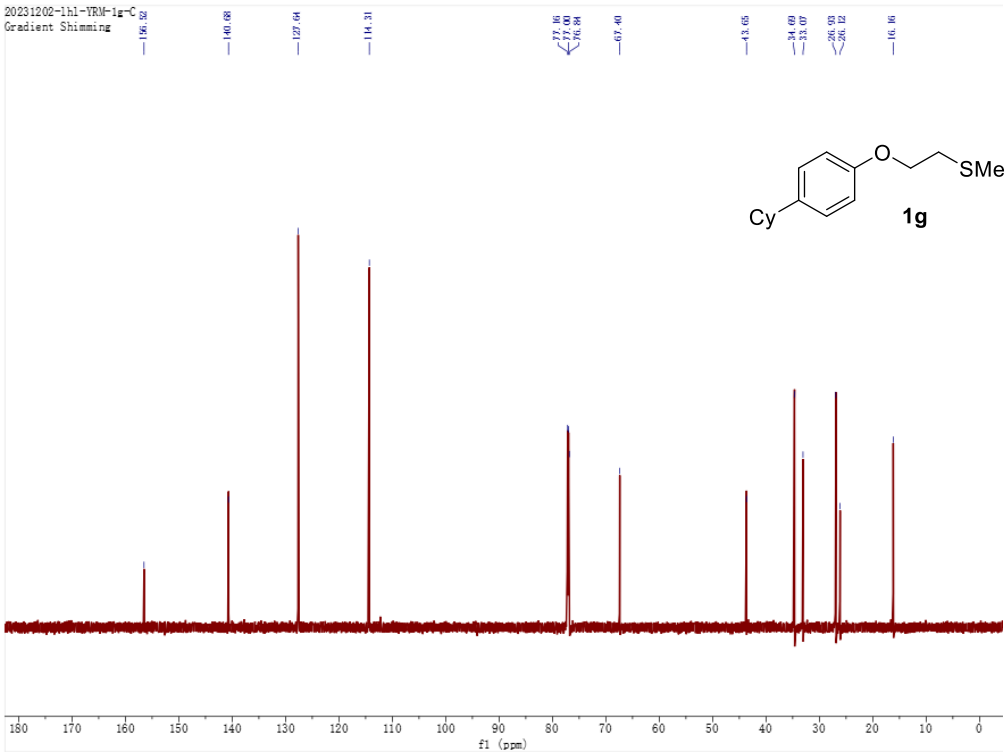
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1f**



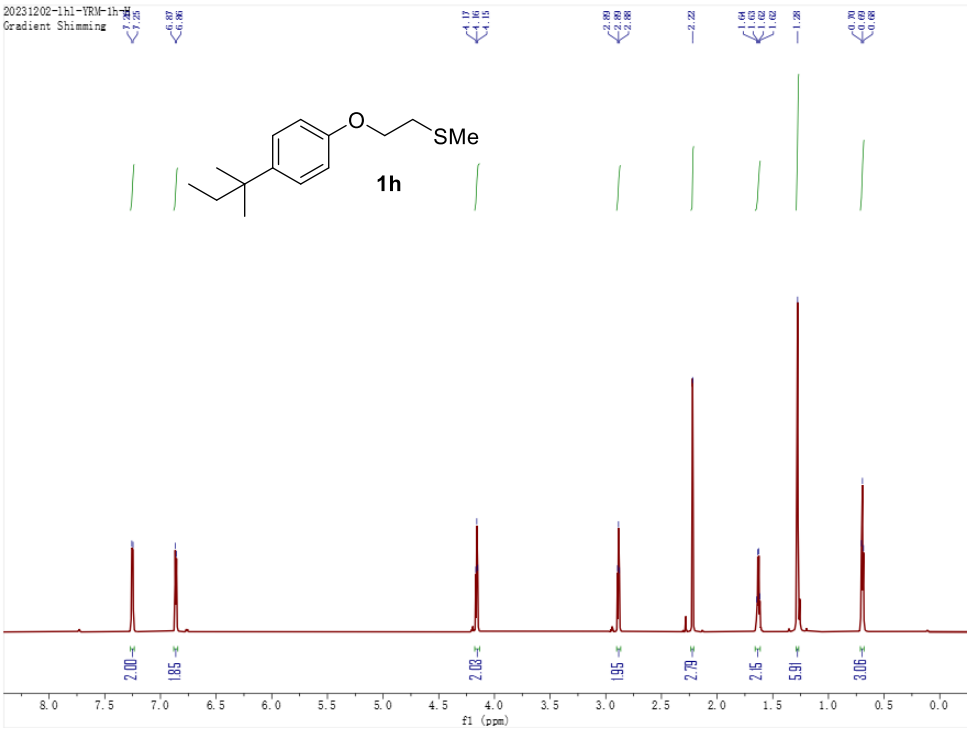



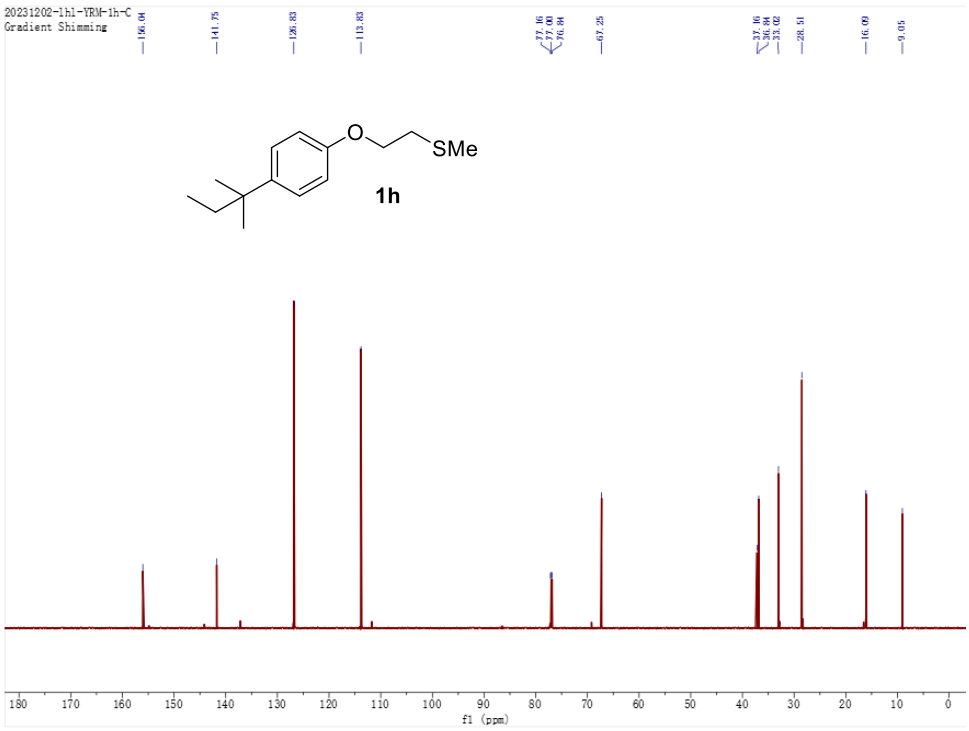
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1g**



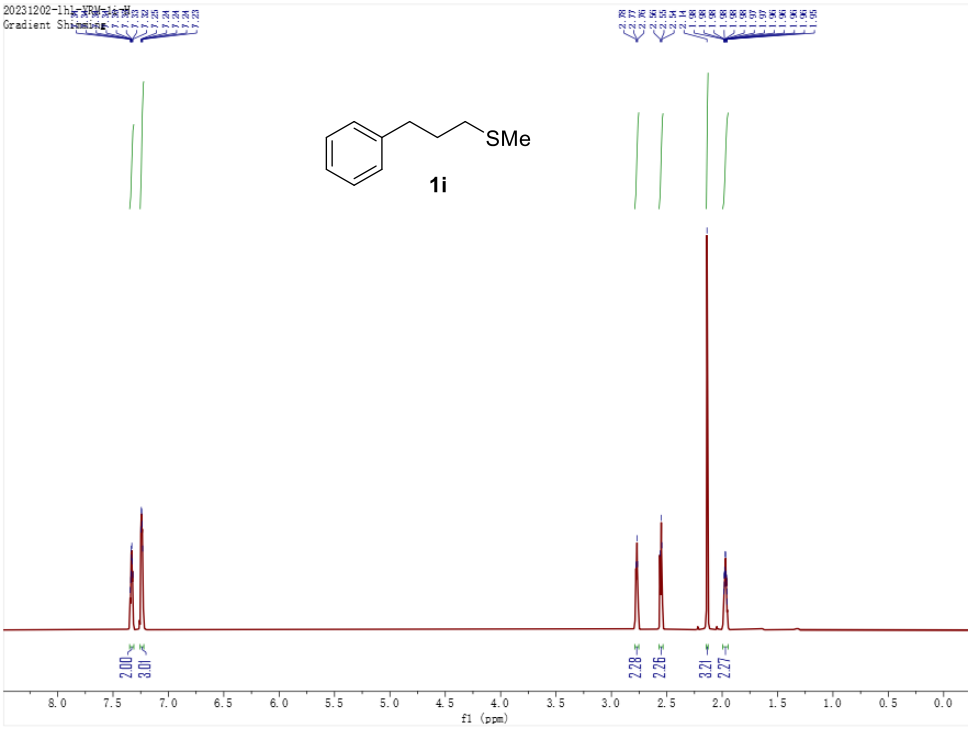



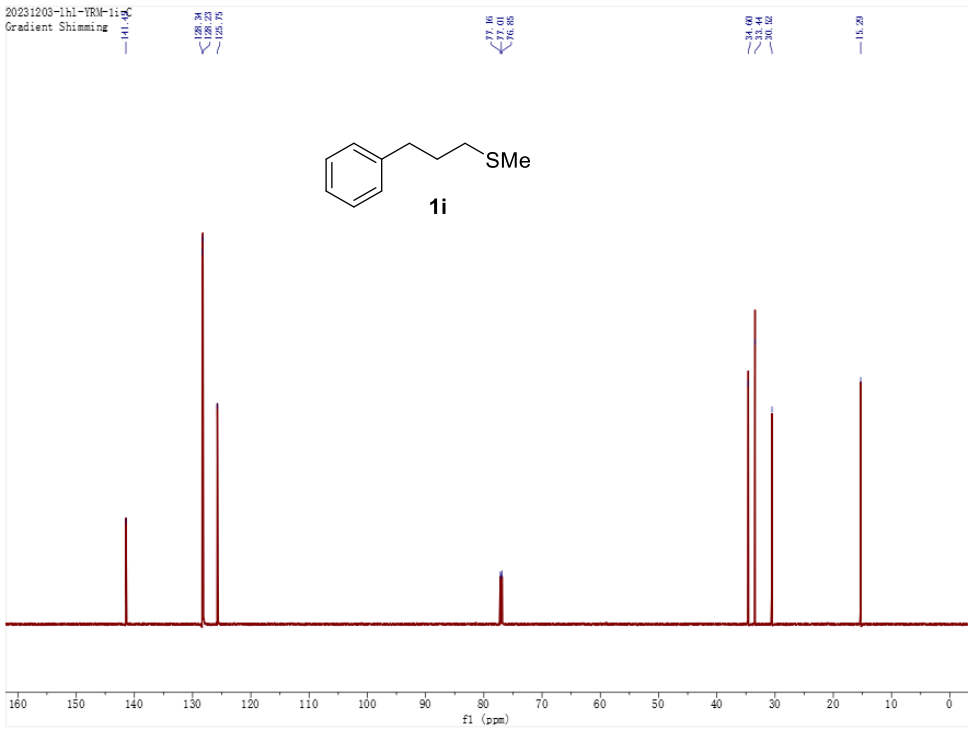
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1h**



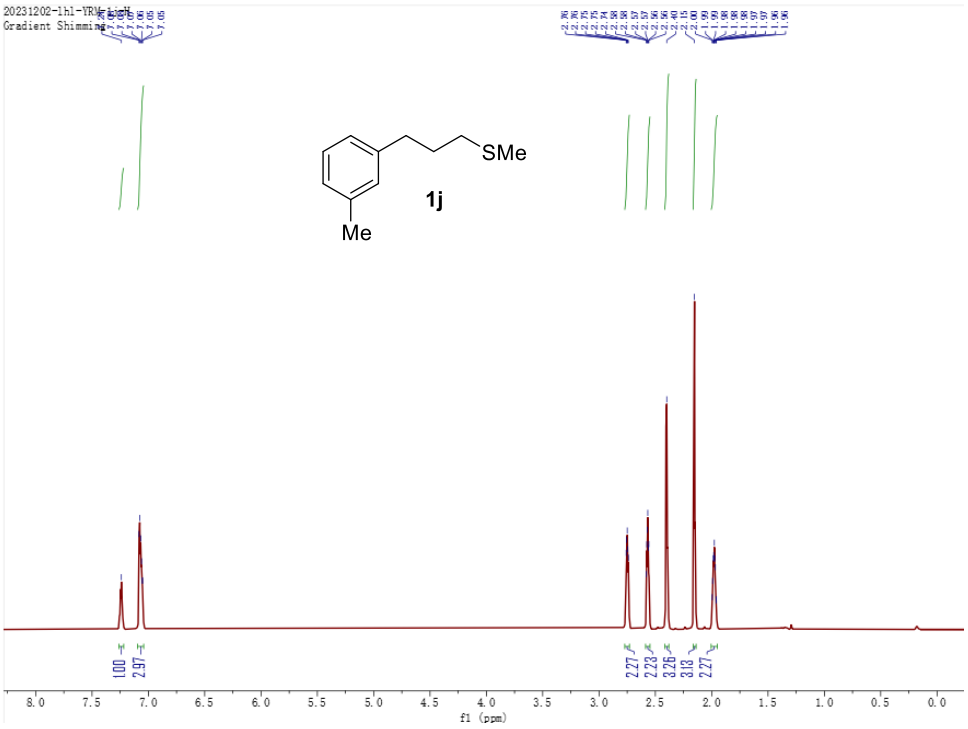



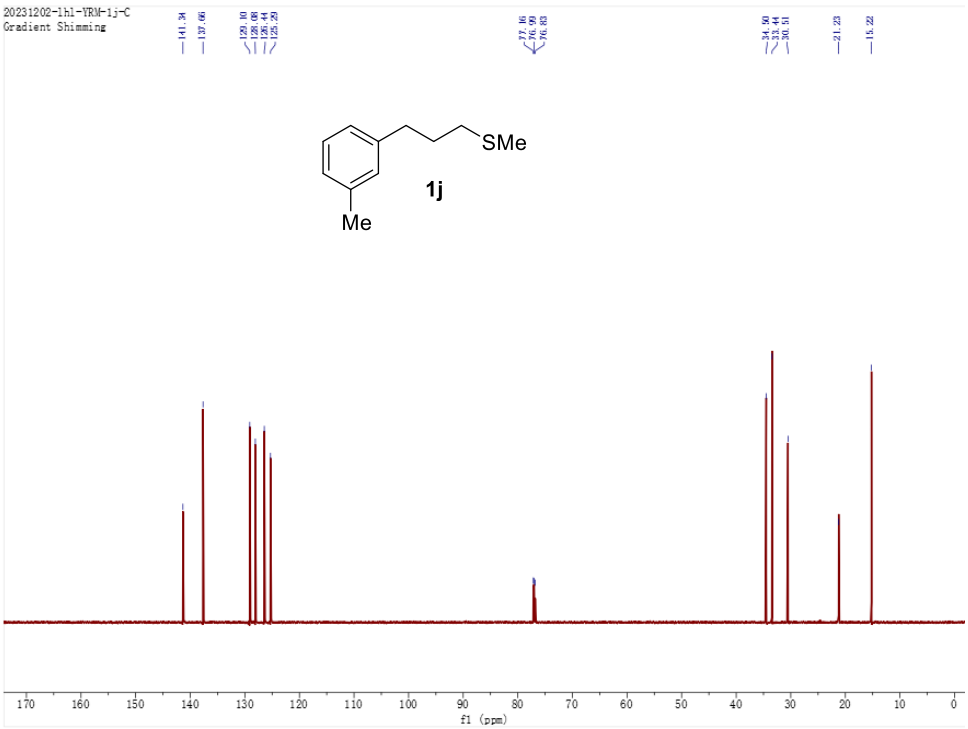
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1i**



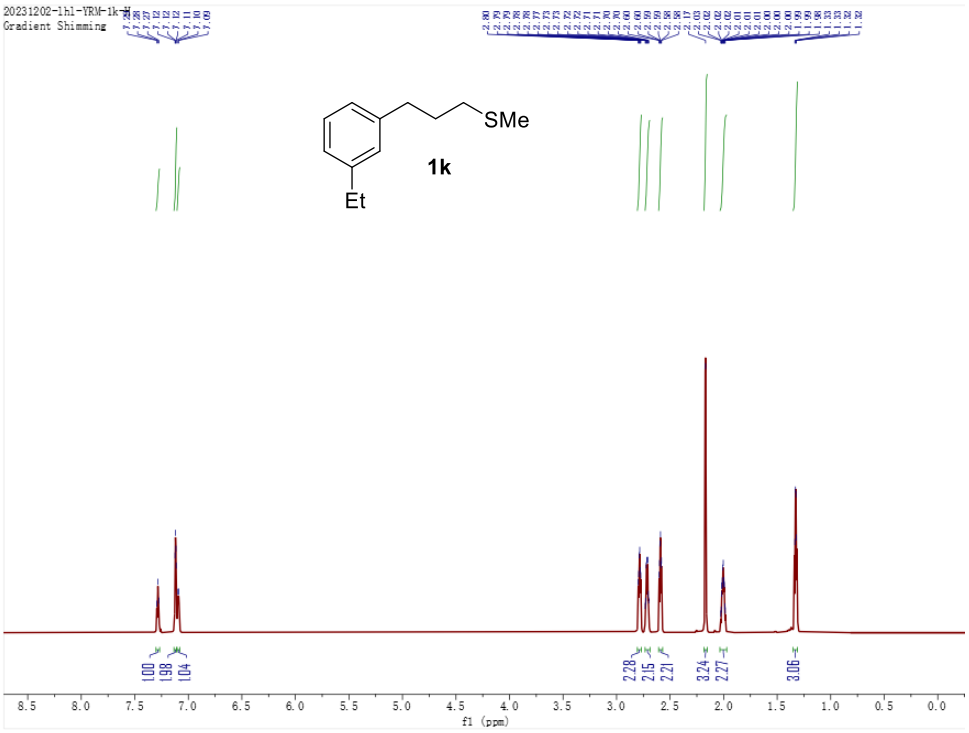



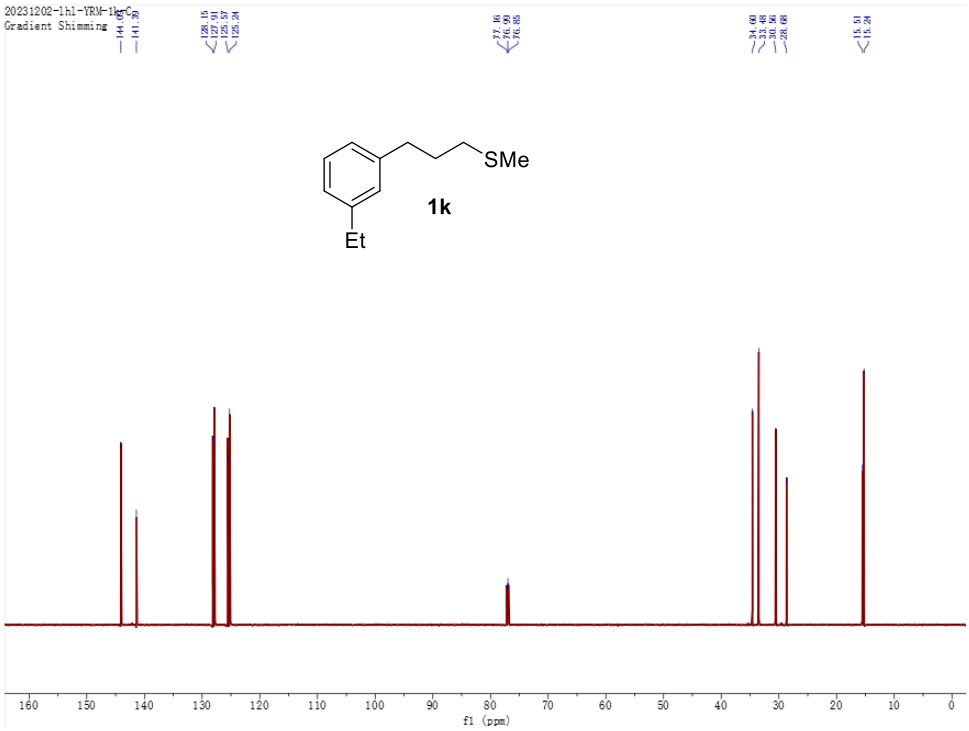
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1j**



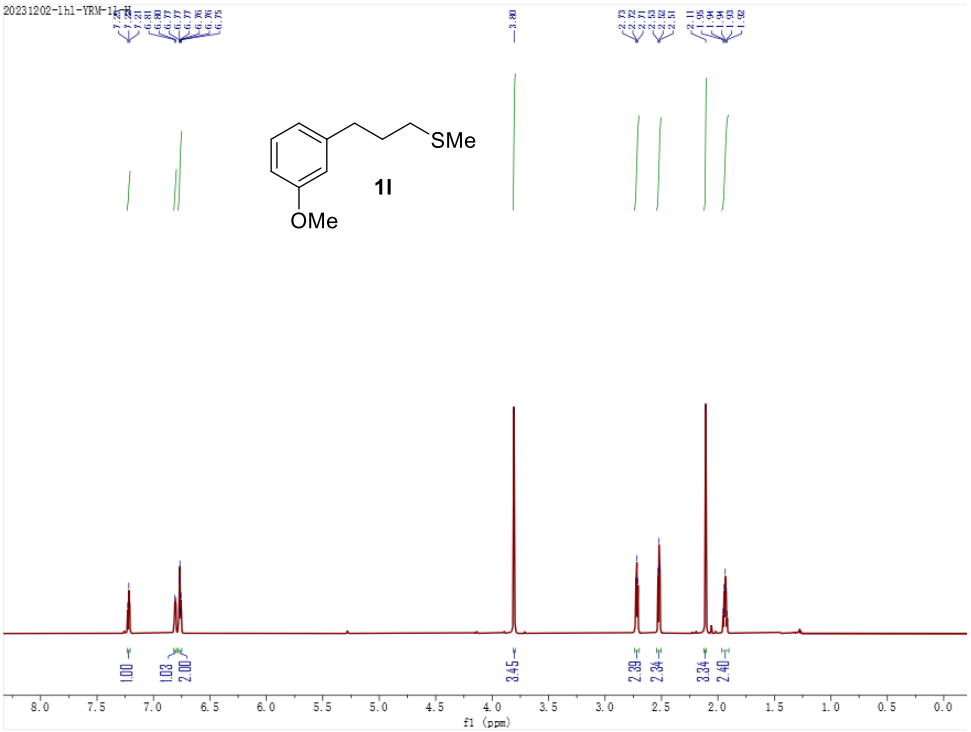



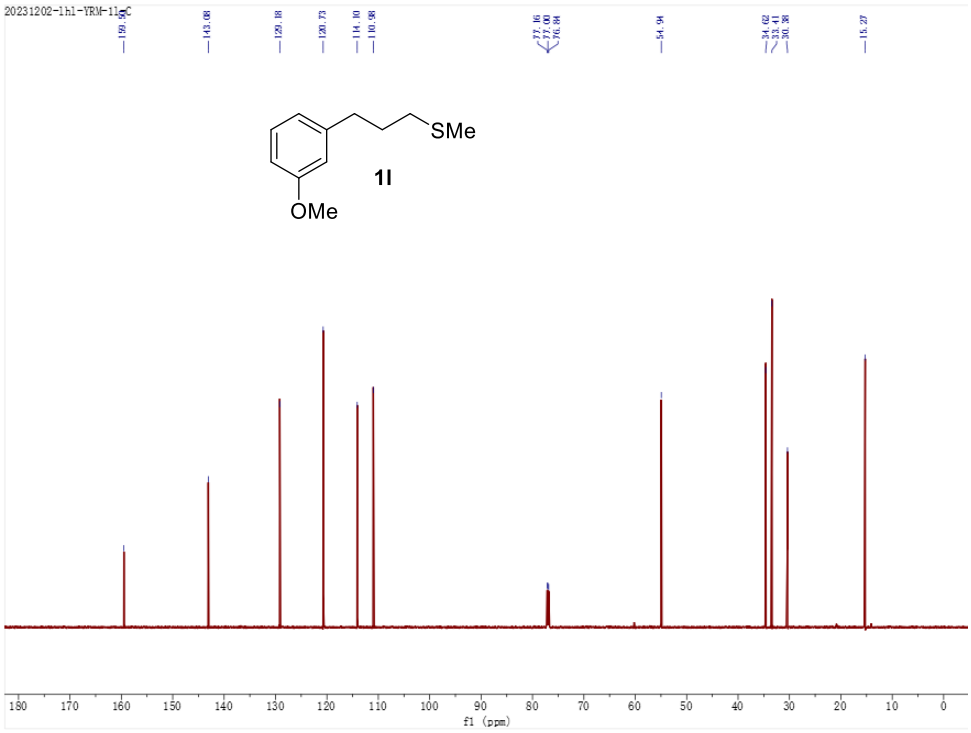
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1k**



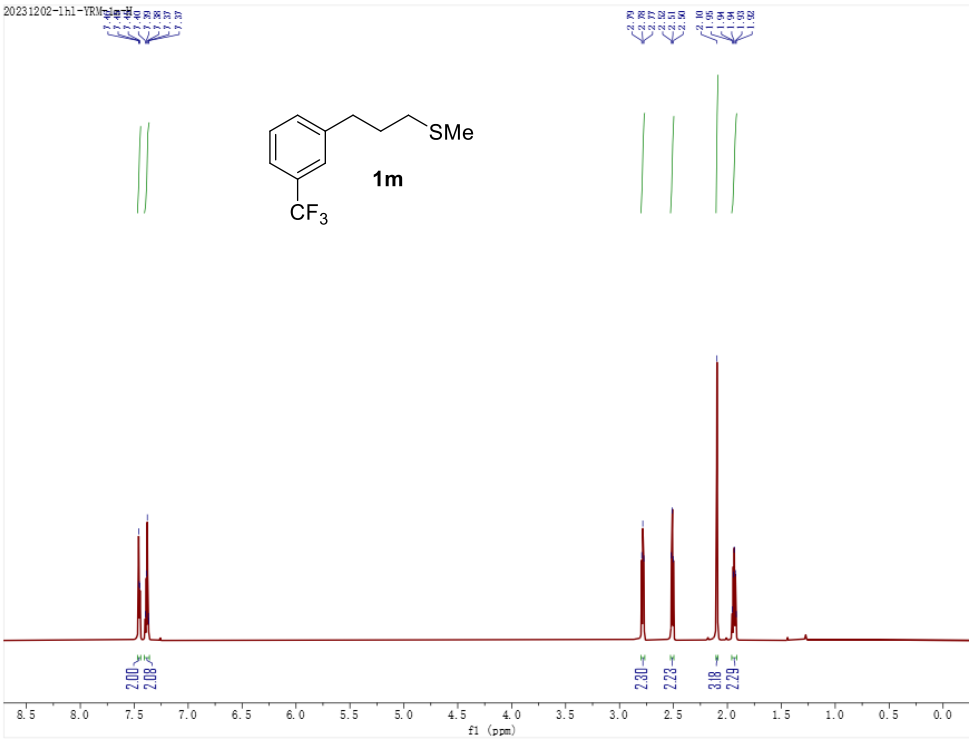



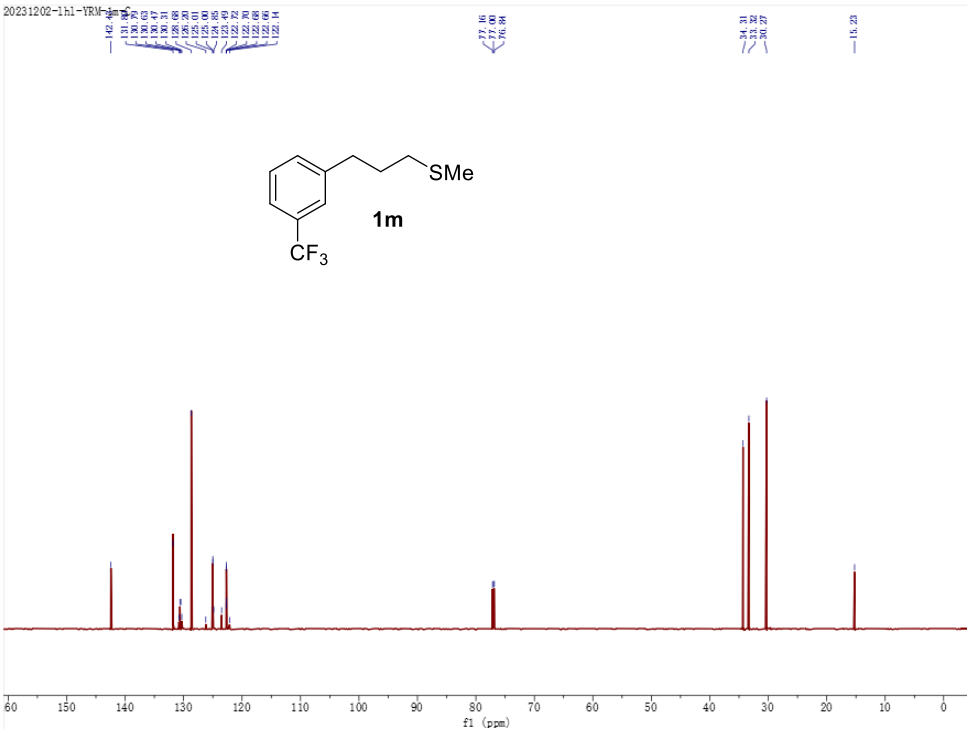
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1l**



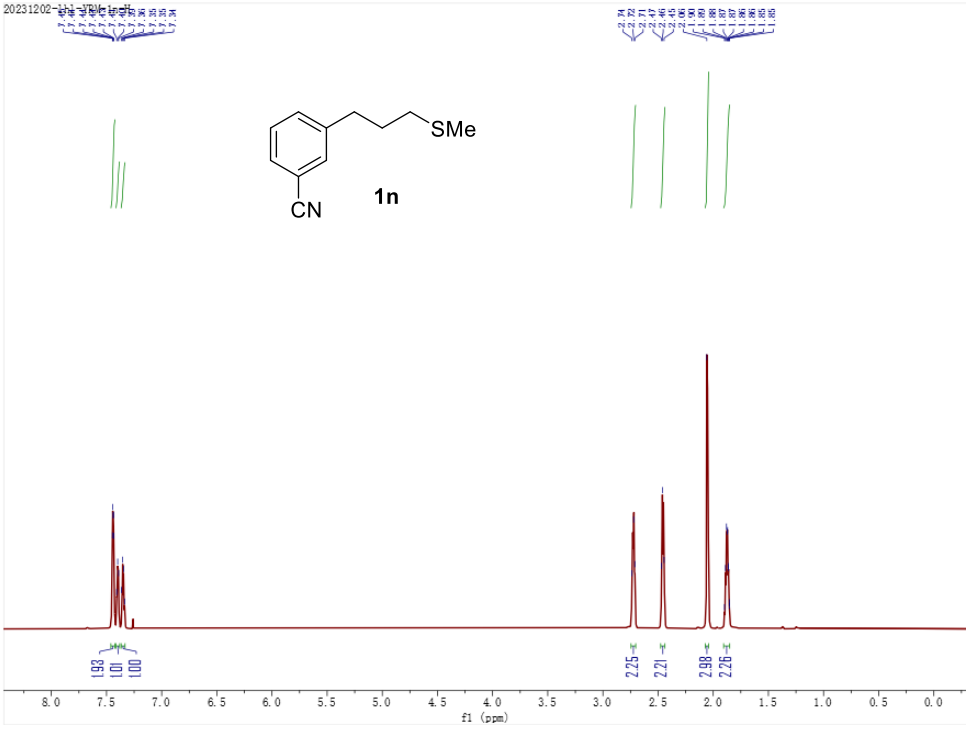



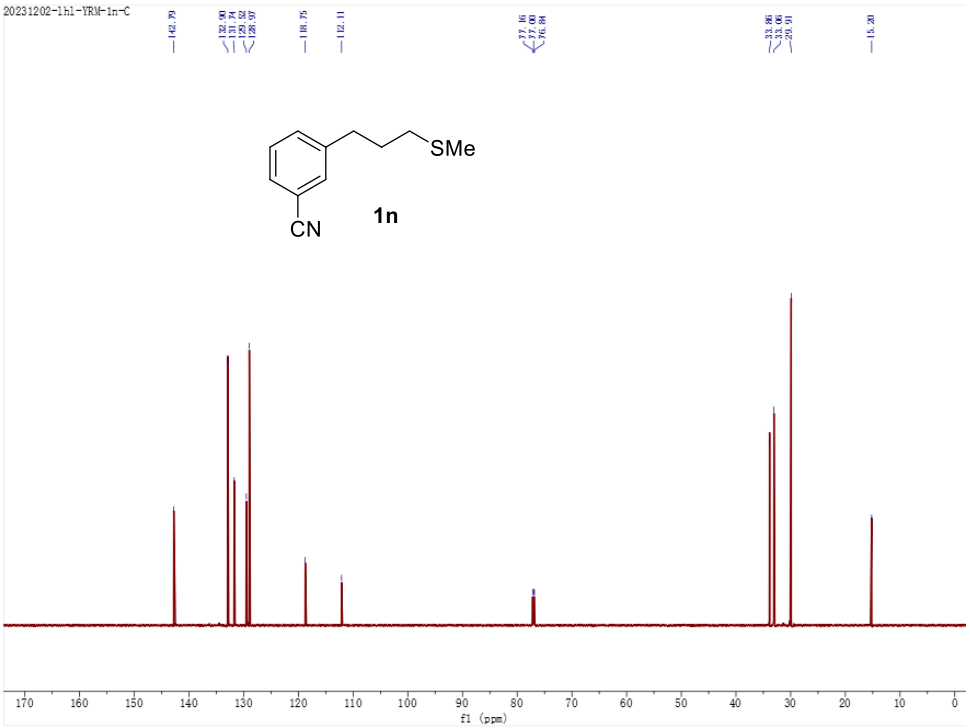
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1m**



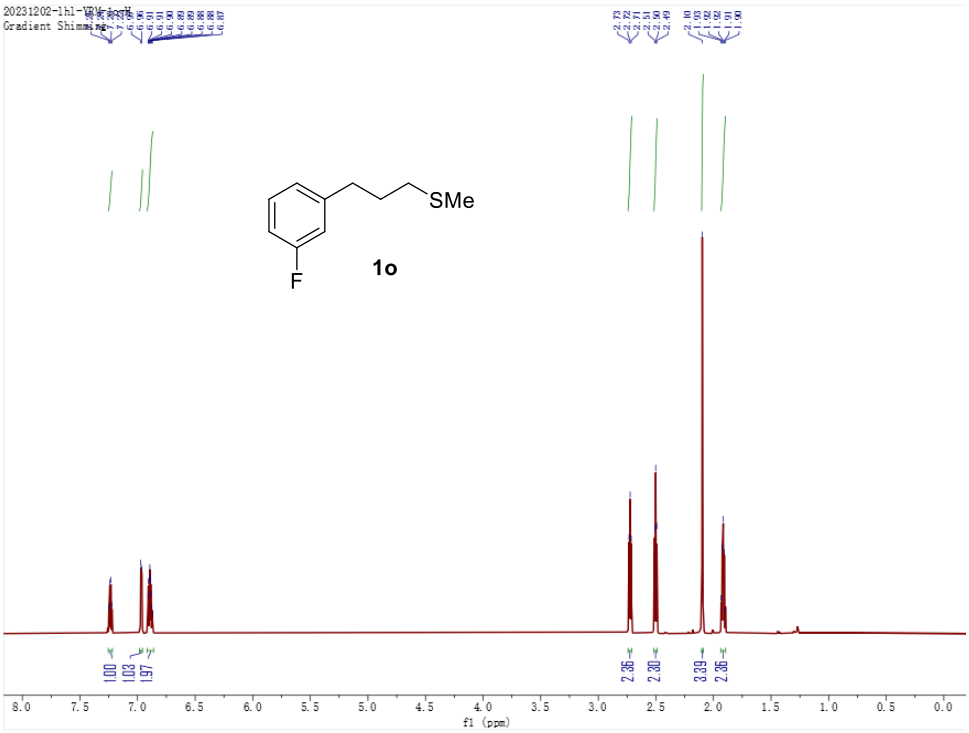



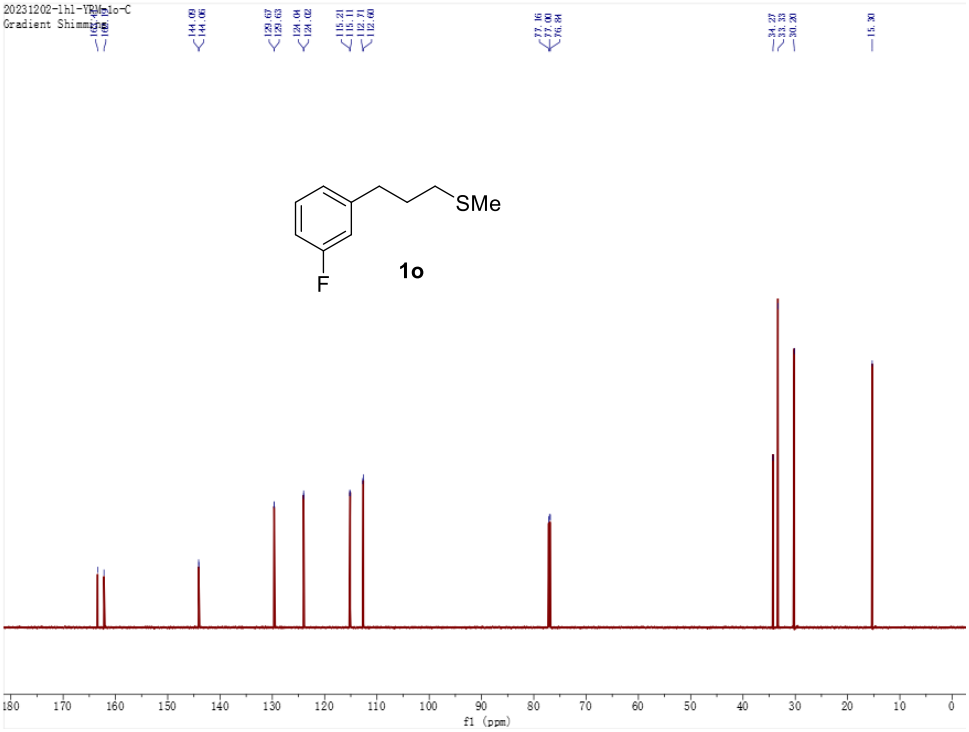
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1n**



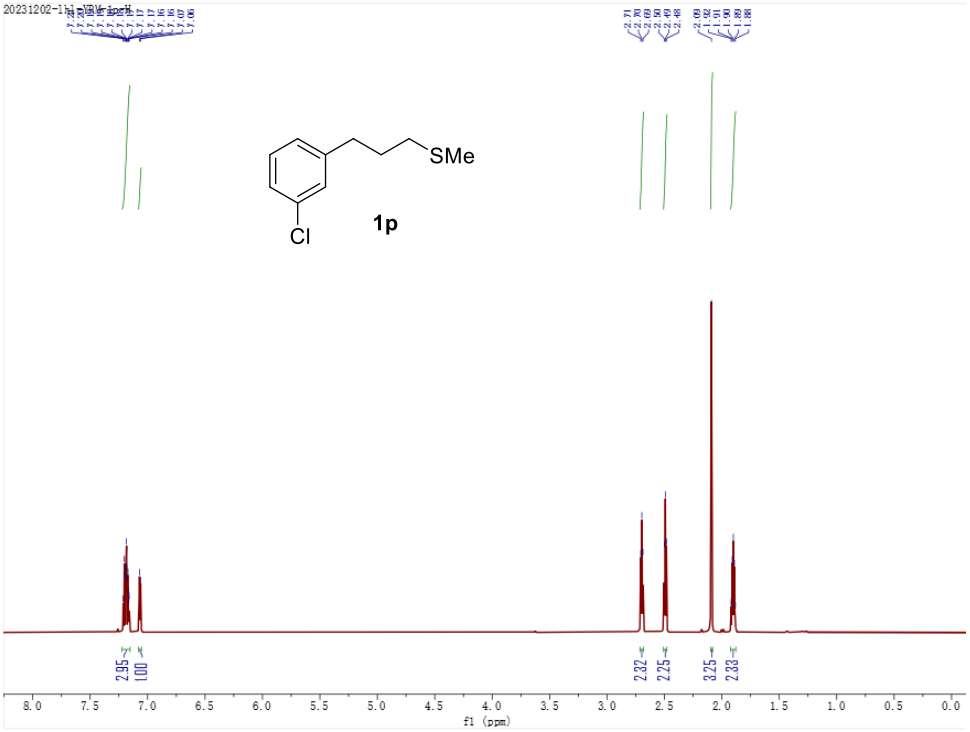



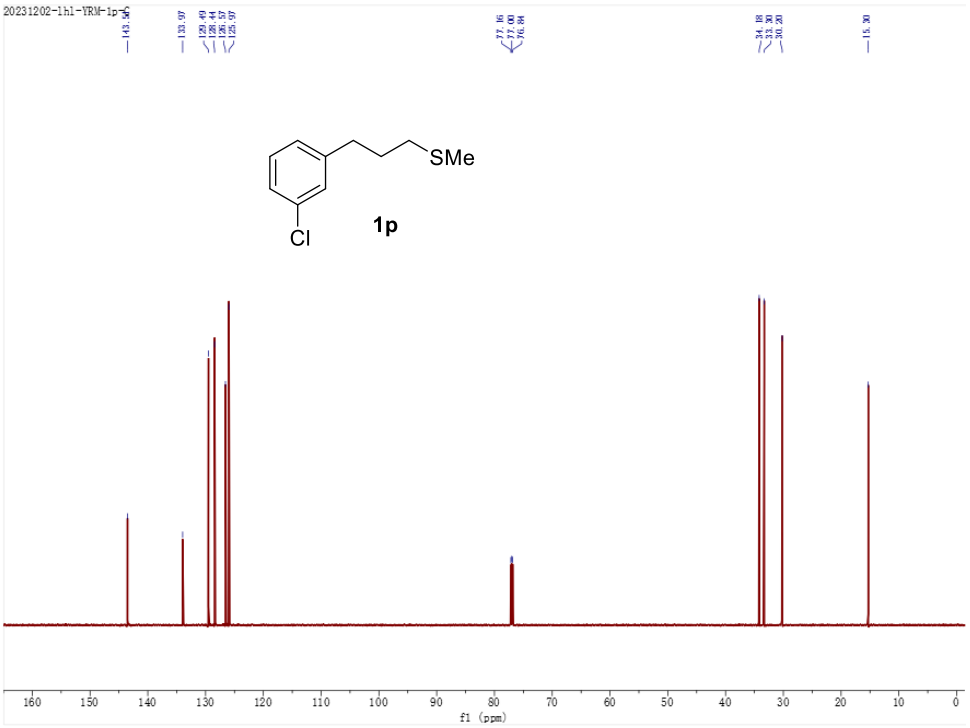
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1o**



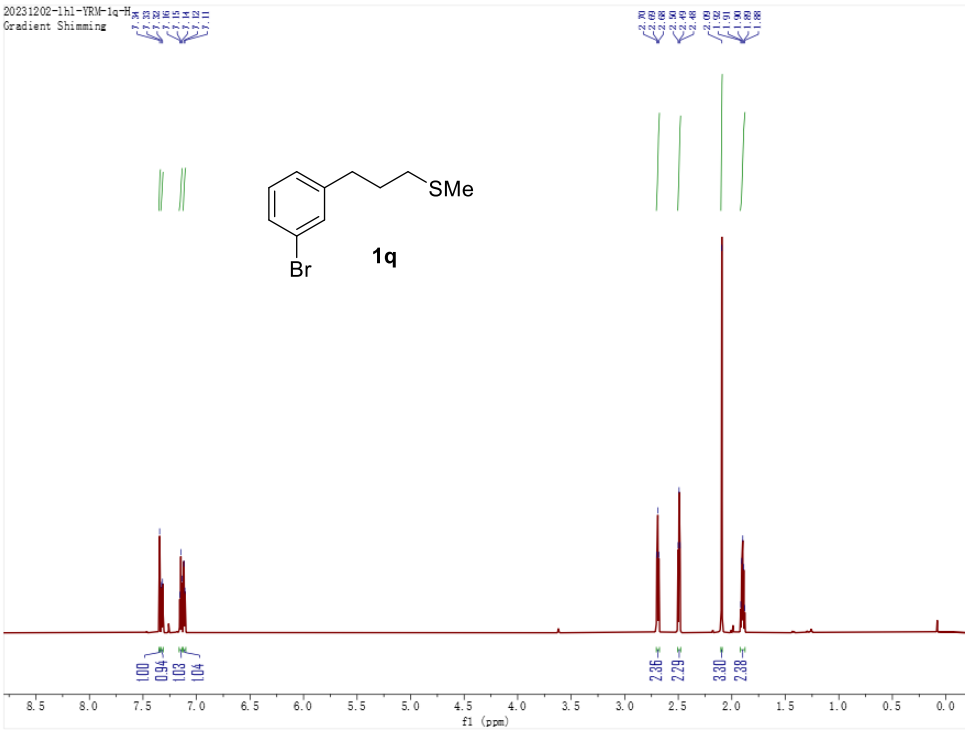



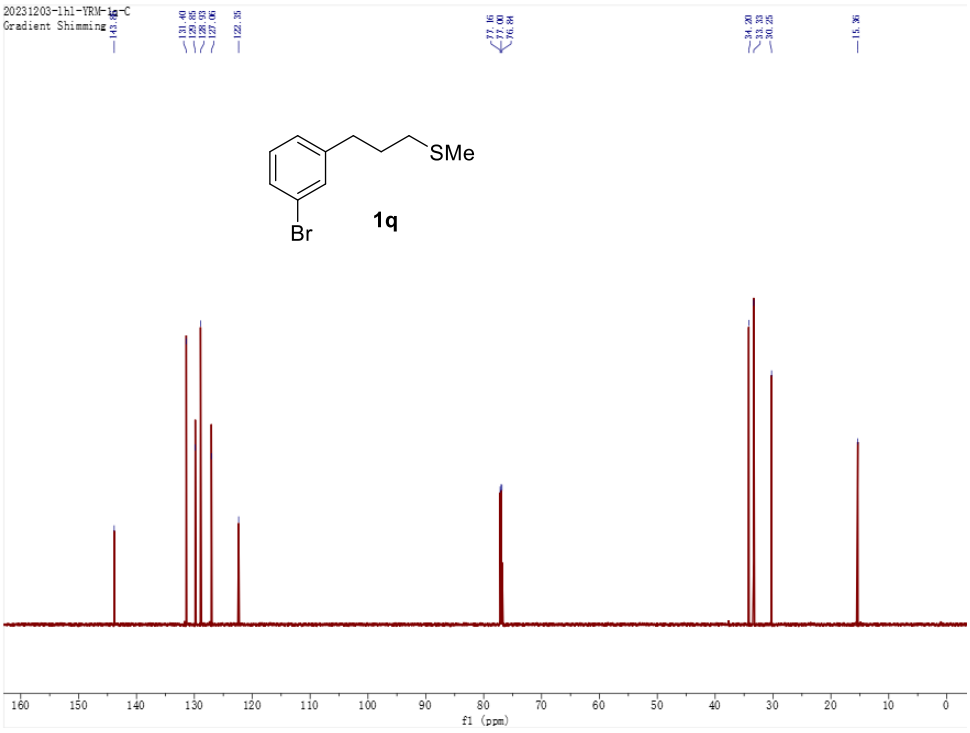
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1p**



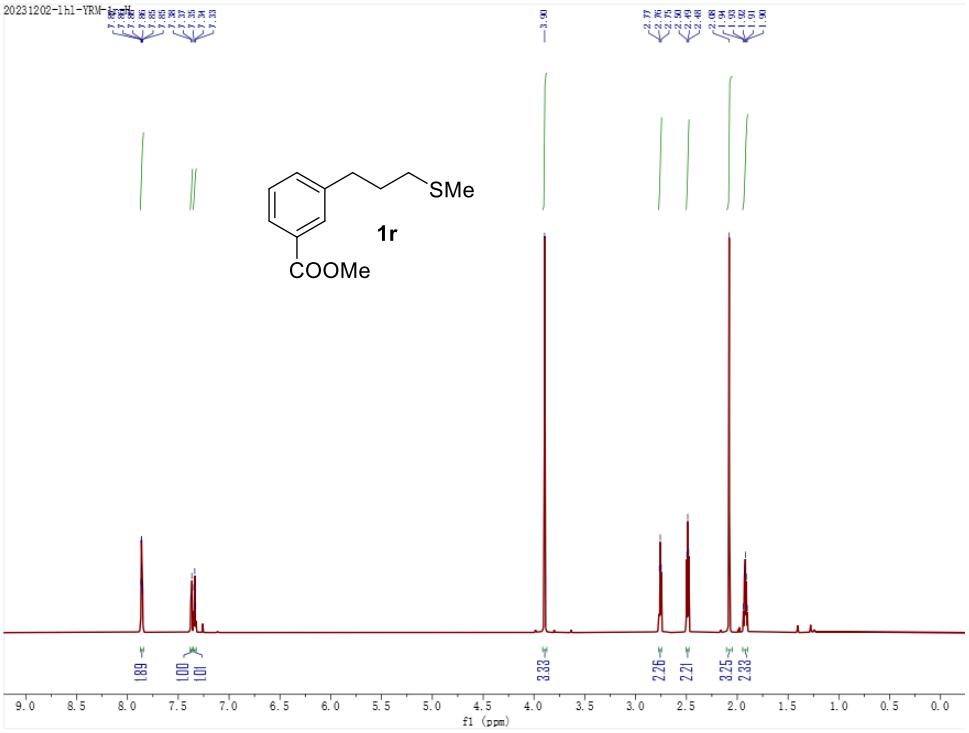



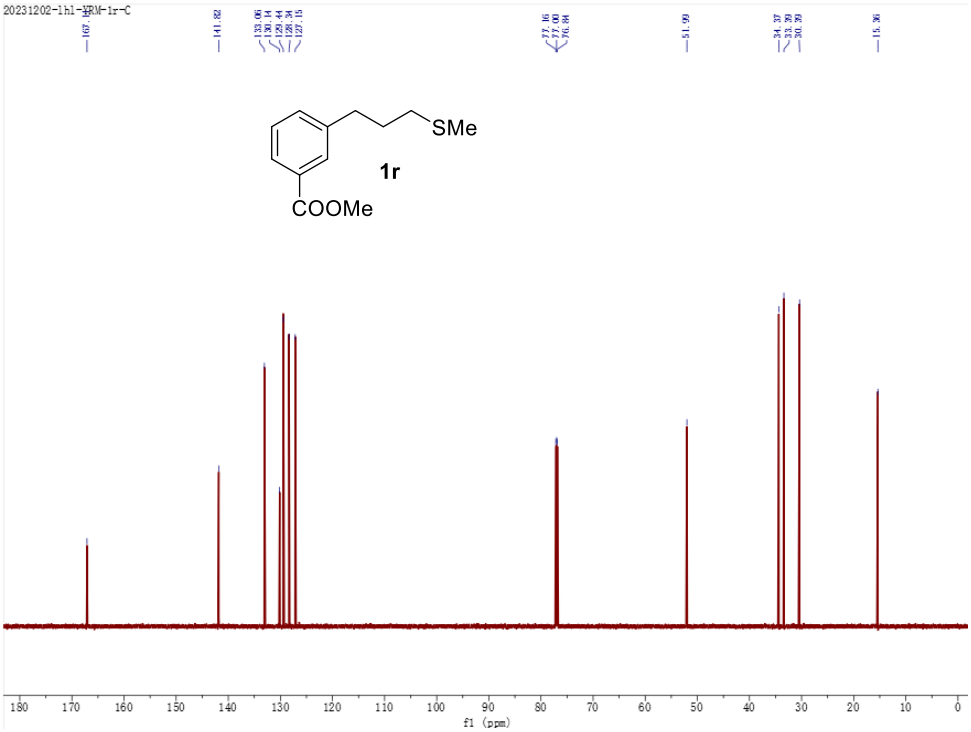
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1q**



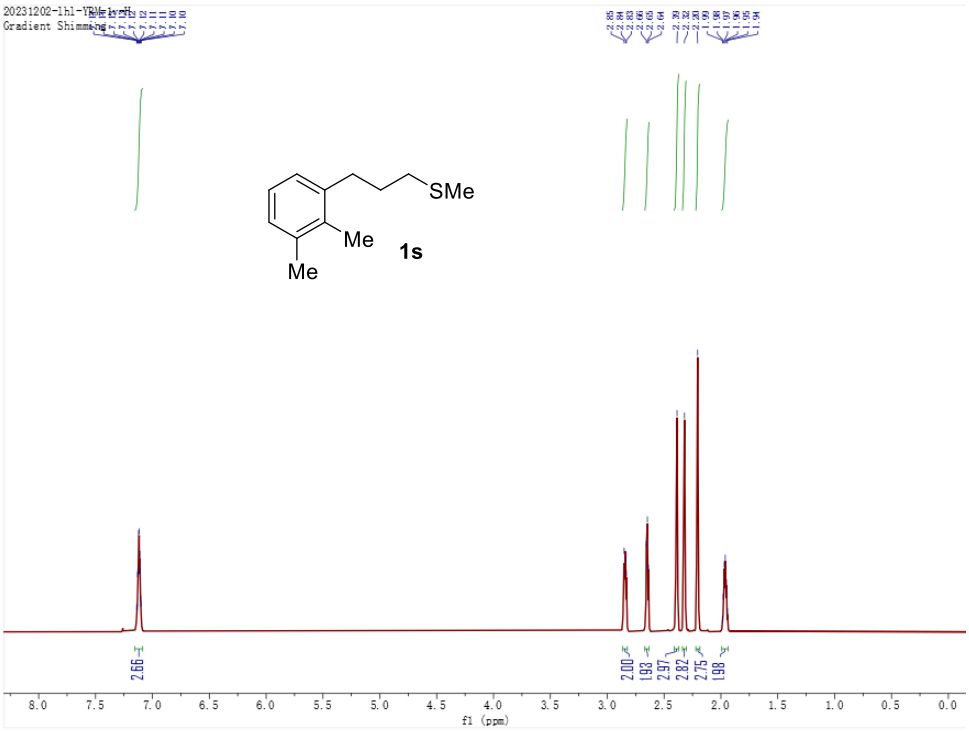



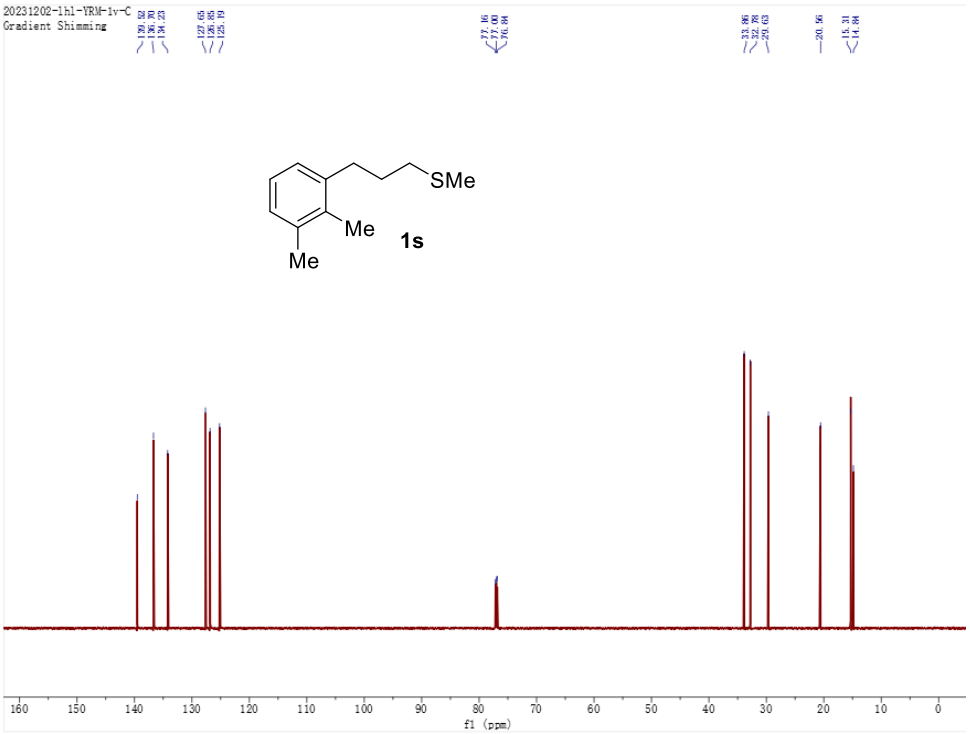
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1r**



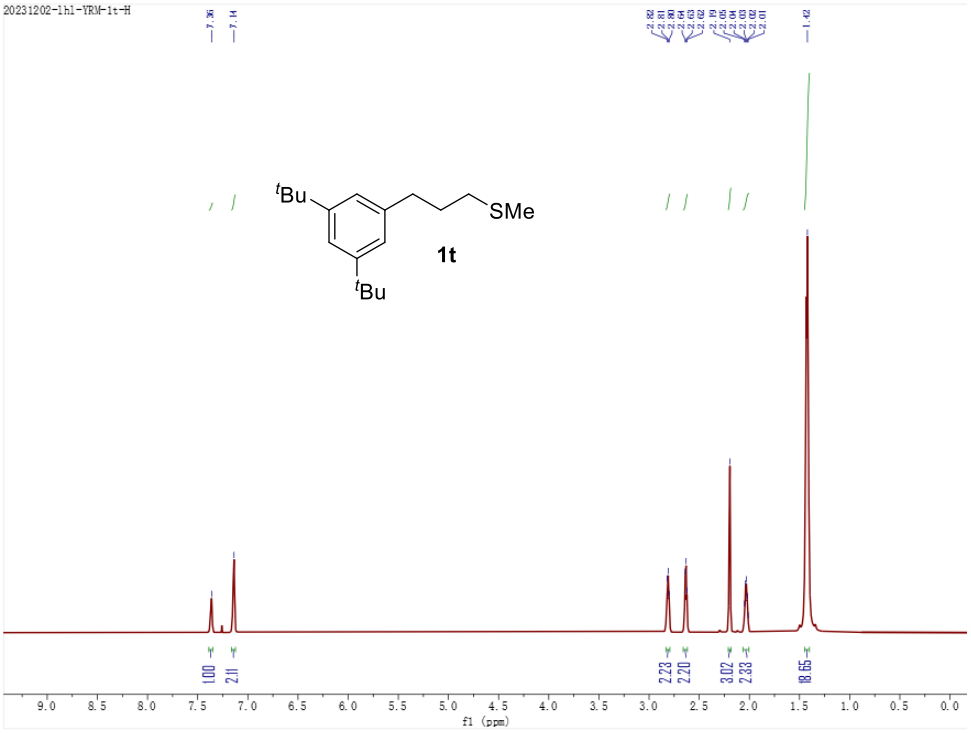



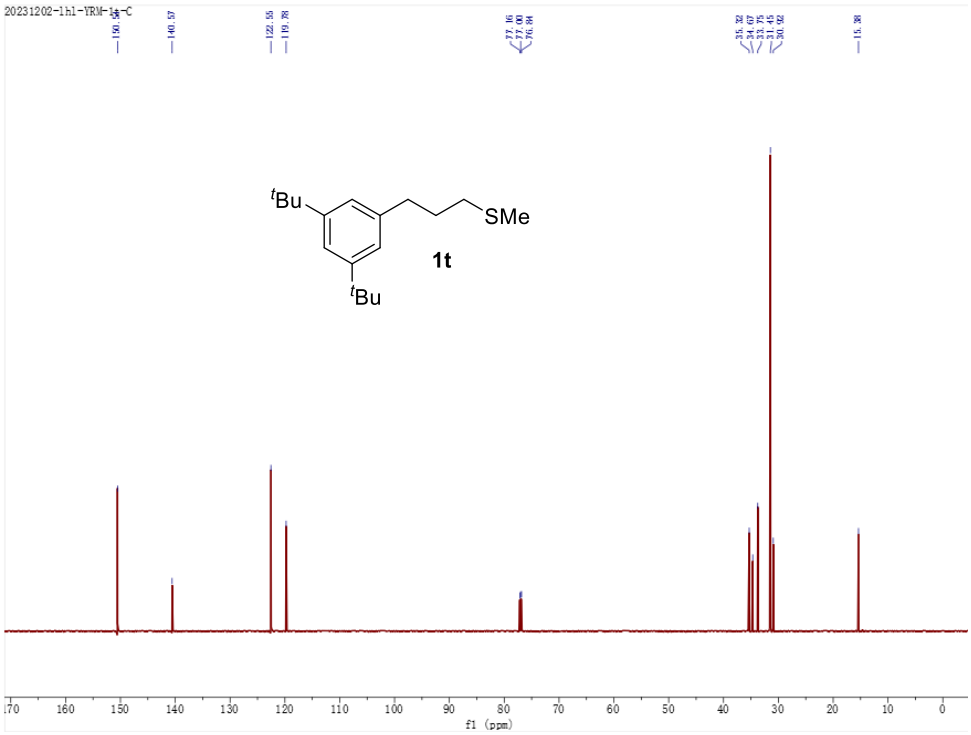
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1s**



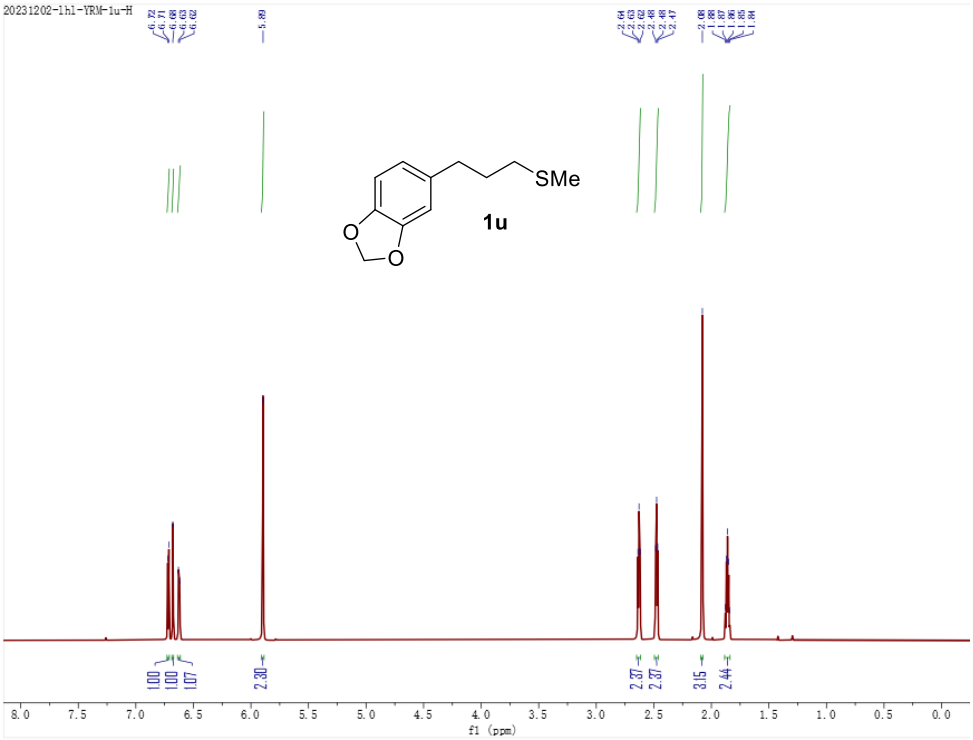



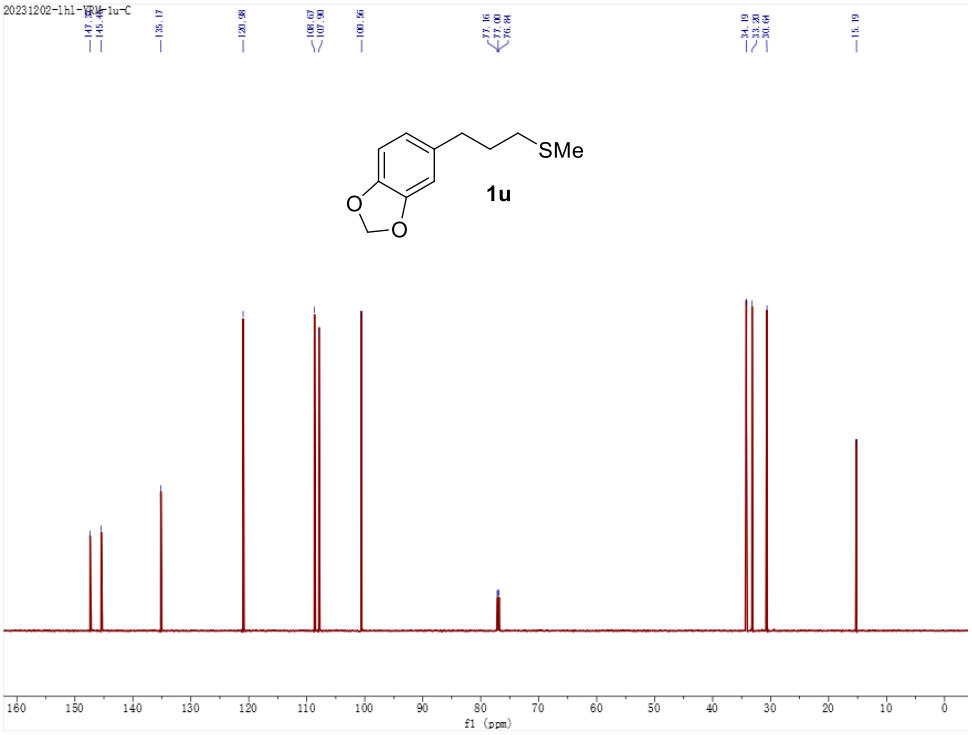
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1t**



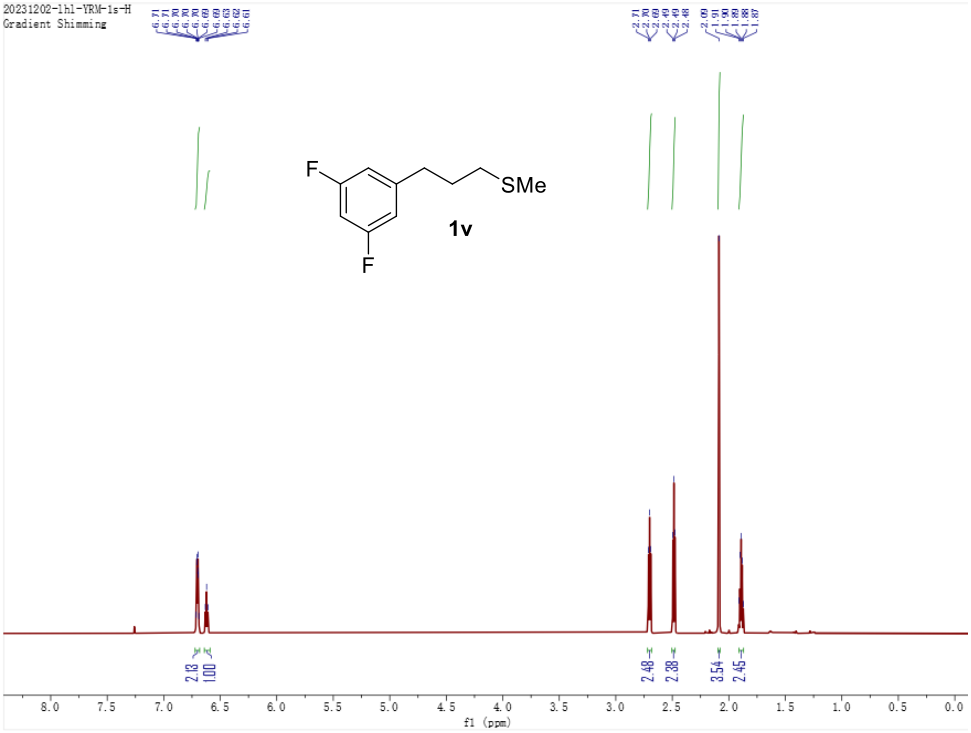



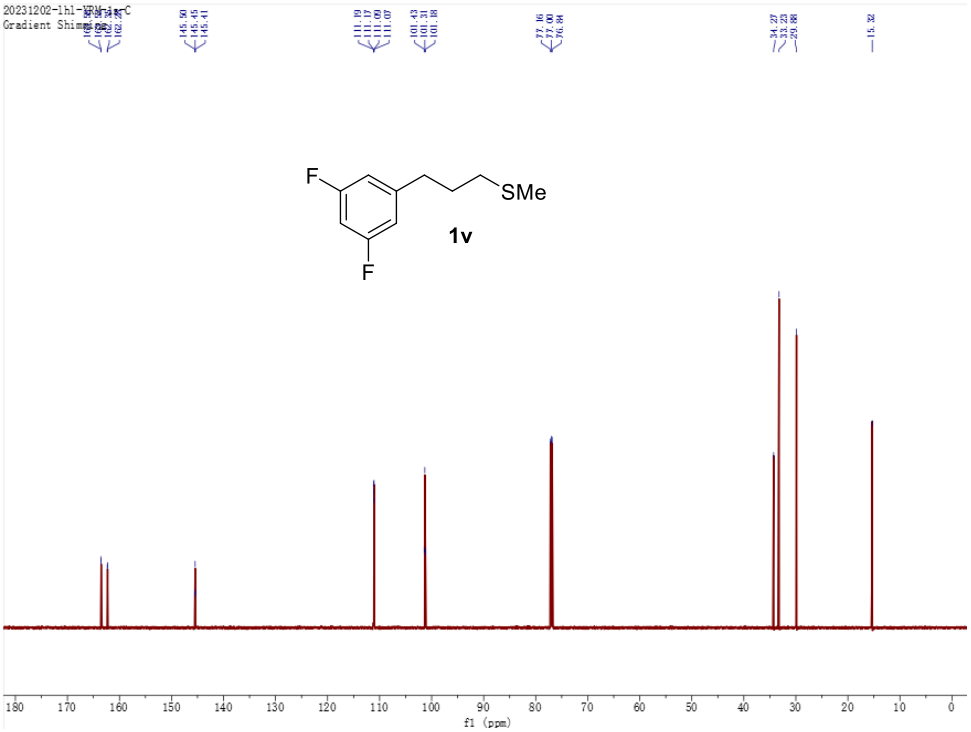
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1u**



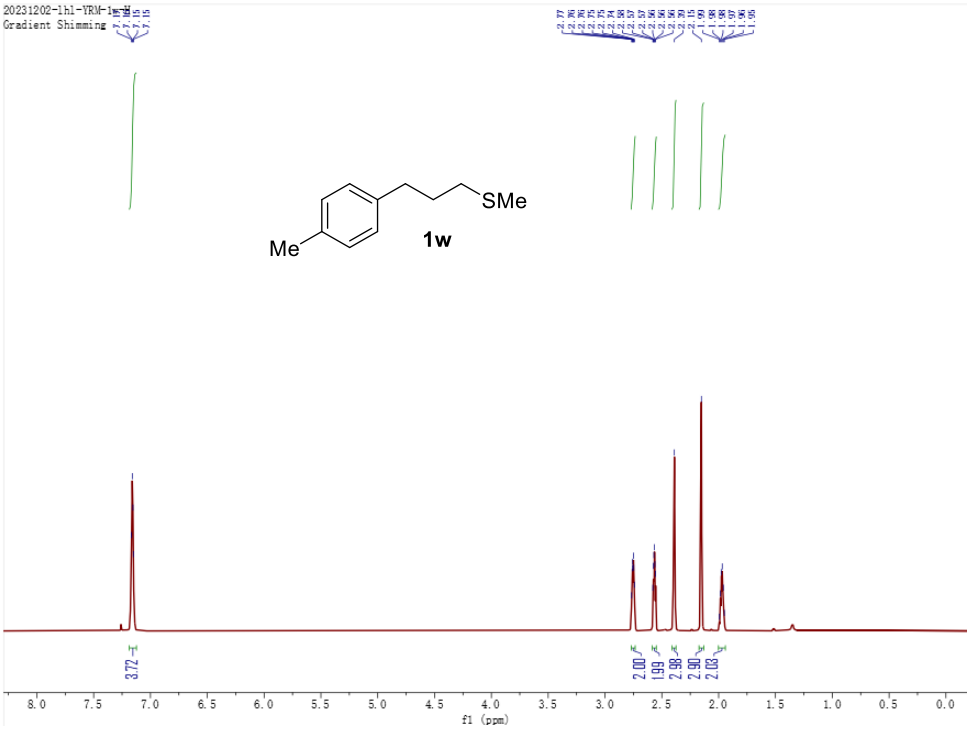



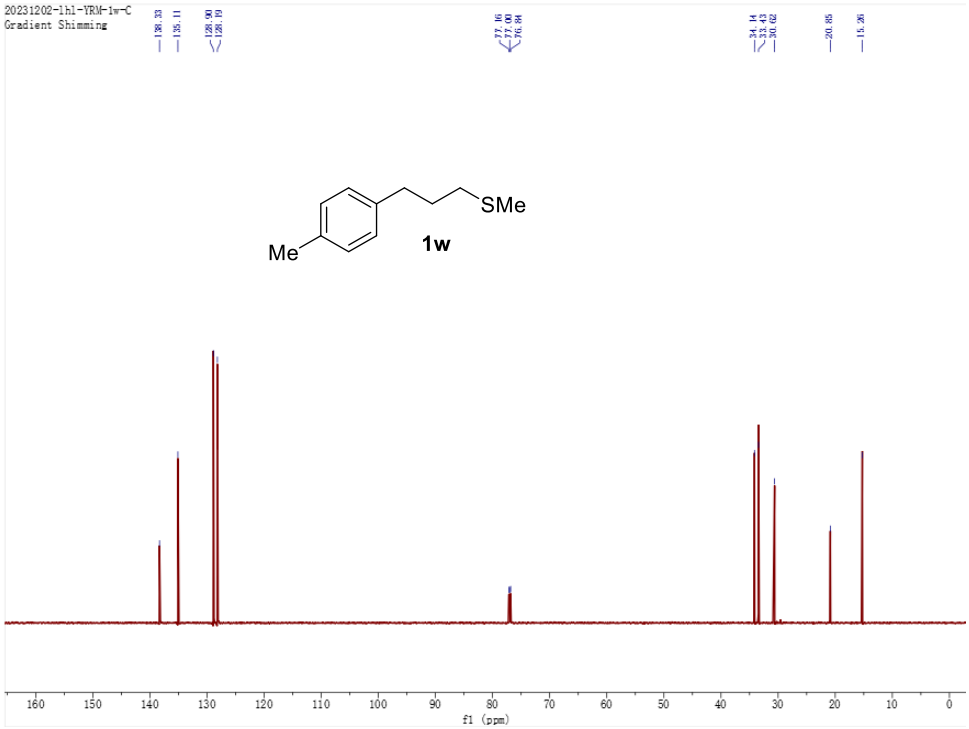
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1v**



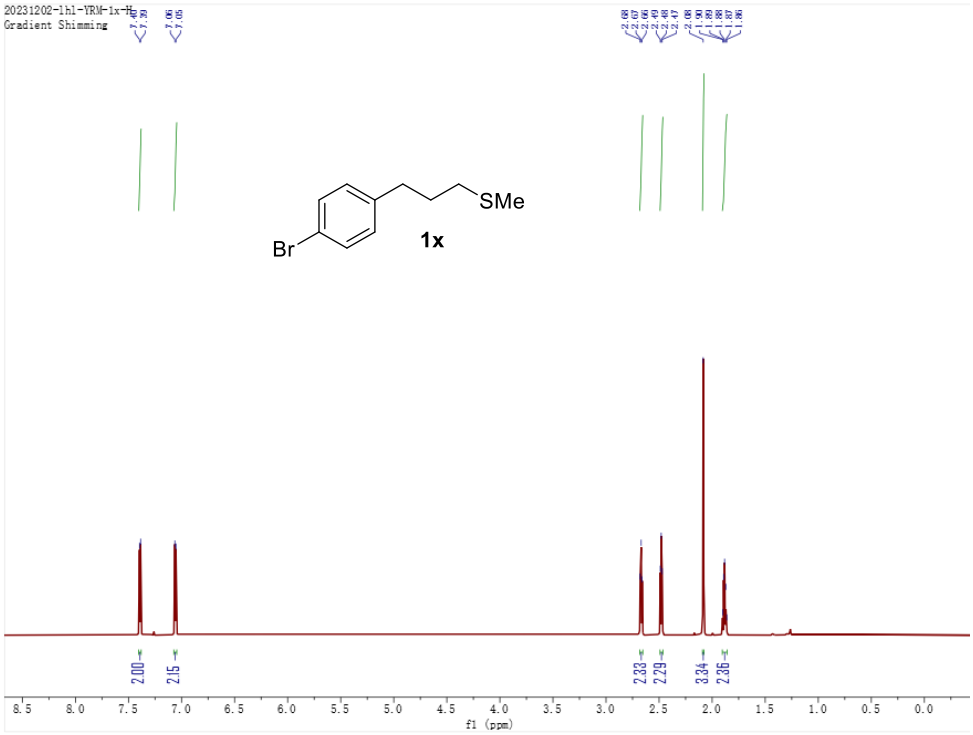



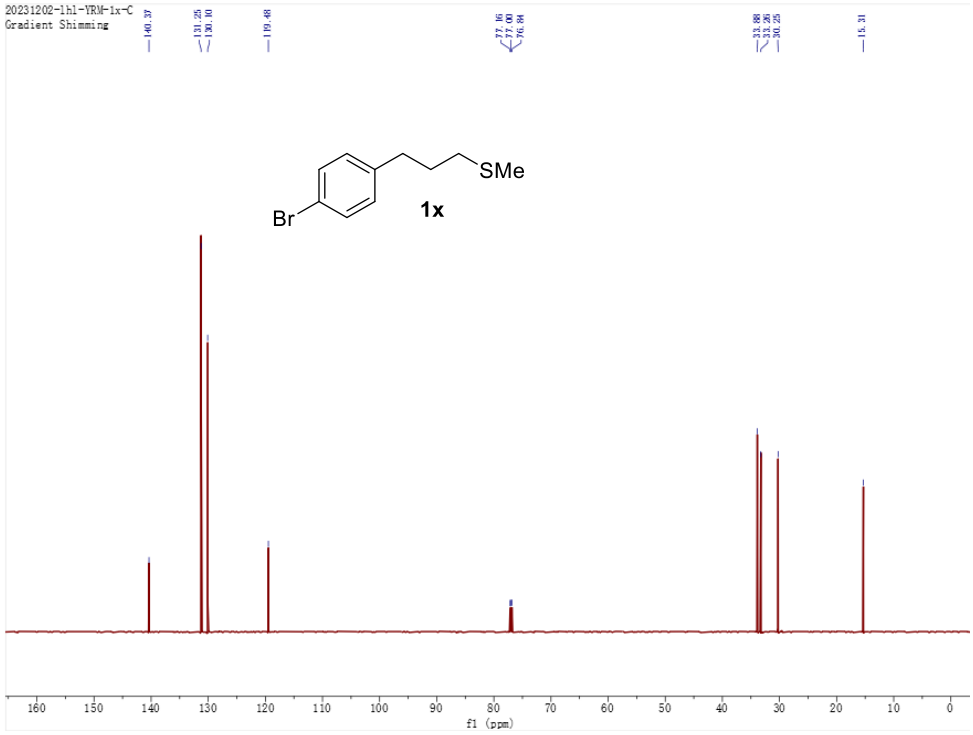
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1w**



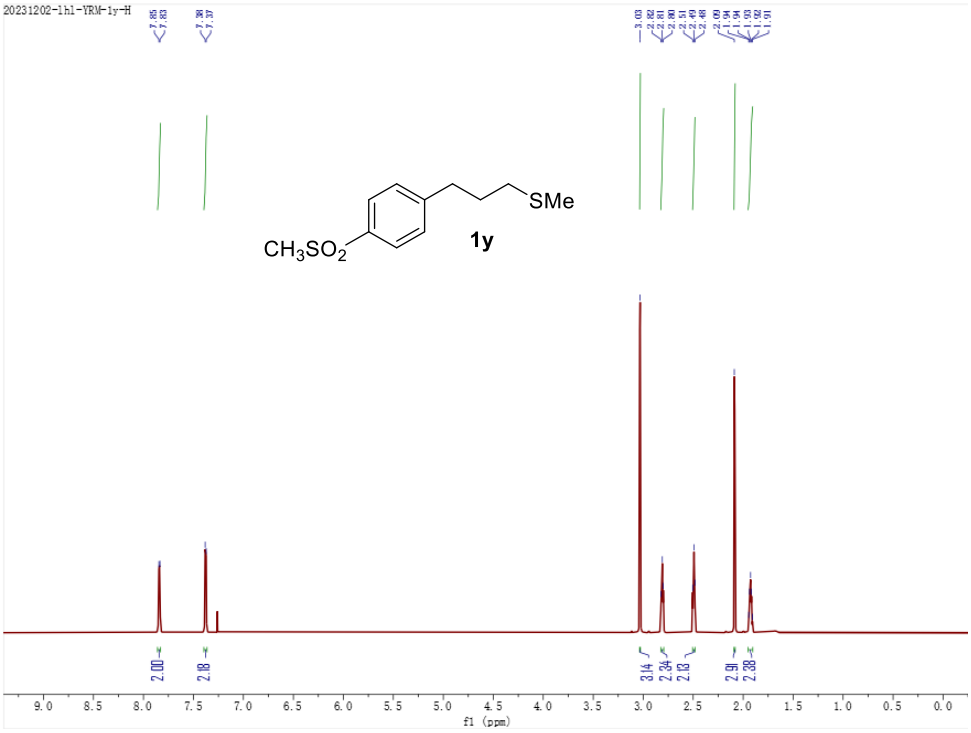



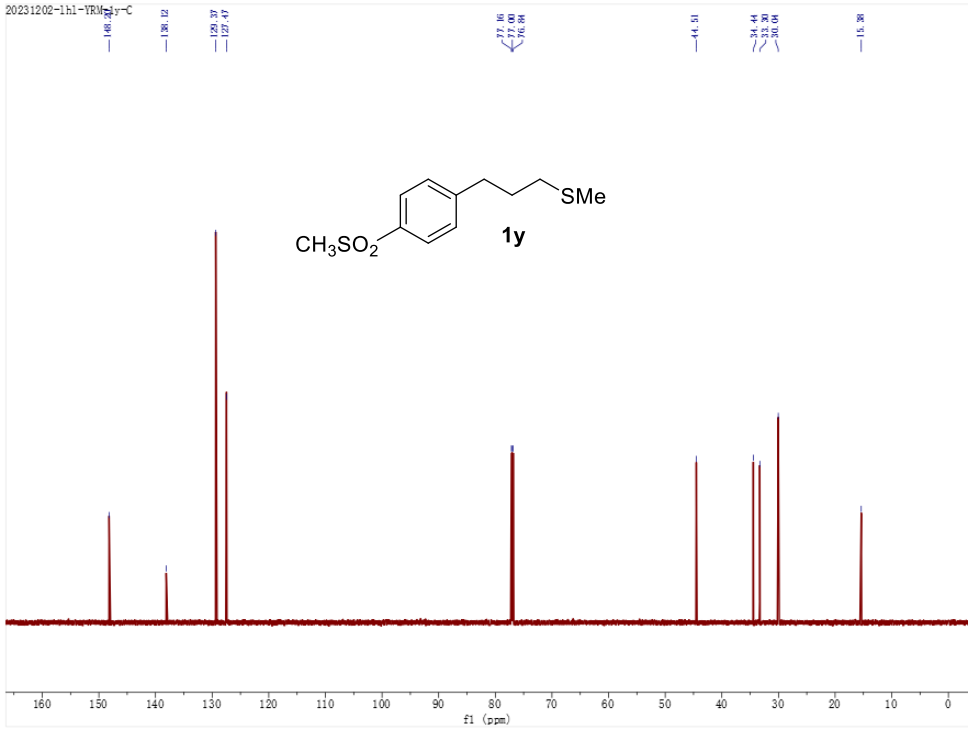
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1x**



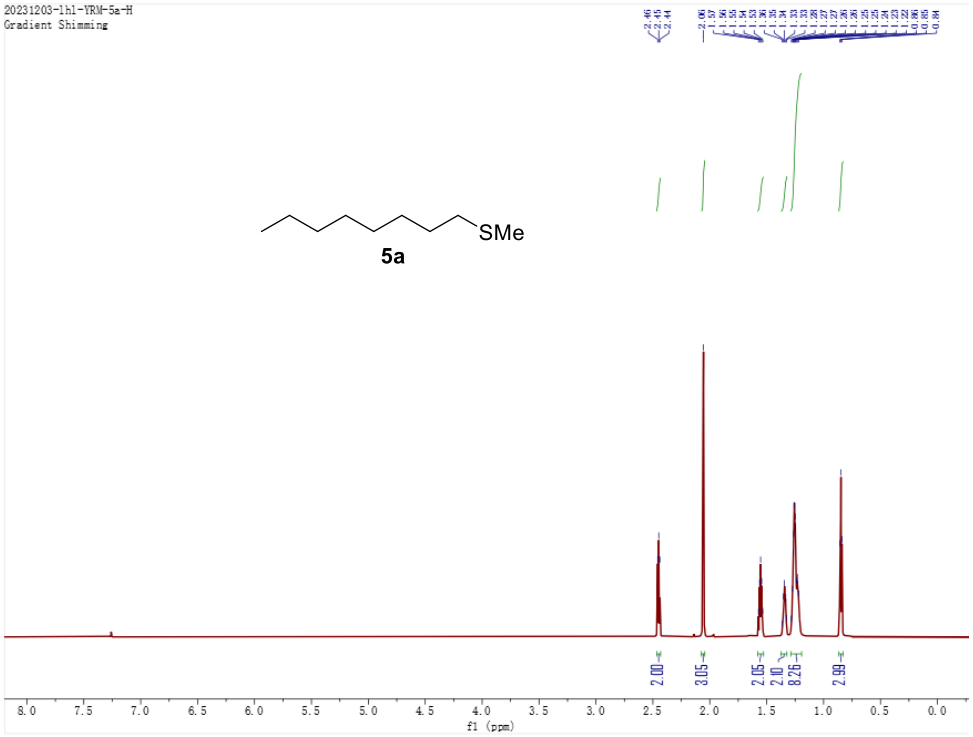



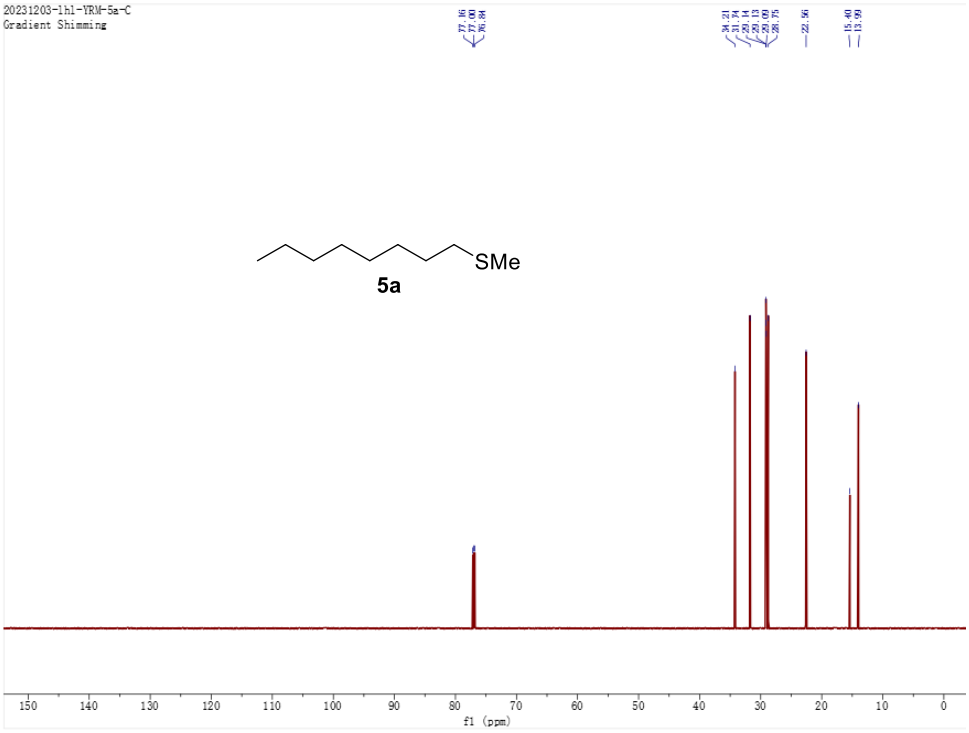
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1y**



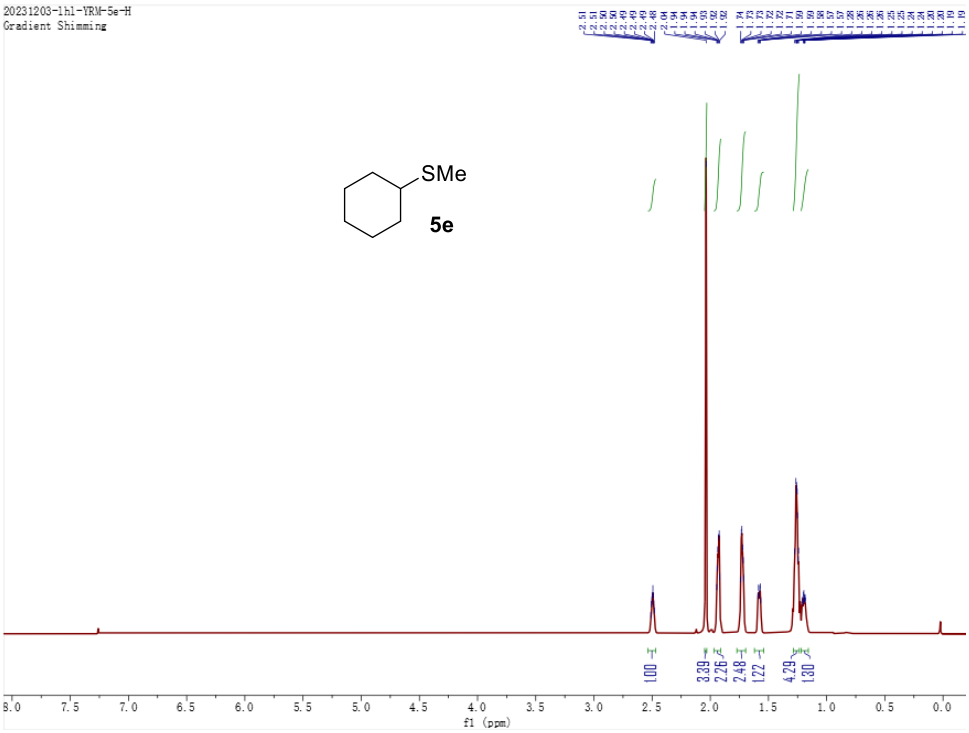



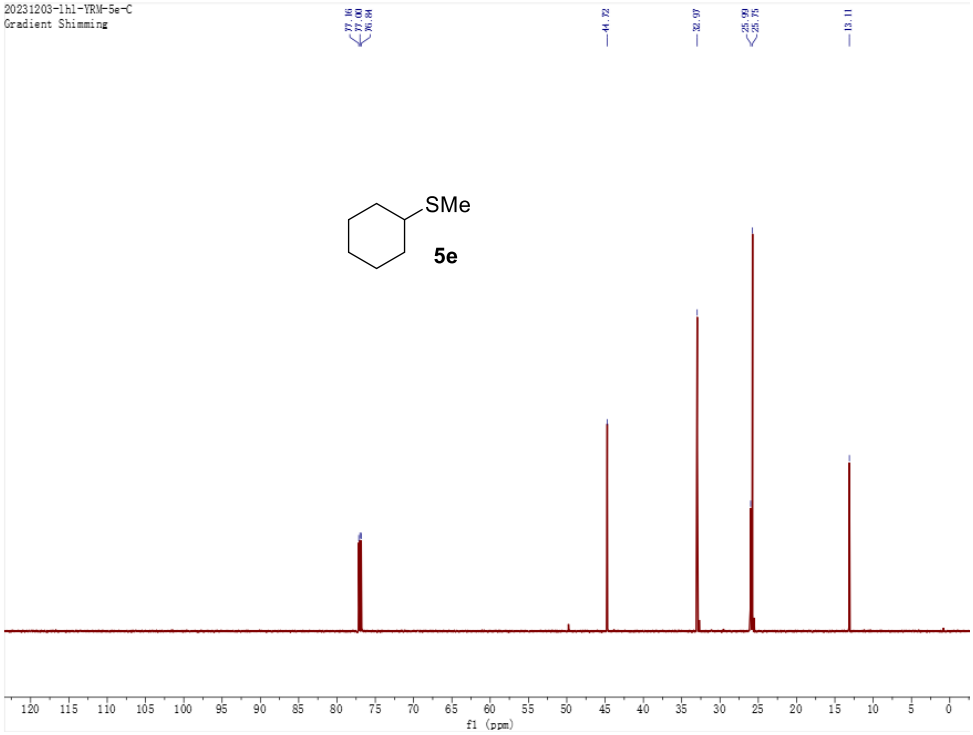
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5a**



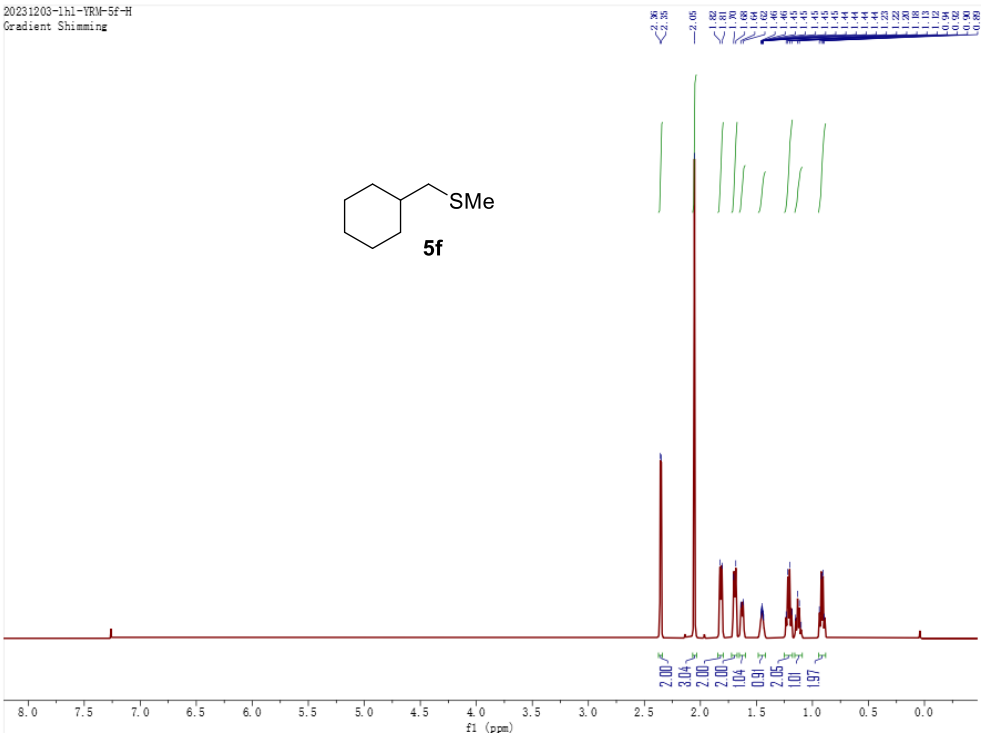



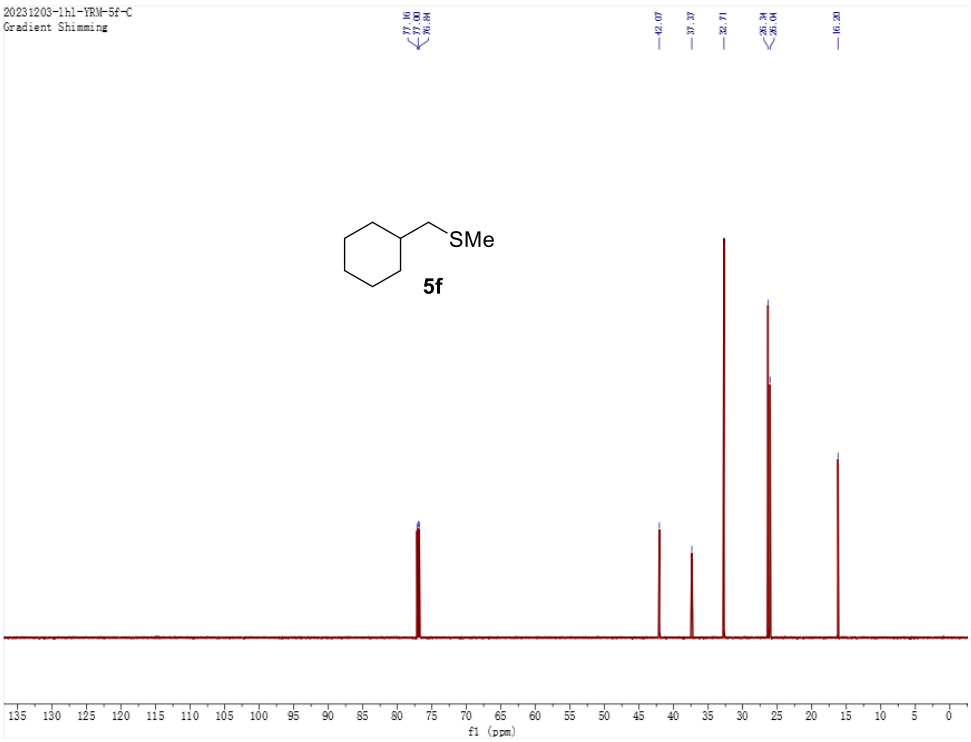
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5e**



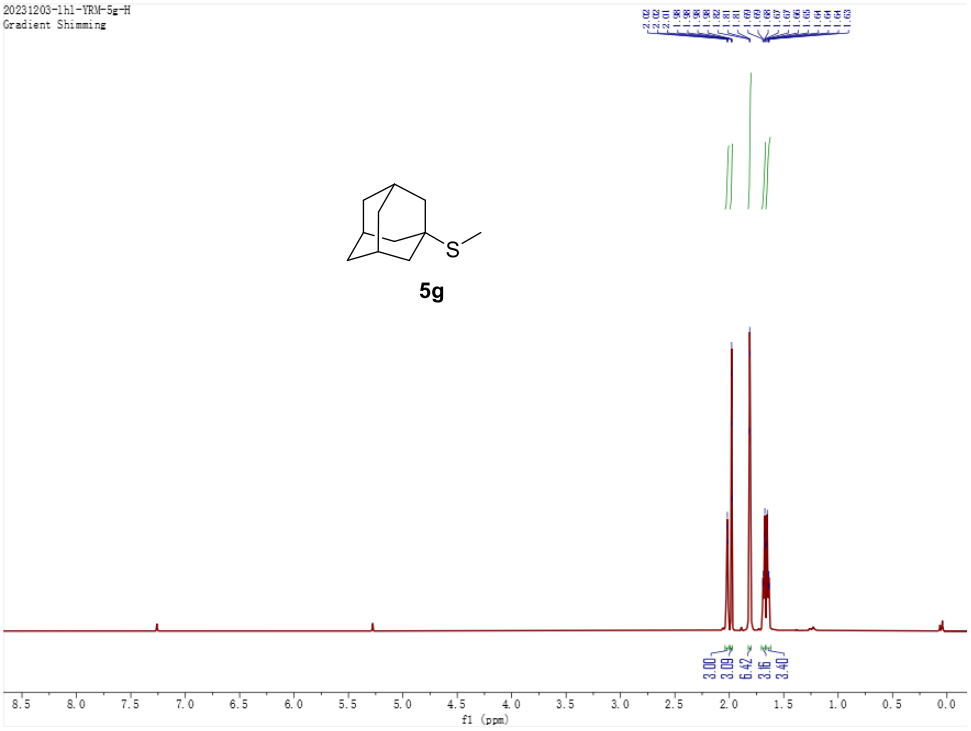



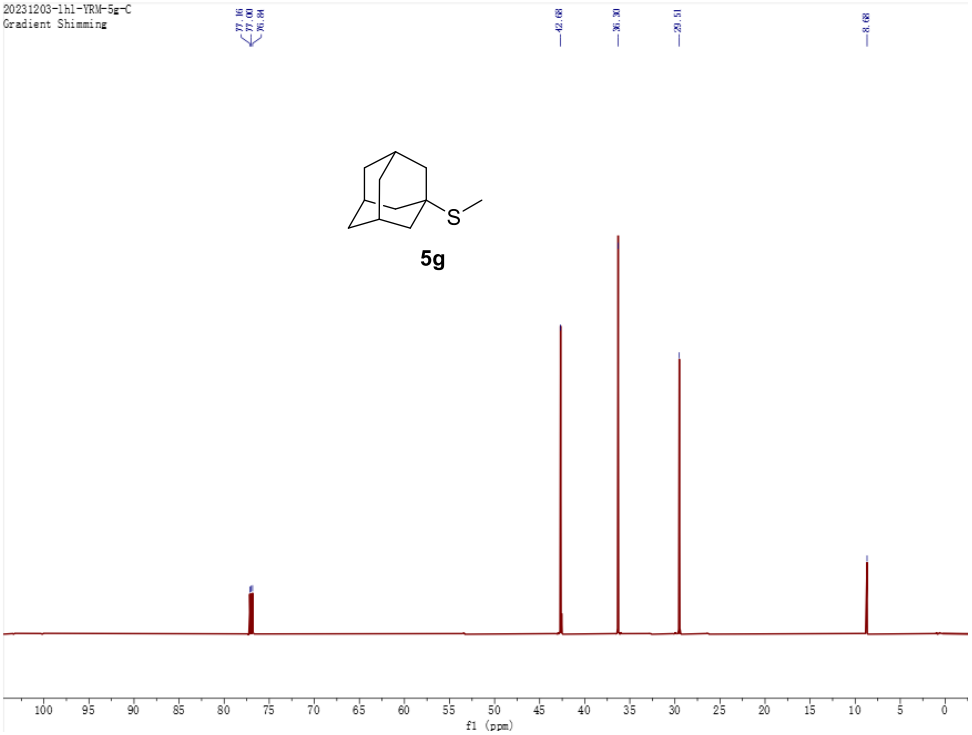
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5f**



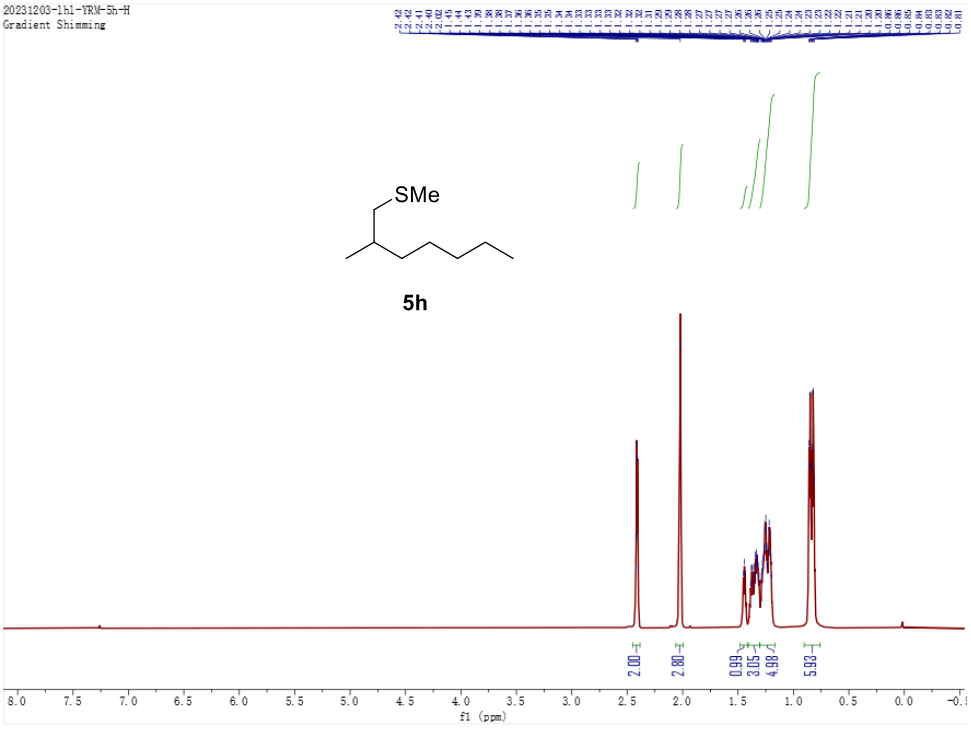



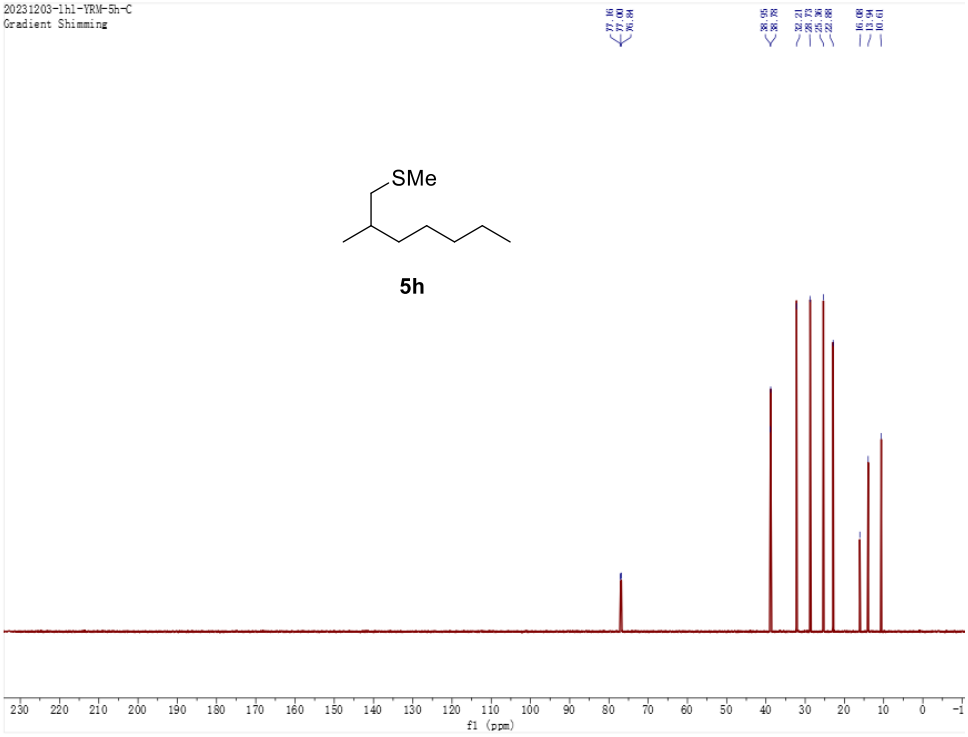
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5g**



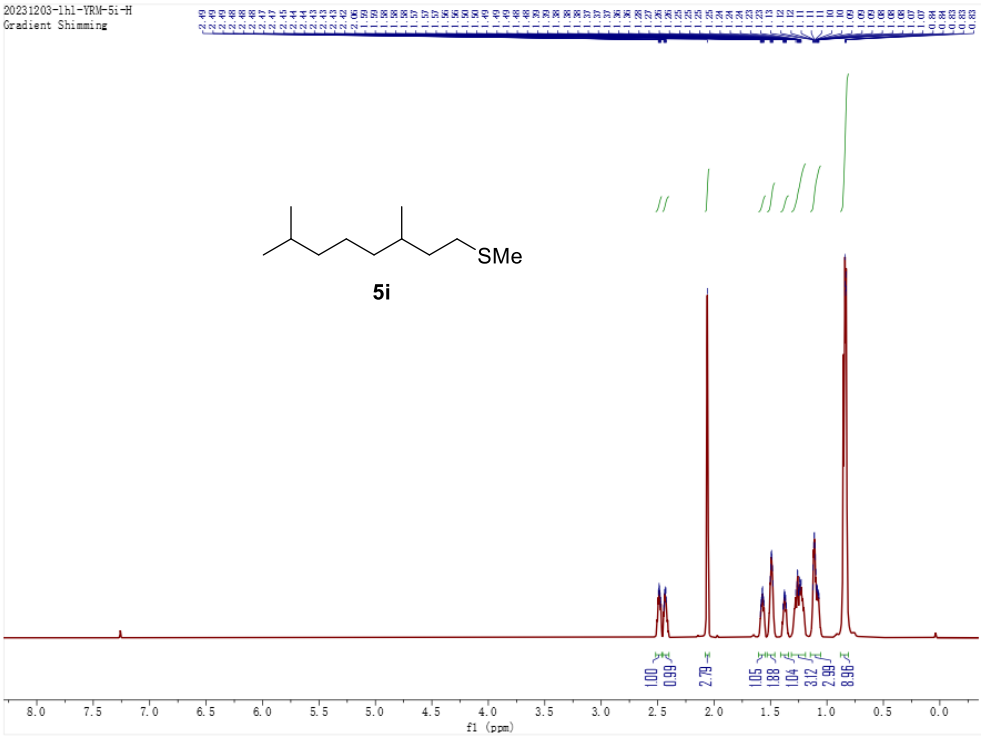



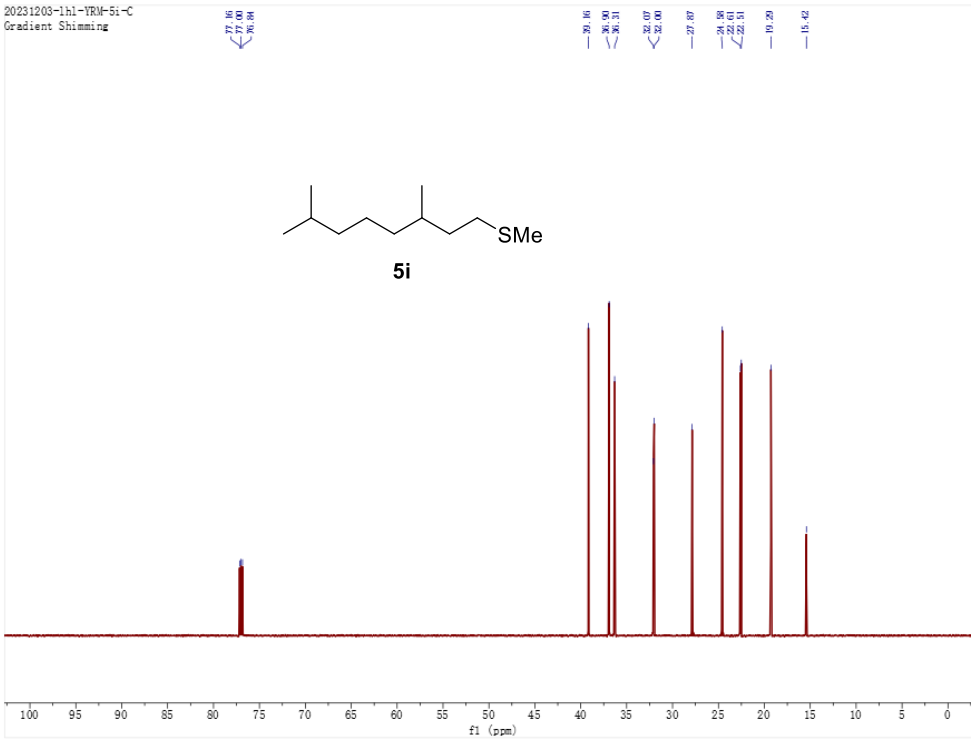
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5h**



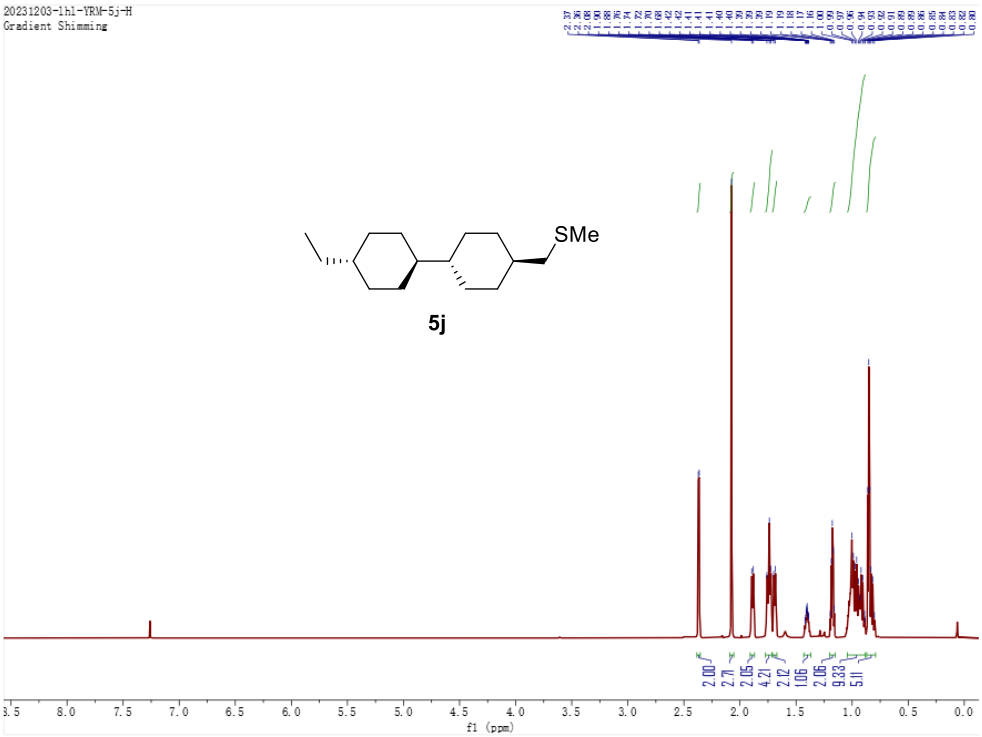



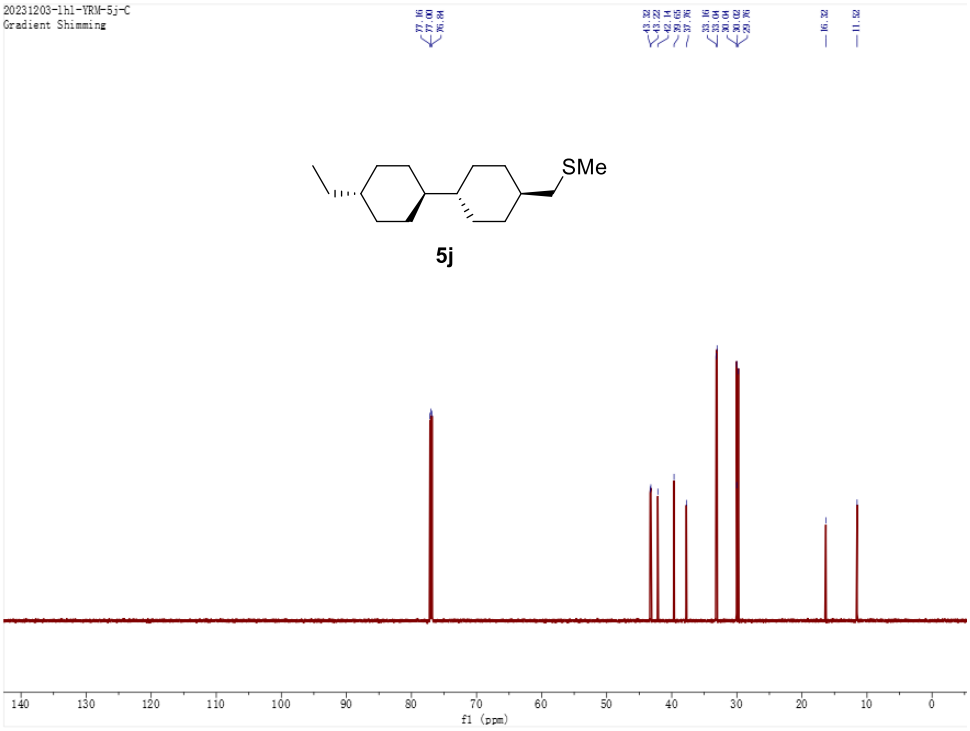
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5i**



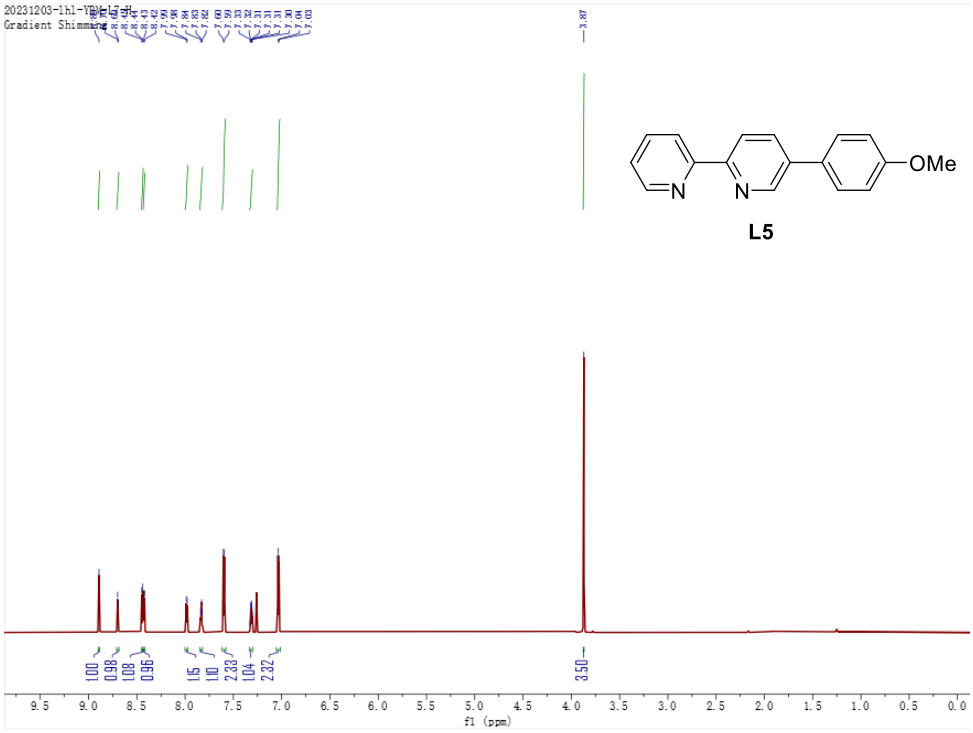



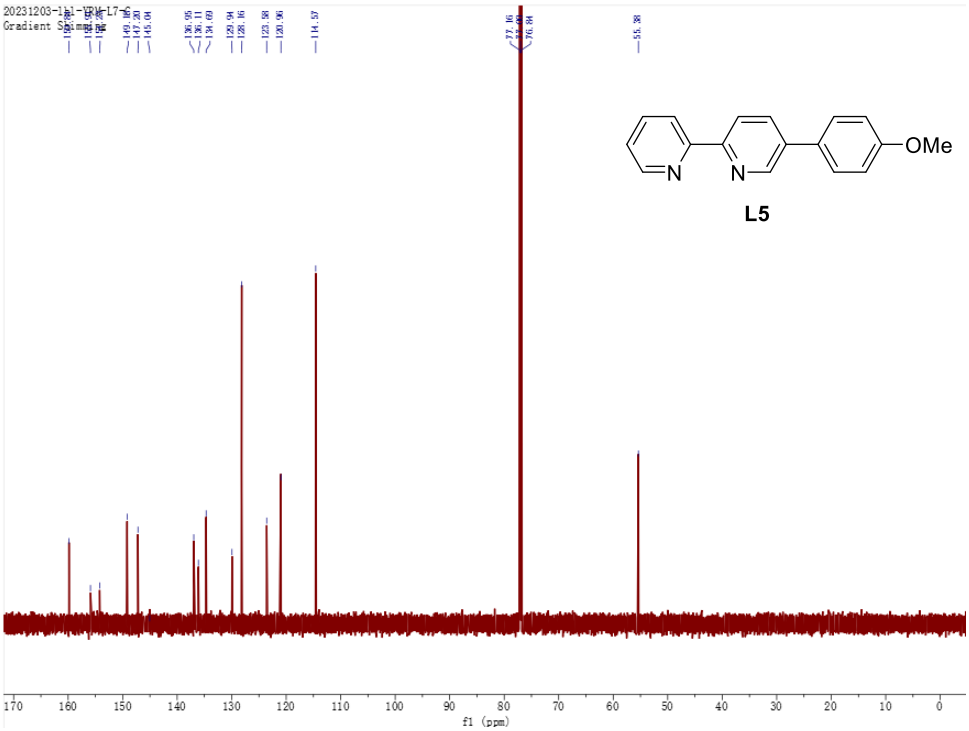
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **5j**



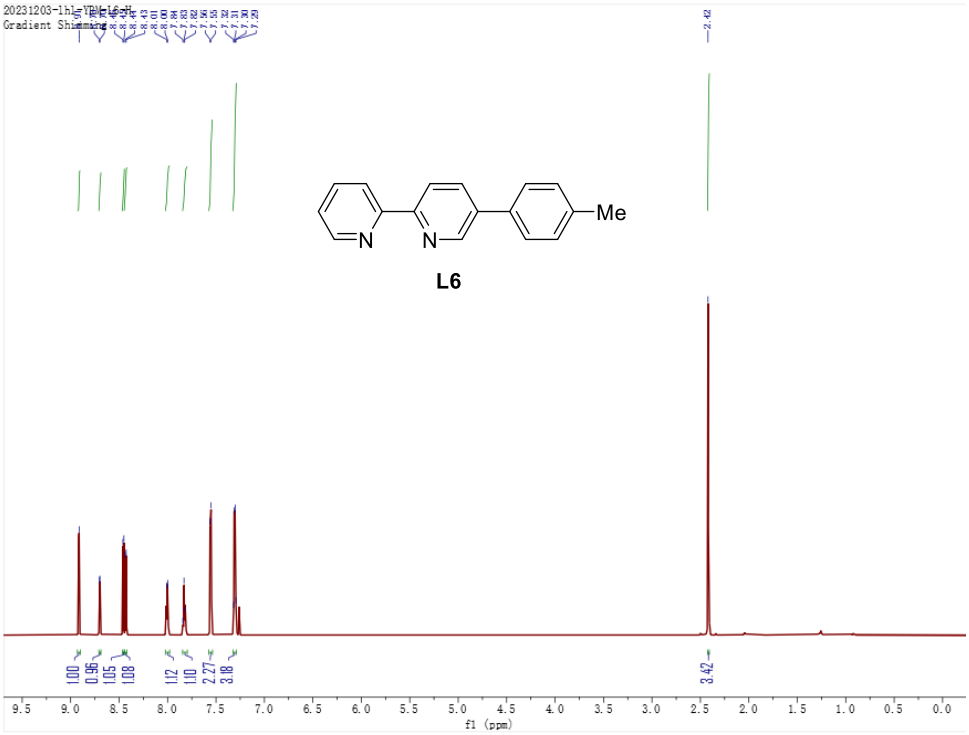



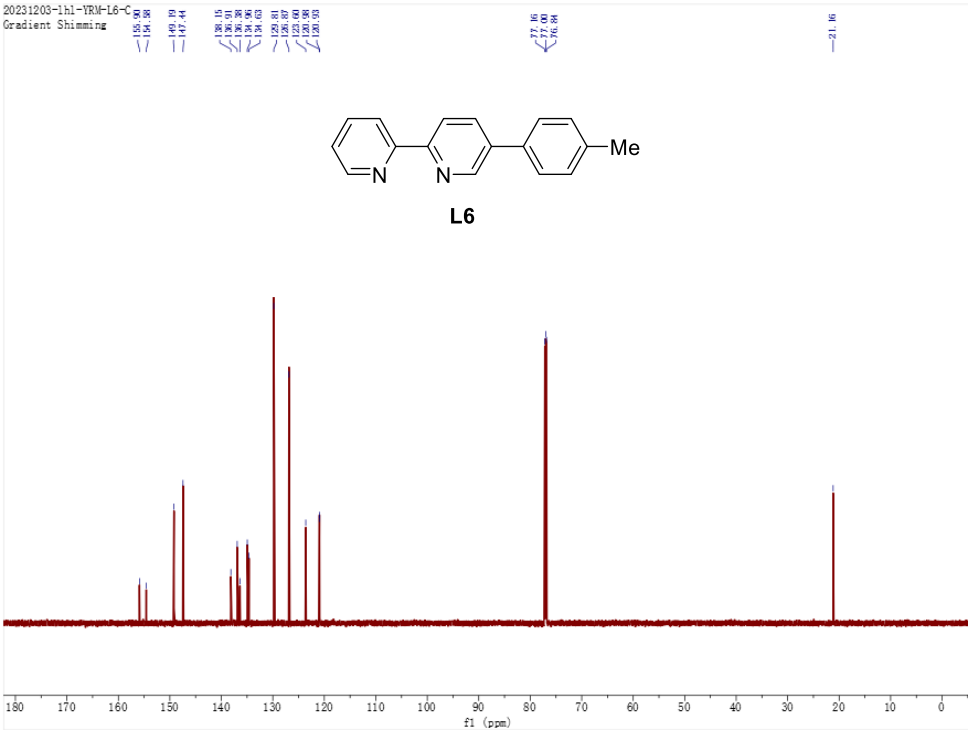
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L5**



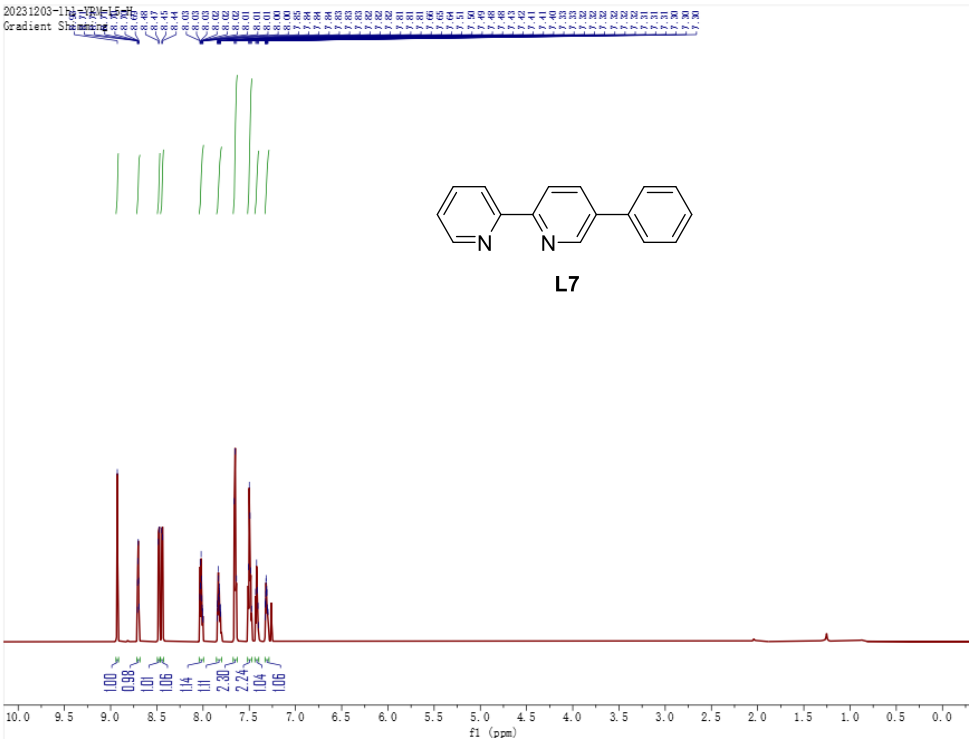



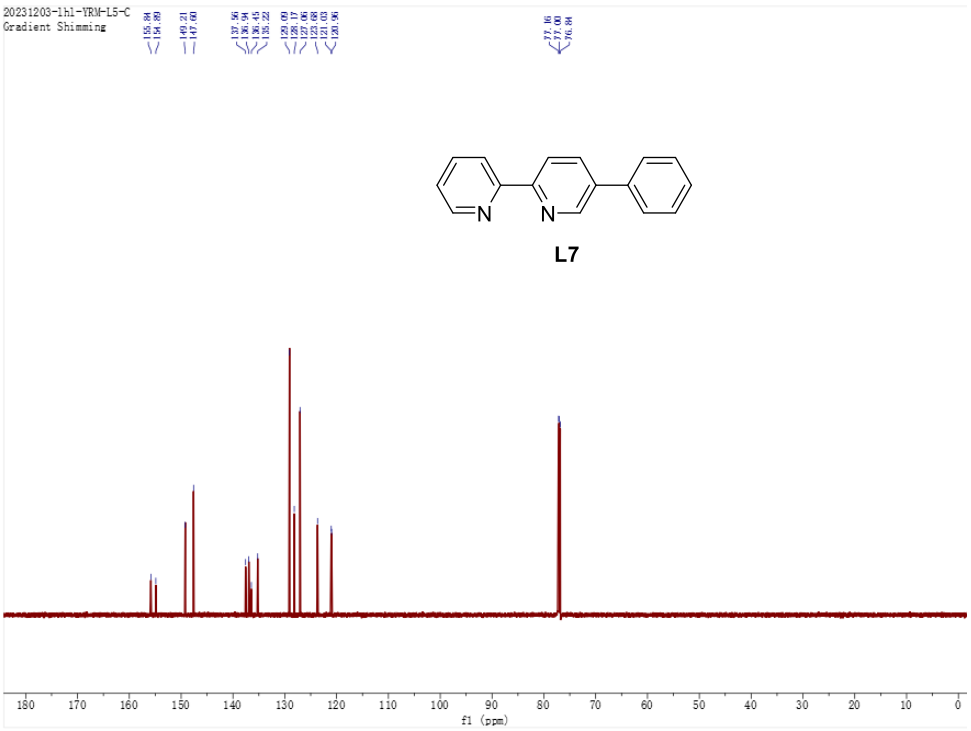
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L6**



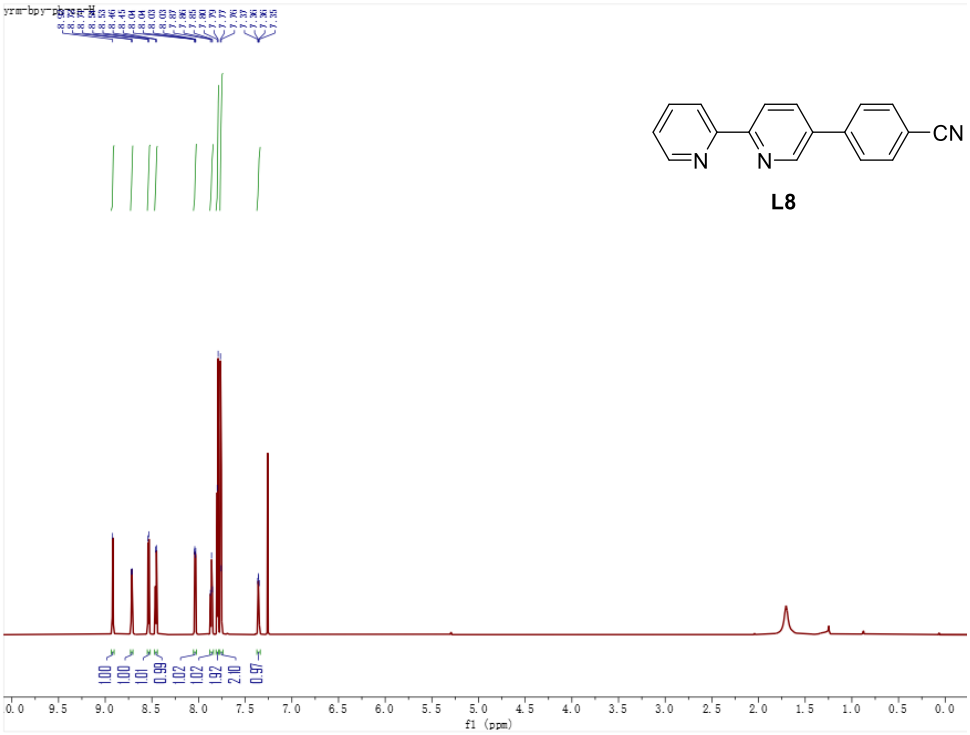



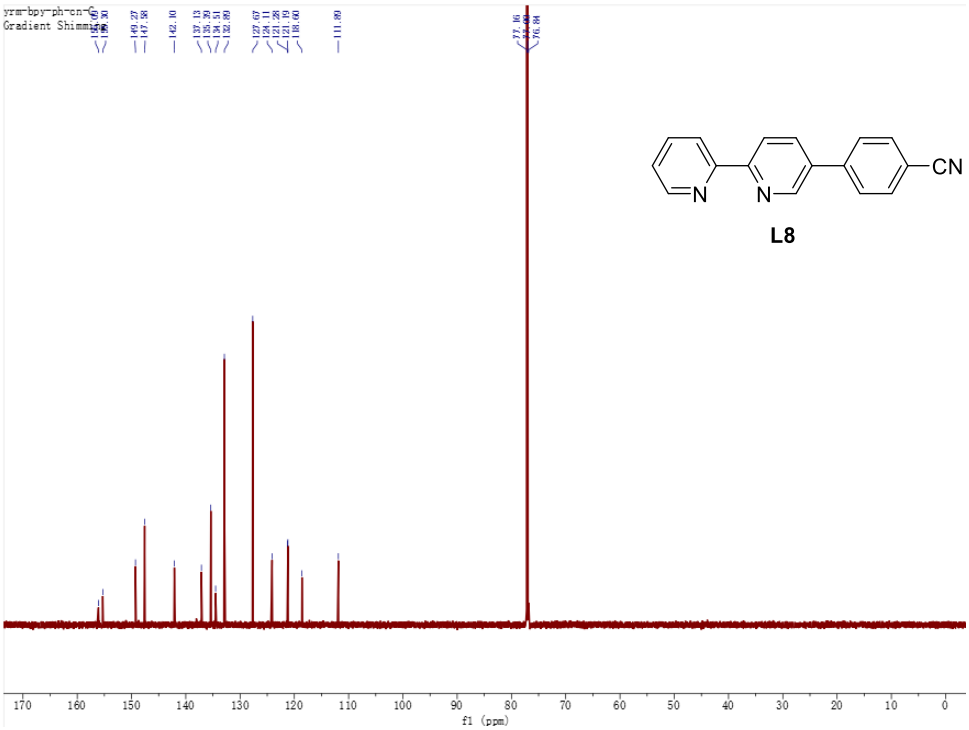
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L7**



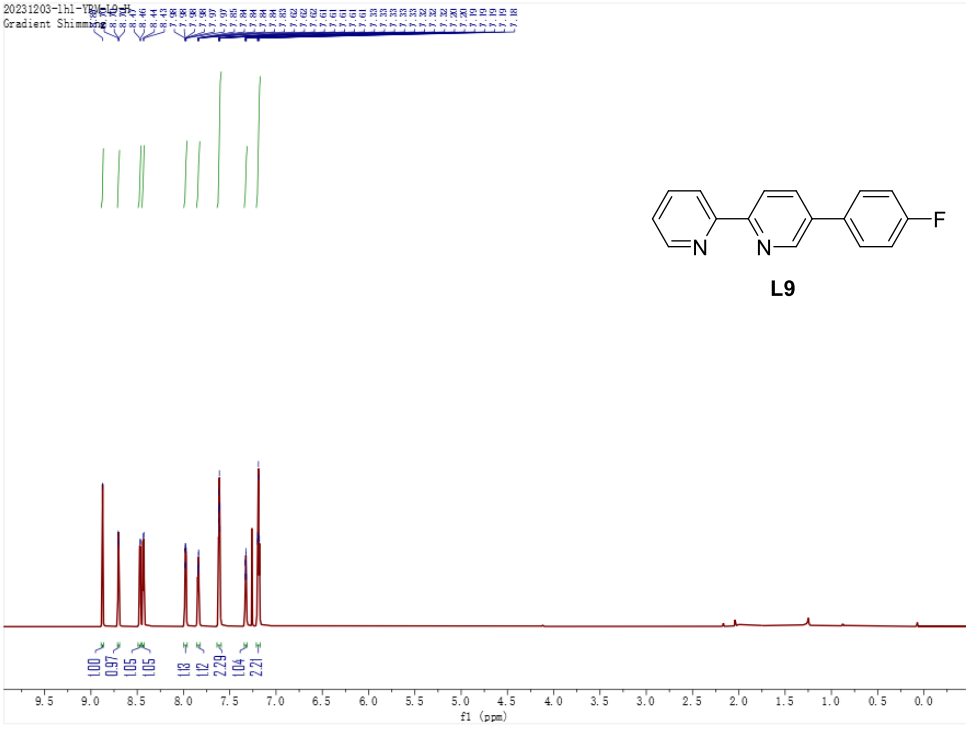



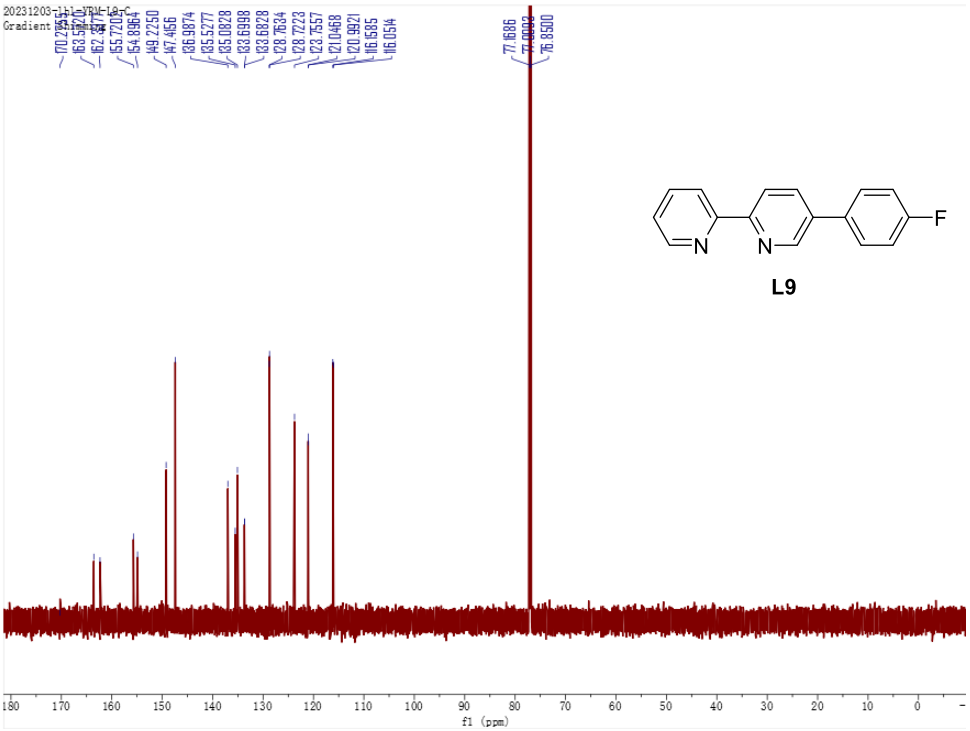
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L8**



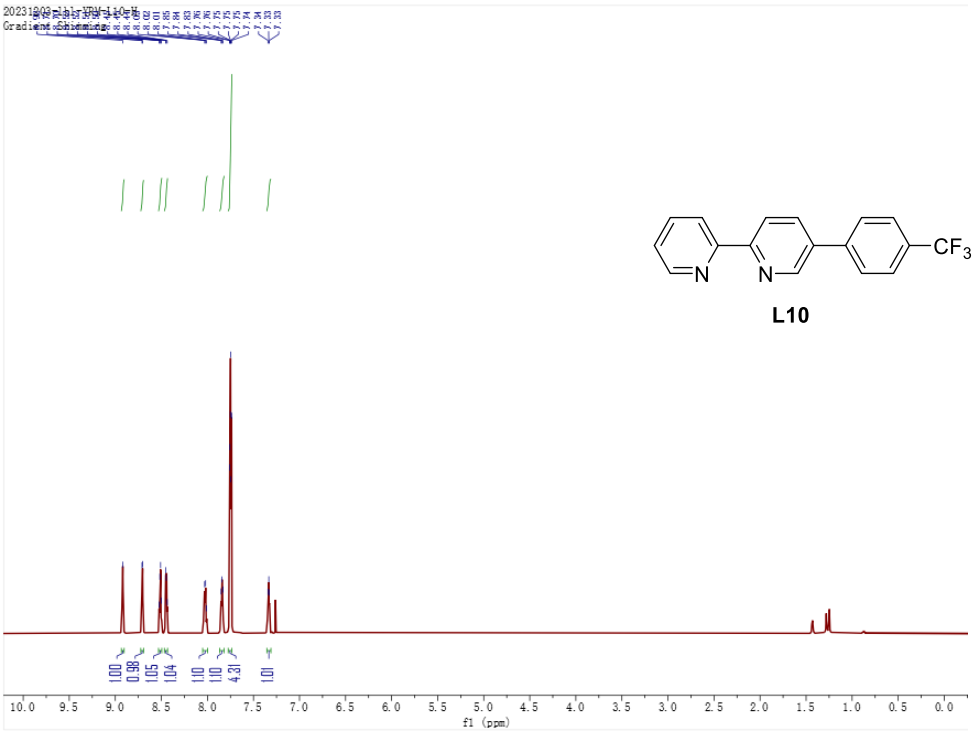



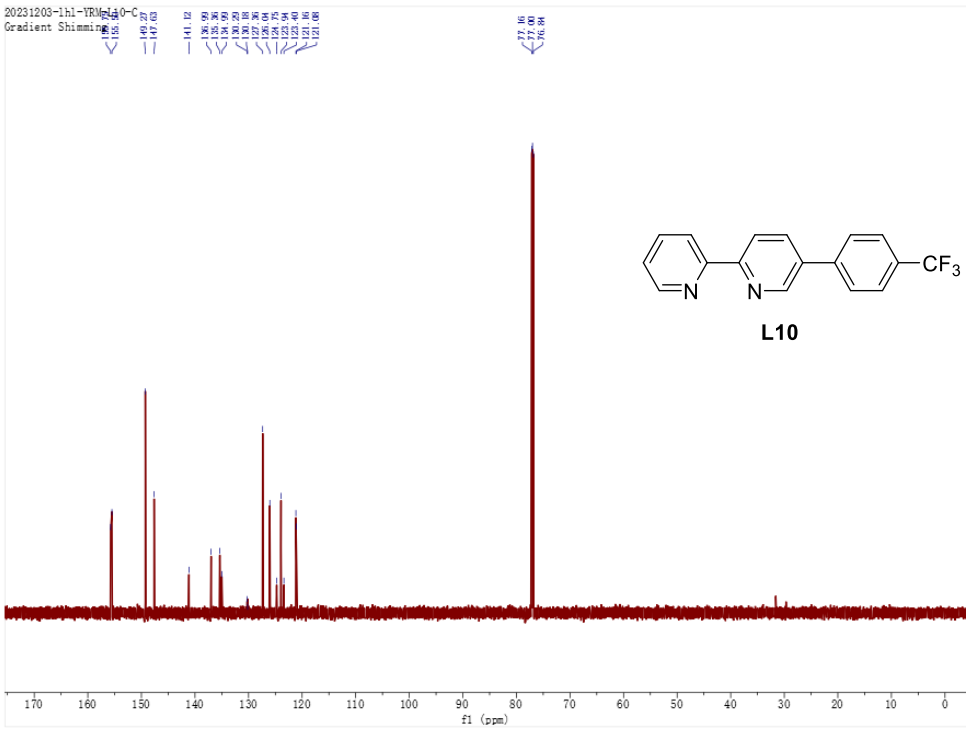
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L9**



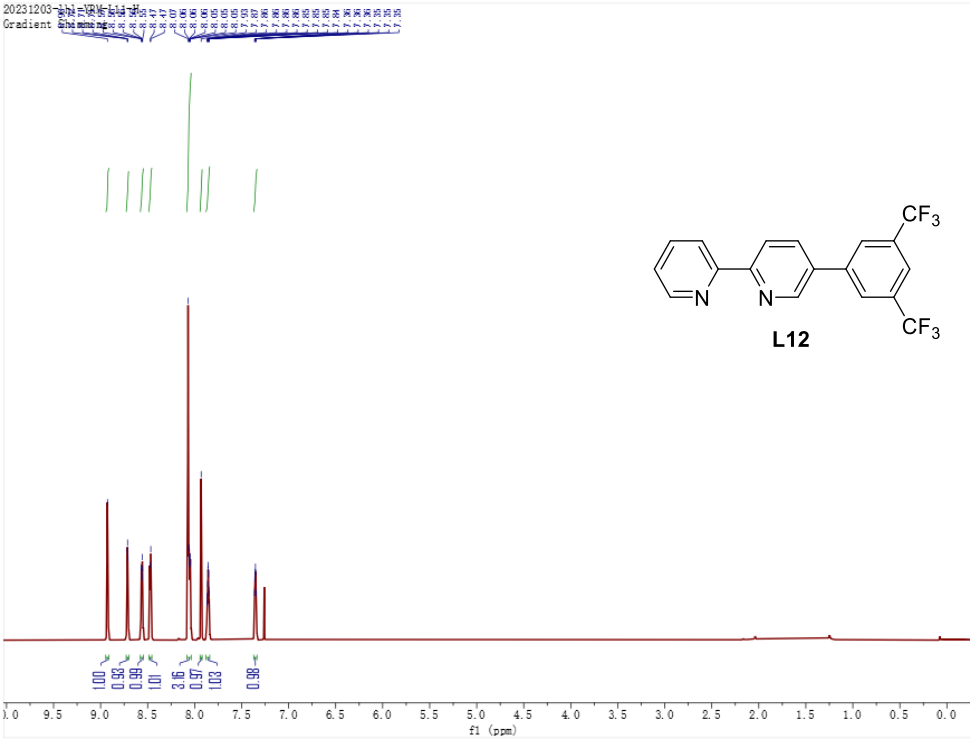



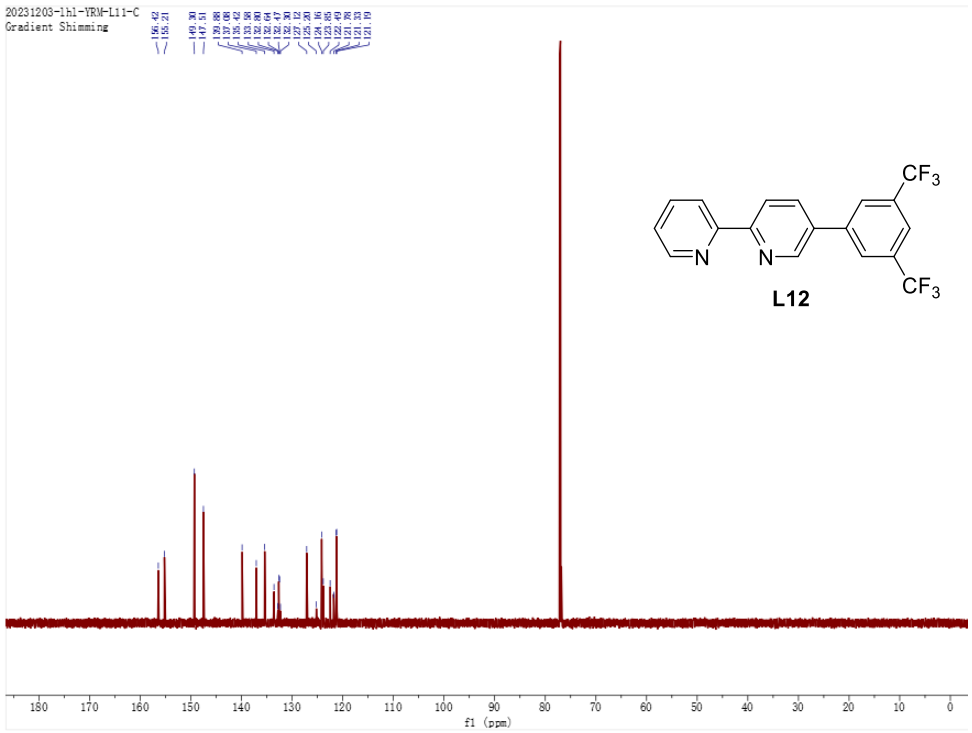
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L10**



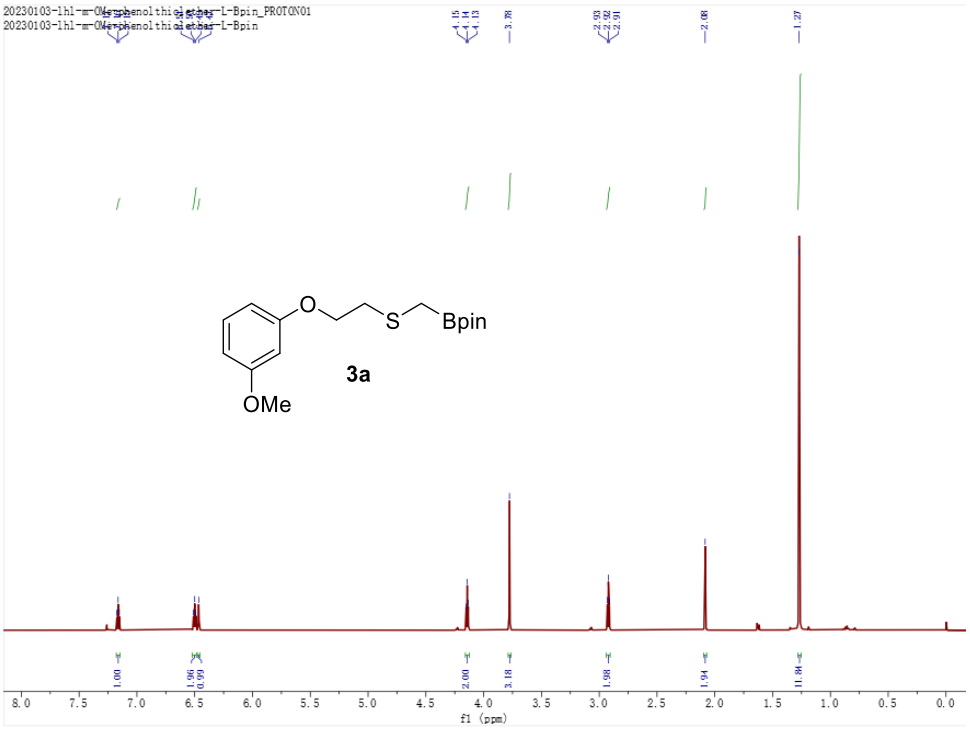



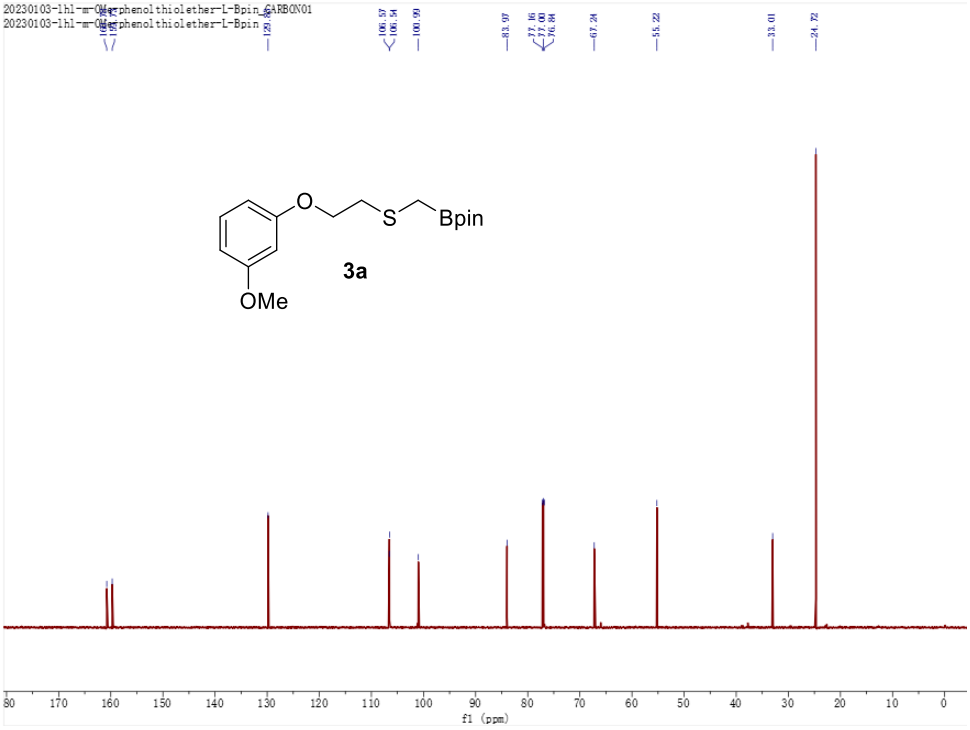
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **L12**



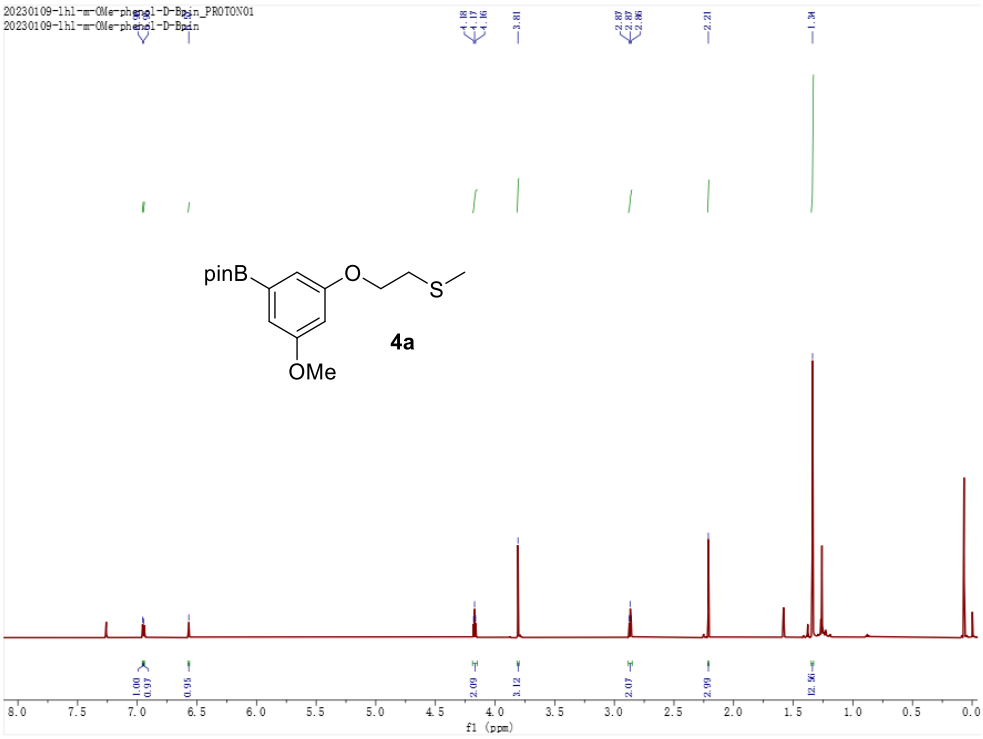



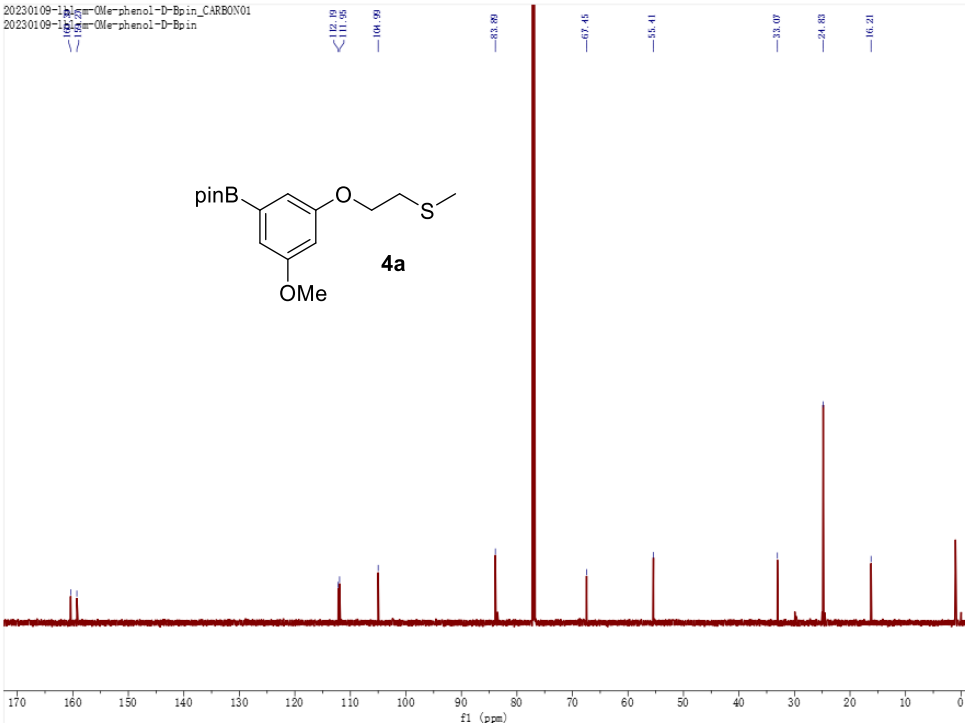
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3a**



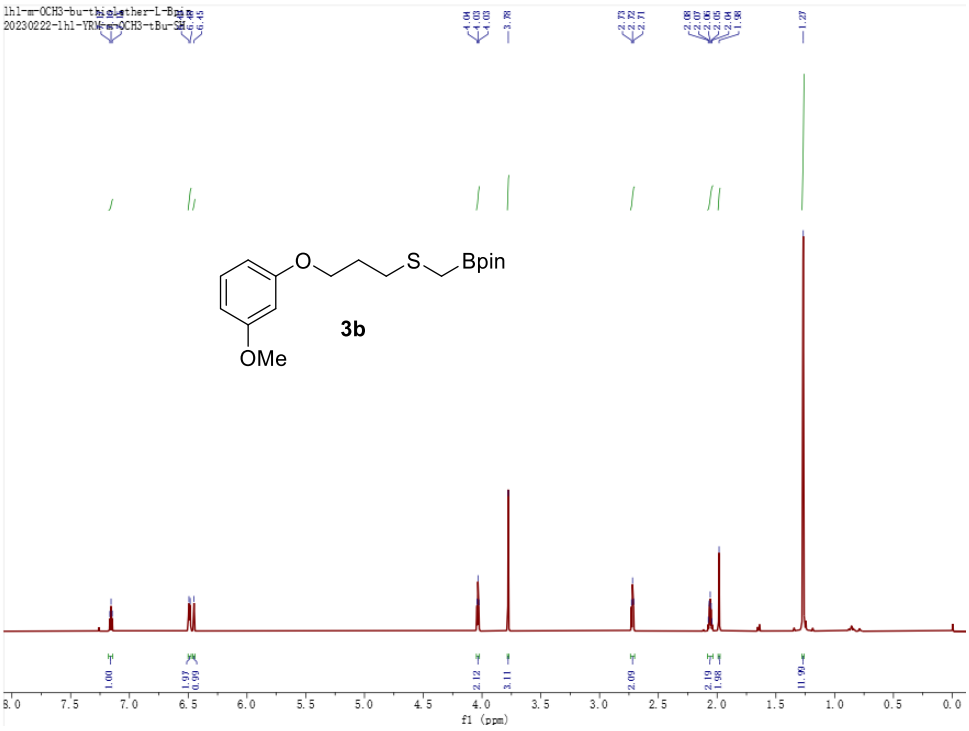



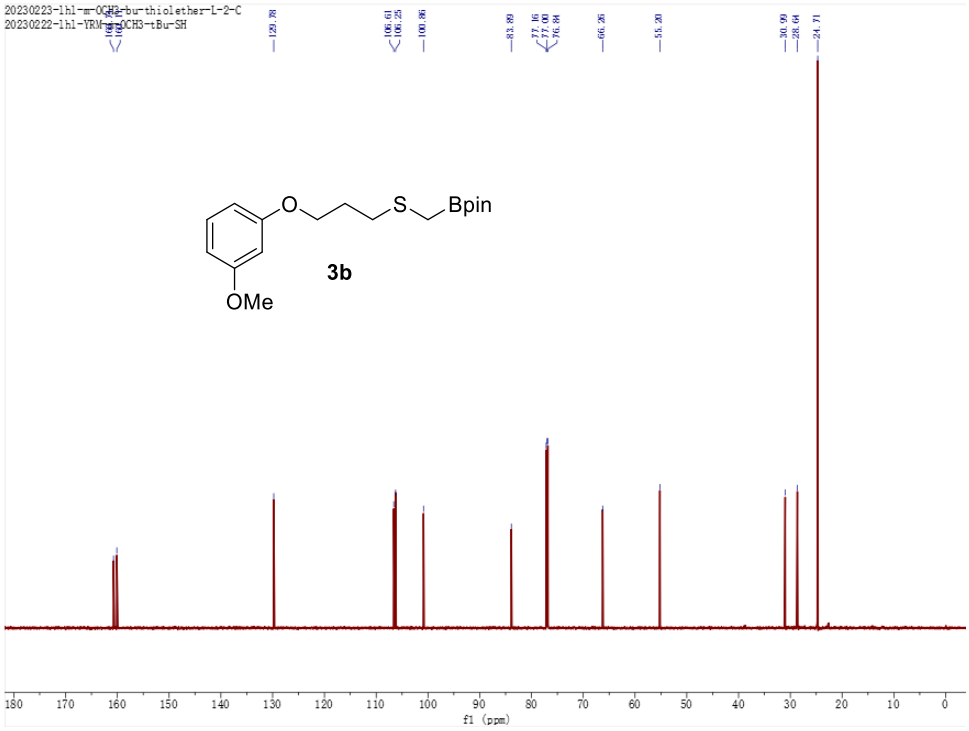
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4a**



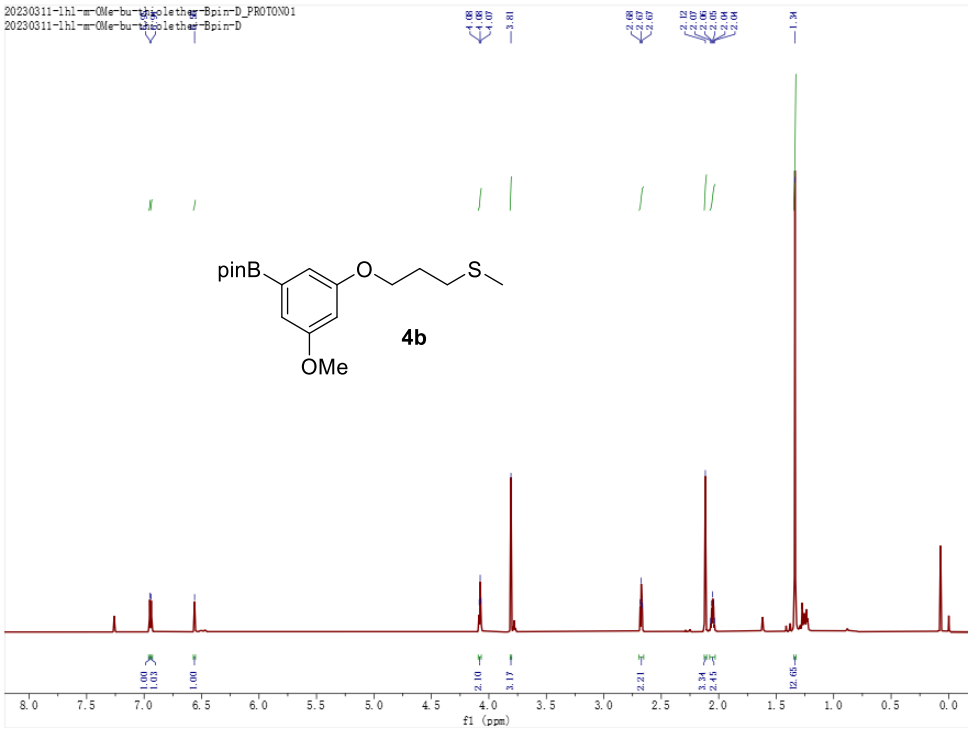



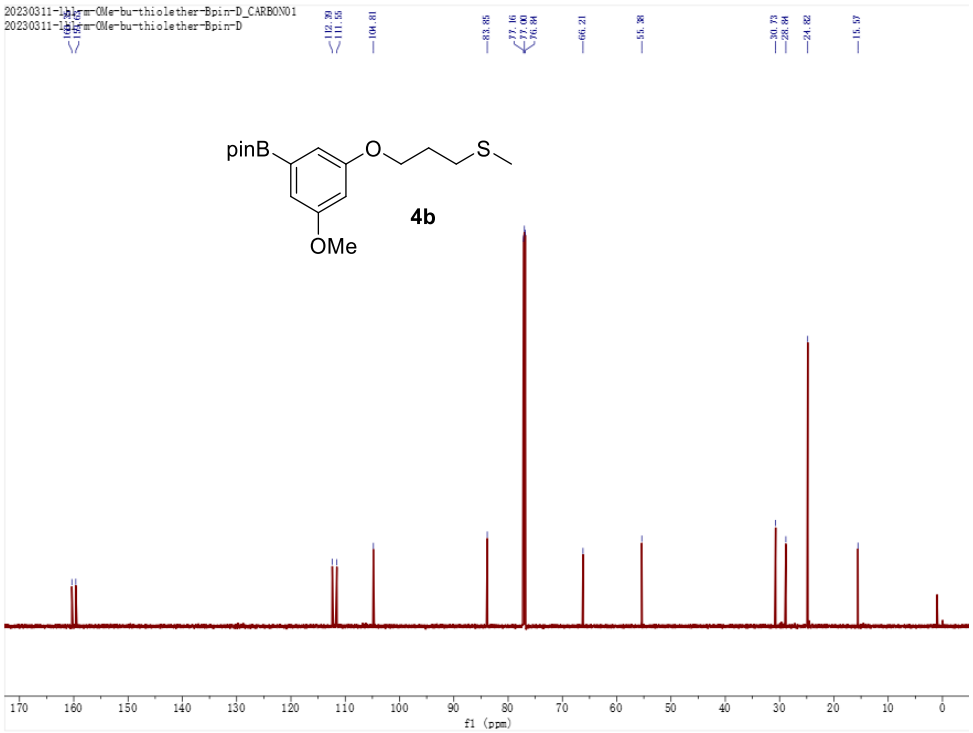
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3b**



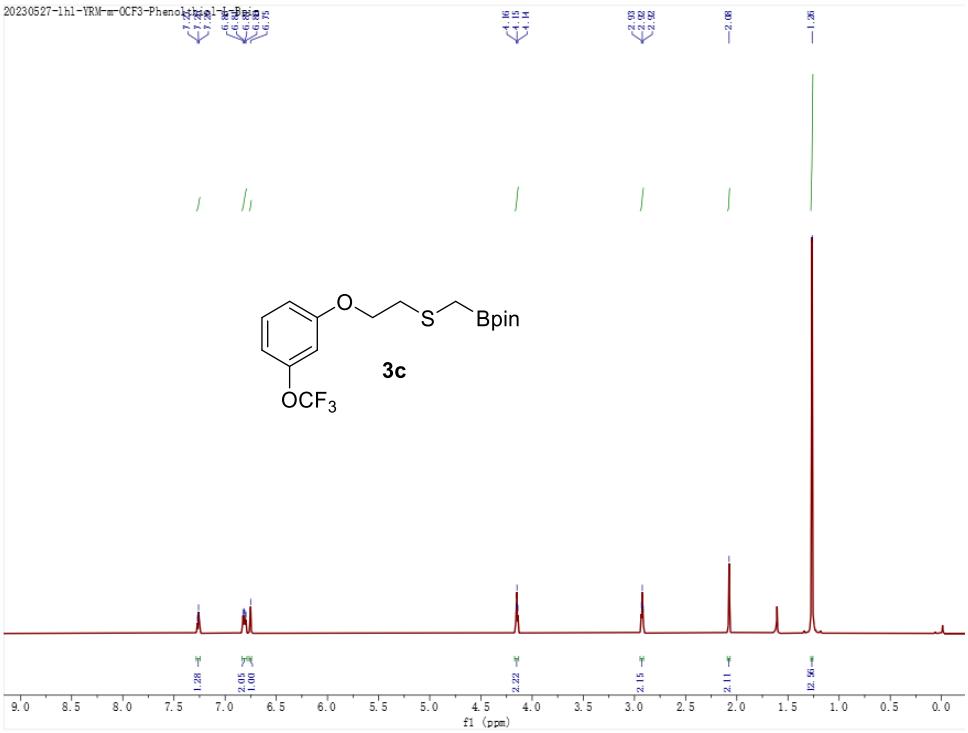



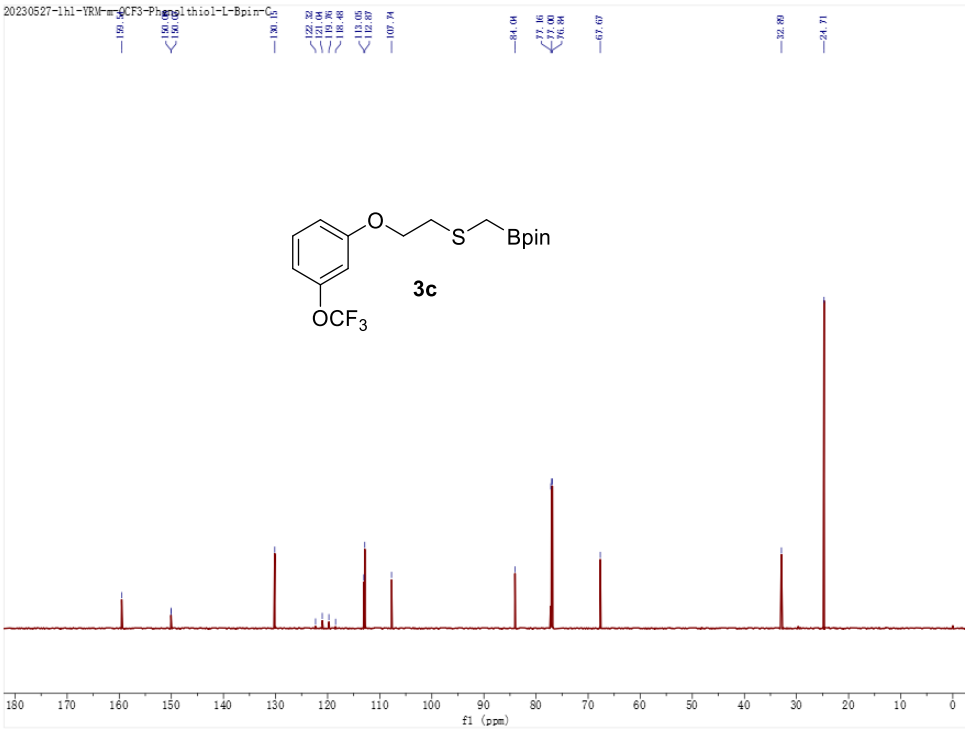
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4b**



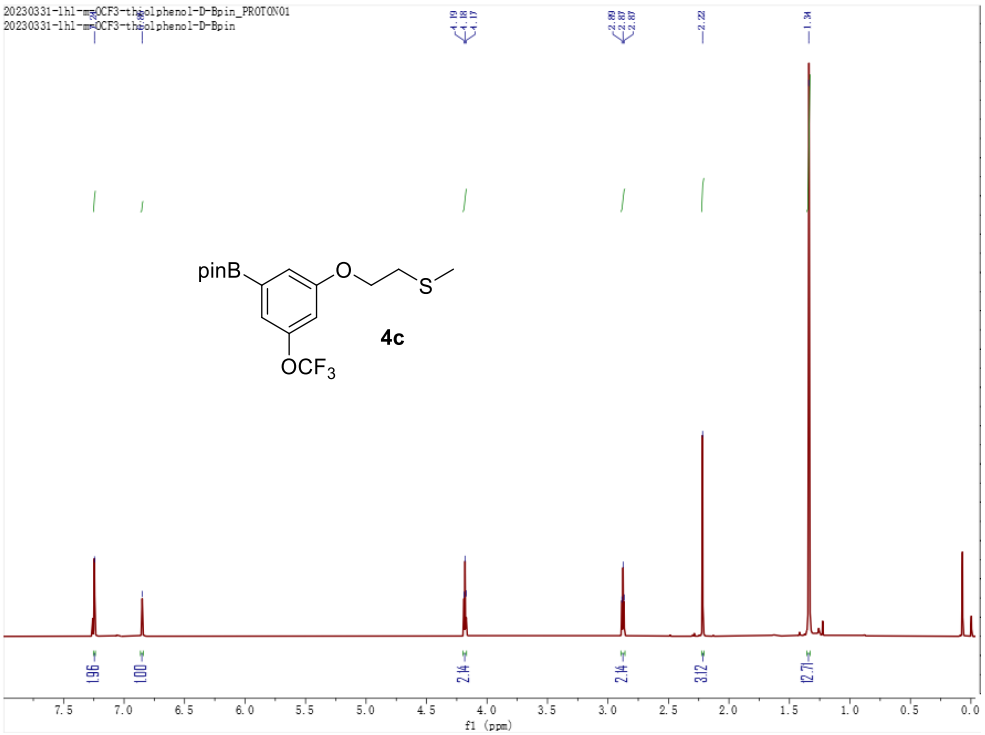



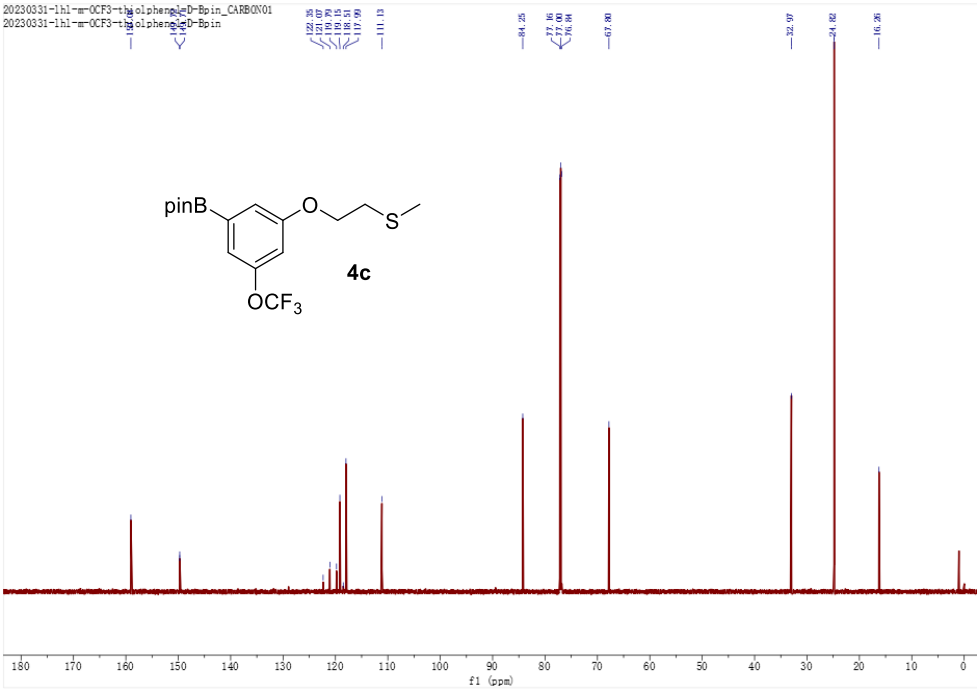
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3c**



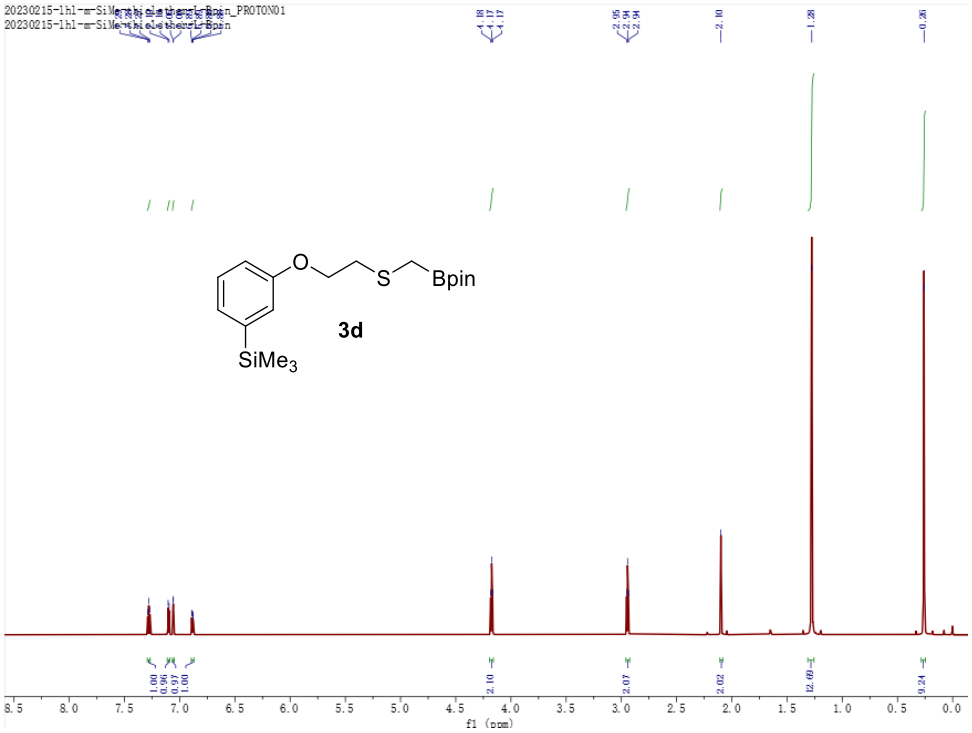



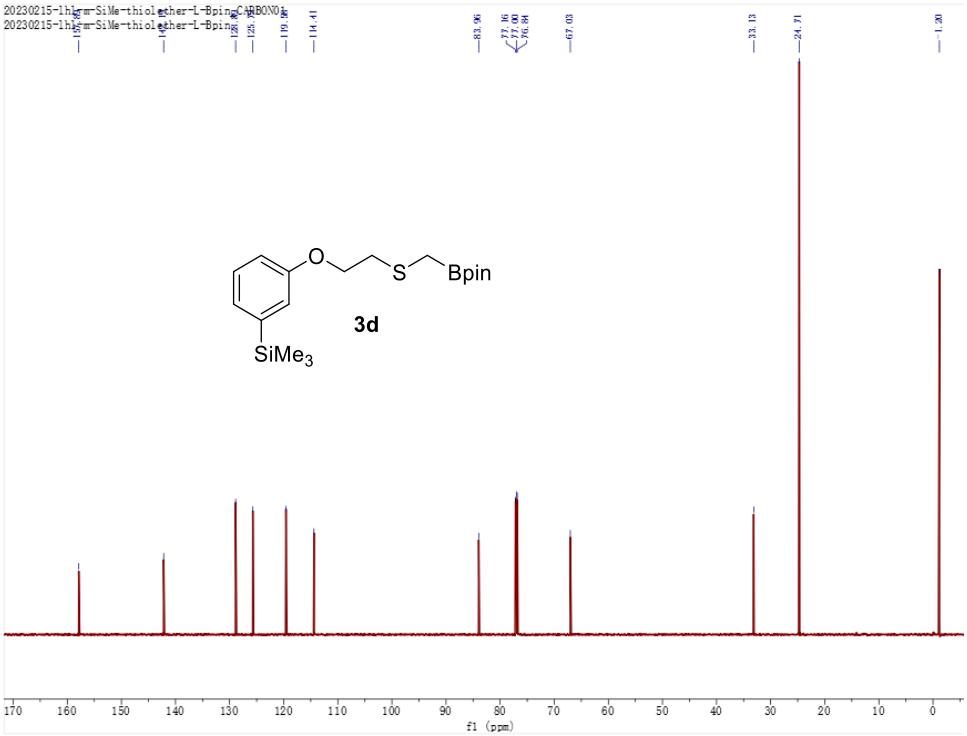
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4c**



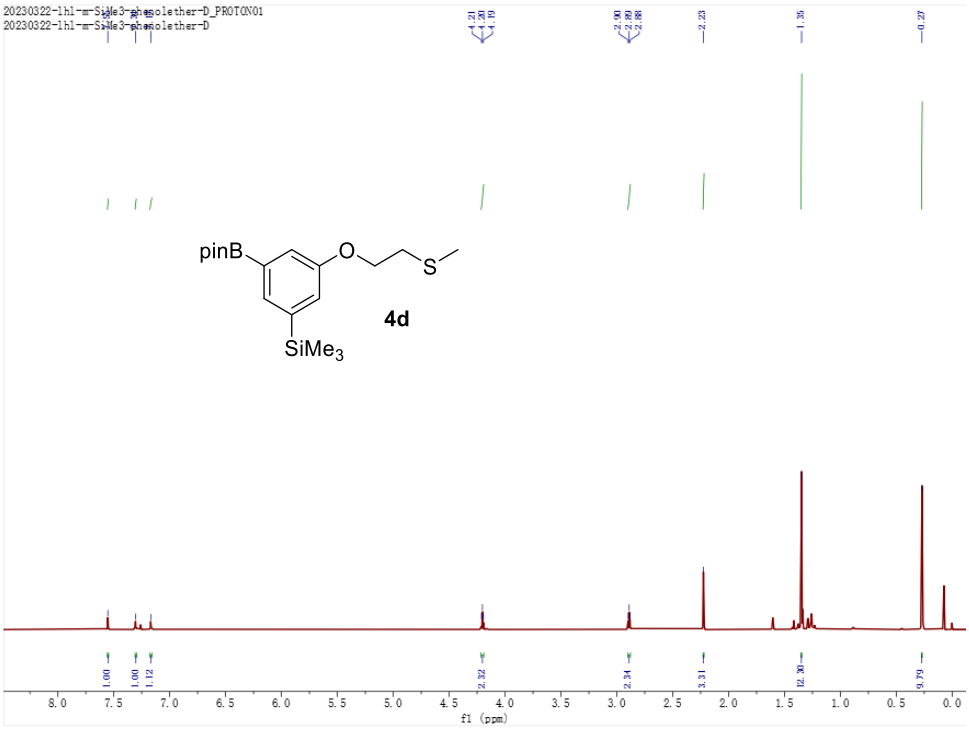



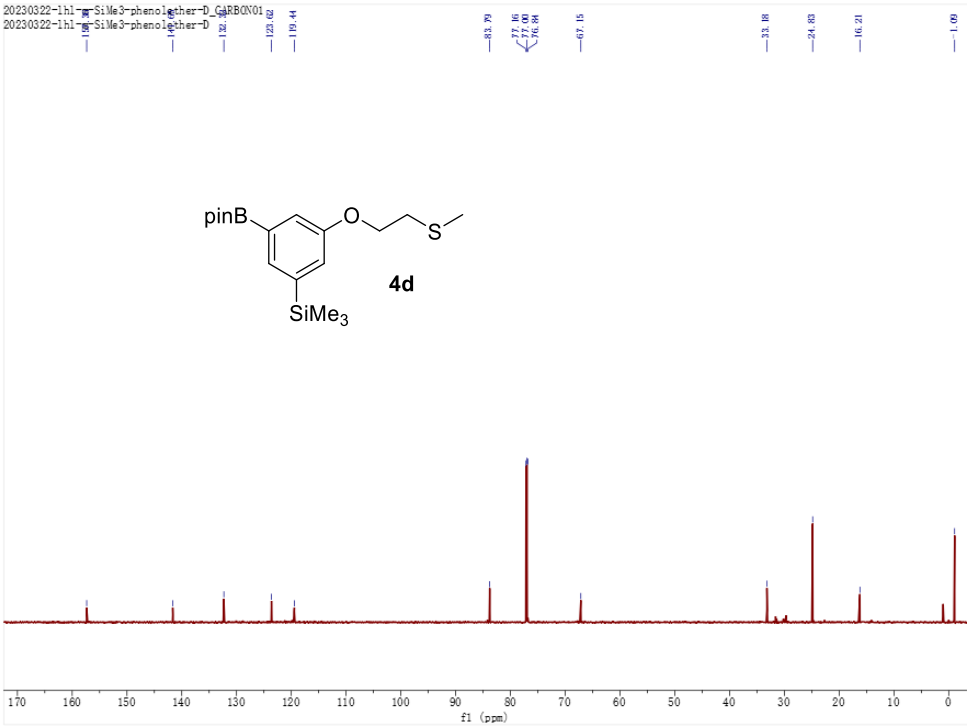
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3d**



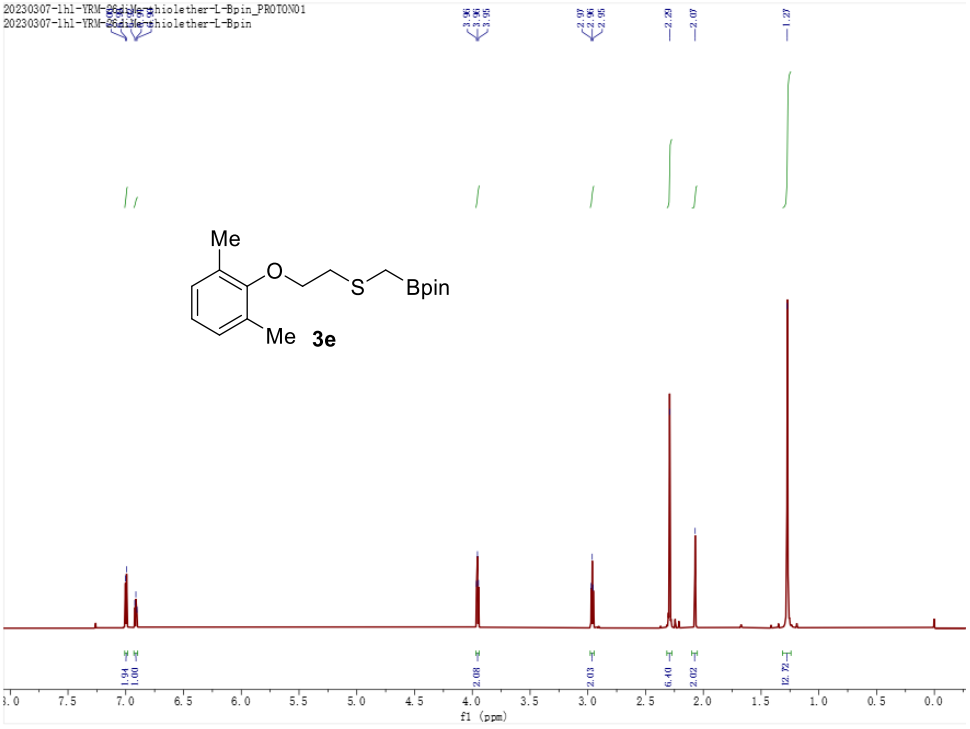



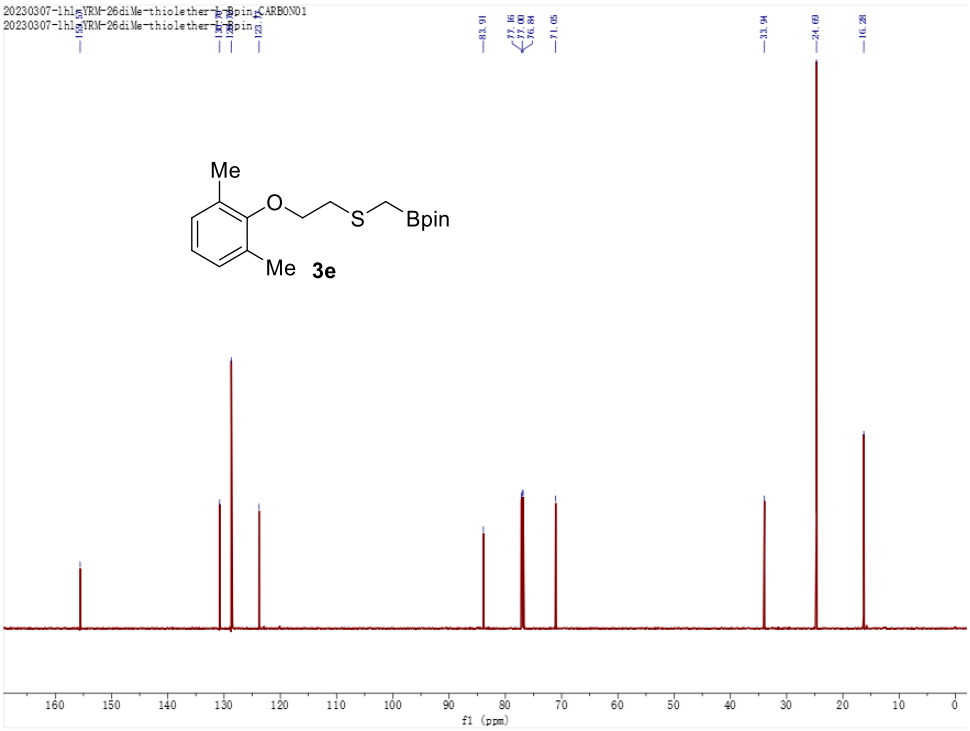
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4d**



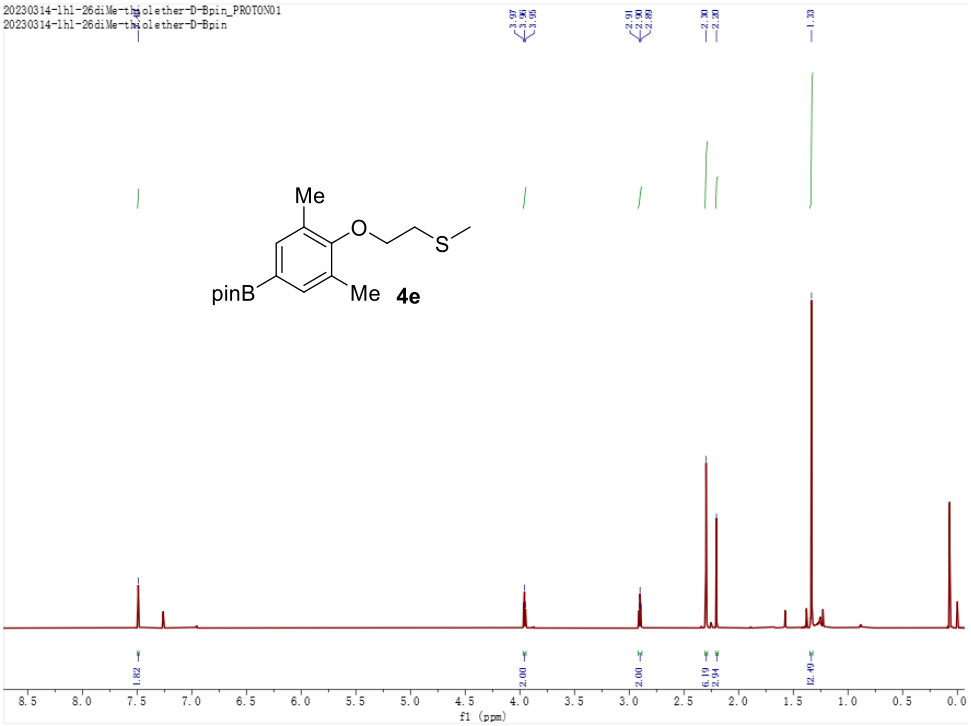



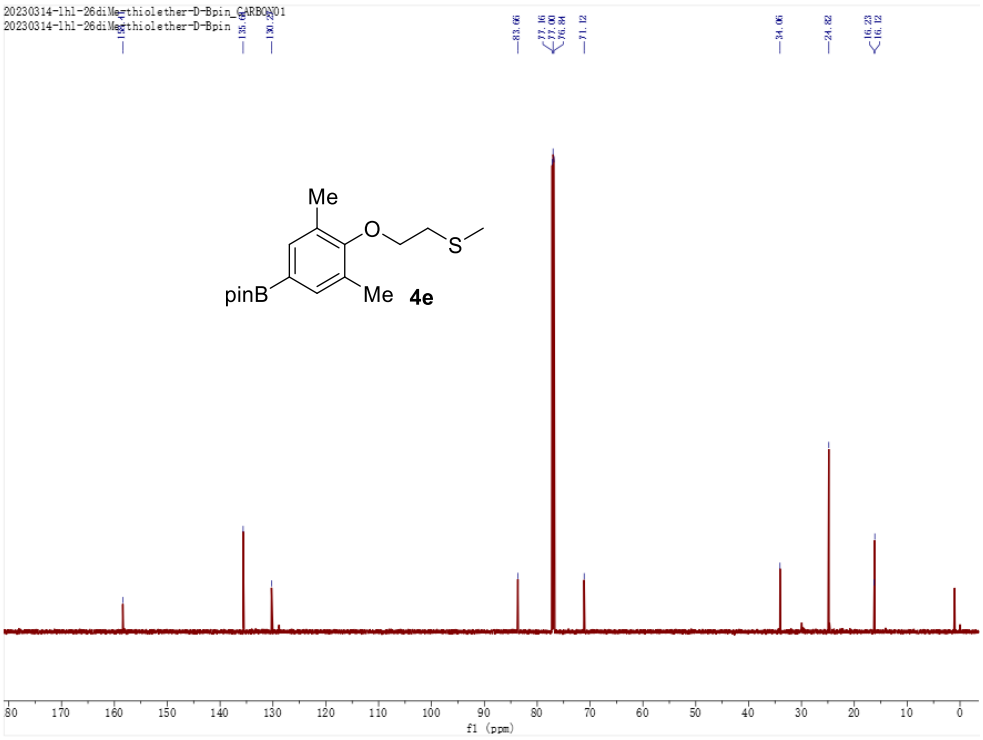
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3e**



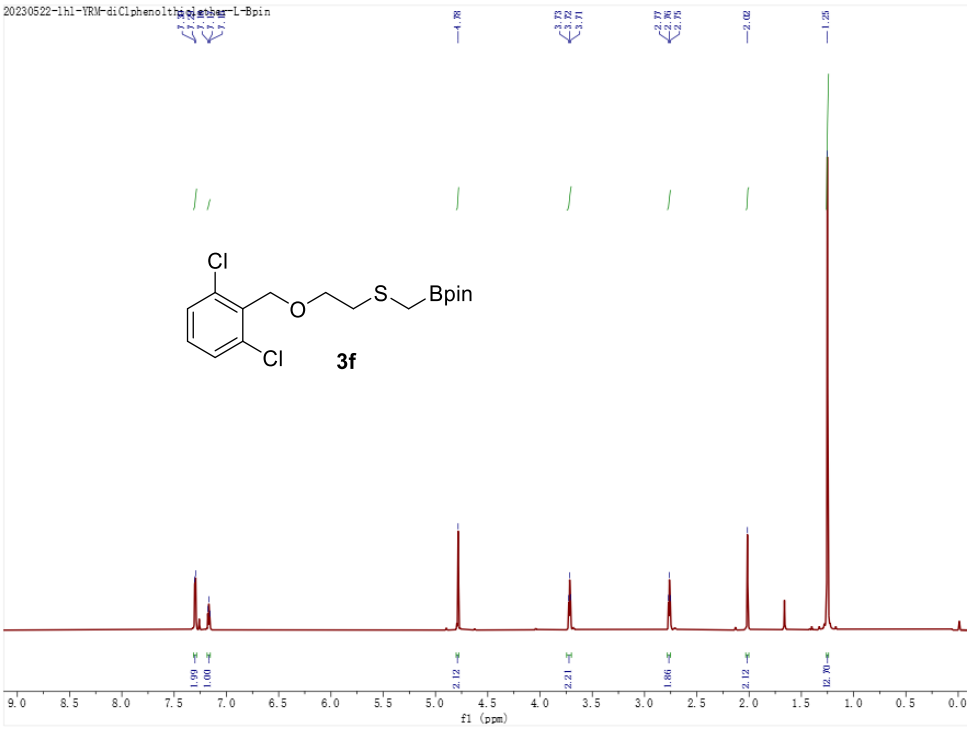



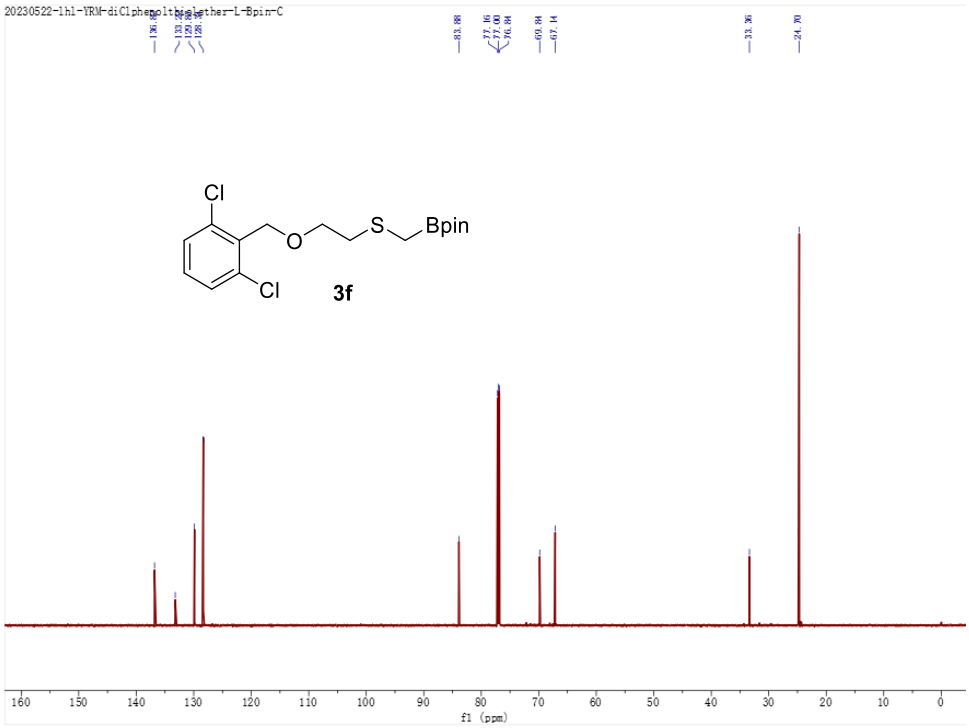
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4e**



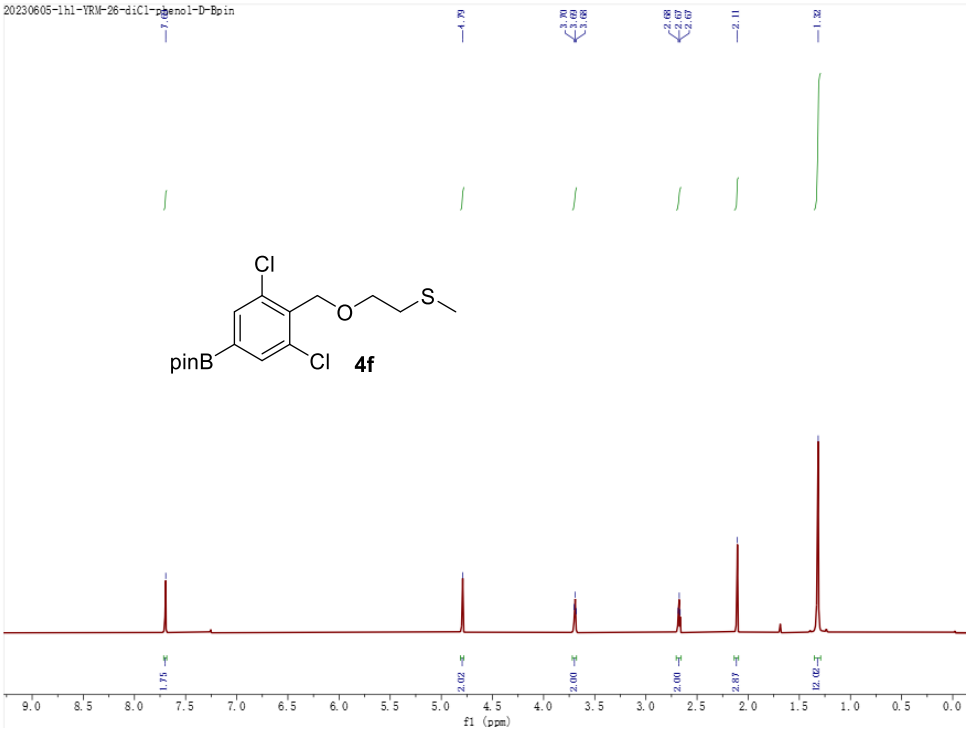



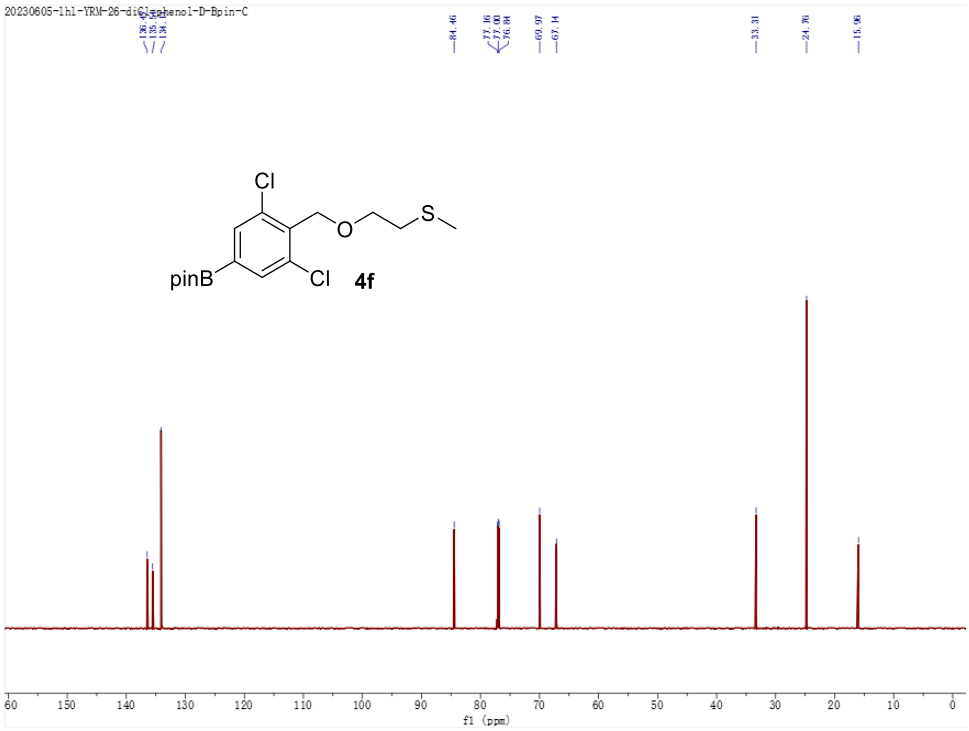
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3f**



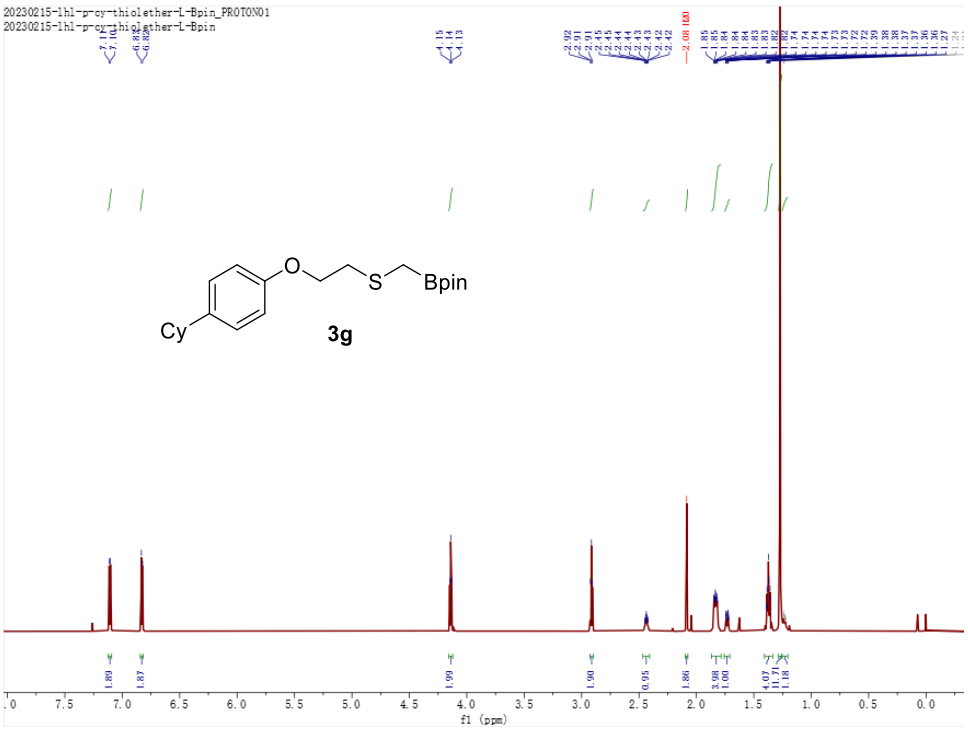



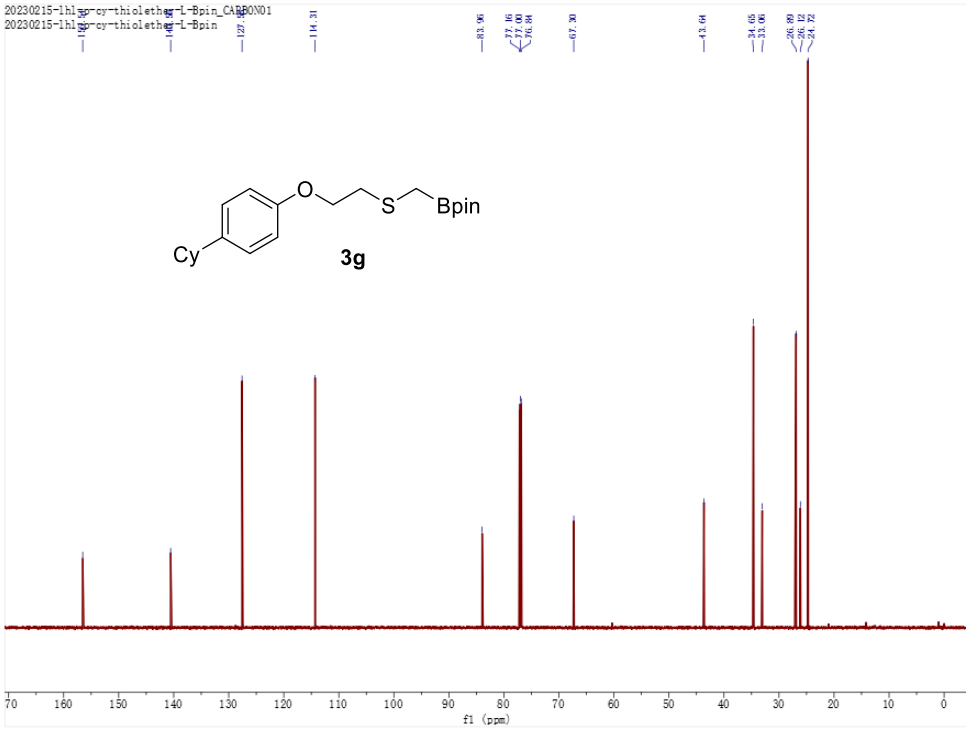
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4f**



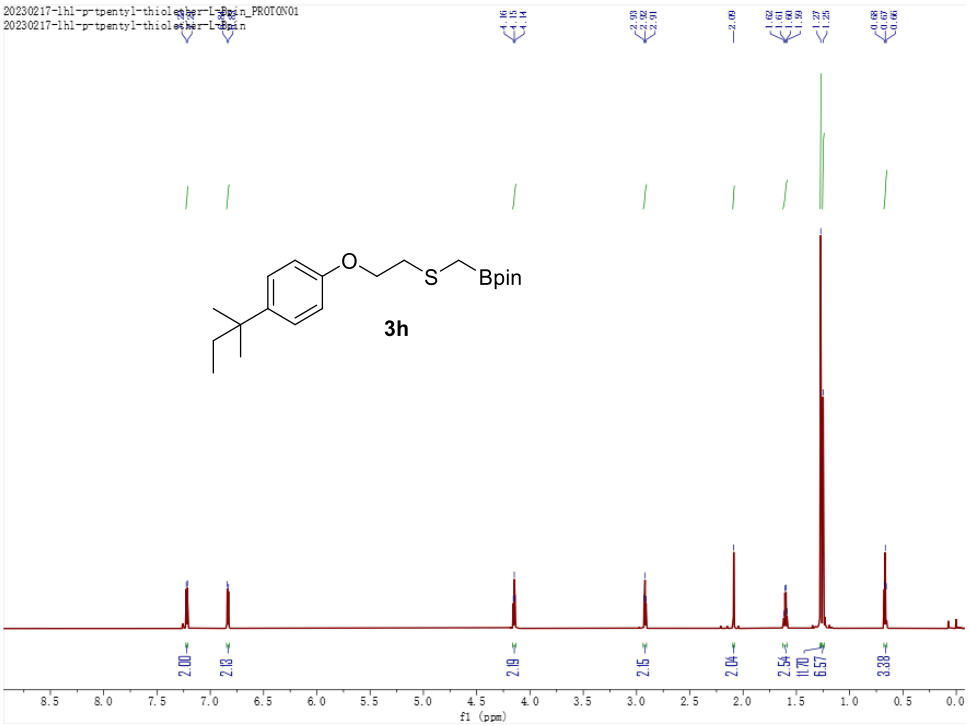



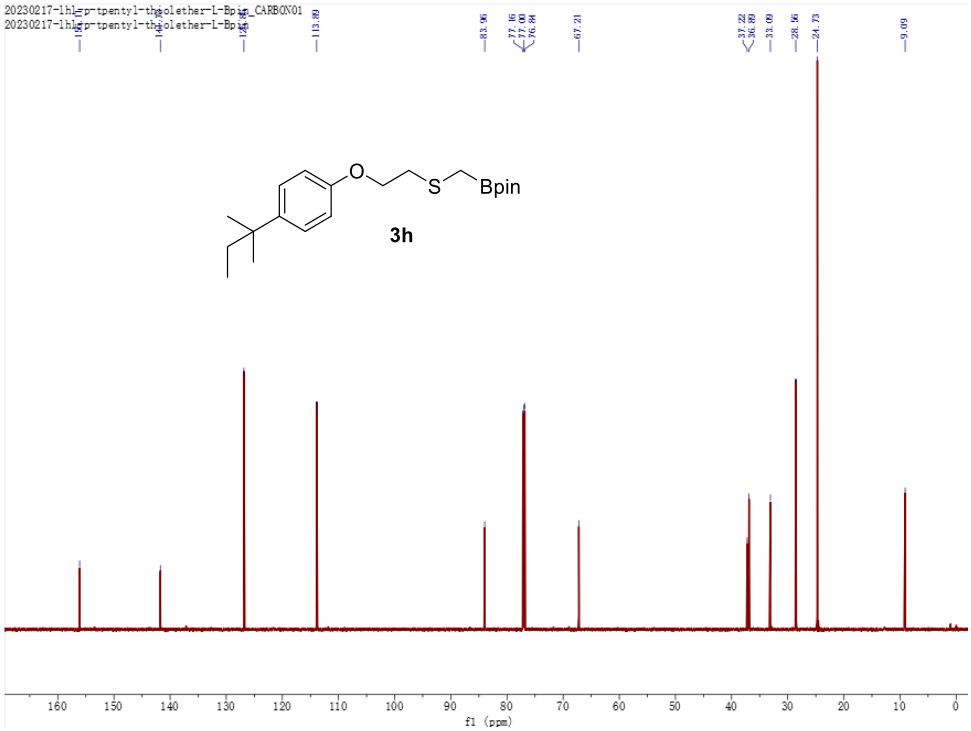
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3g**



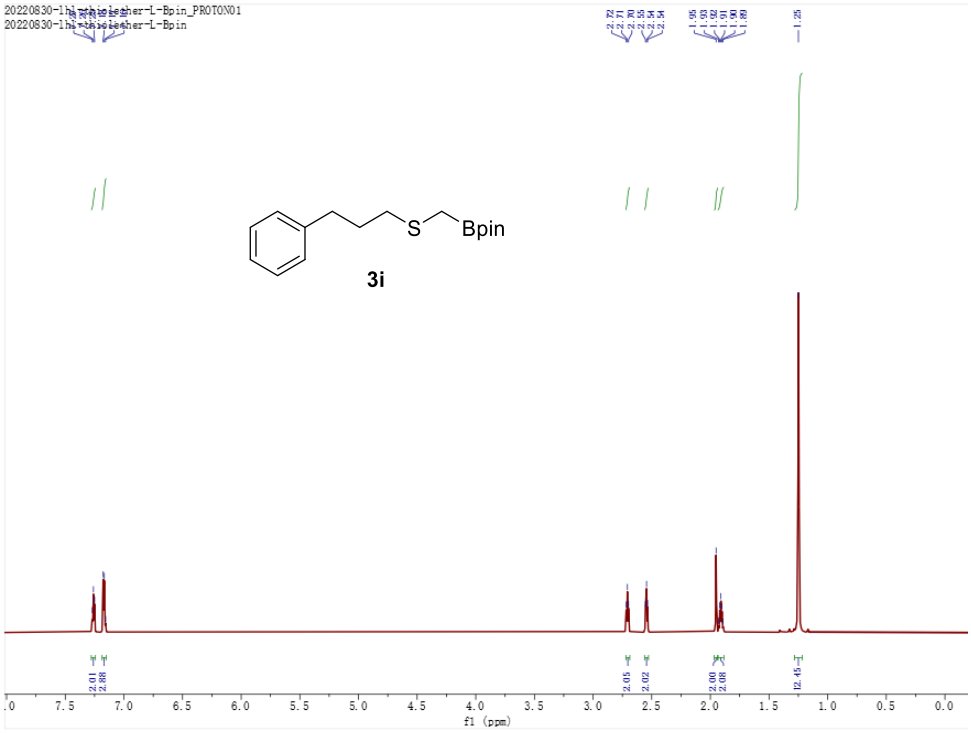



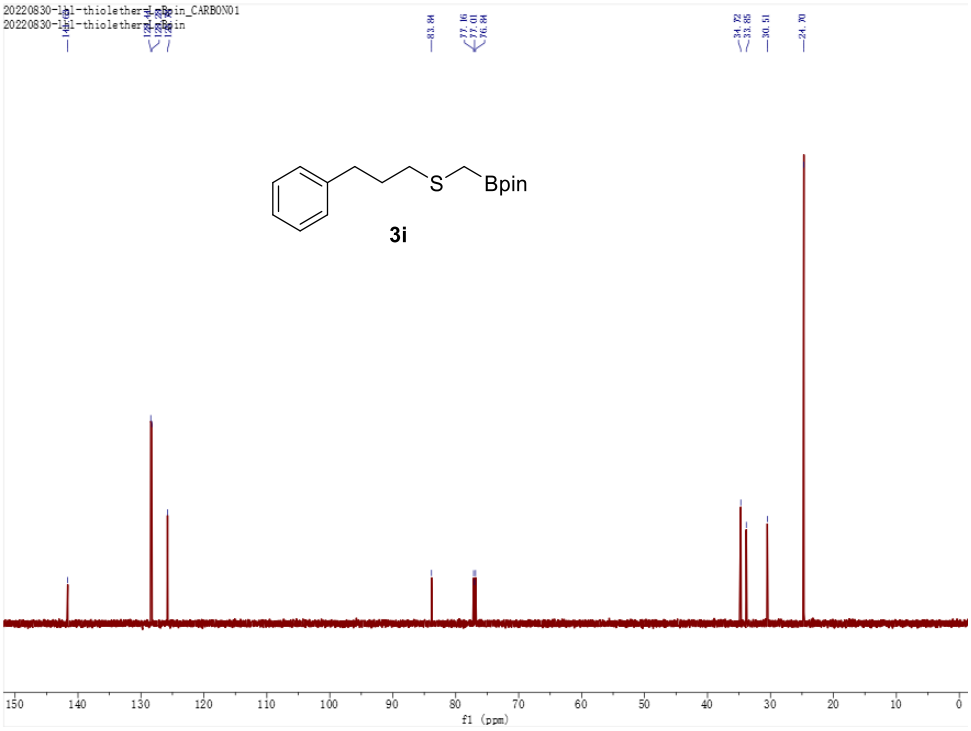
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3h**



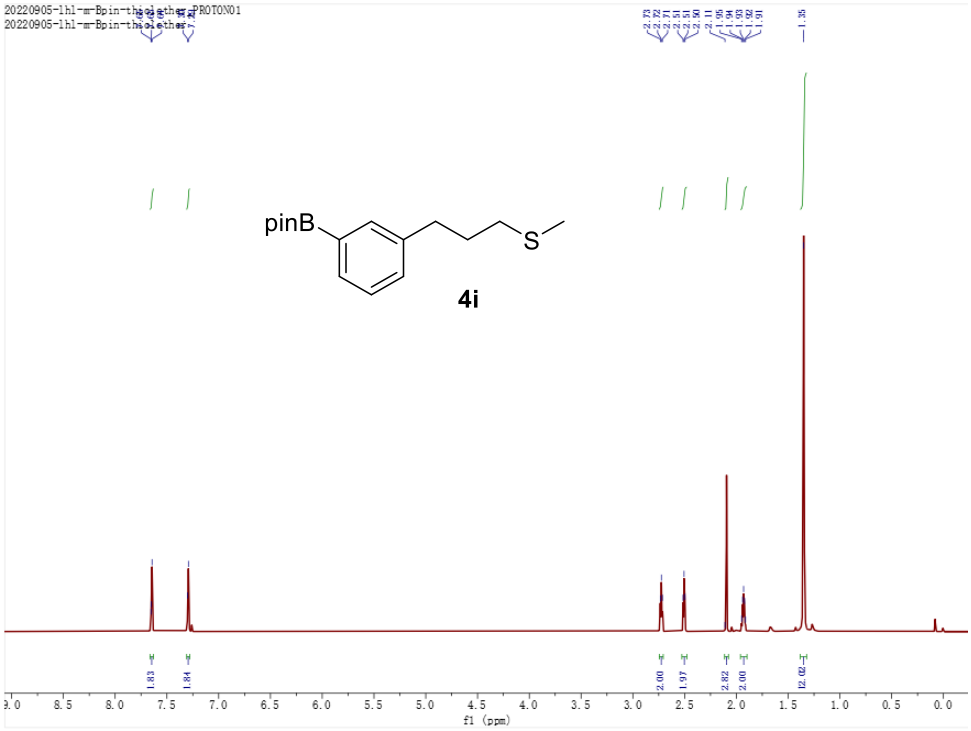



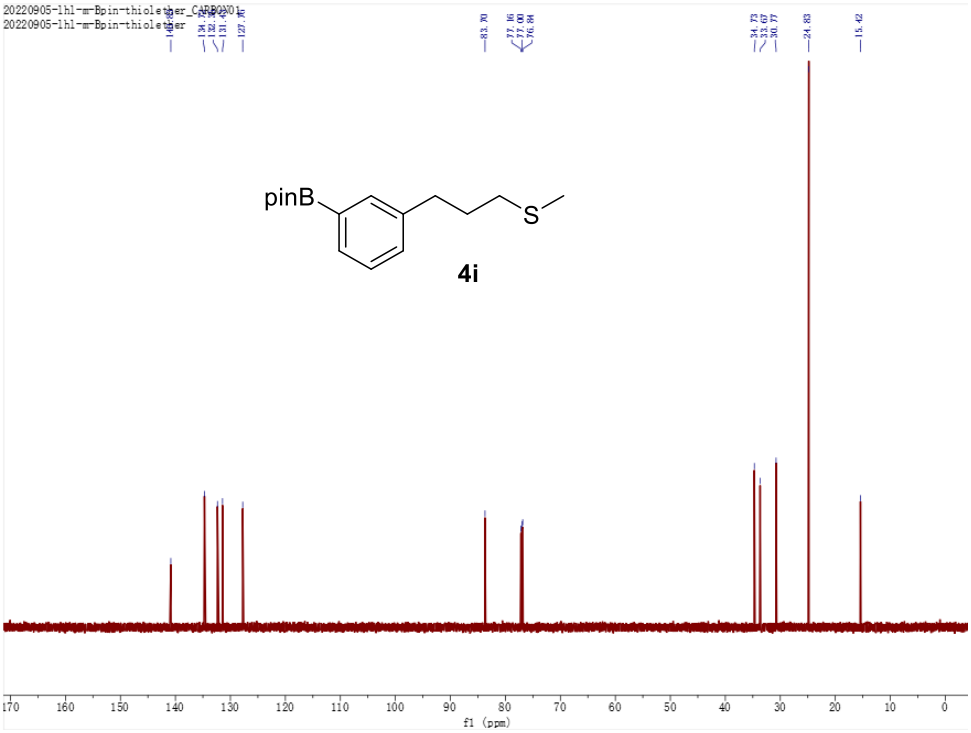
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3i**



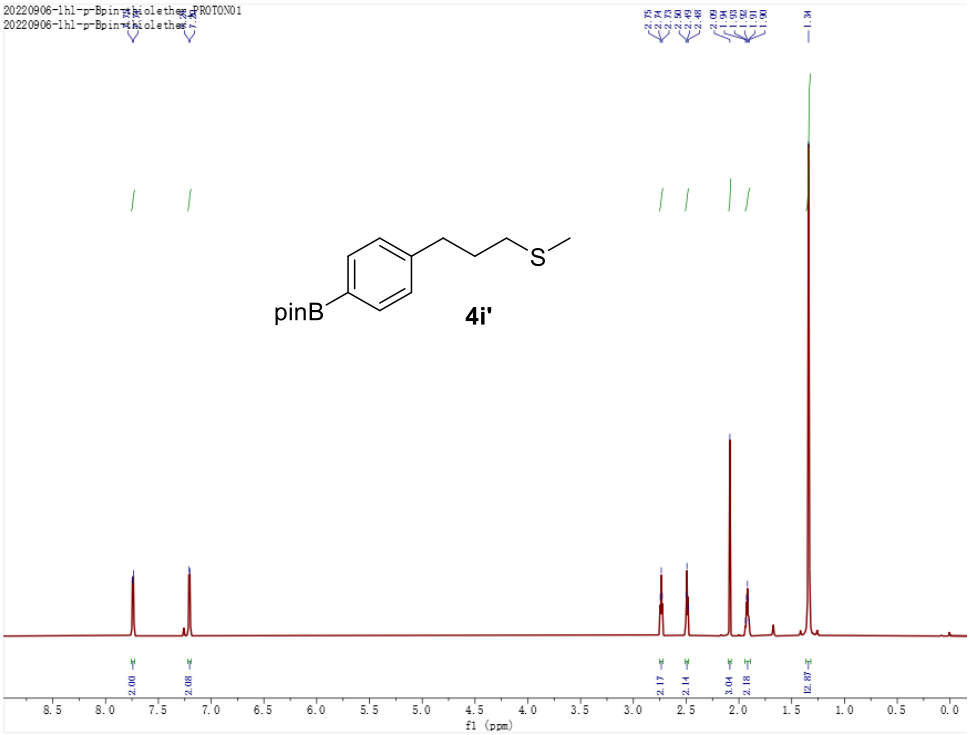



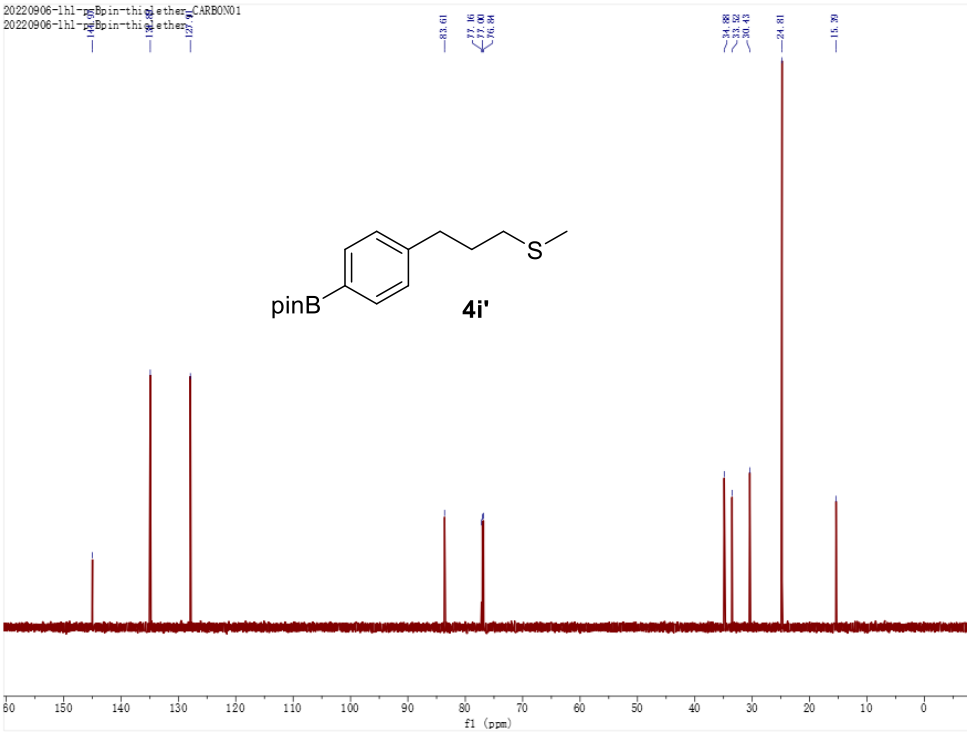
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4i**



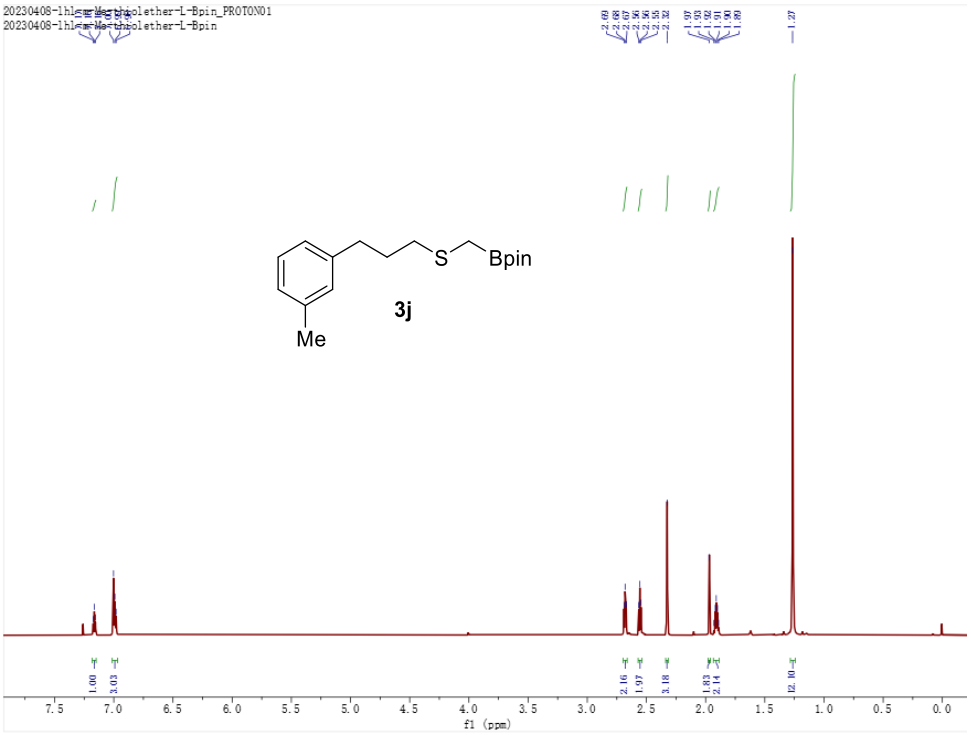



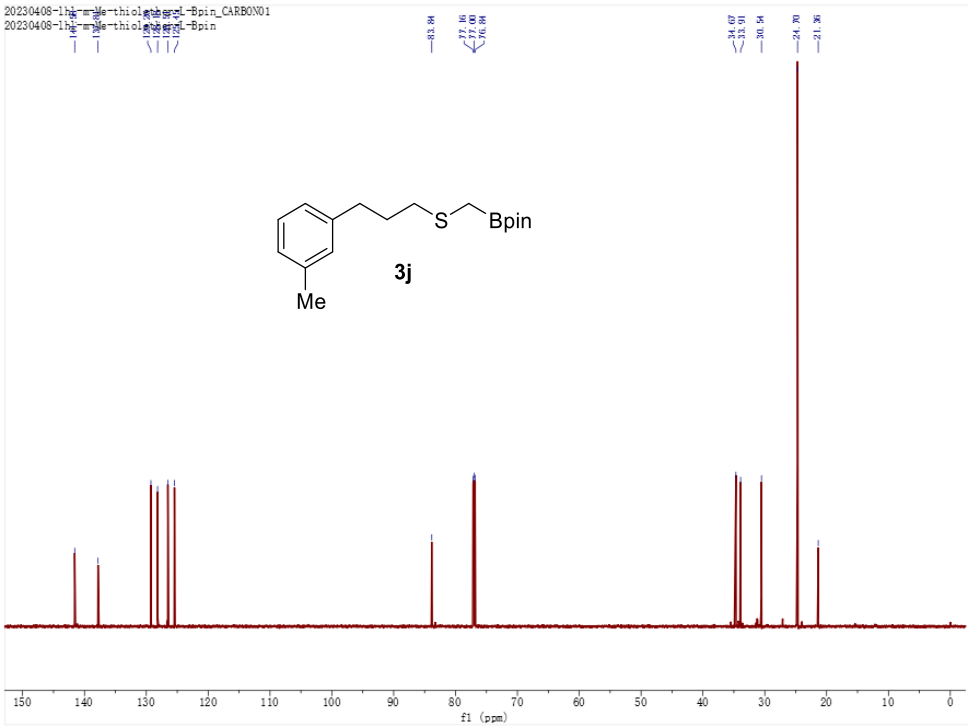
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4i'**



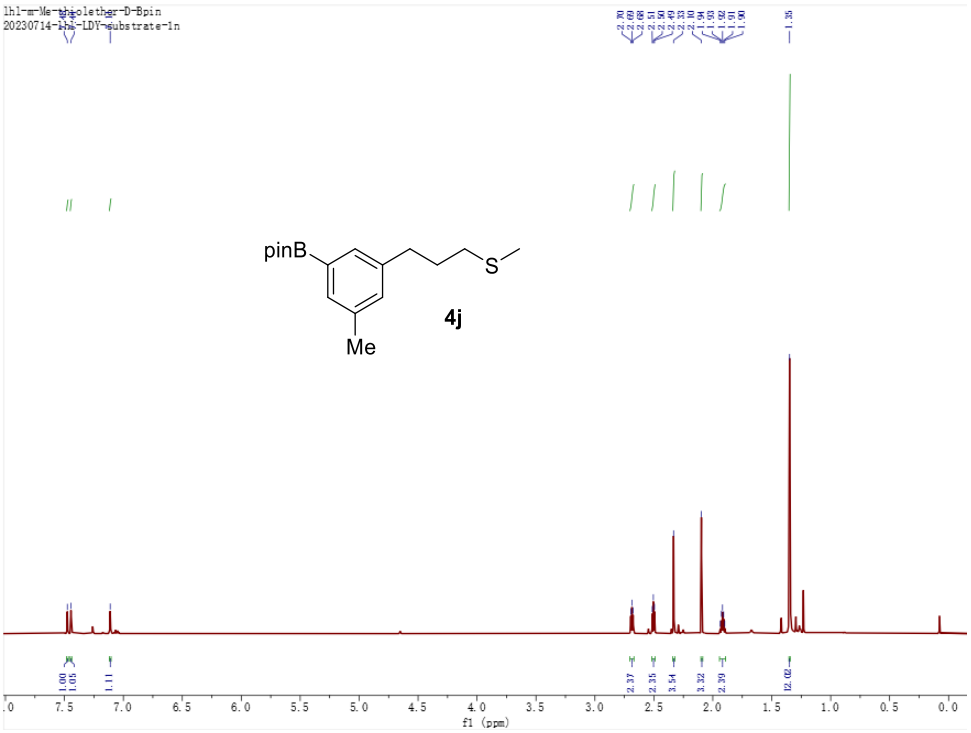



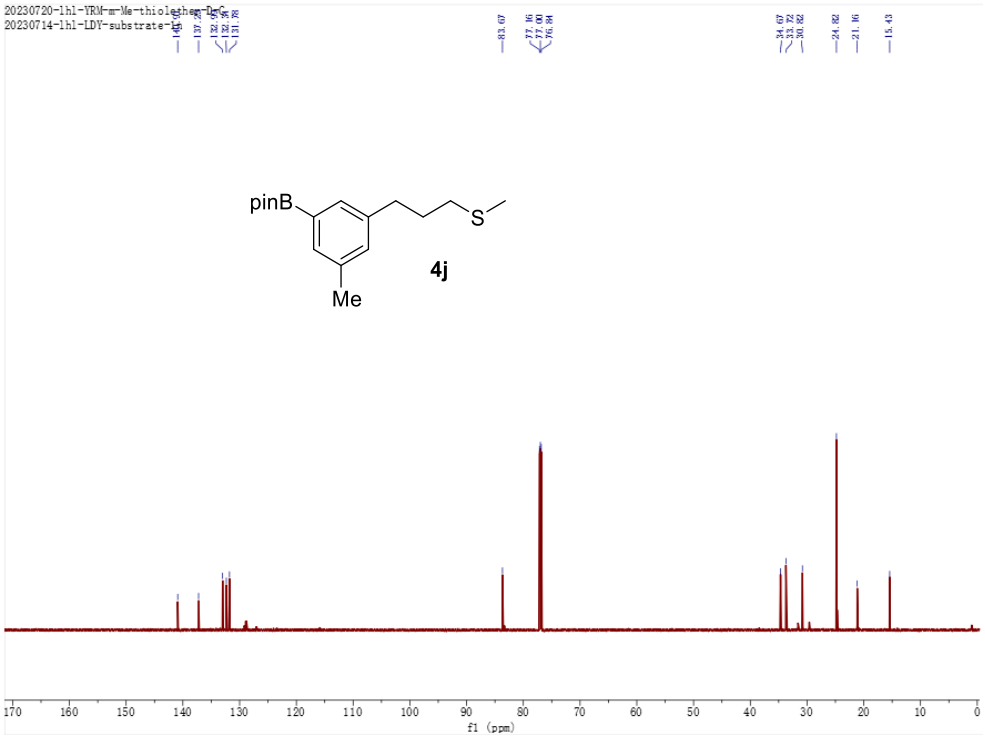
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3j**



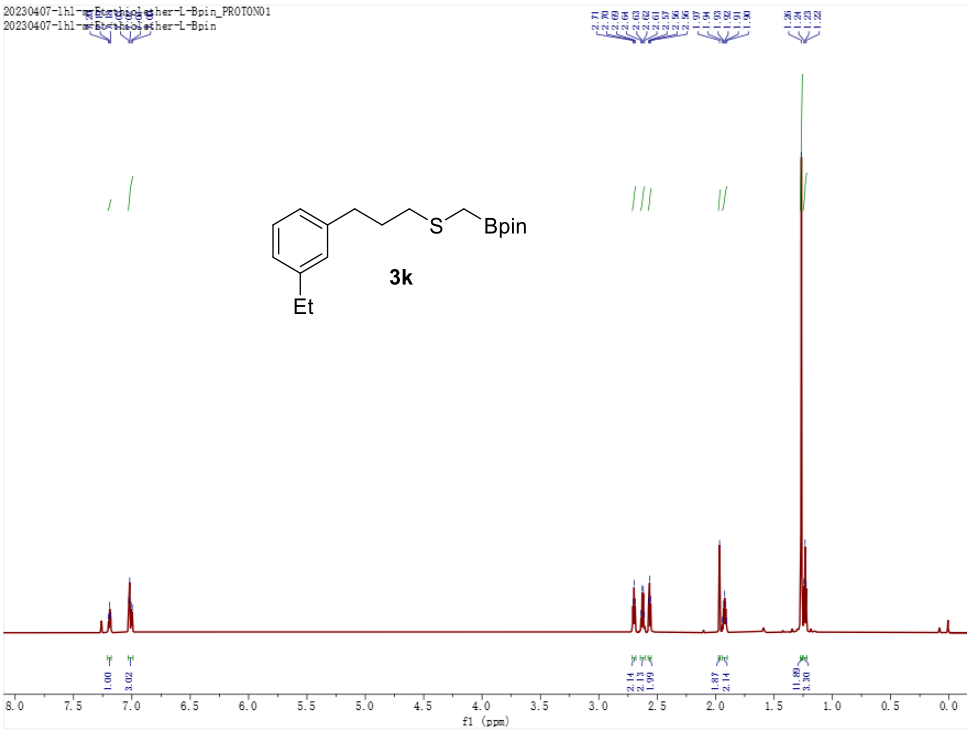



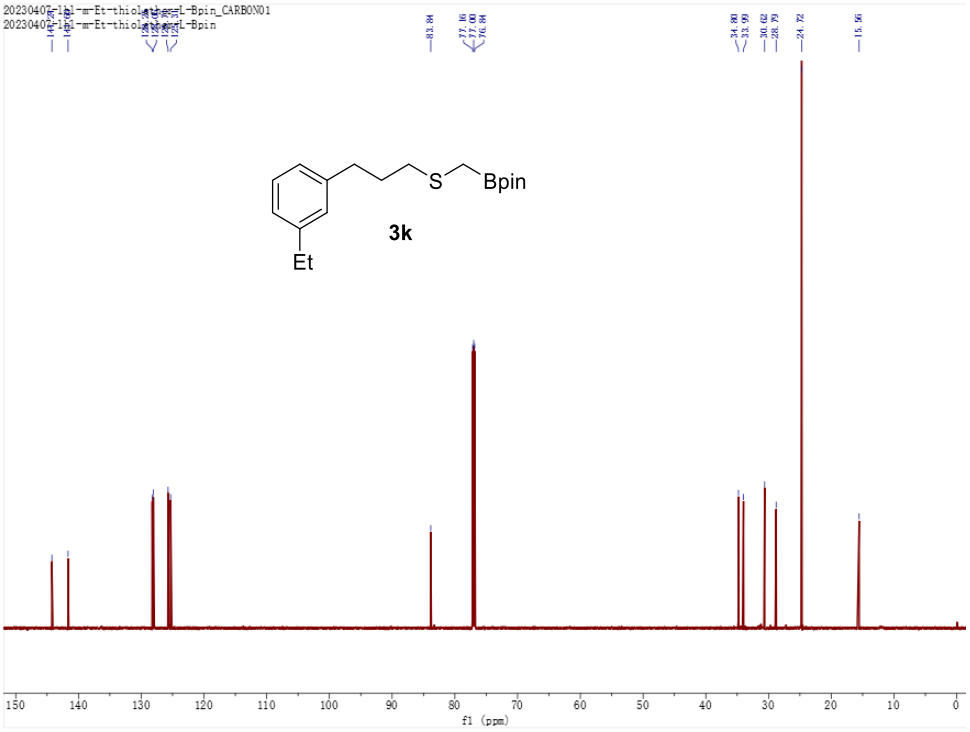
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4j**



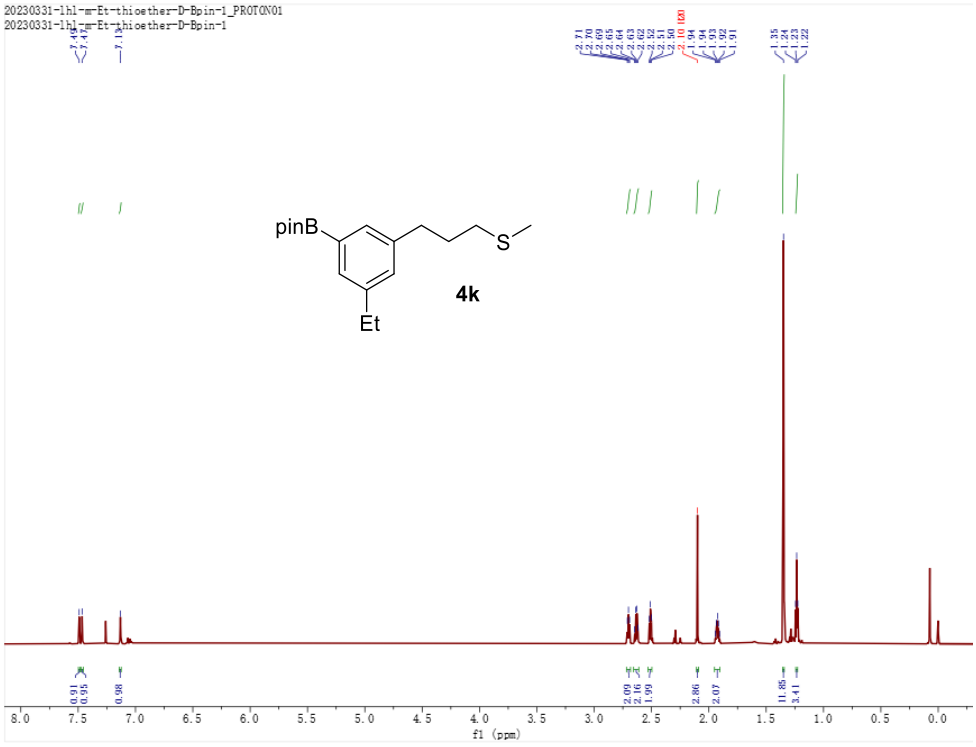



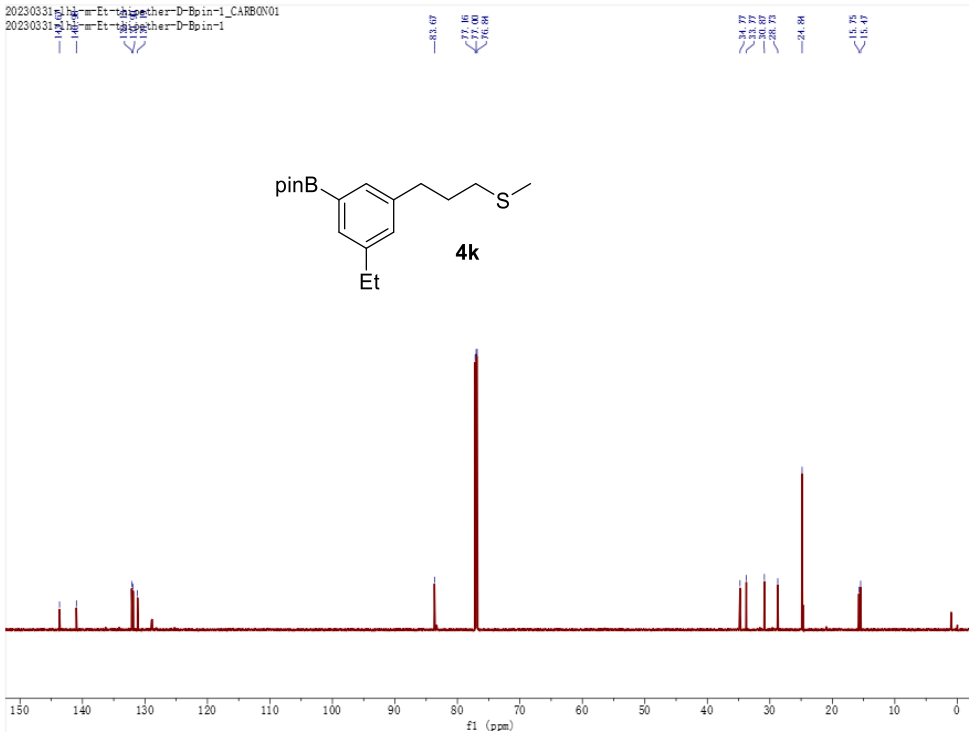
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3k**



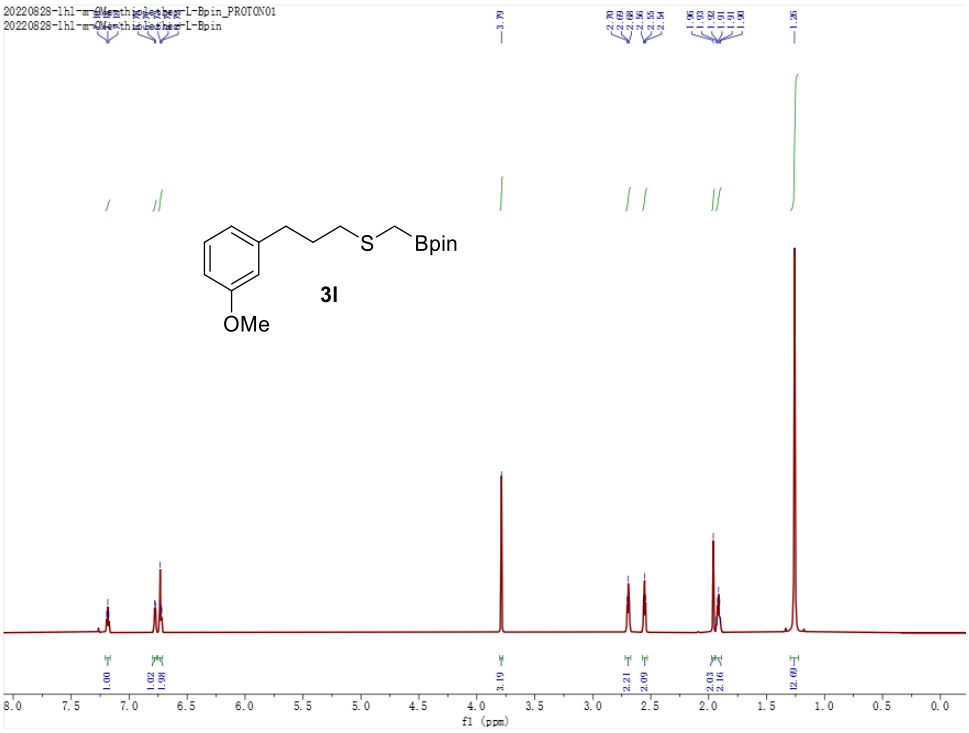



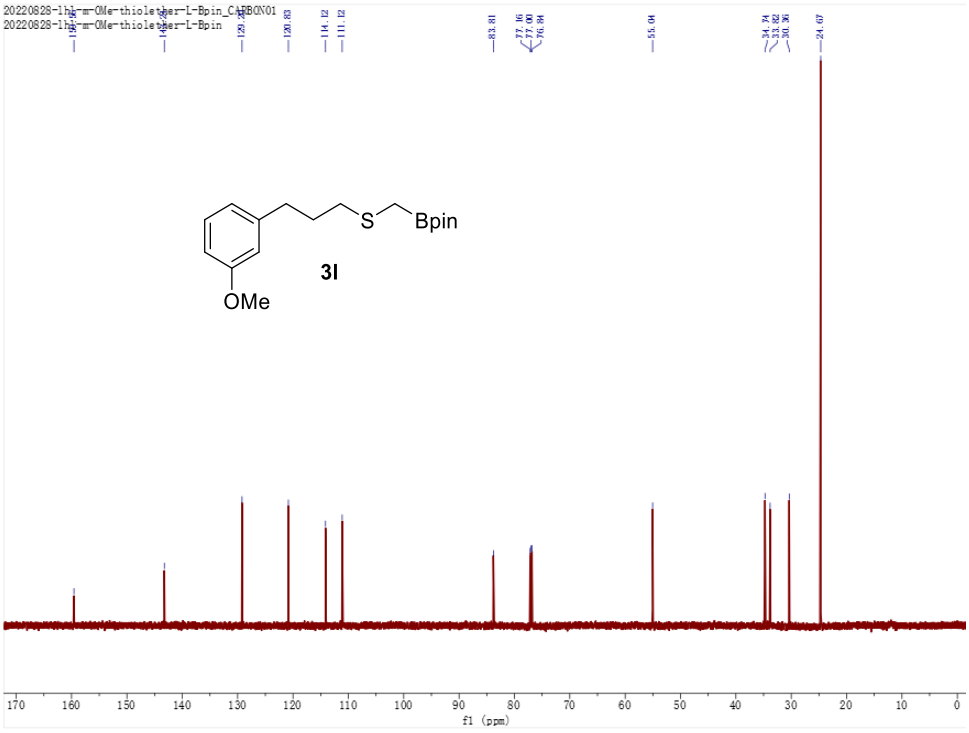
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4k**



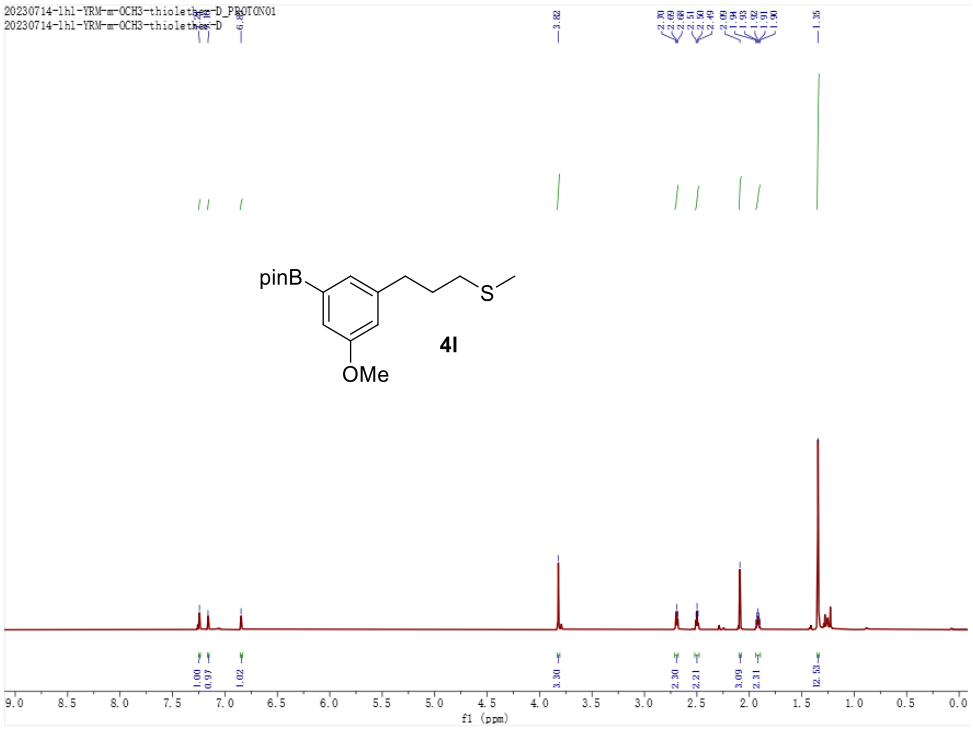



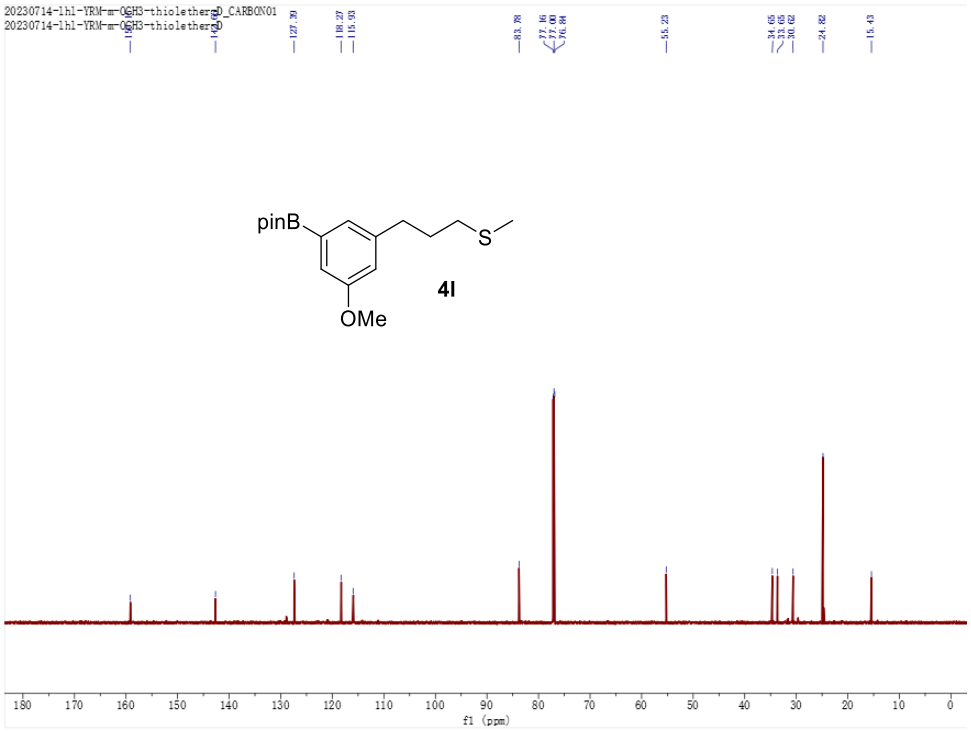
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3l**



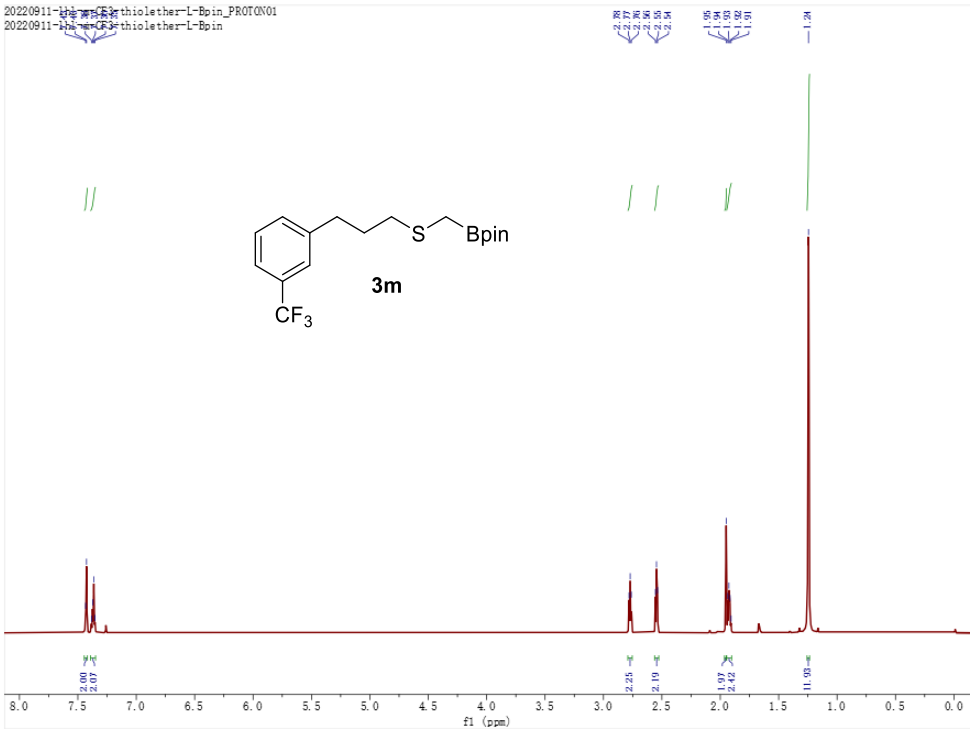



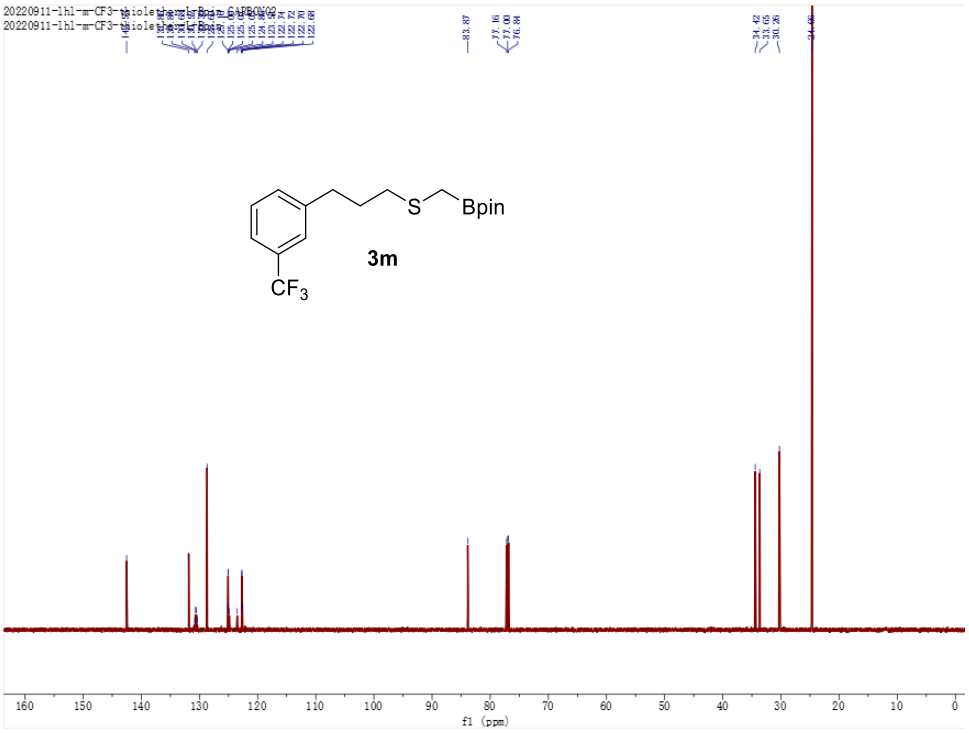
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4l**



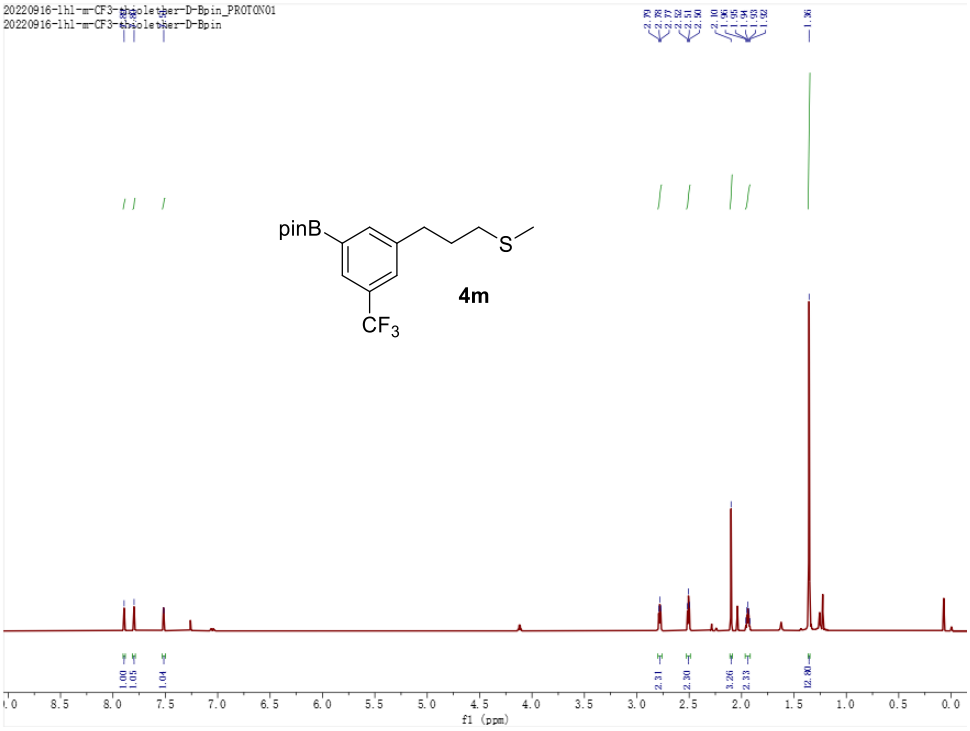



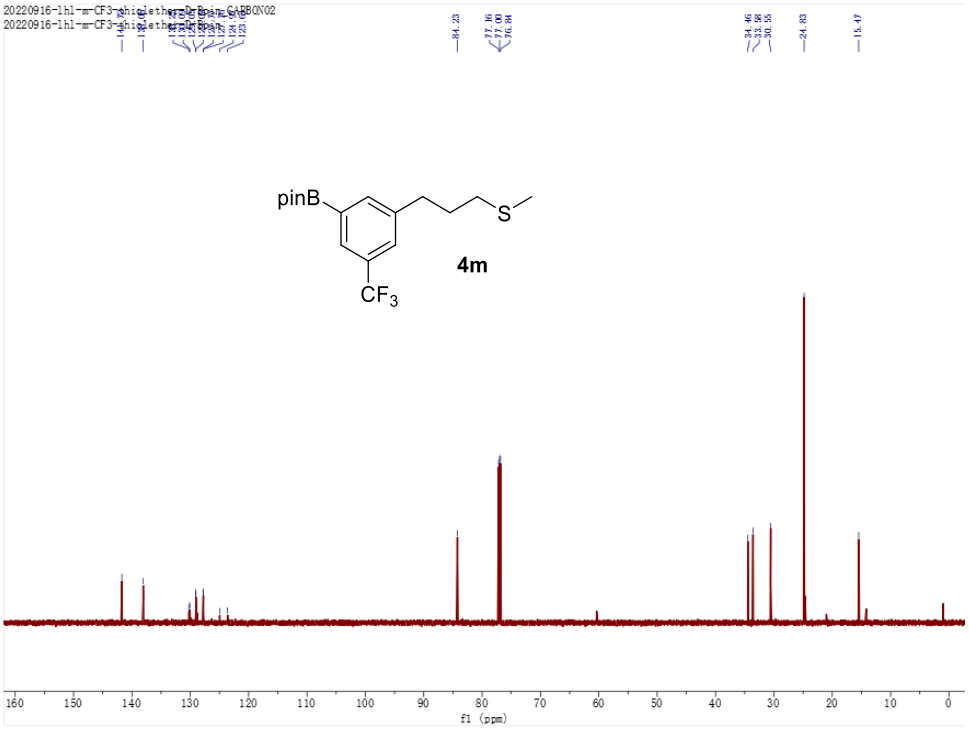
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3m**



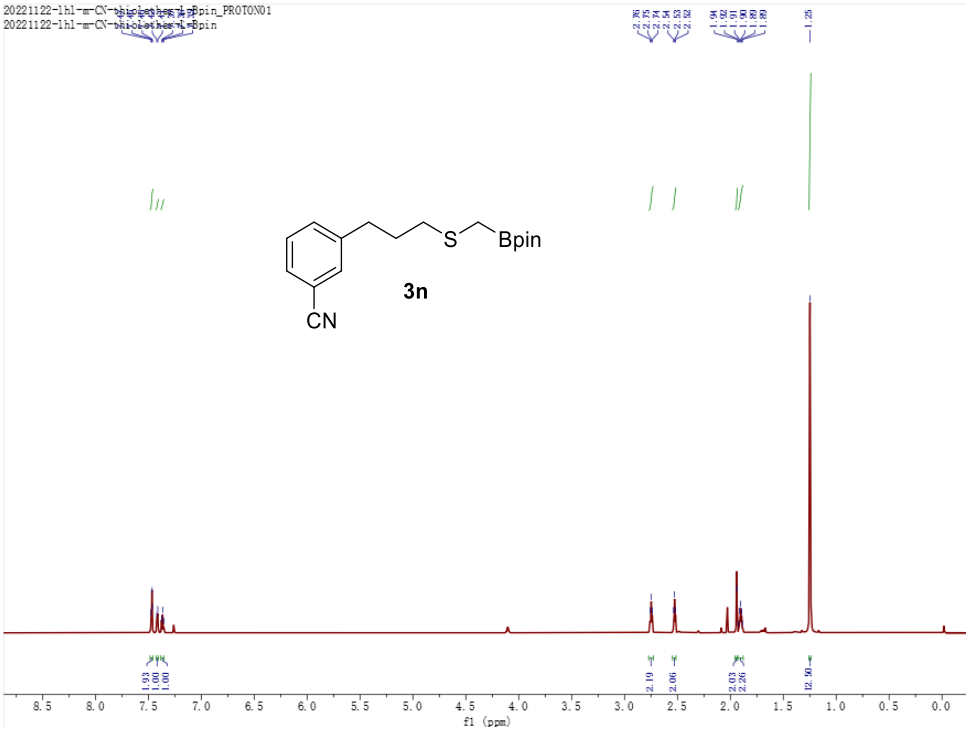



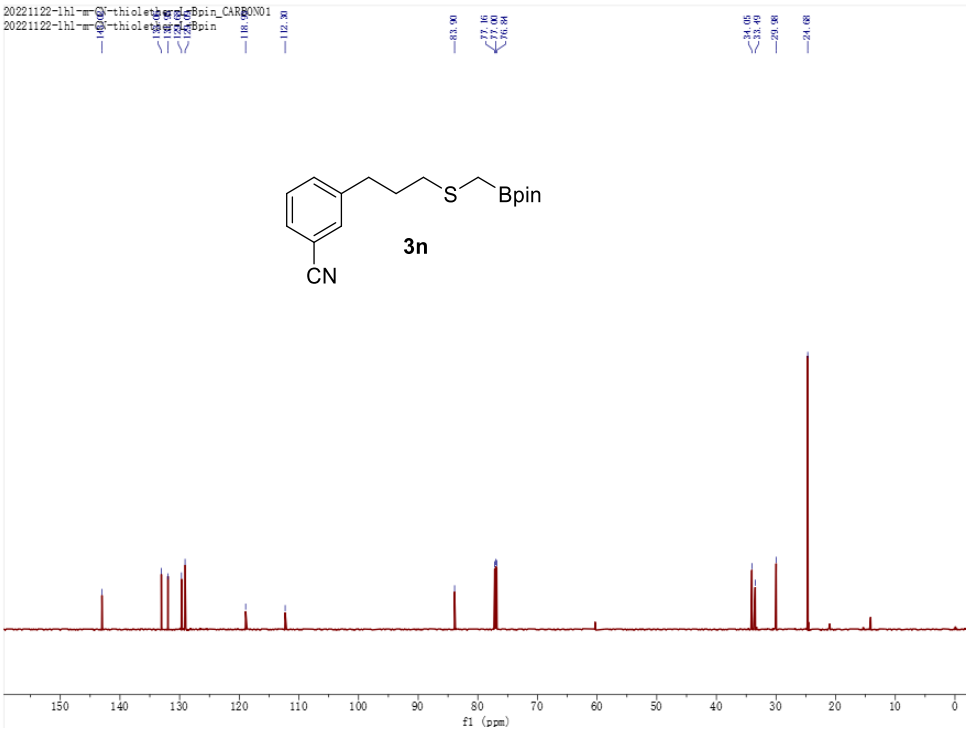
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4m**



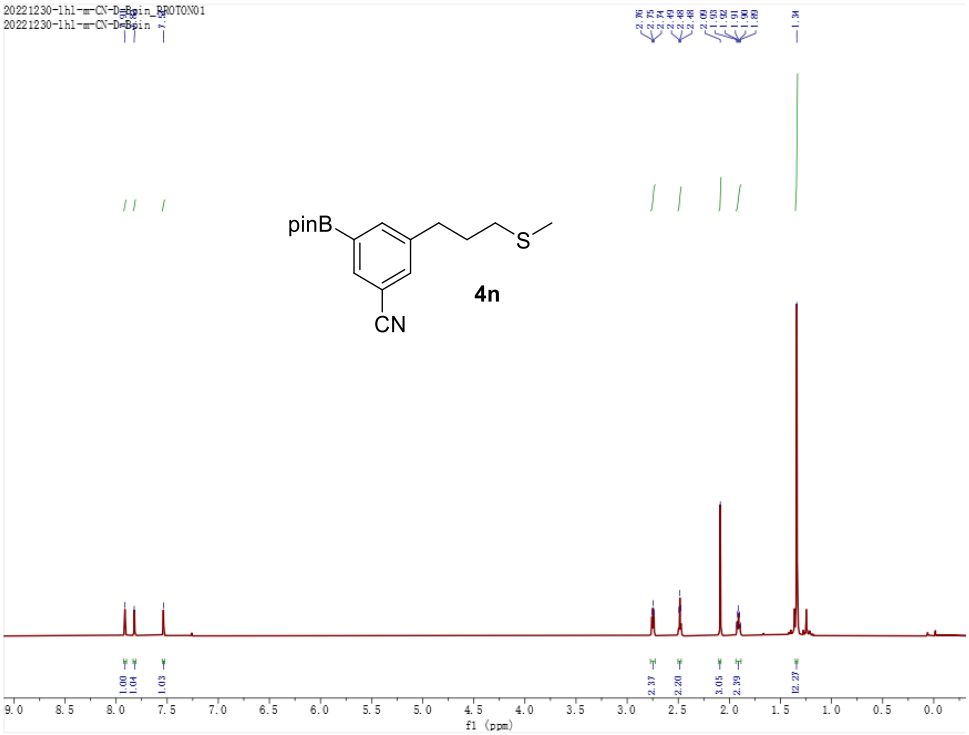



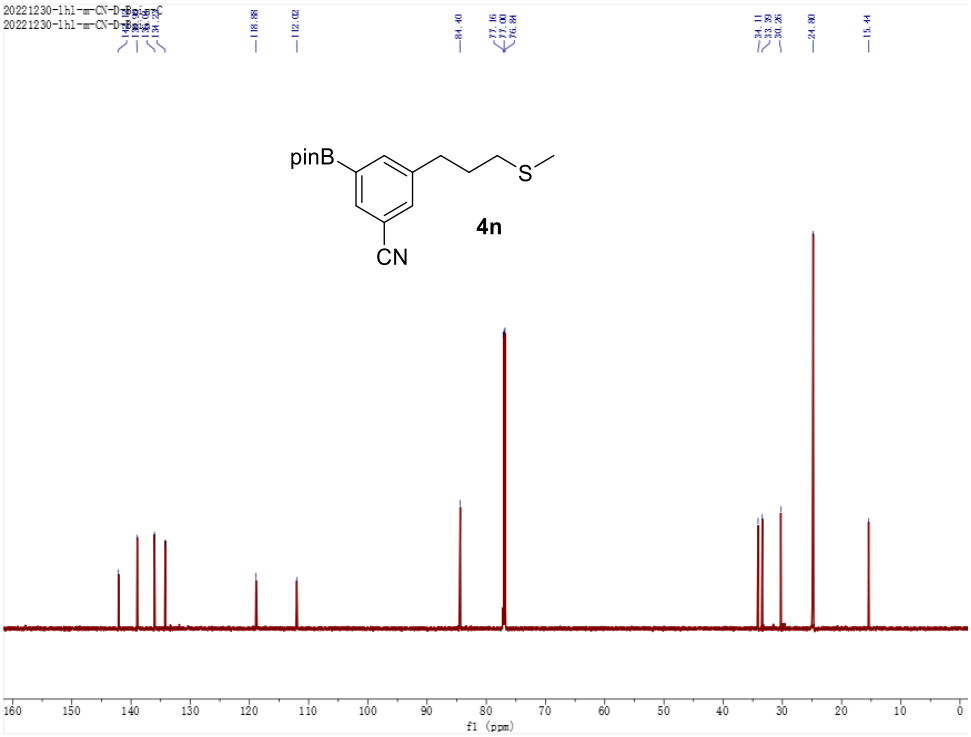
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3n**



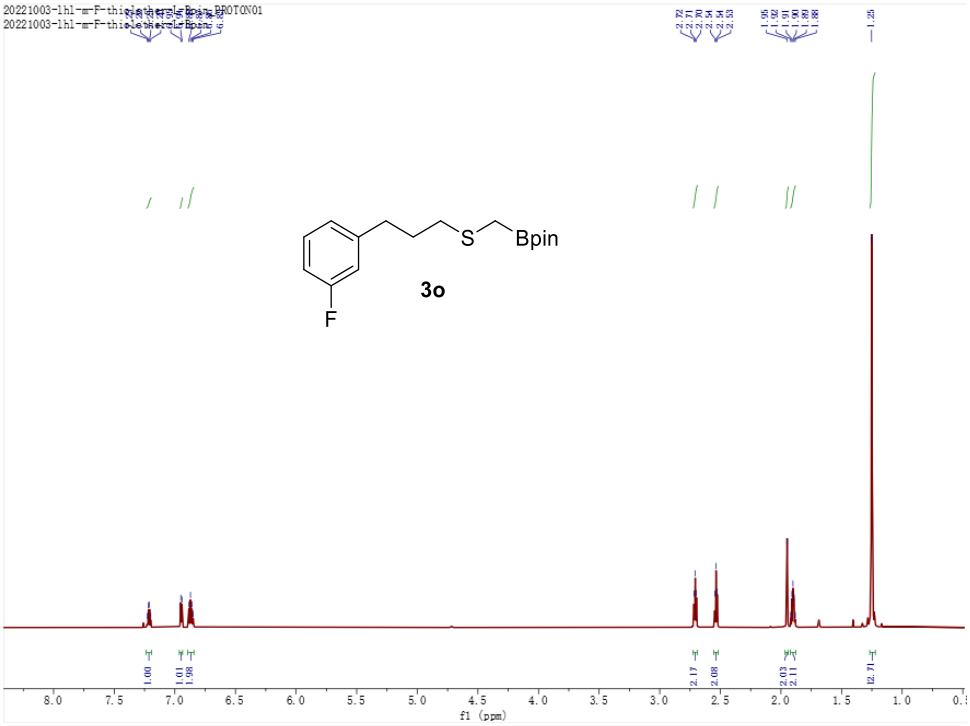



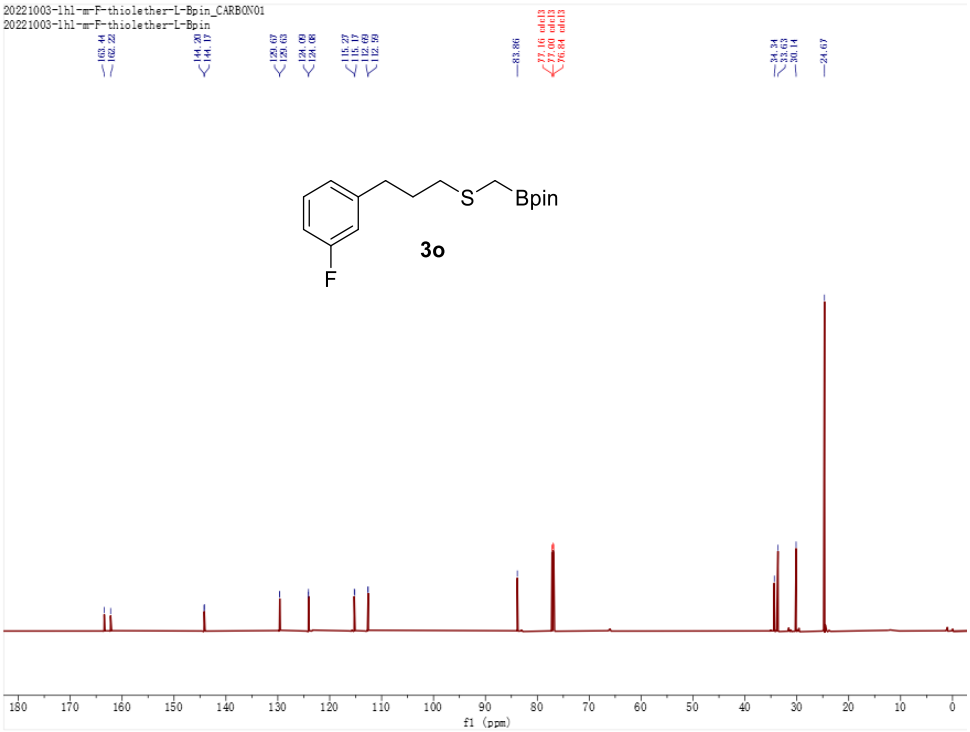
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4n**



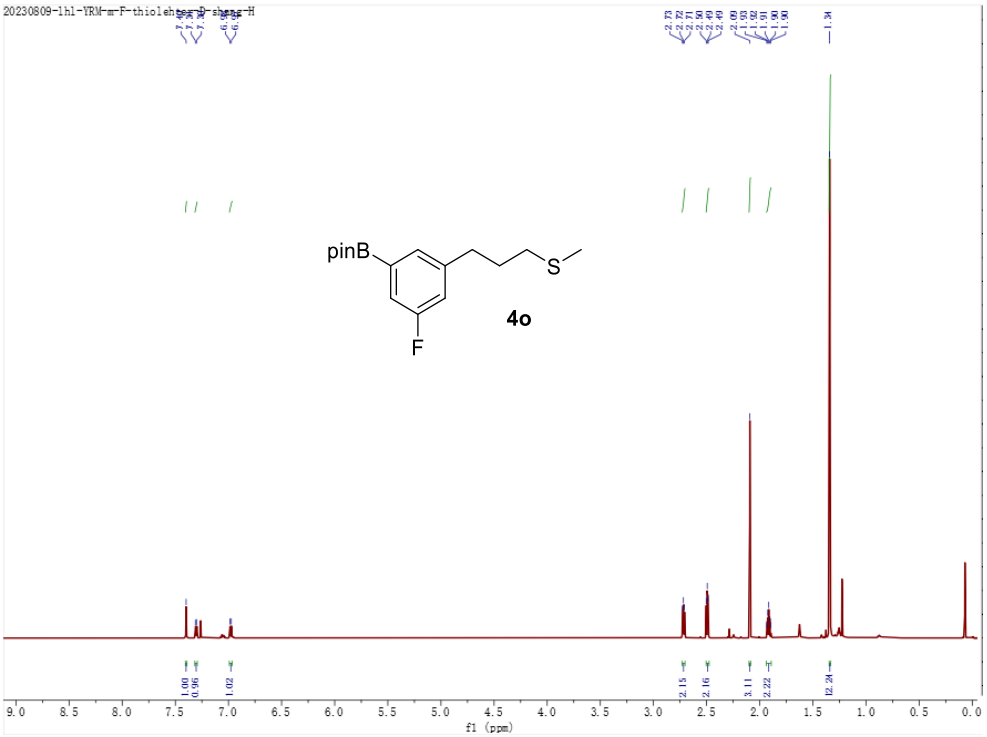



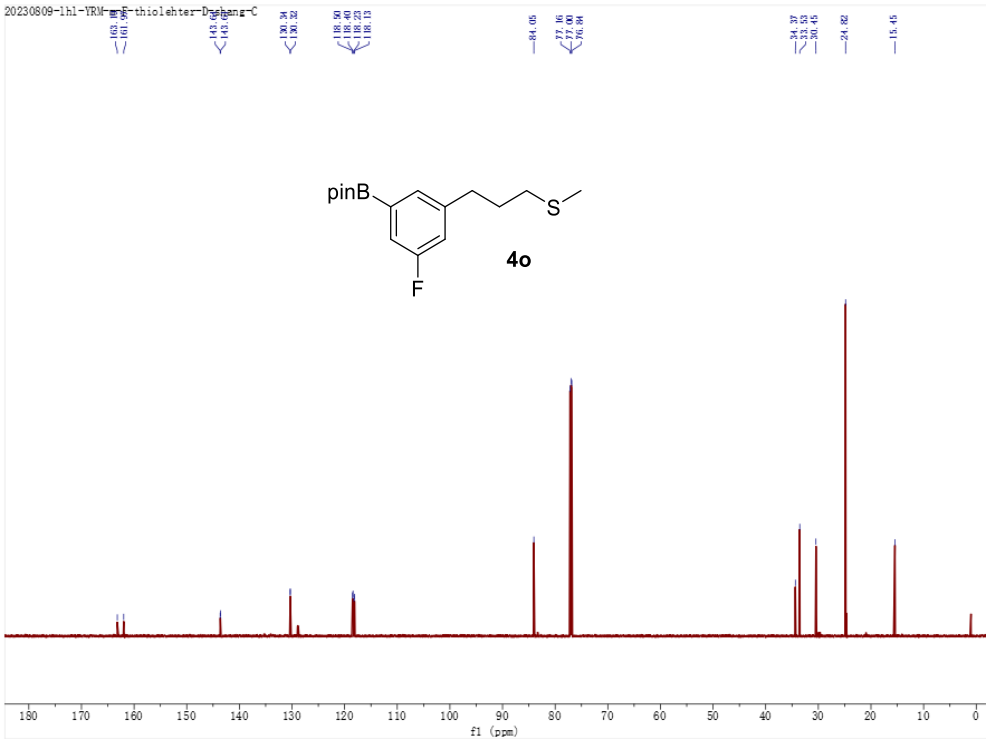
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3o**



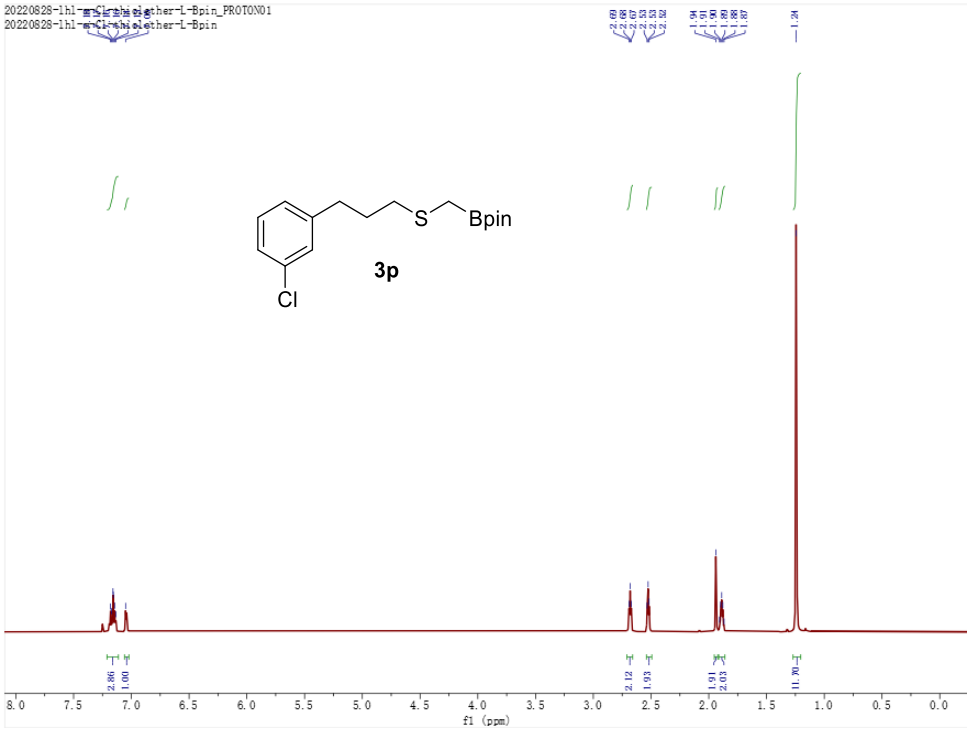



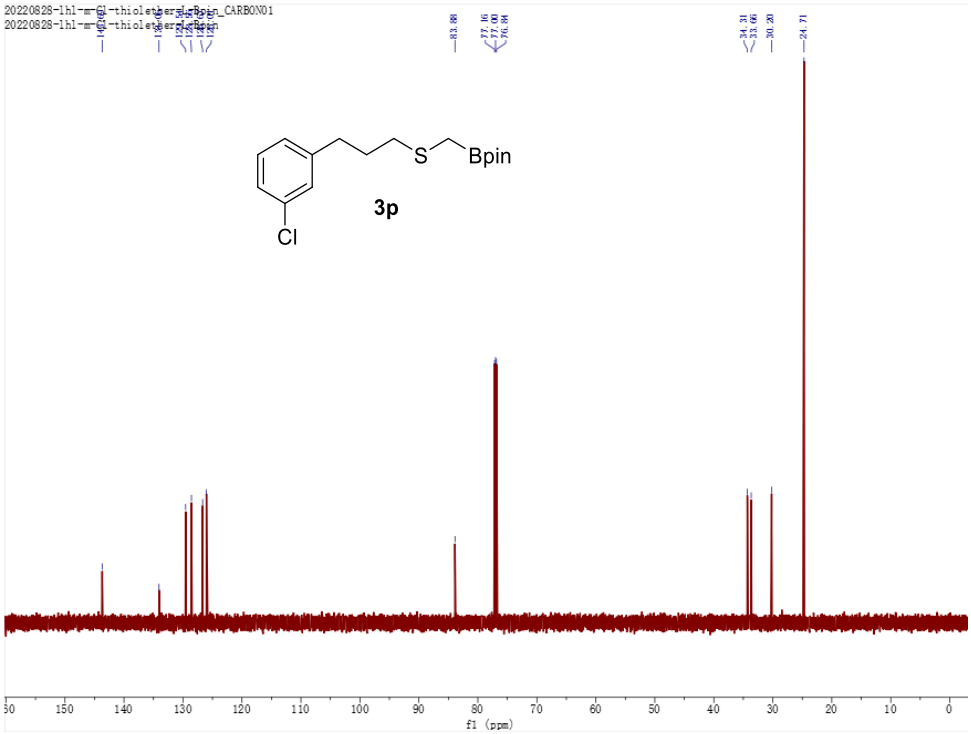
$^{1}H$ NMR (800 MHz, $CDCl_3$) and $^{13}C$ NMR (201MHz, $CDCl_3$) for **4o**



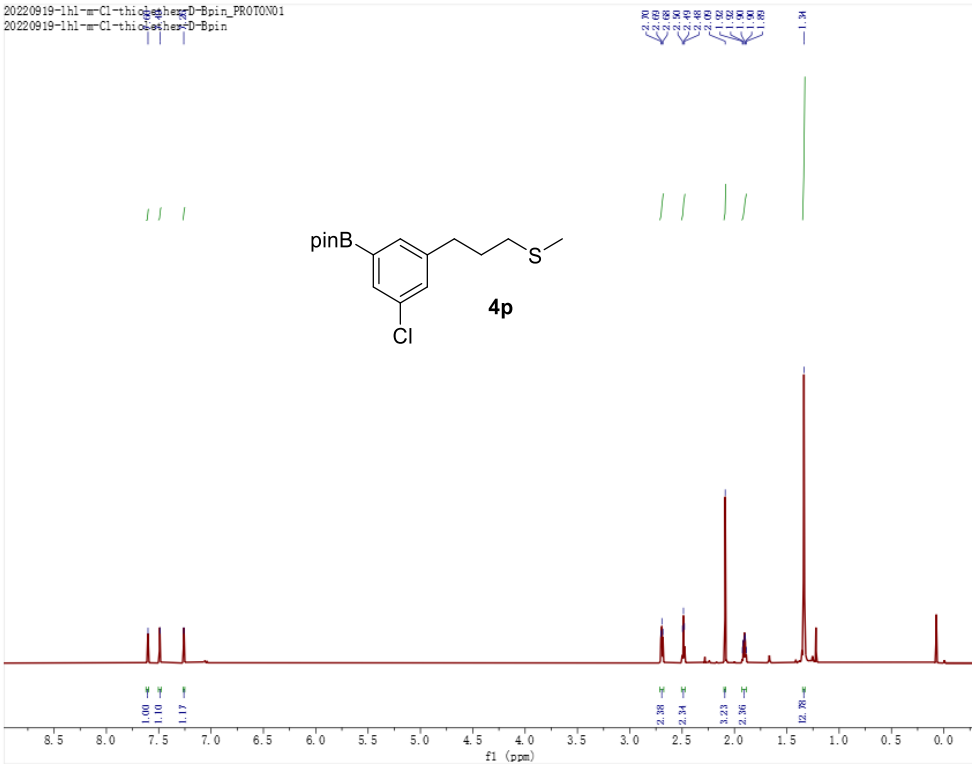



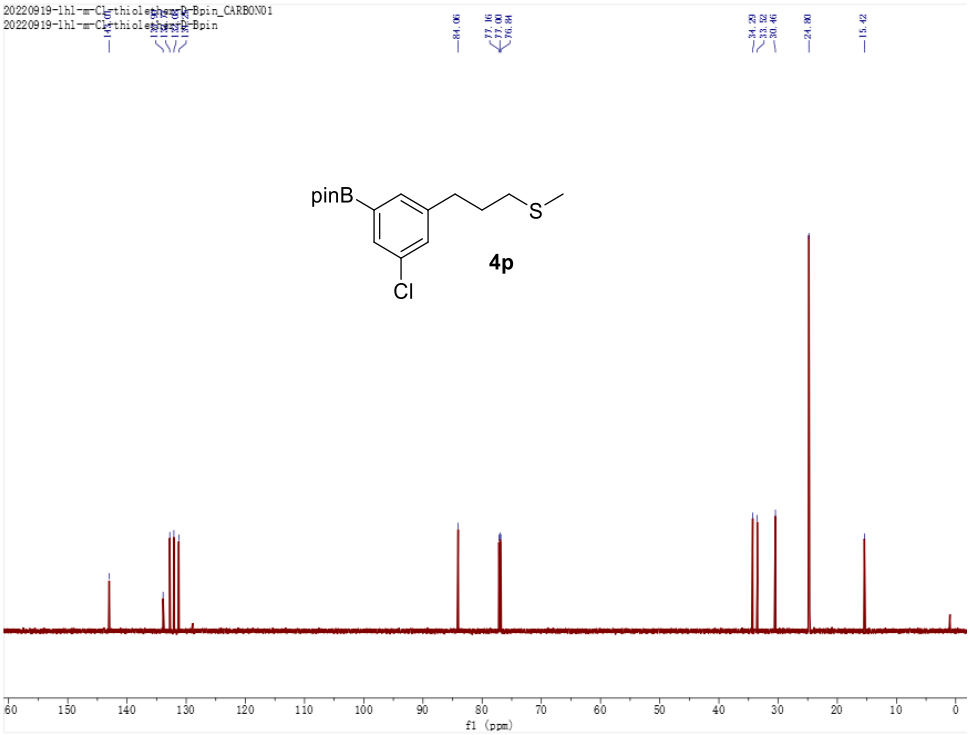
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3p**



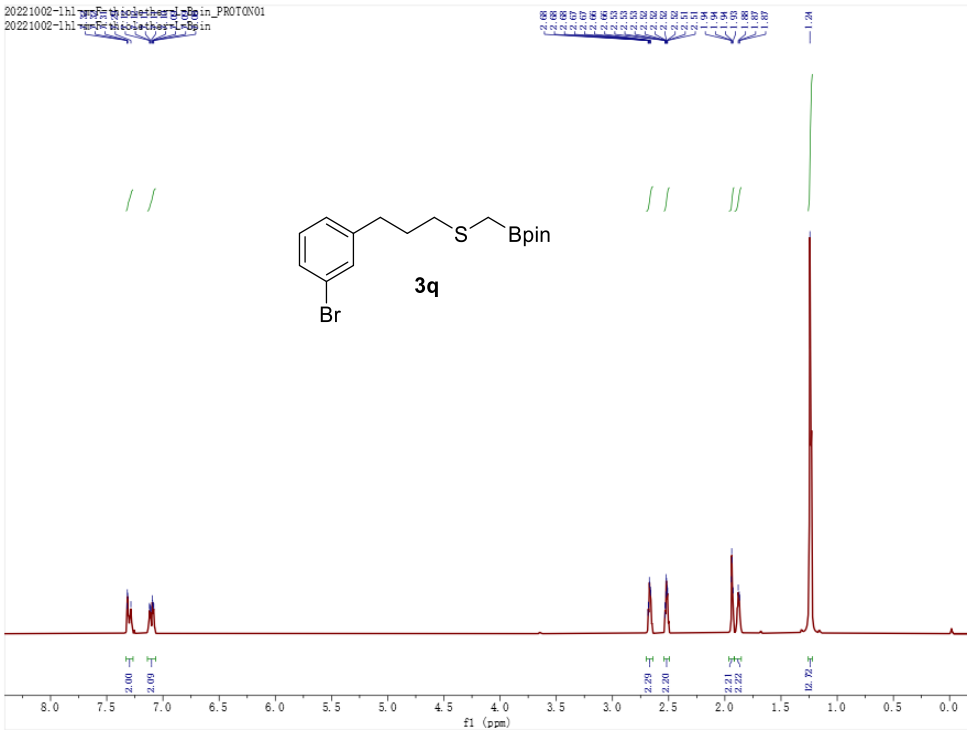



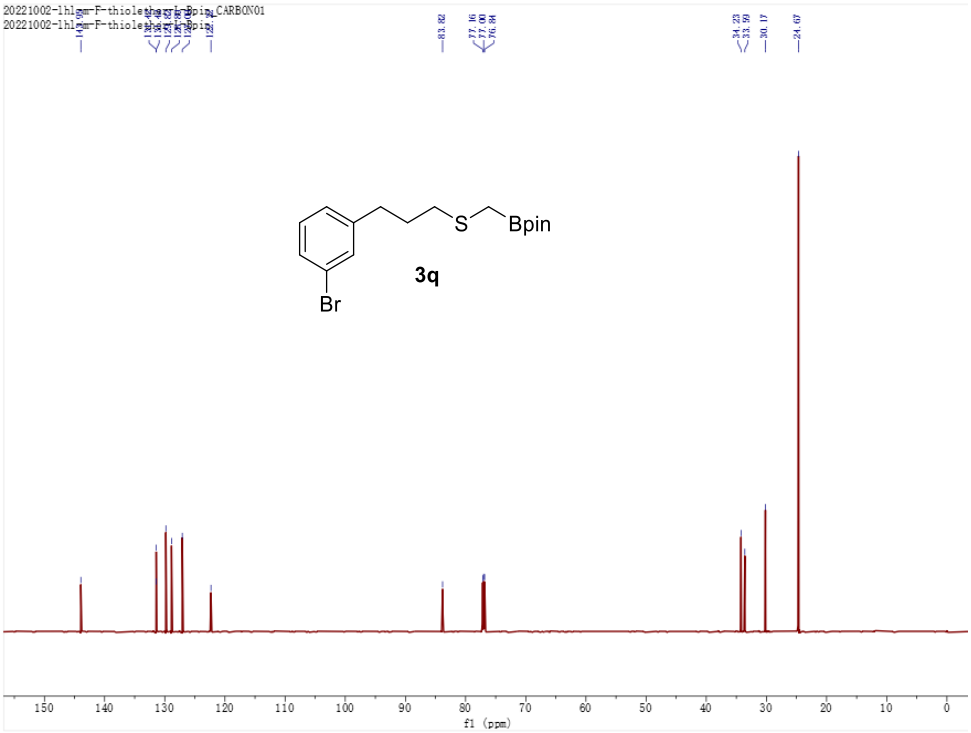
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4p**



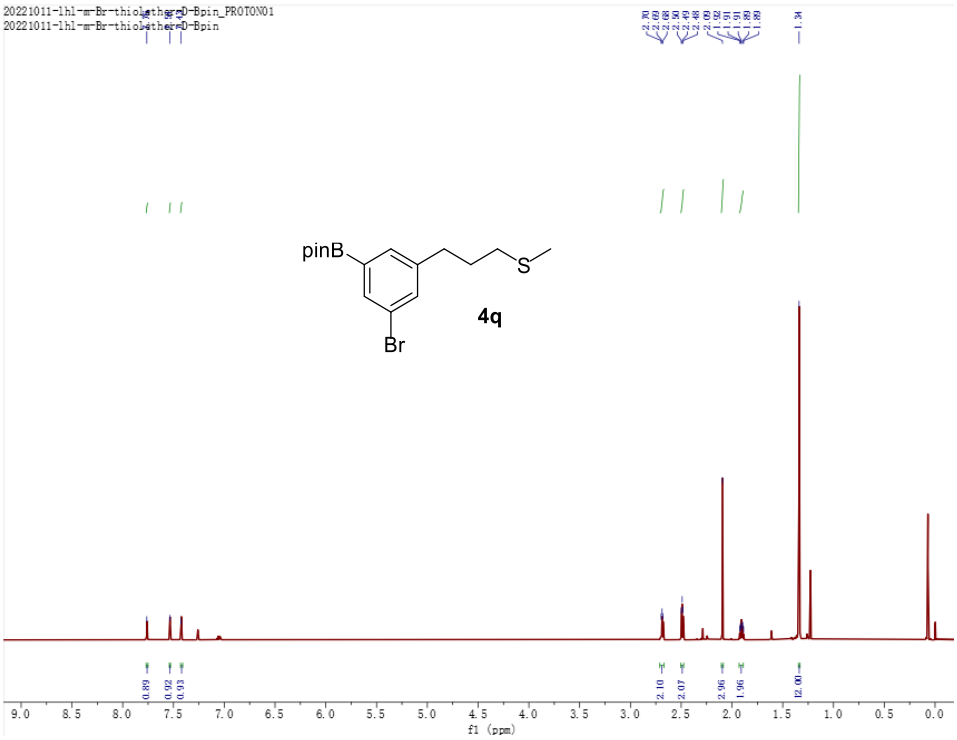



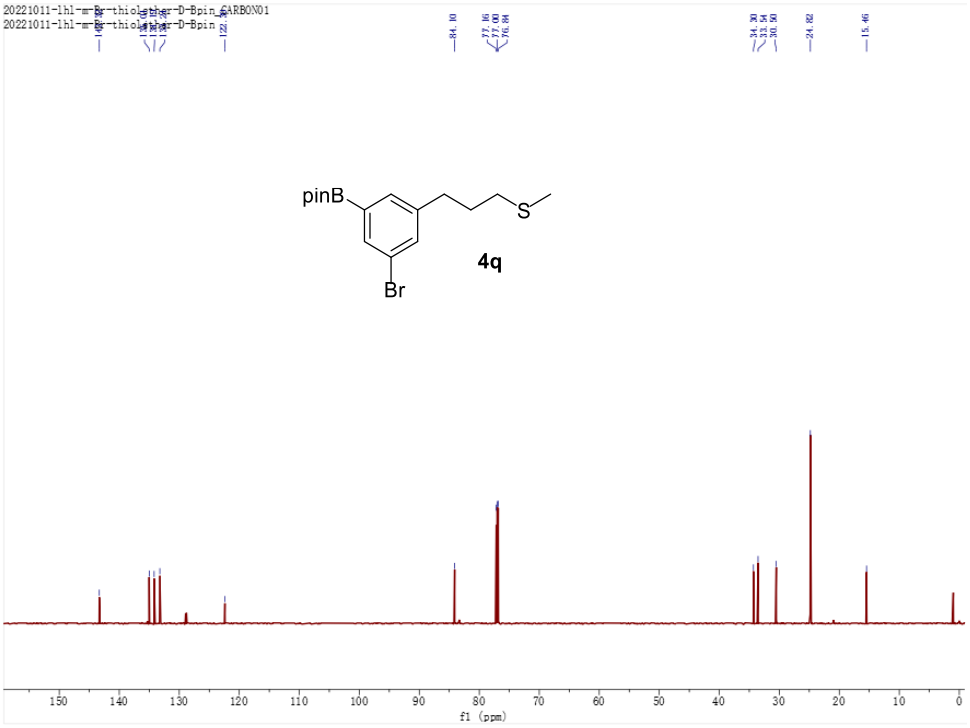
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3q**



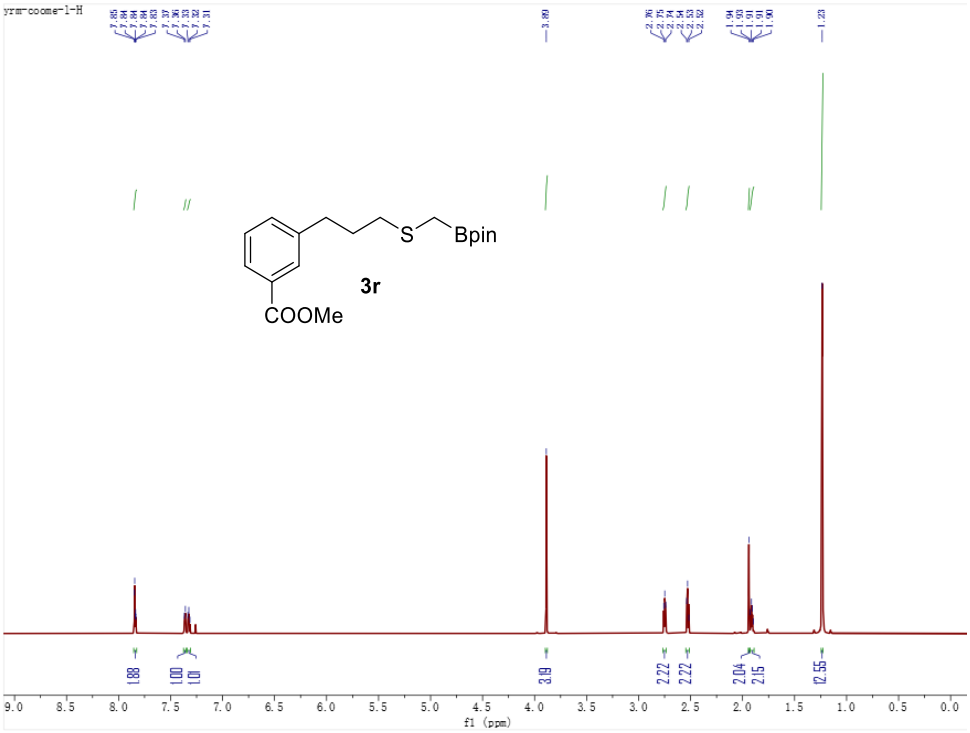



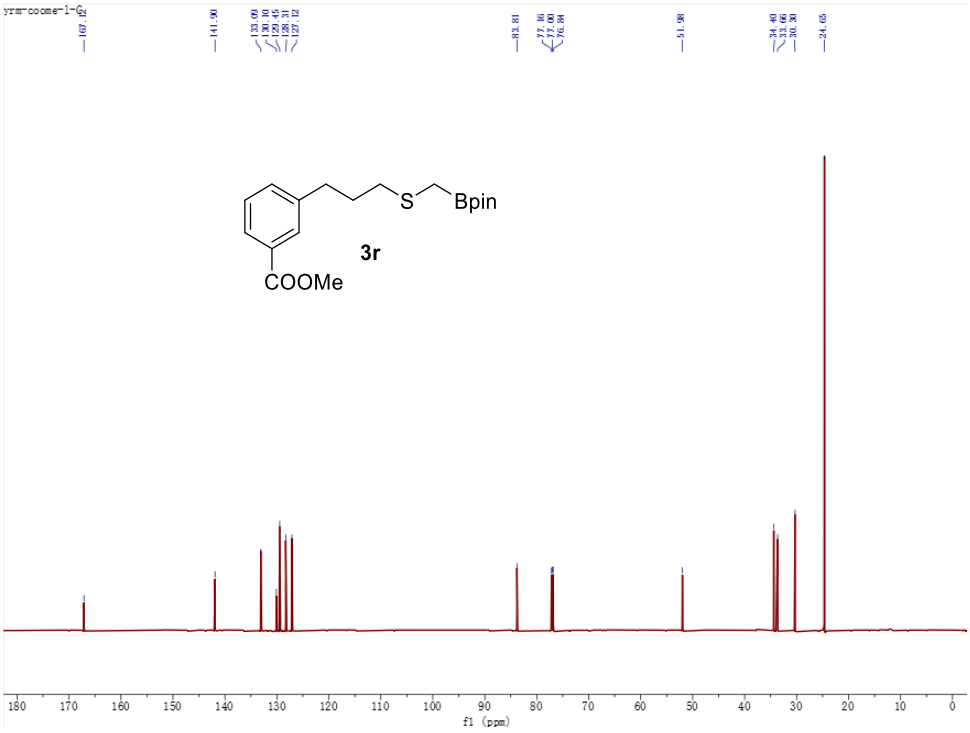
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4q**



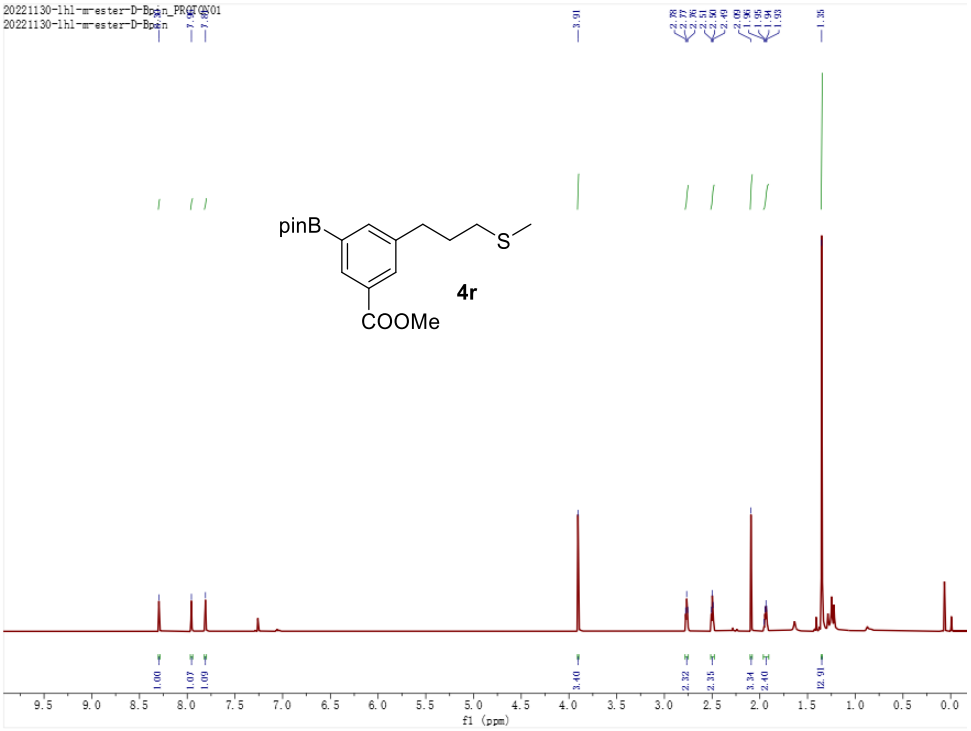



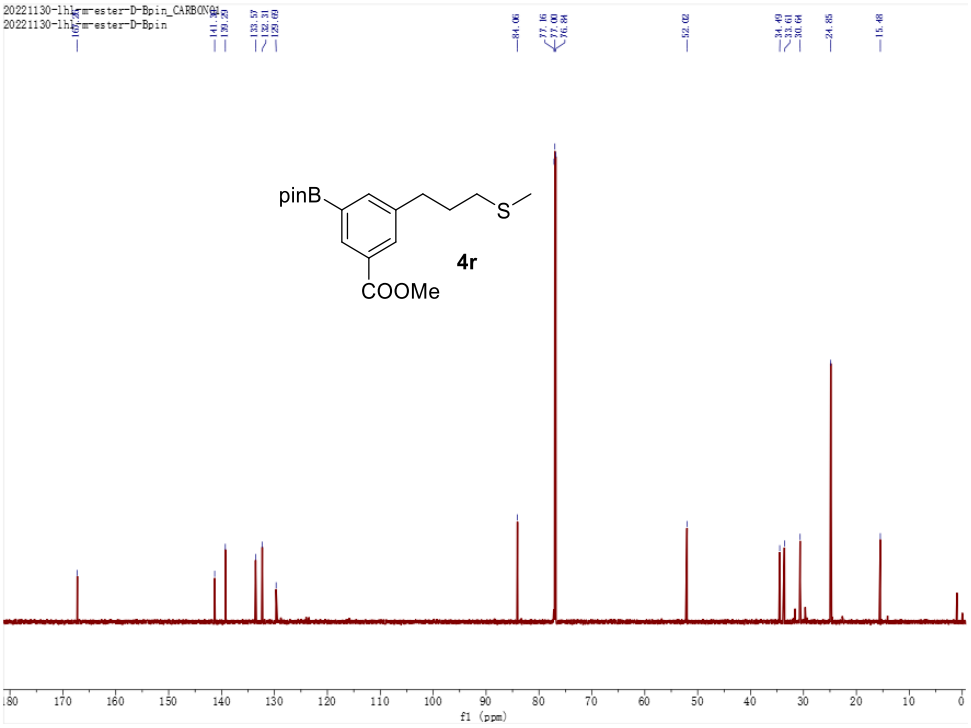
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3r**



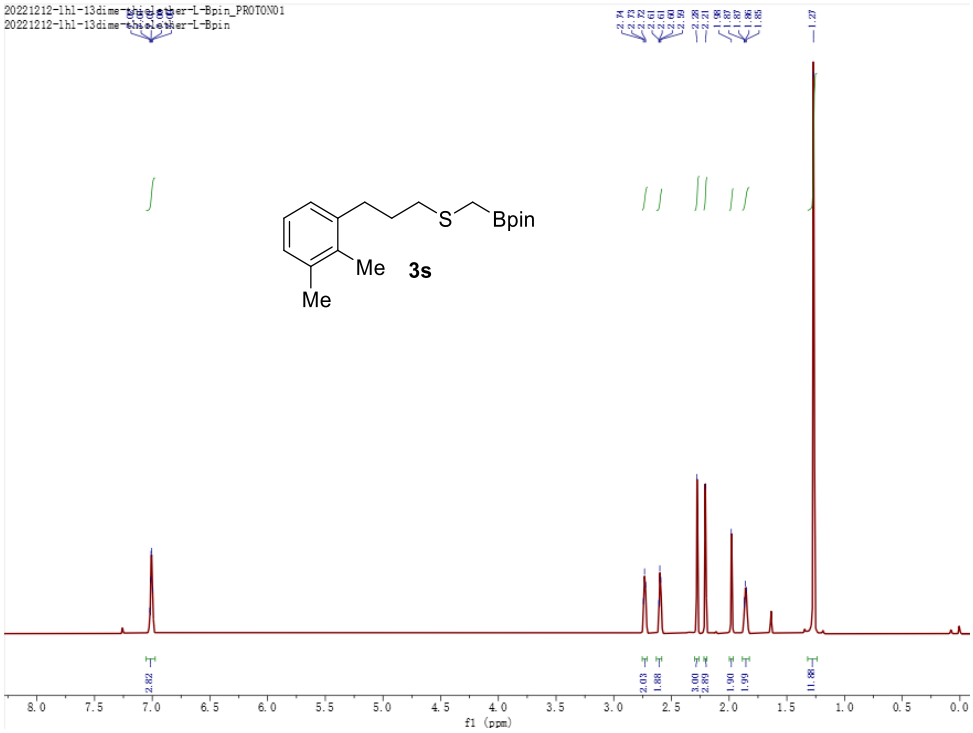



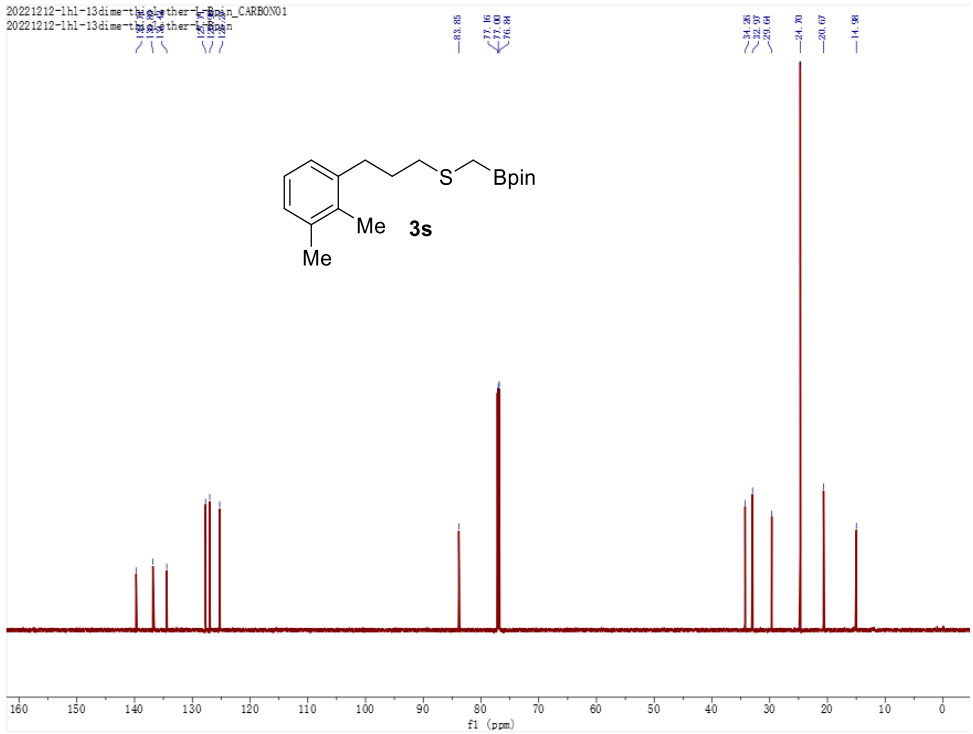
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4r**



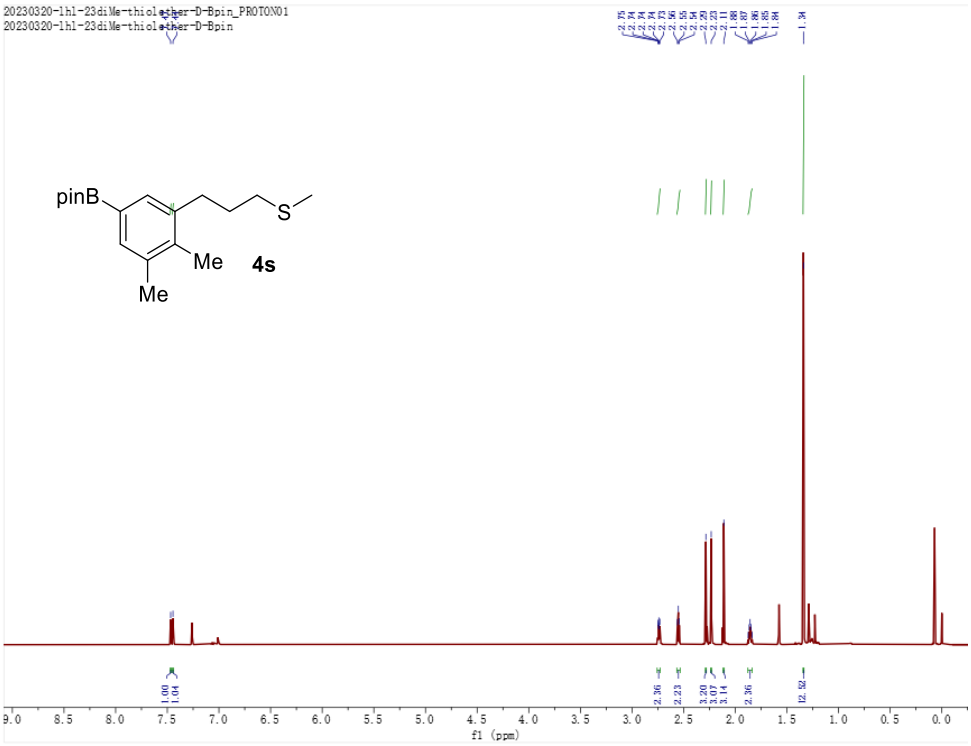



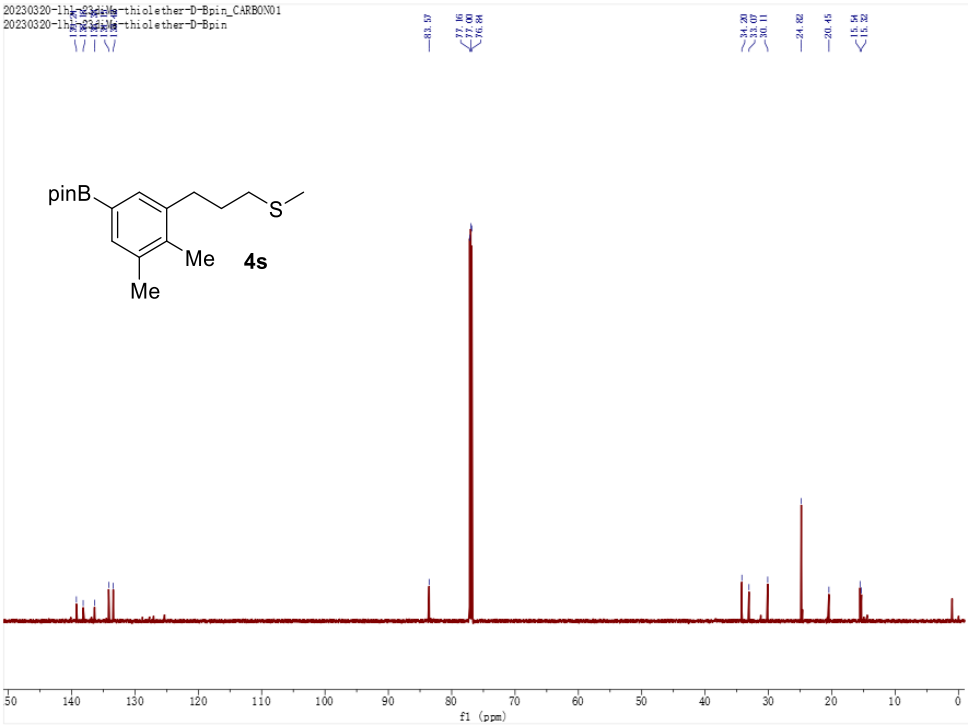
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3s**



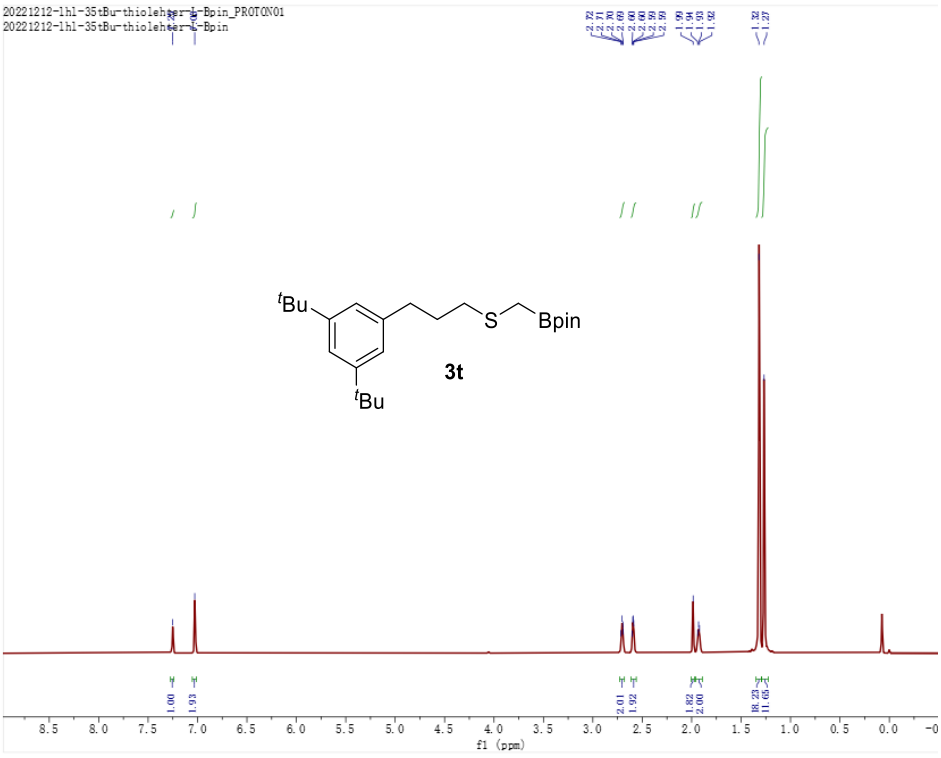



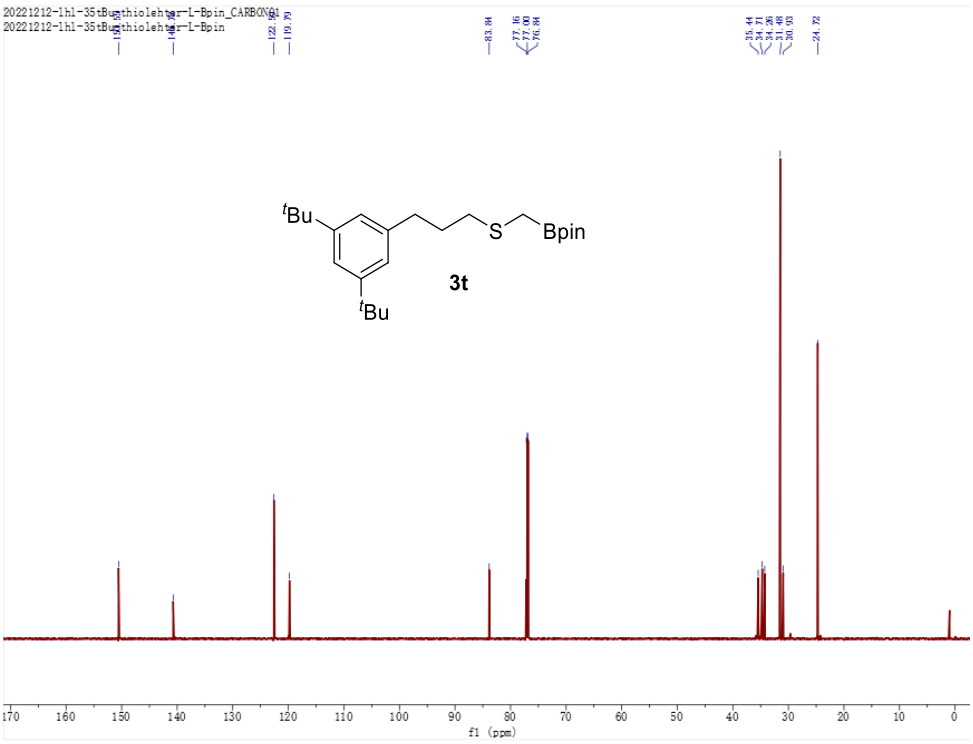
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4s**



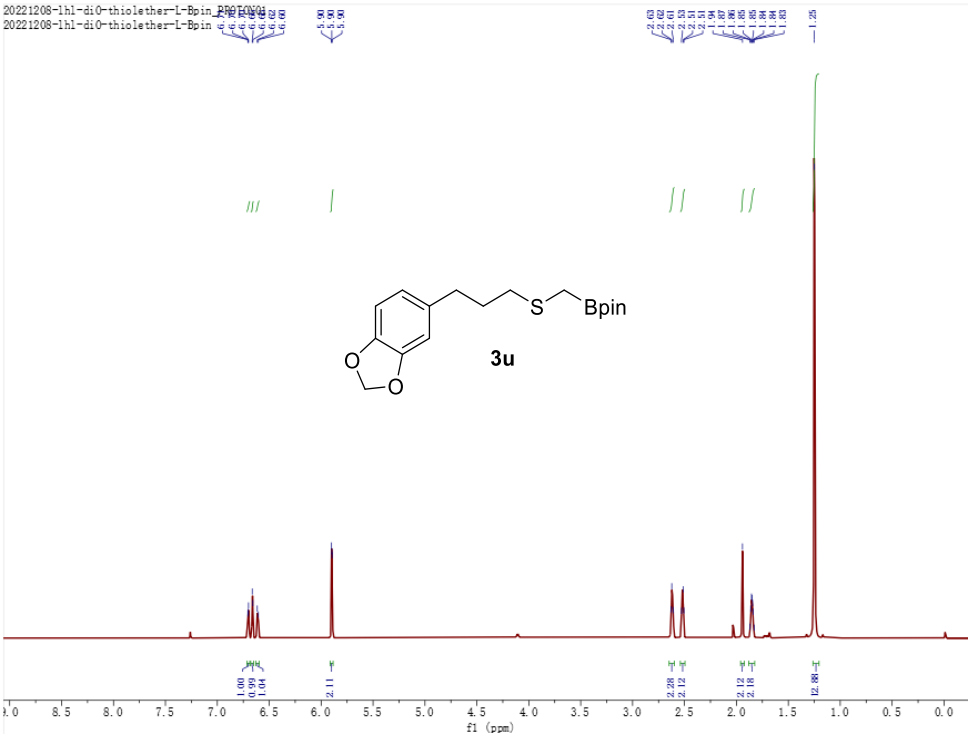



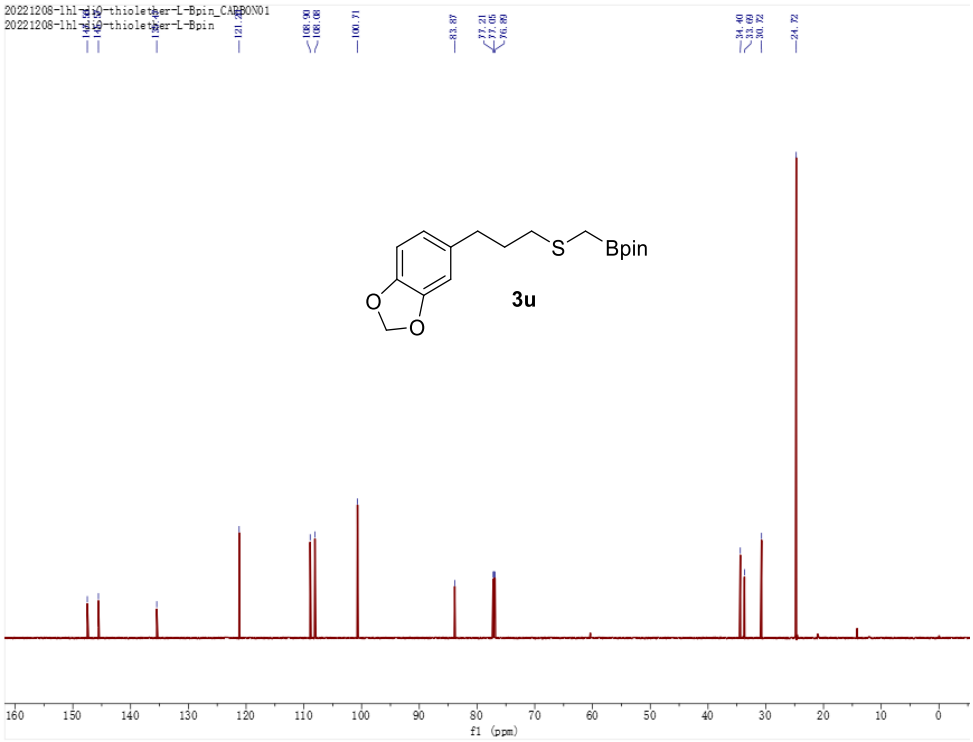
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3t**



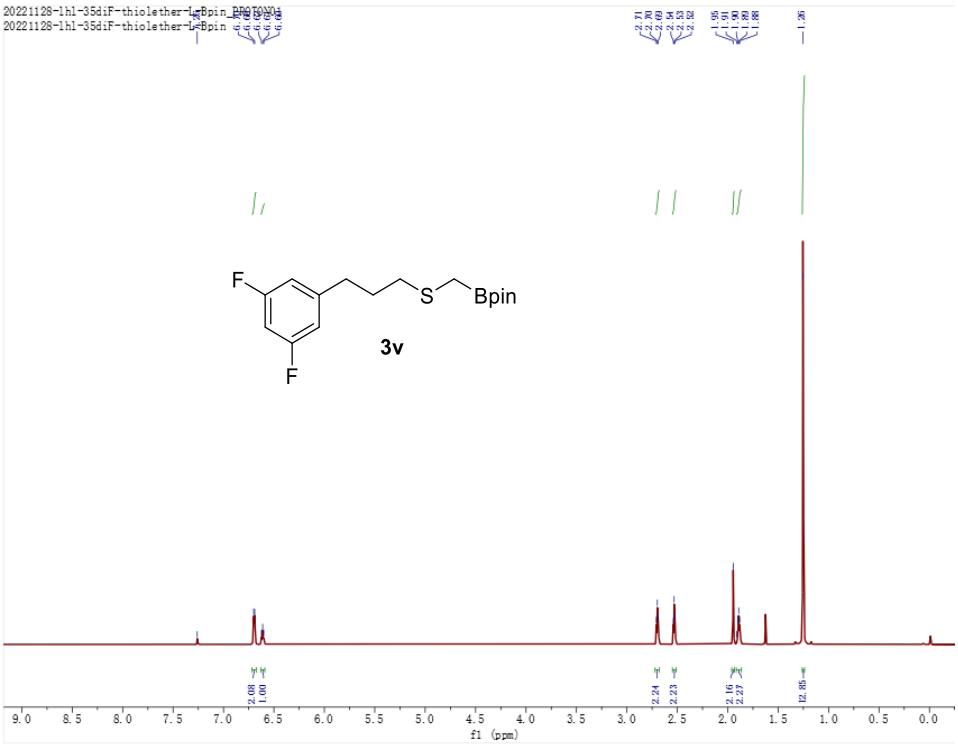



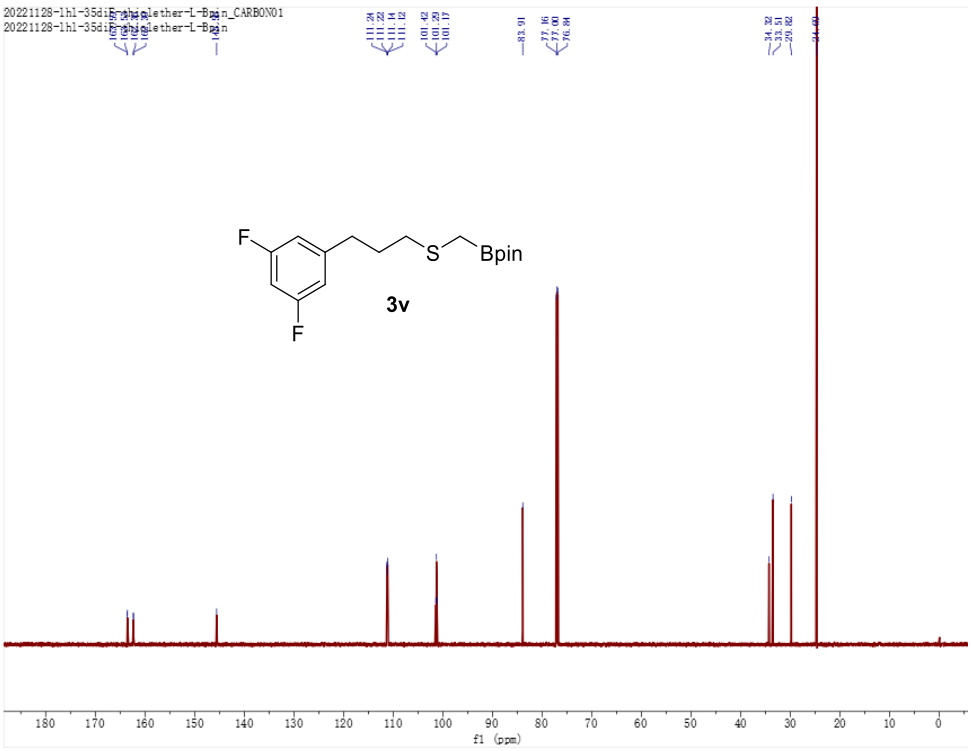
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3u**



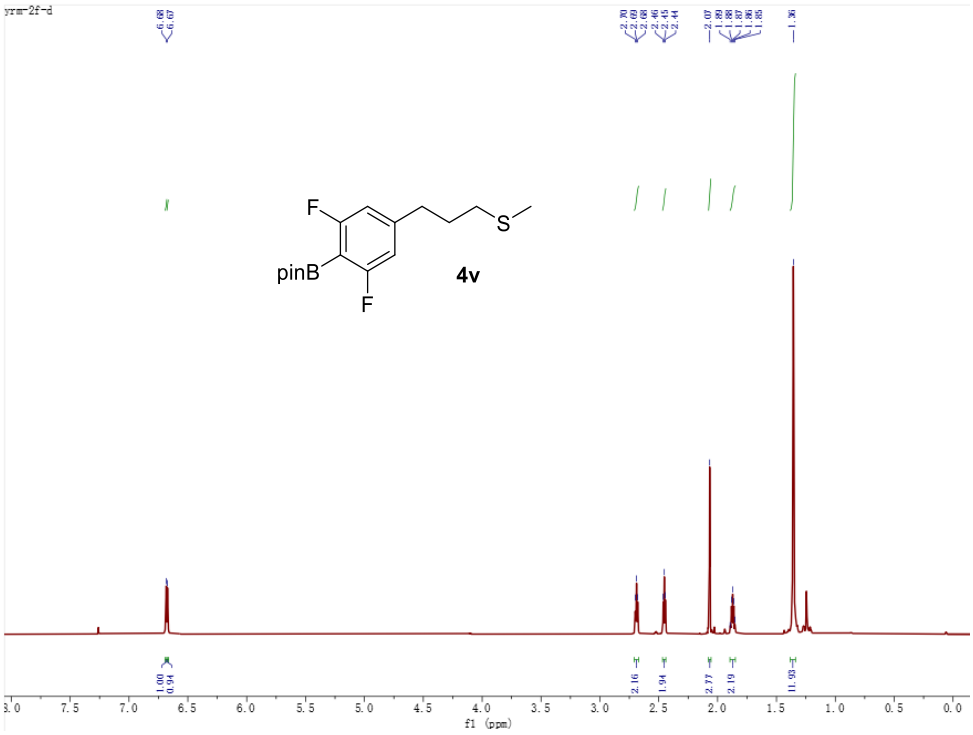



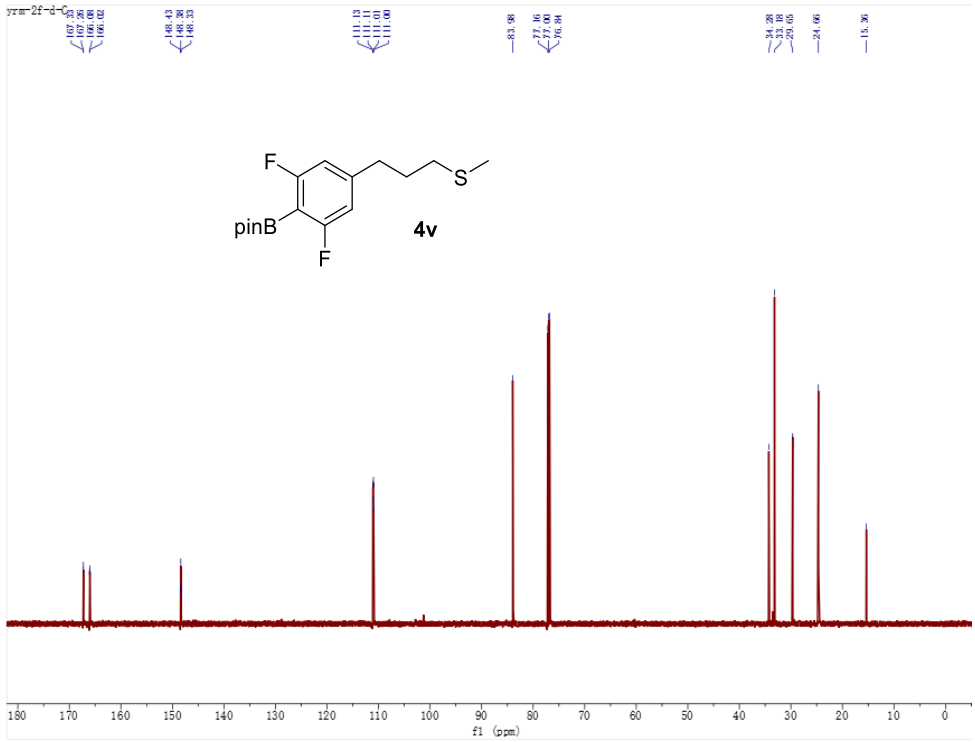
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3v**



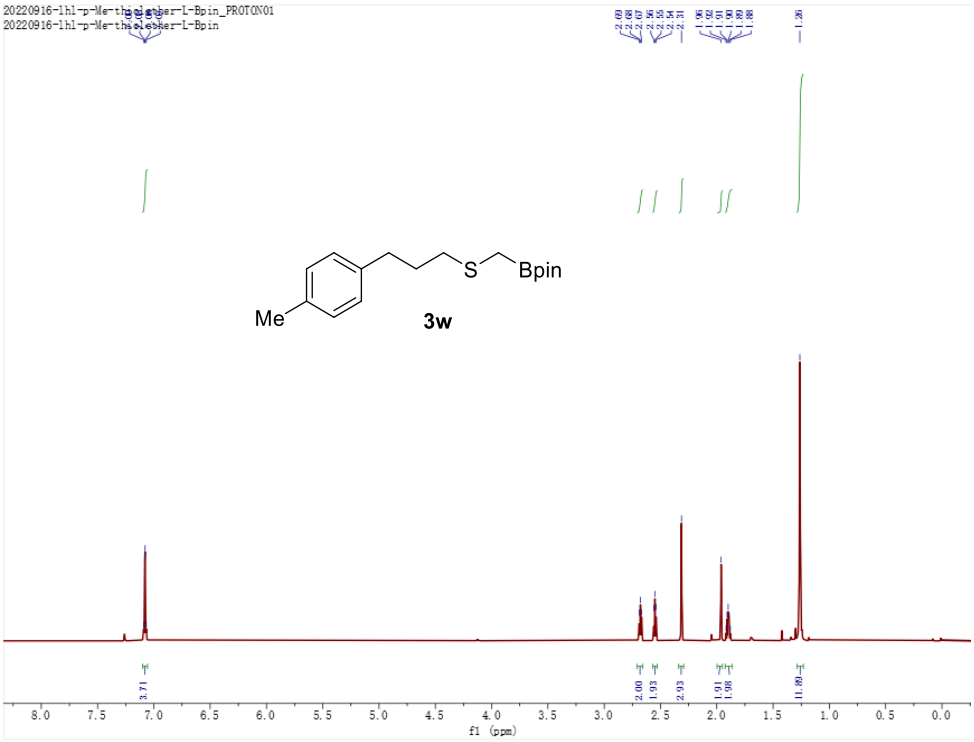



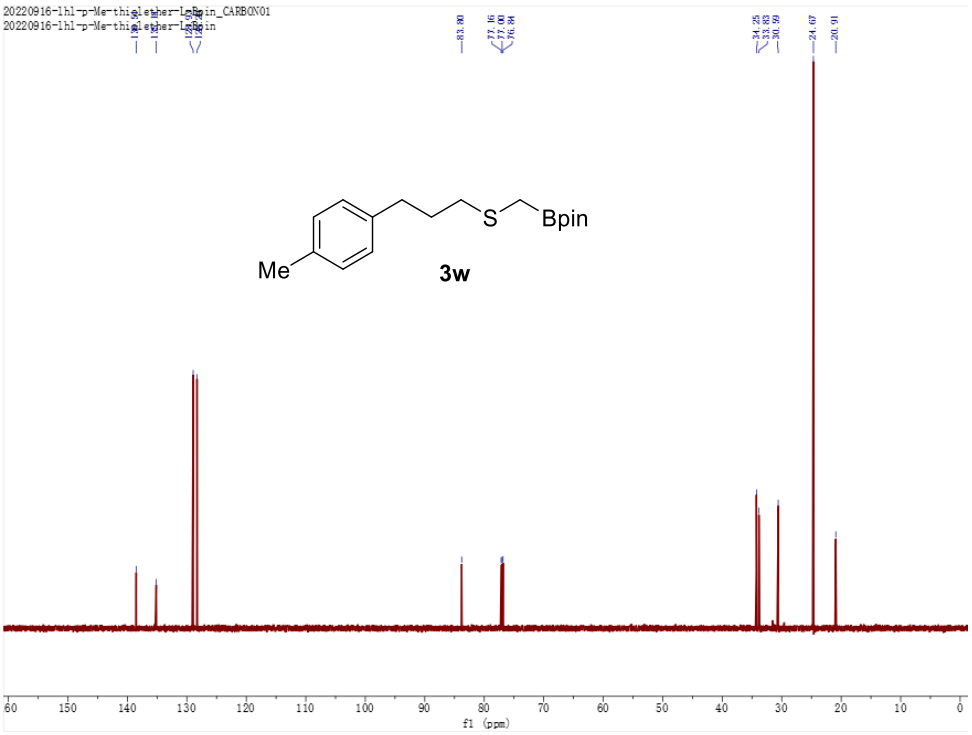
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4v**



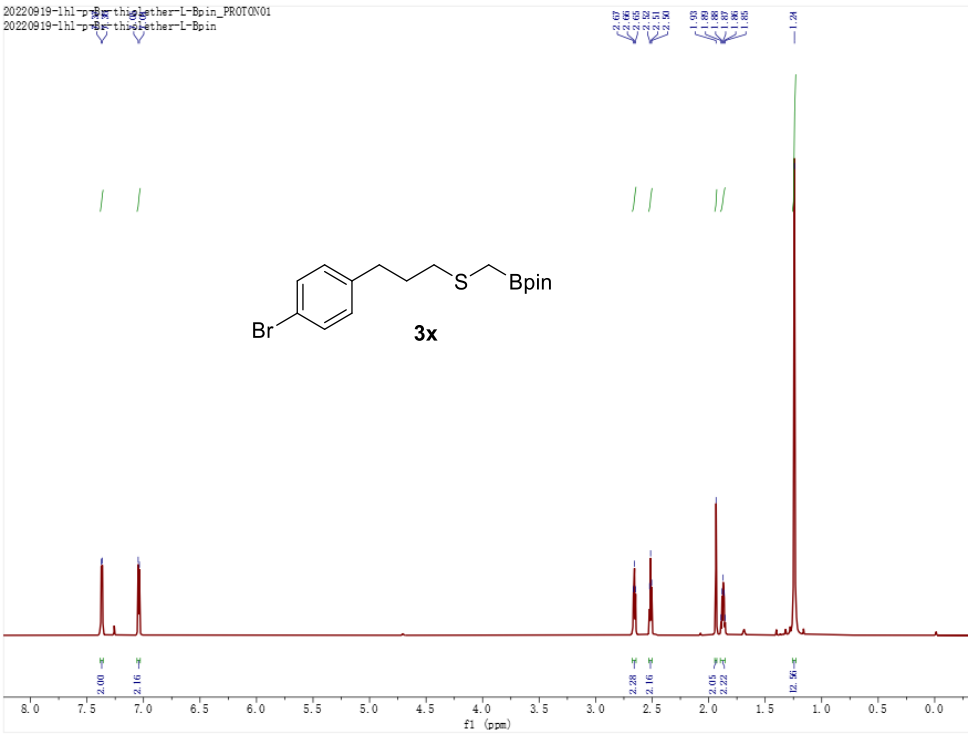



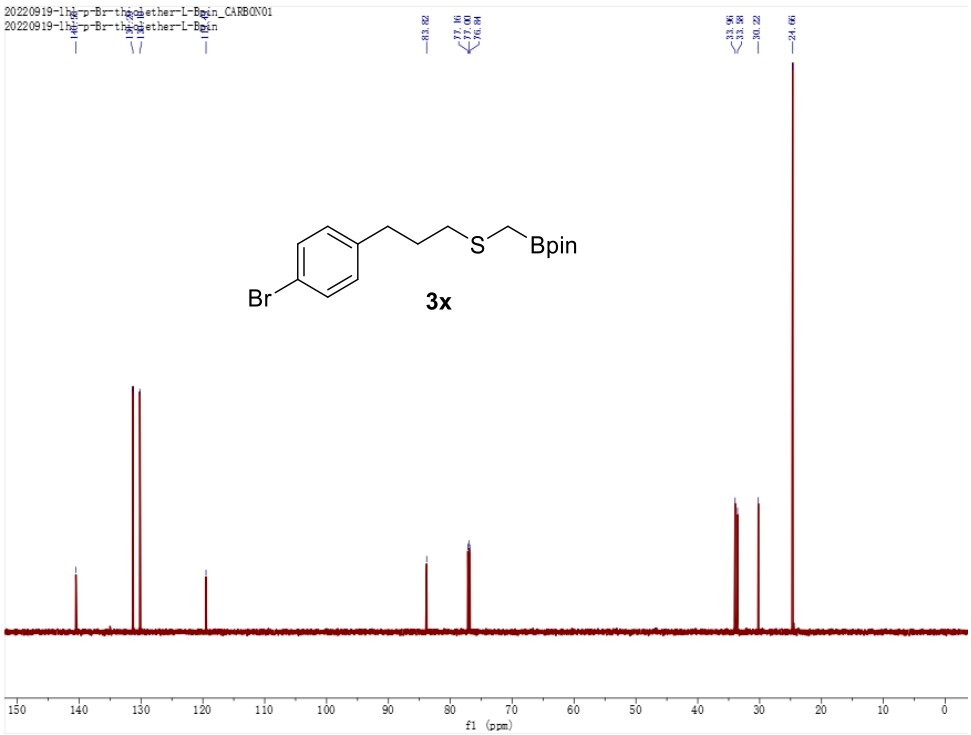
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3w**



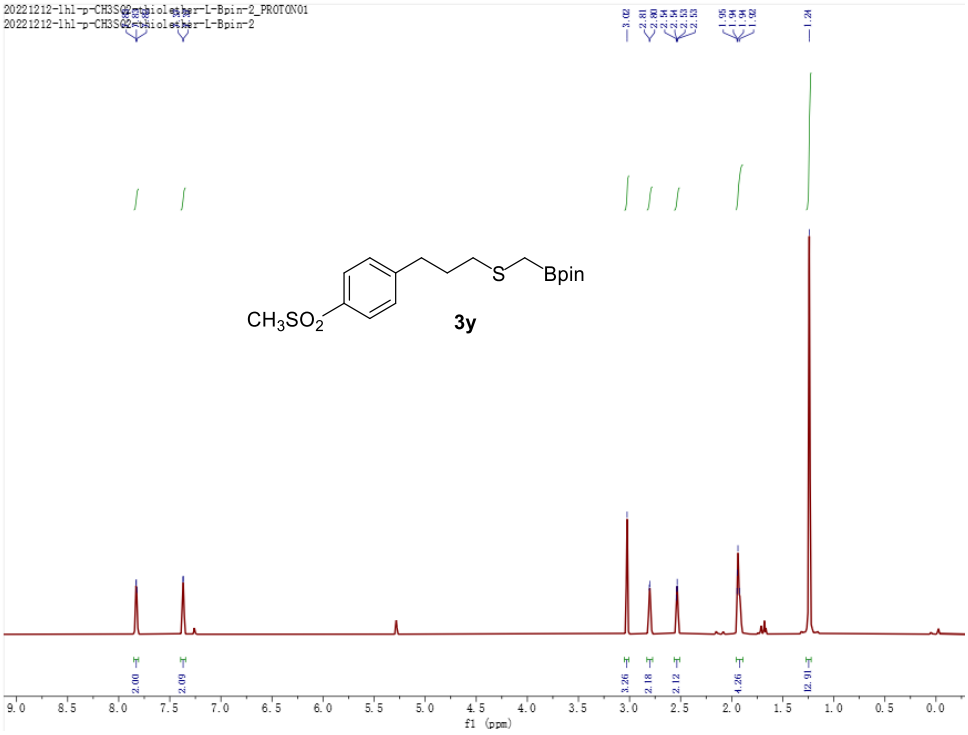



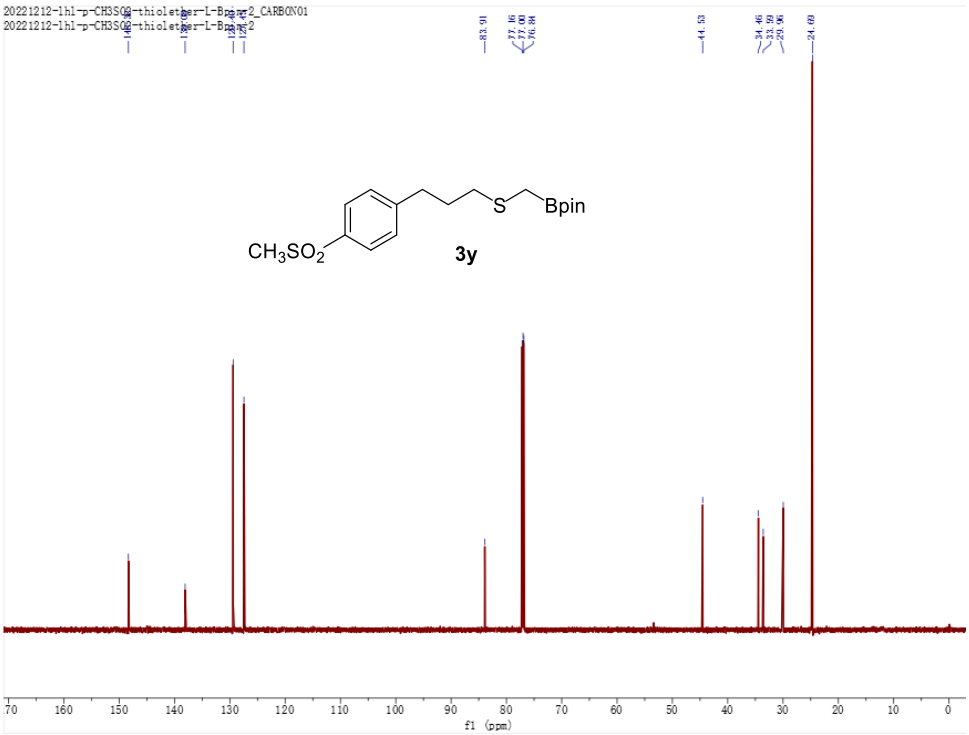
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3x**



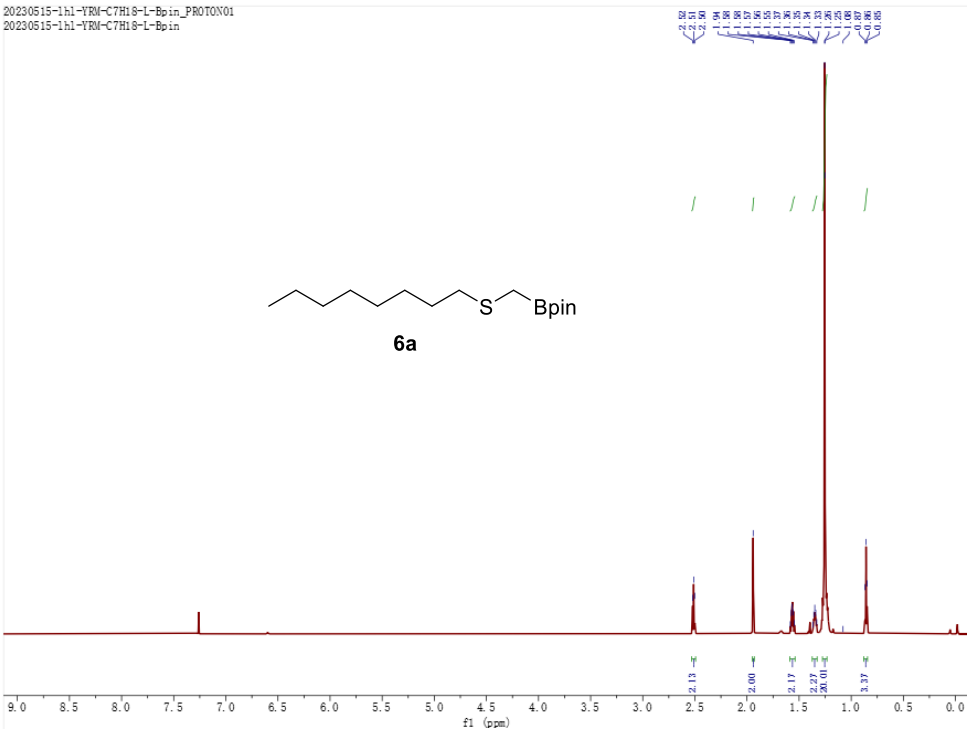



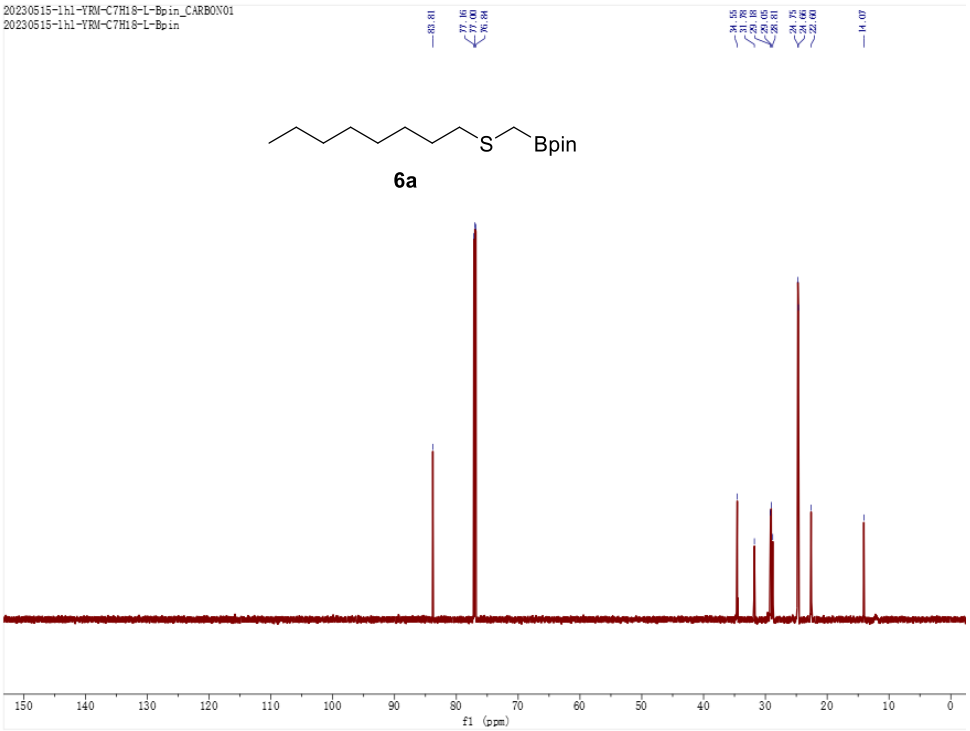
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3y**



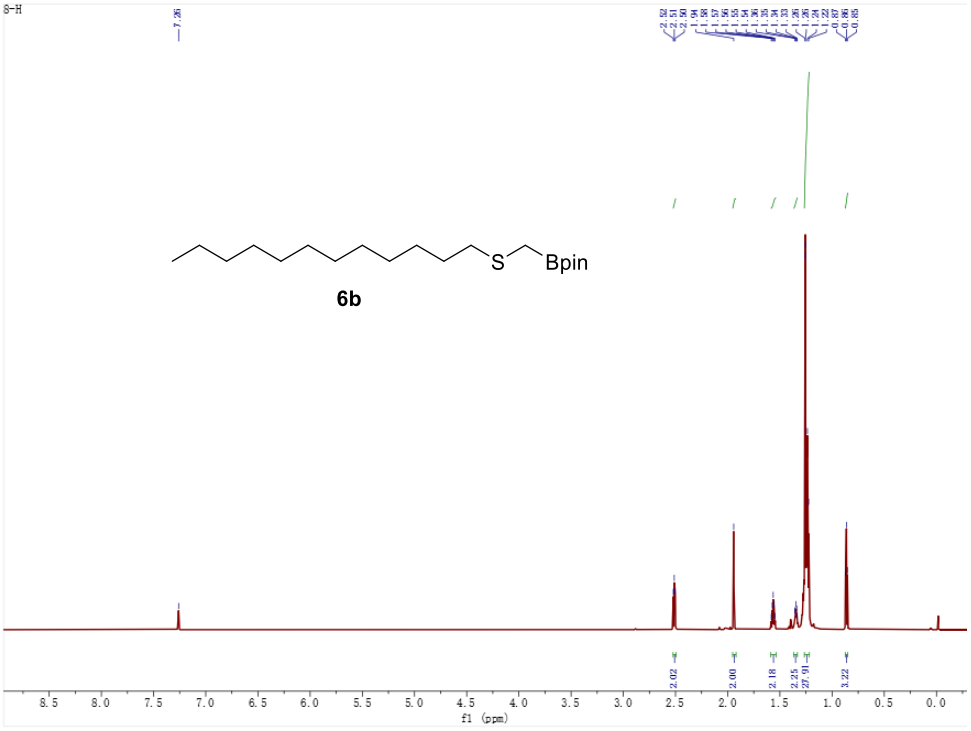



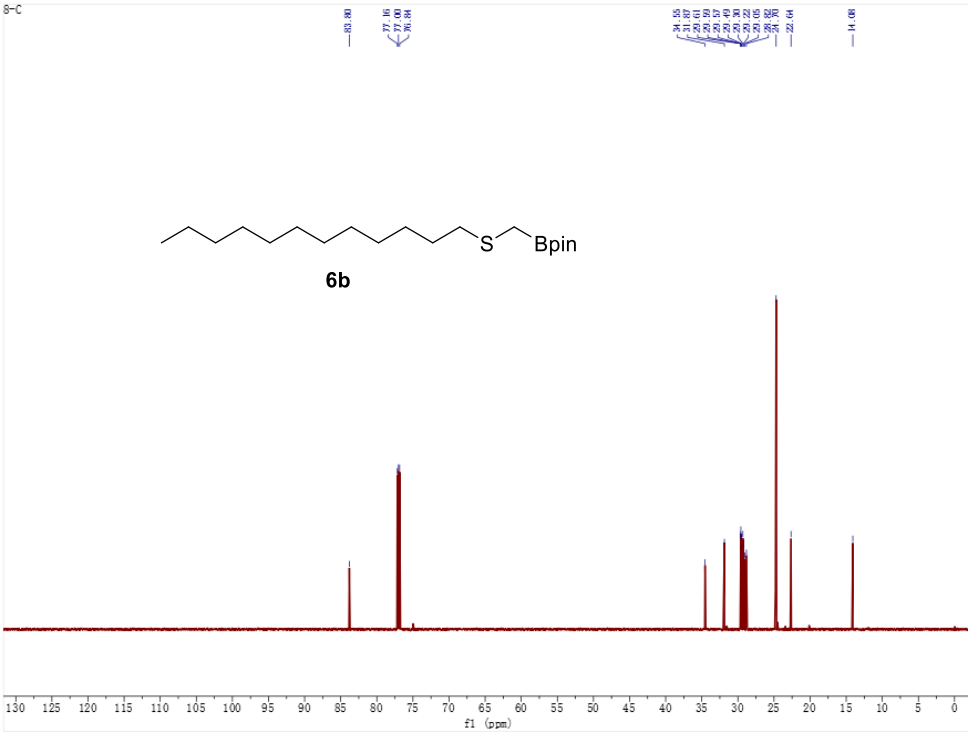
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6a**



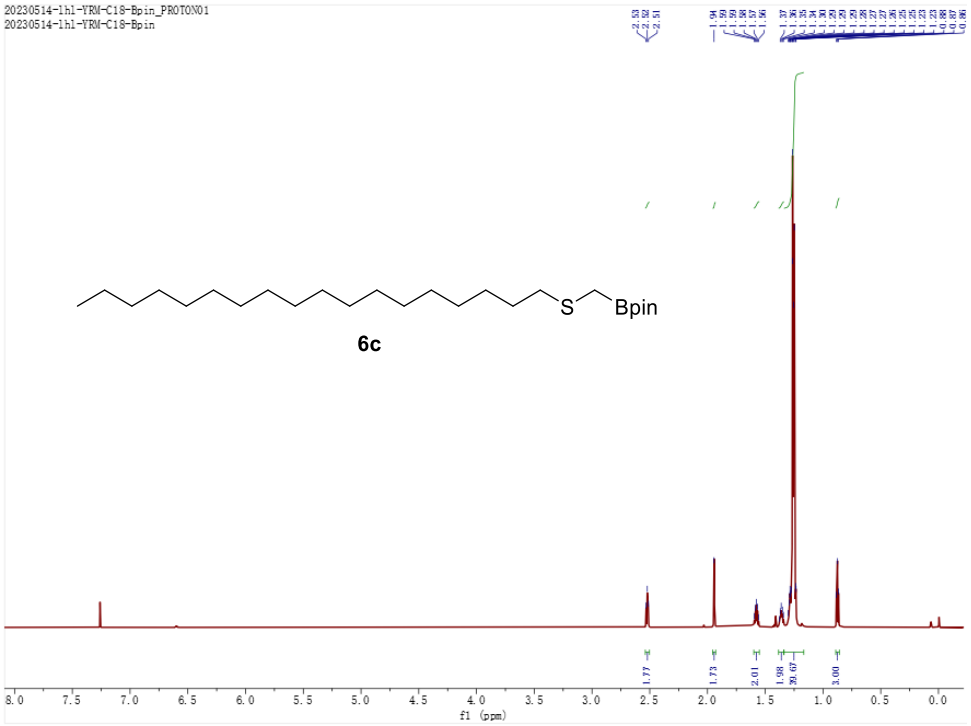



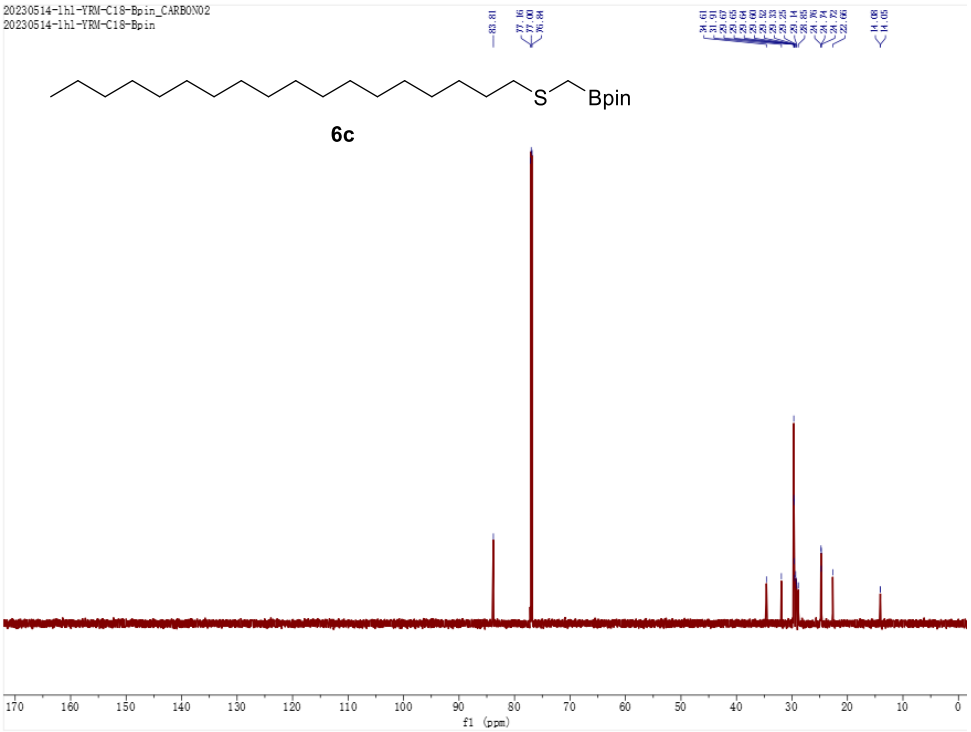
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6b**



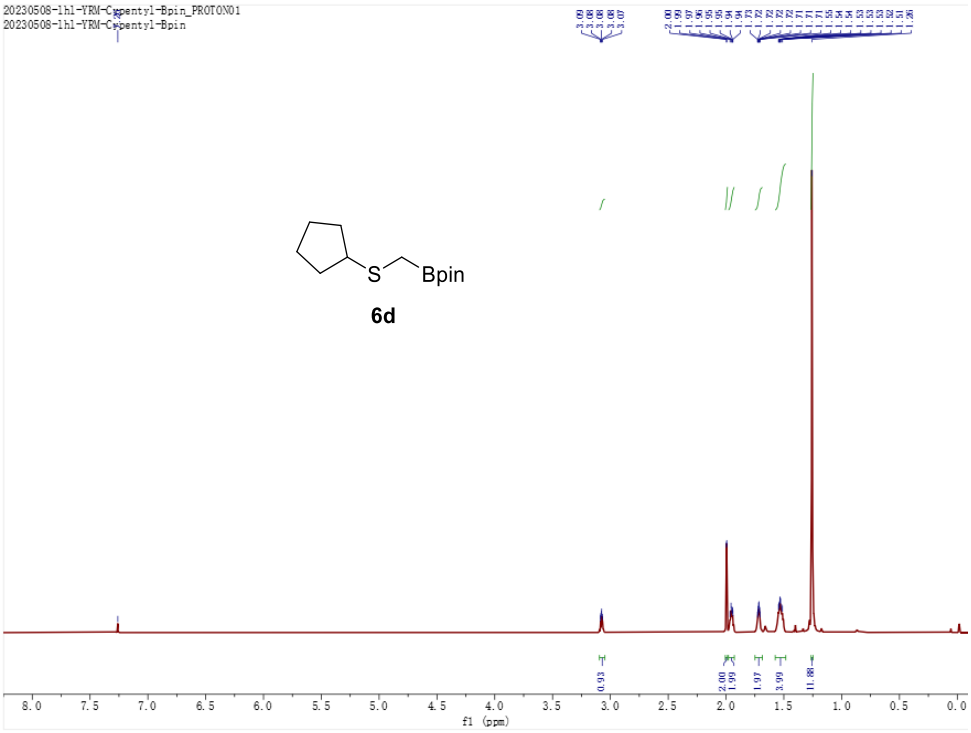



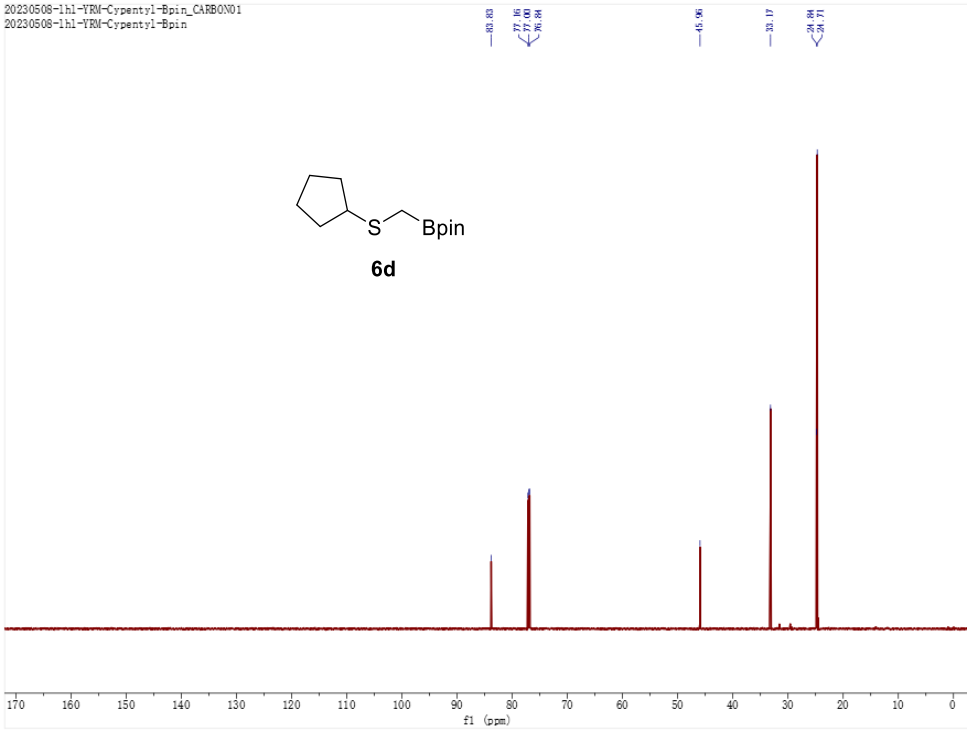
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6c**



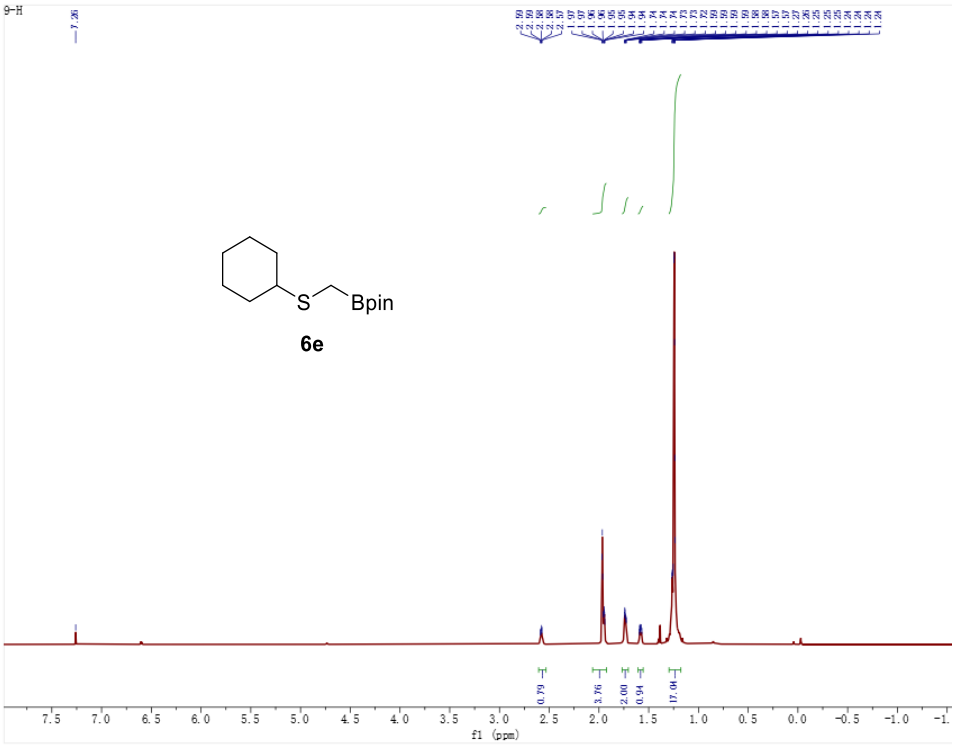



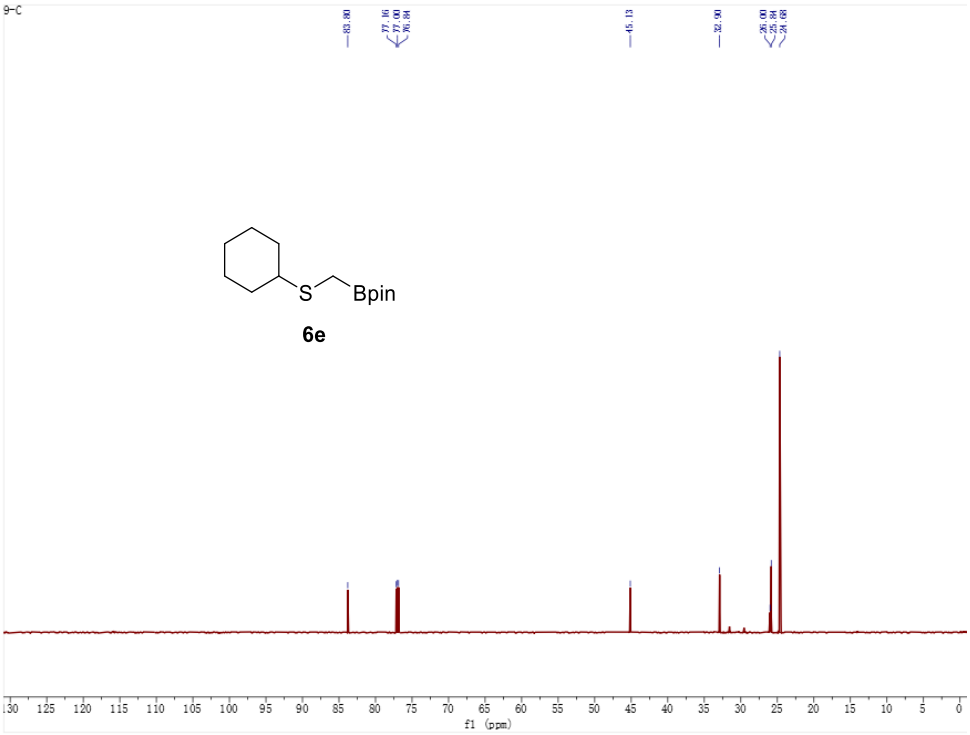
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6d**



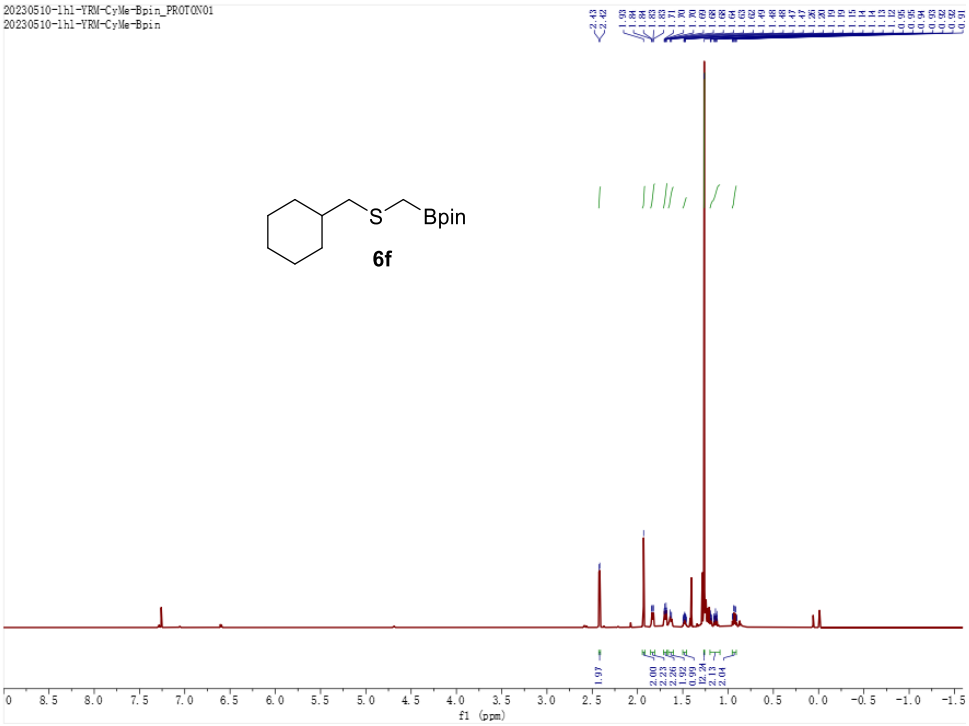



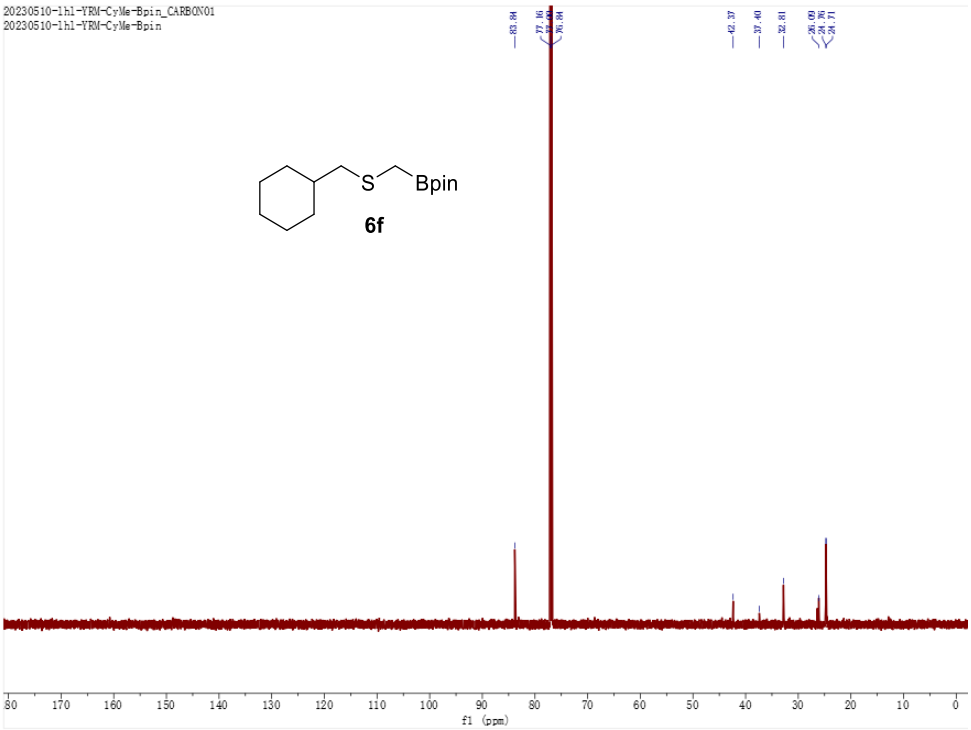
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6e**



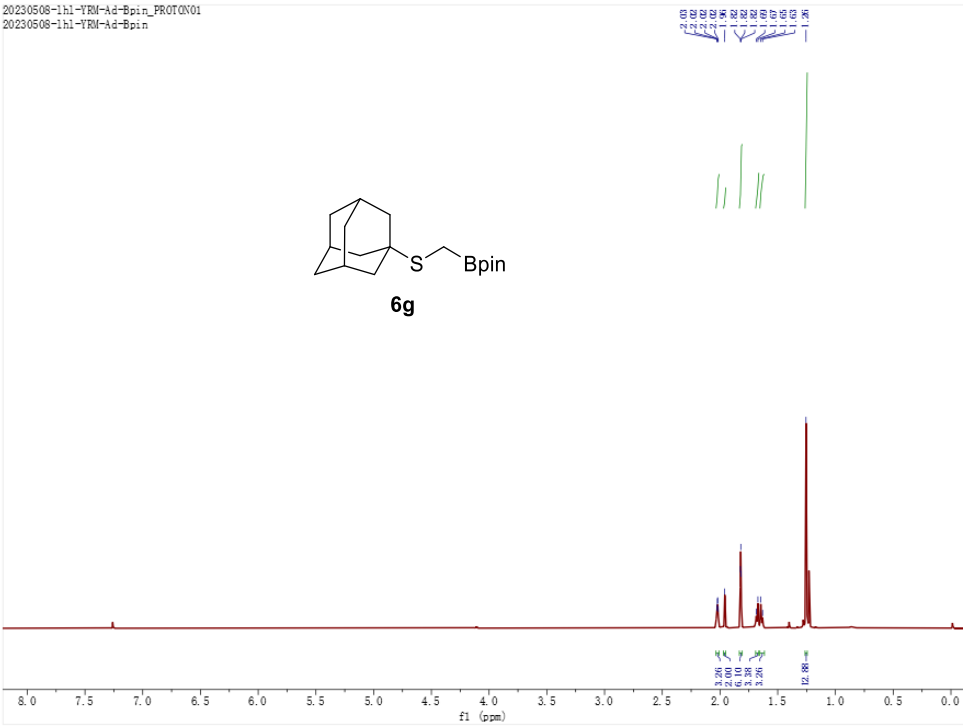



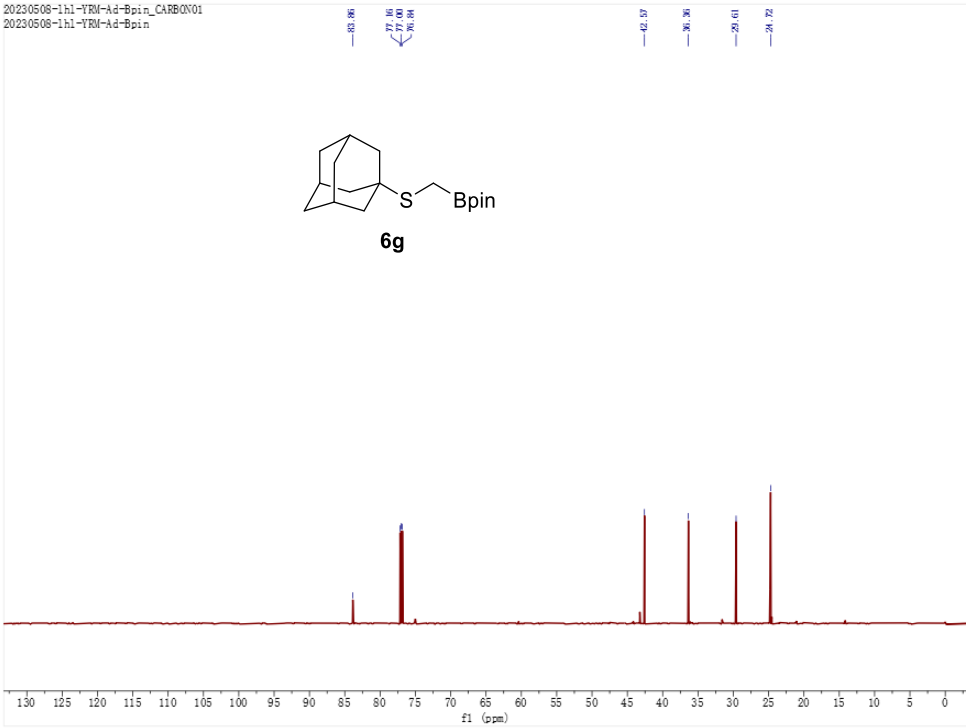
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6f**



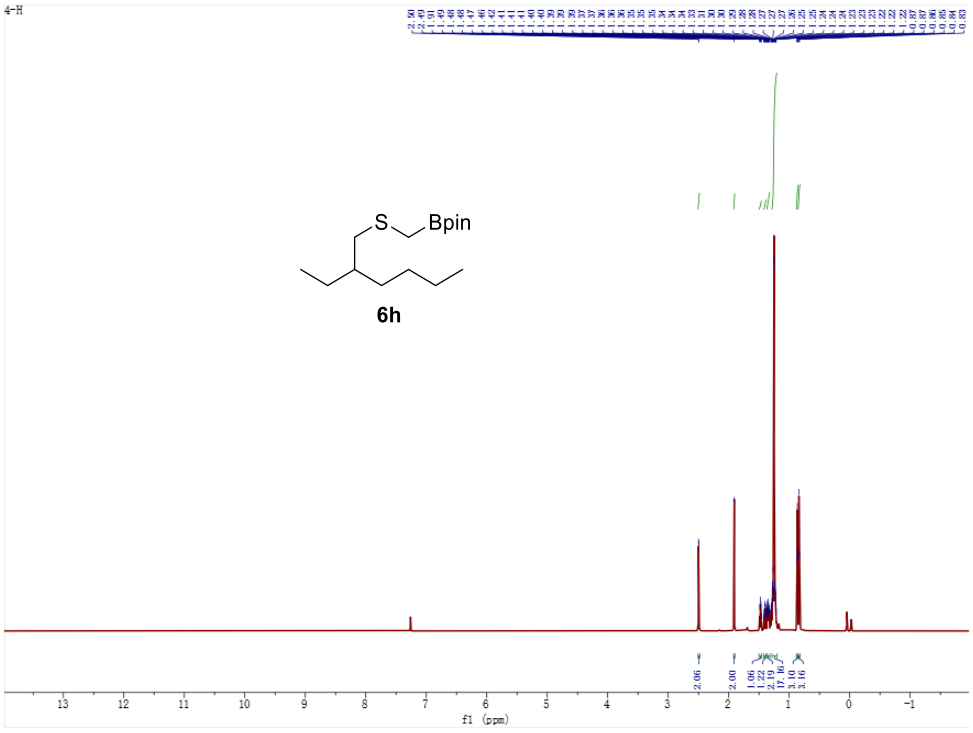



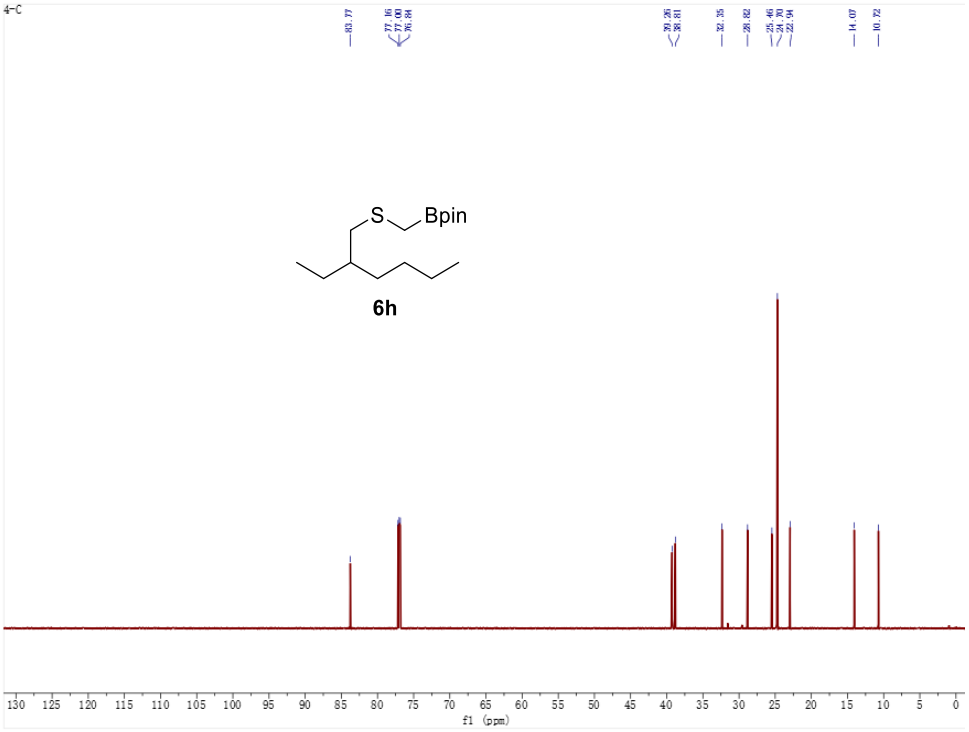
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6g**



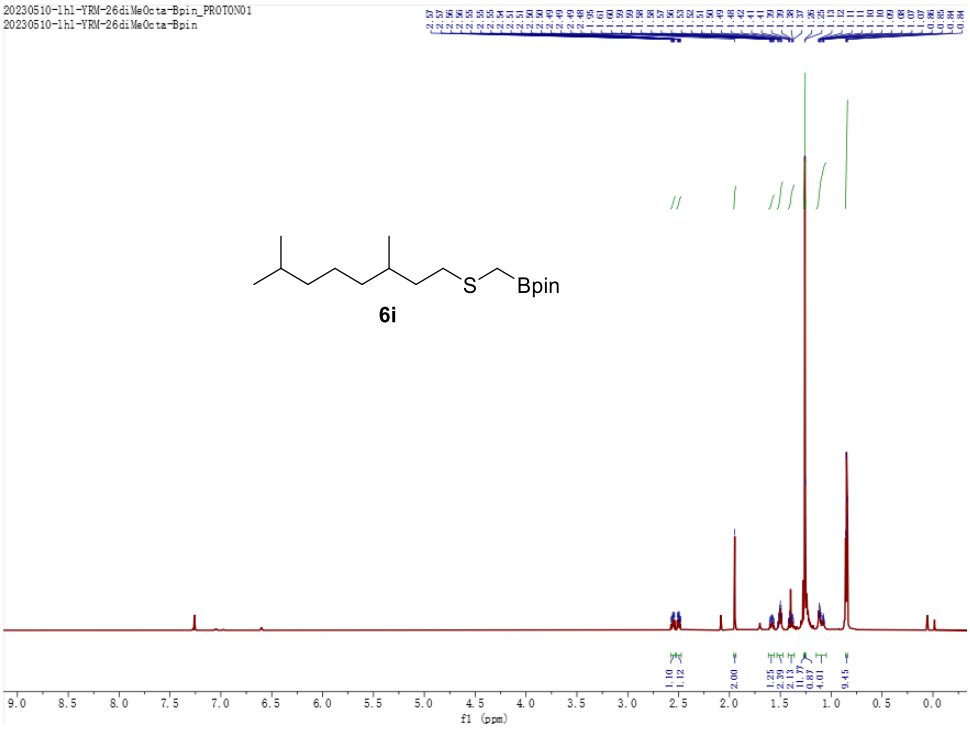



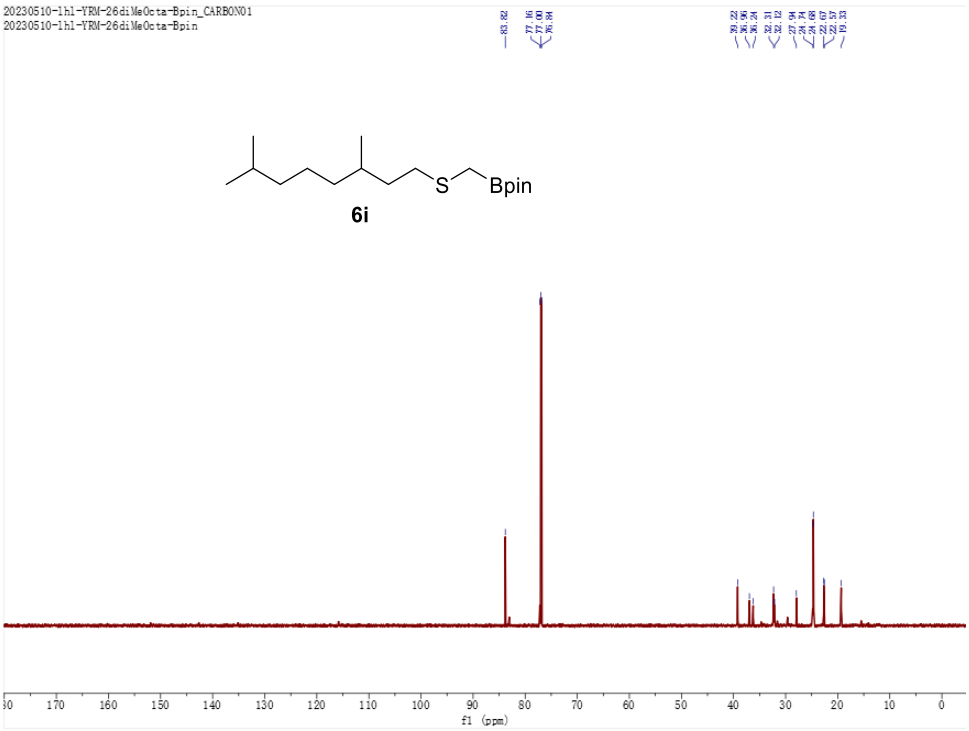
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6h**



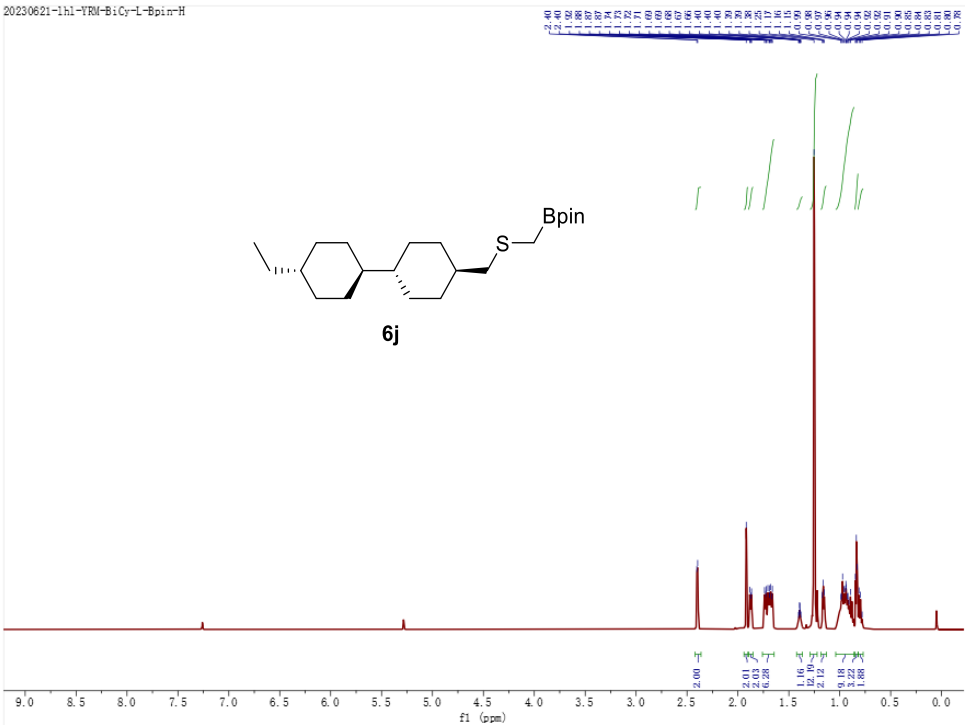



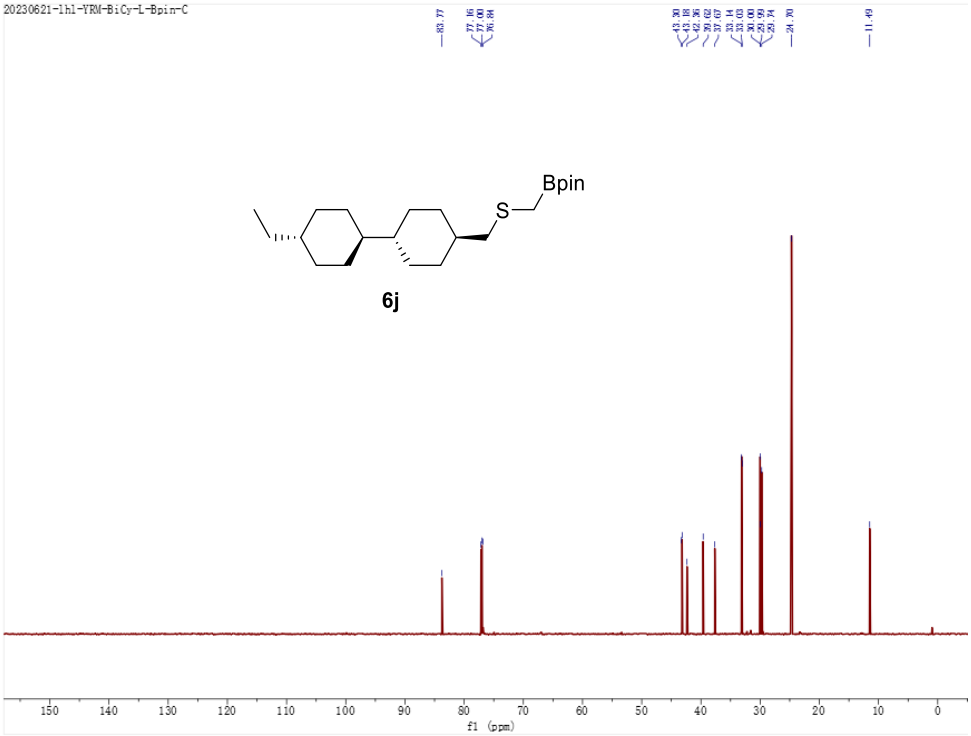
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6i**



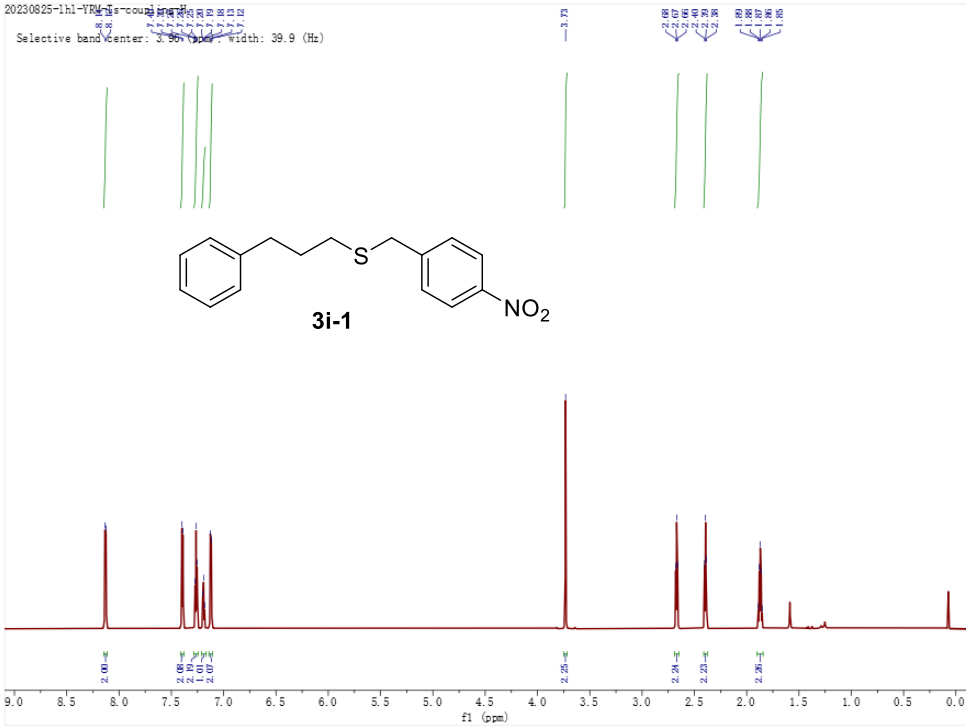



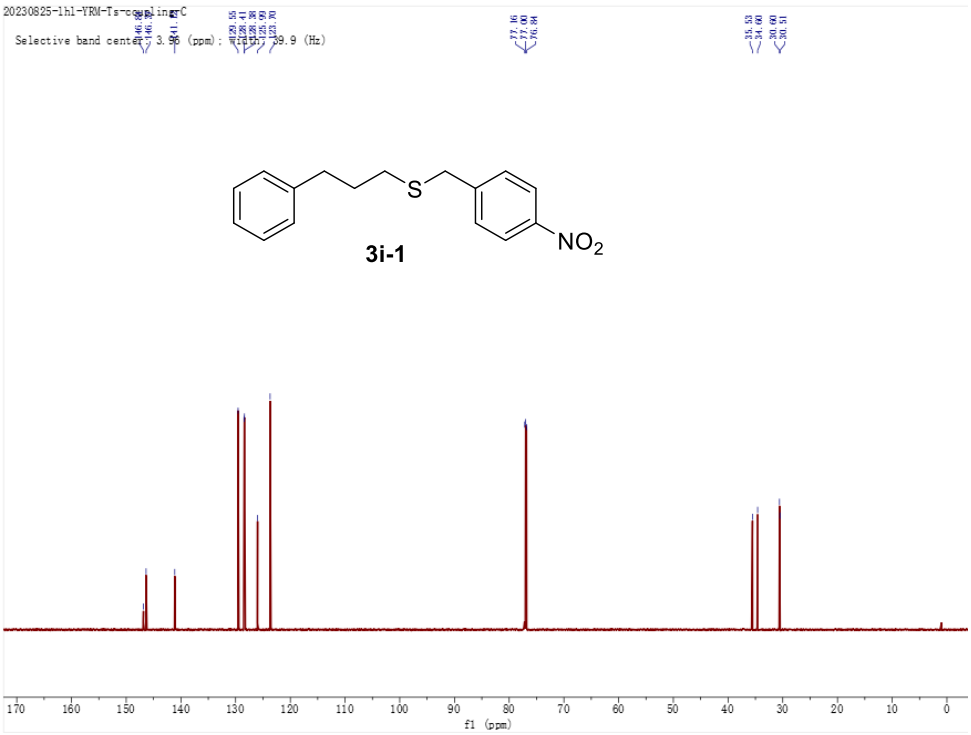
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **6j**



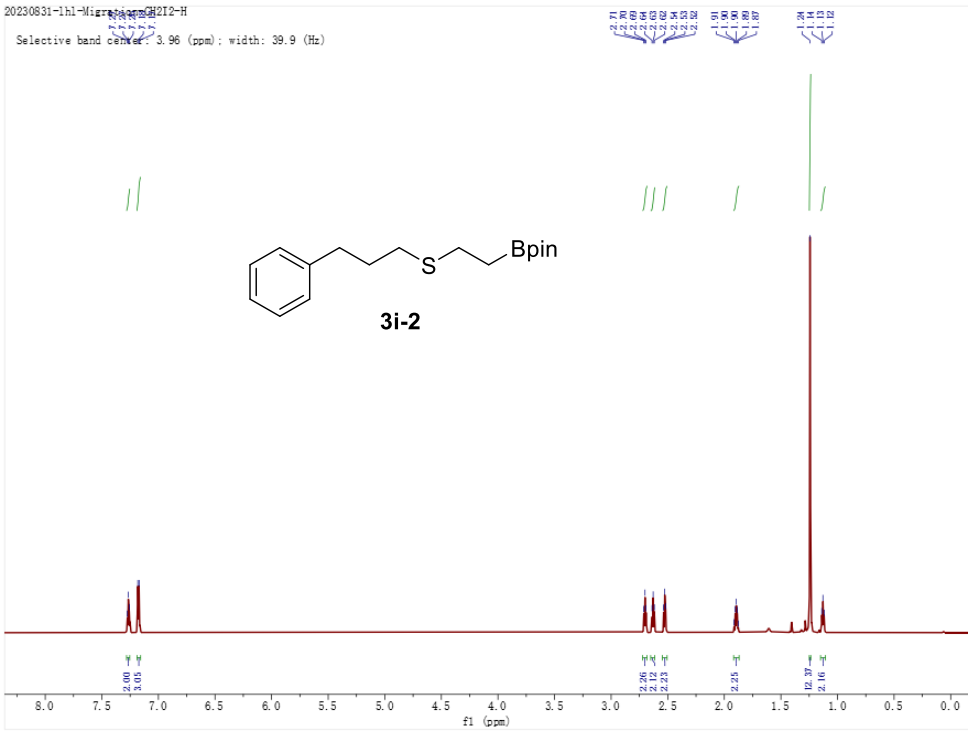



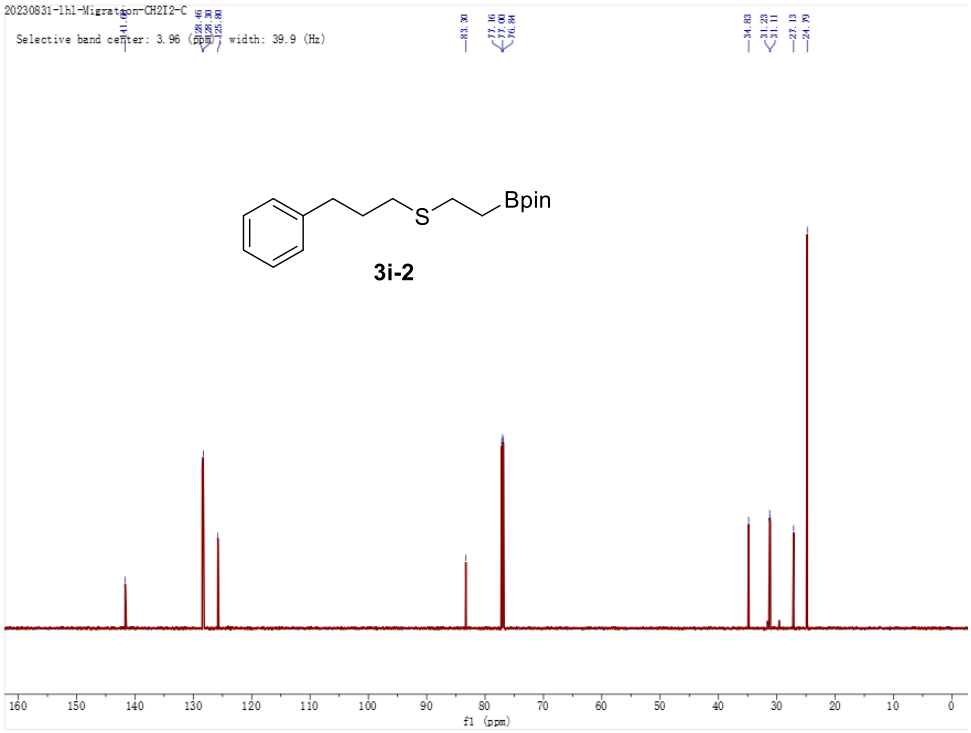
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3i-1**



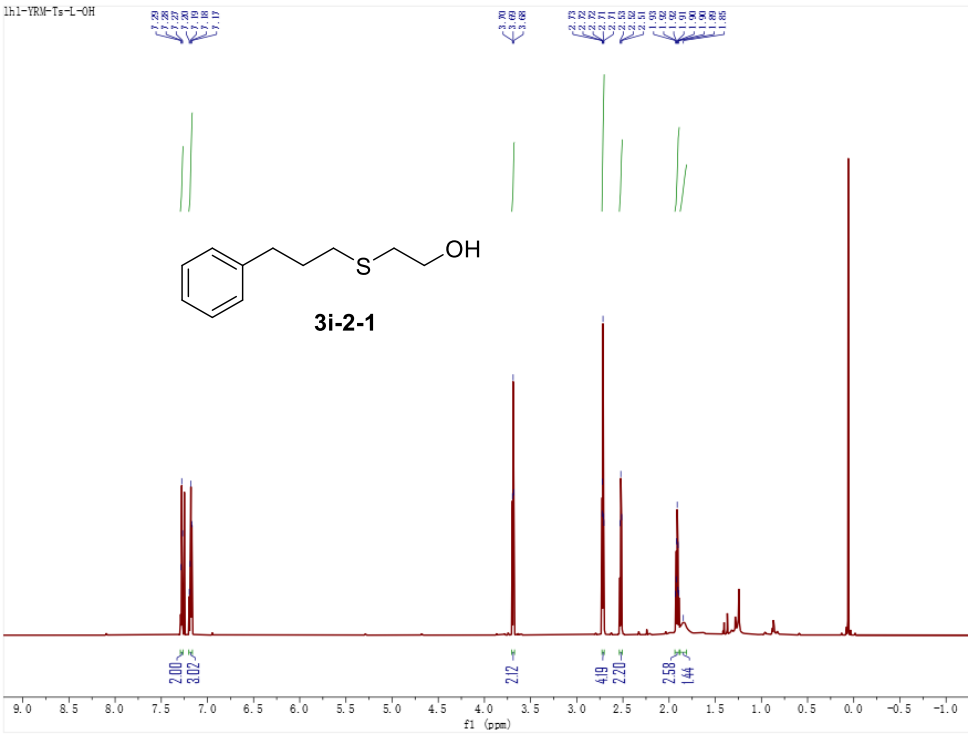



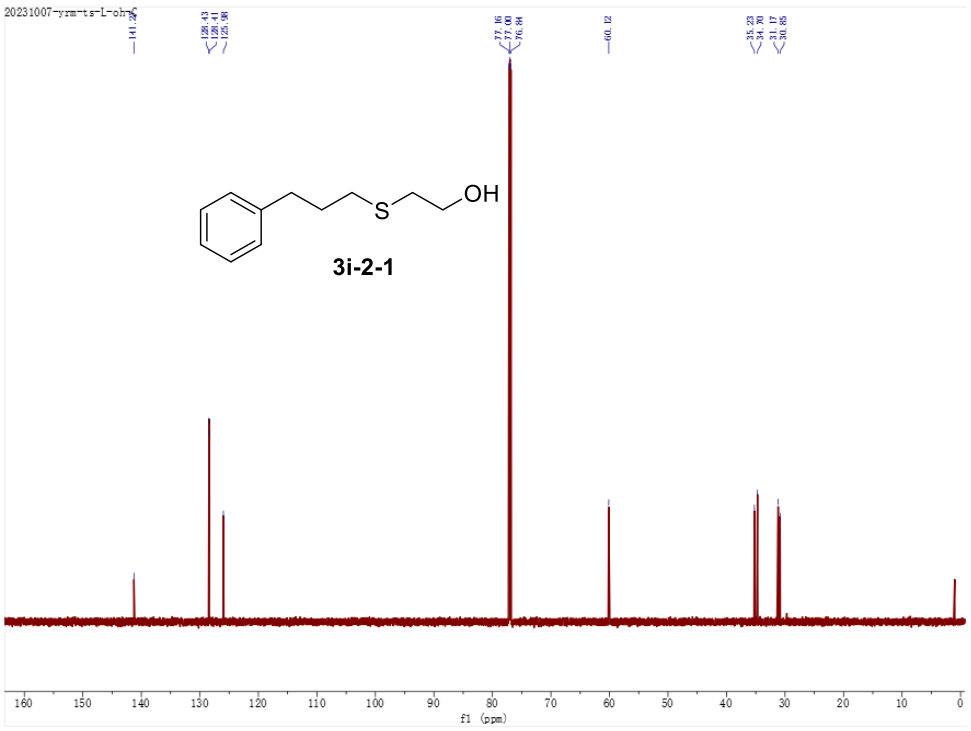
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3i-2**



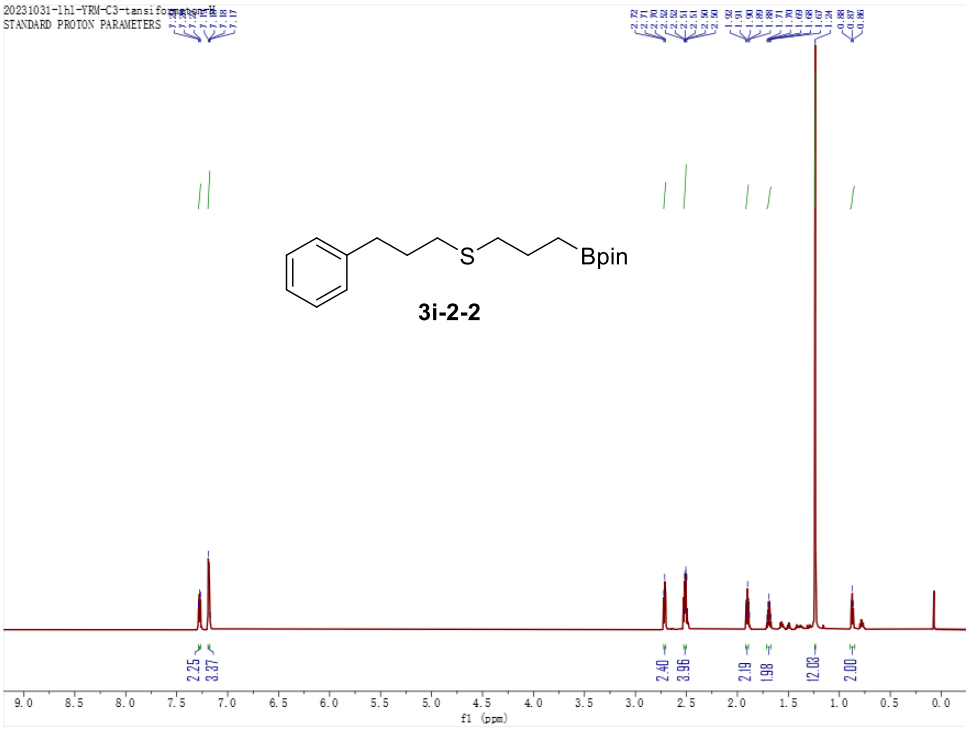



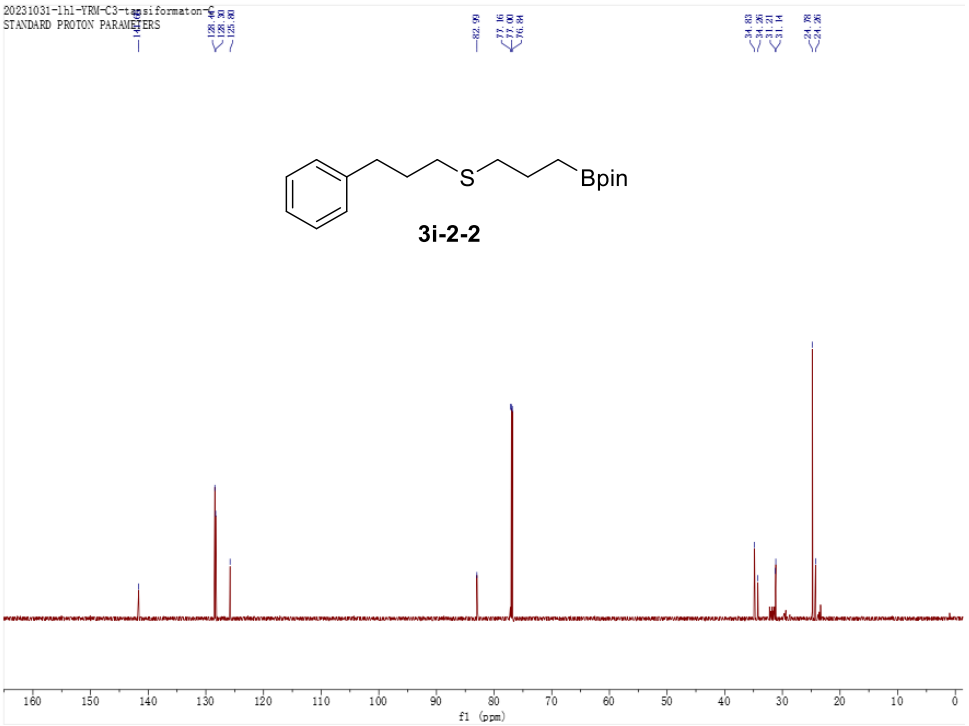
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3i-2-1**



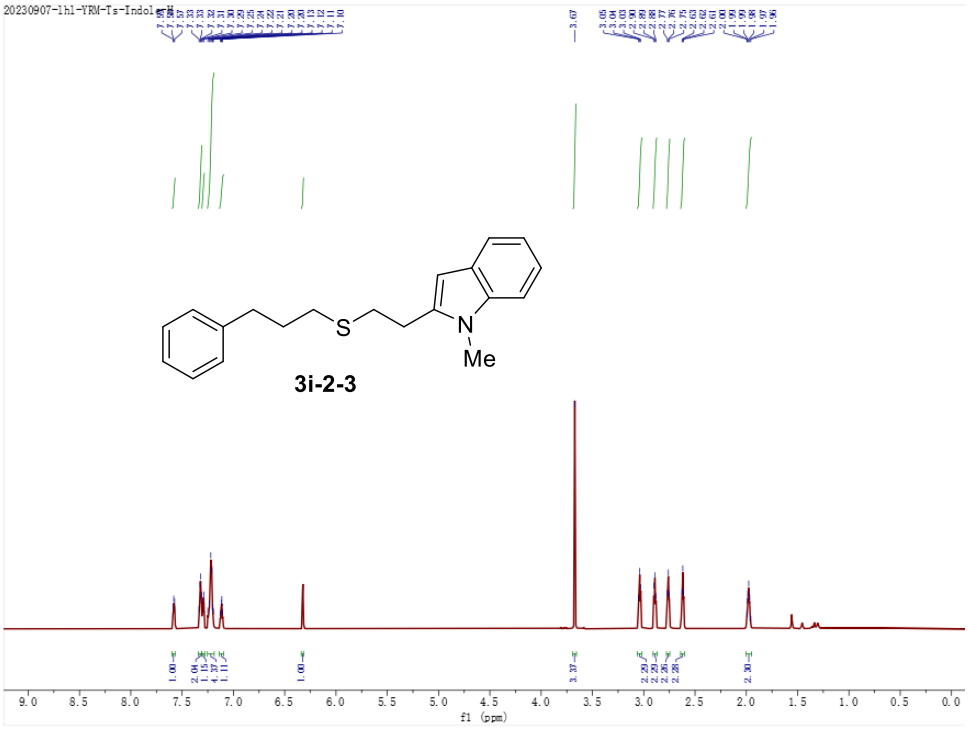



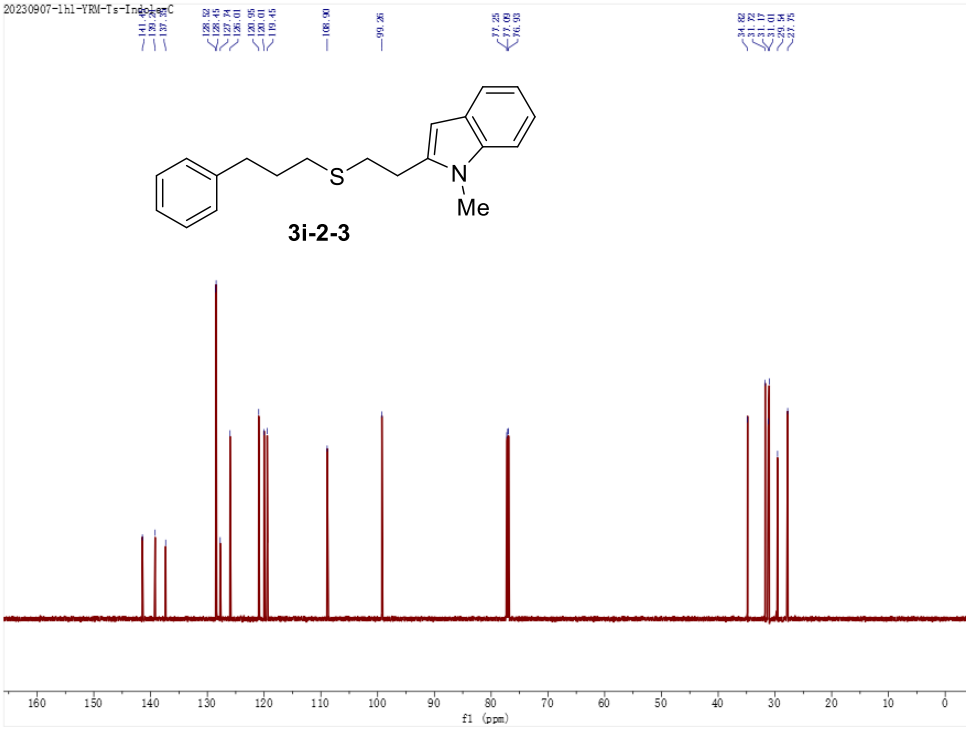
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3i-2-2**



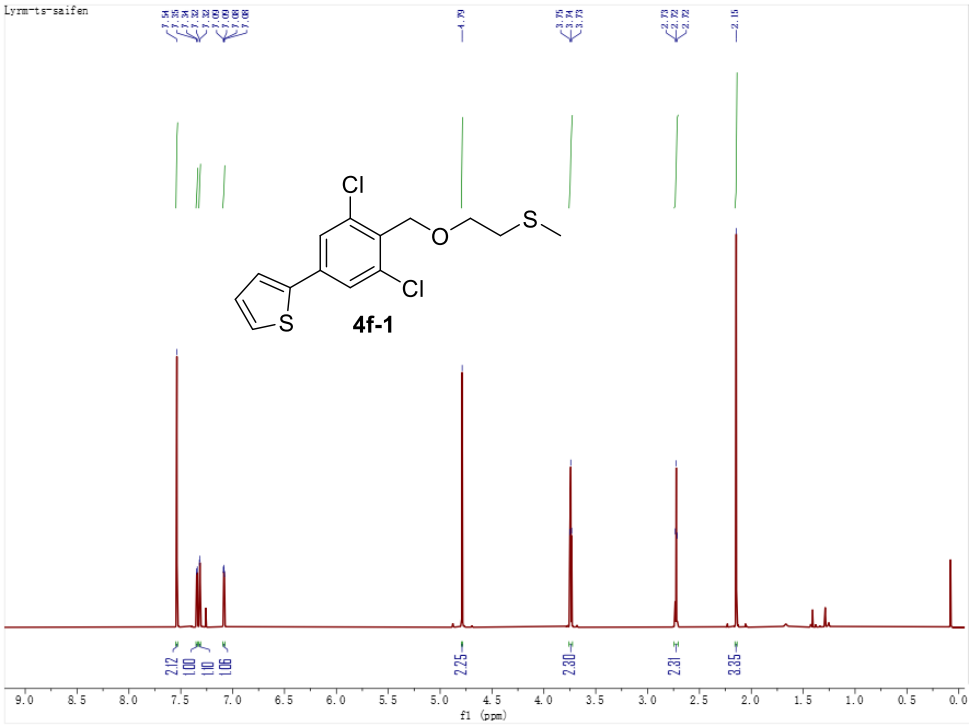



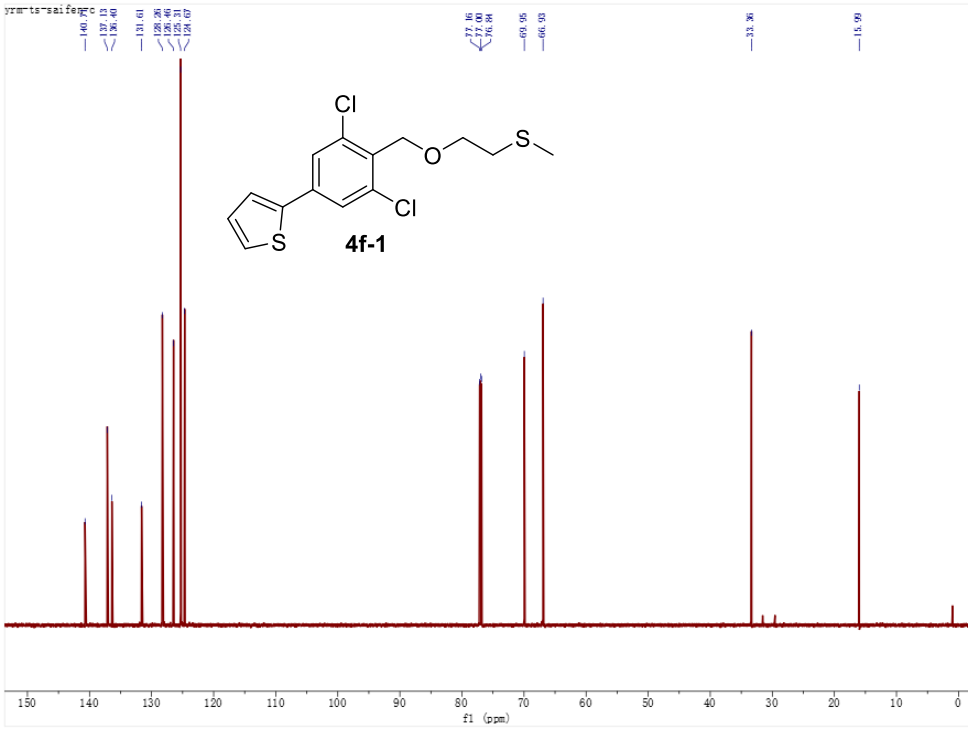
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **3i-2-3**



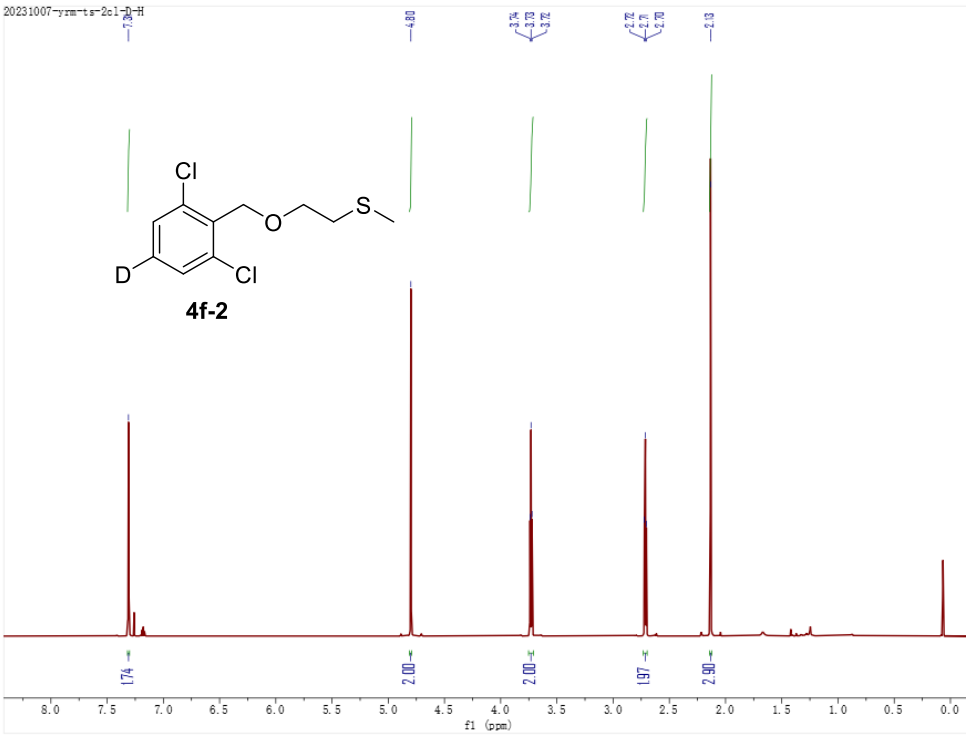



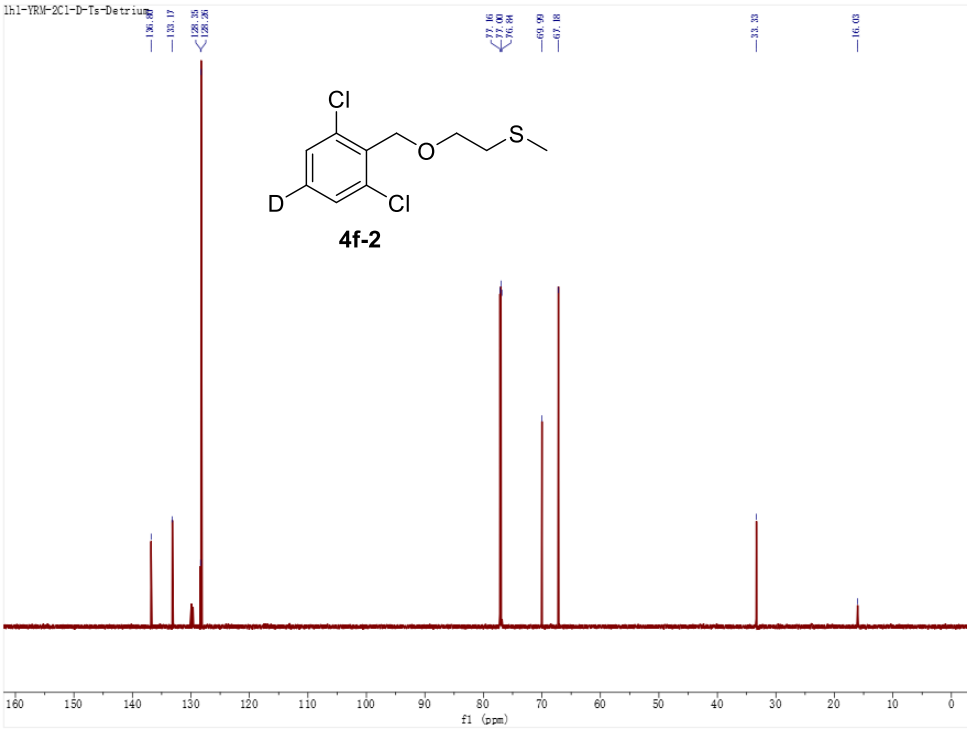
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4f-1**



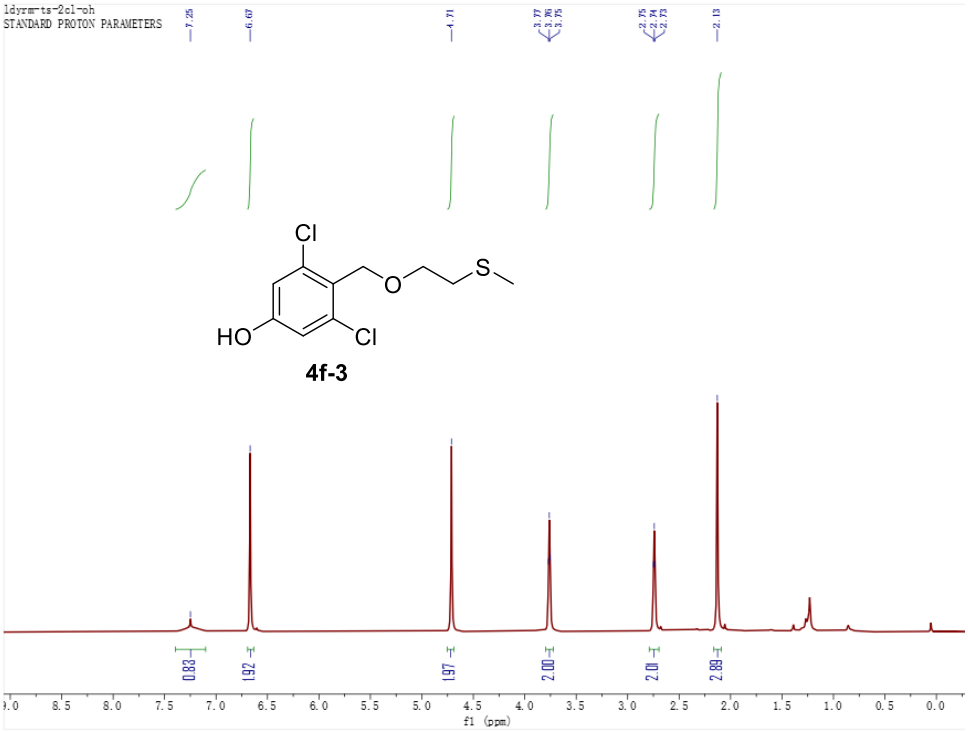



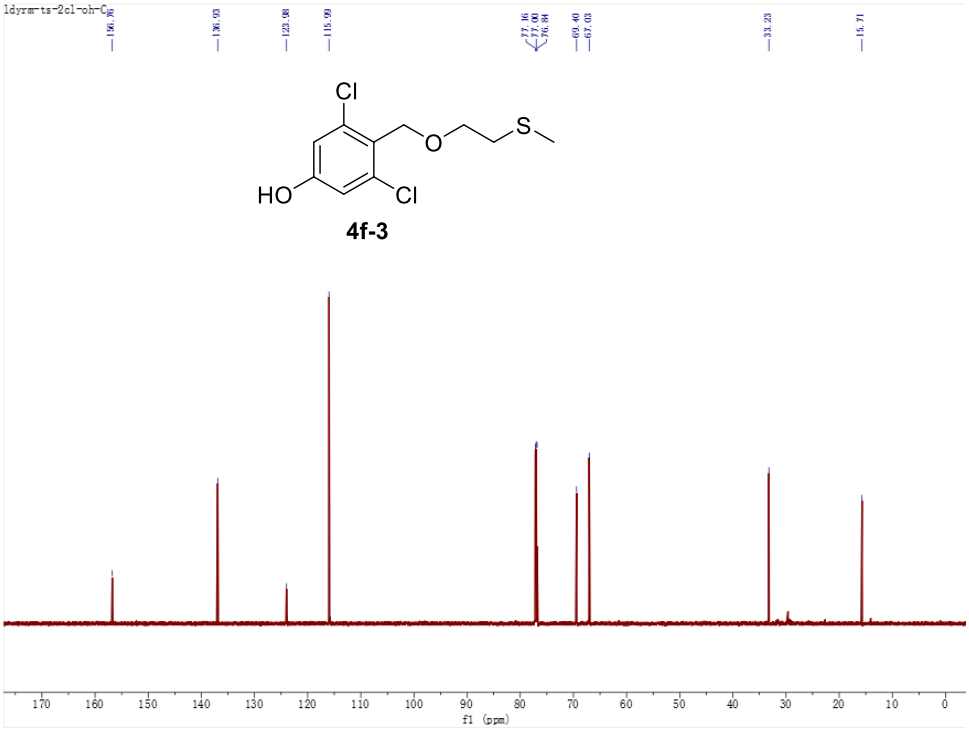
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4f-2**



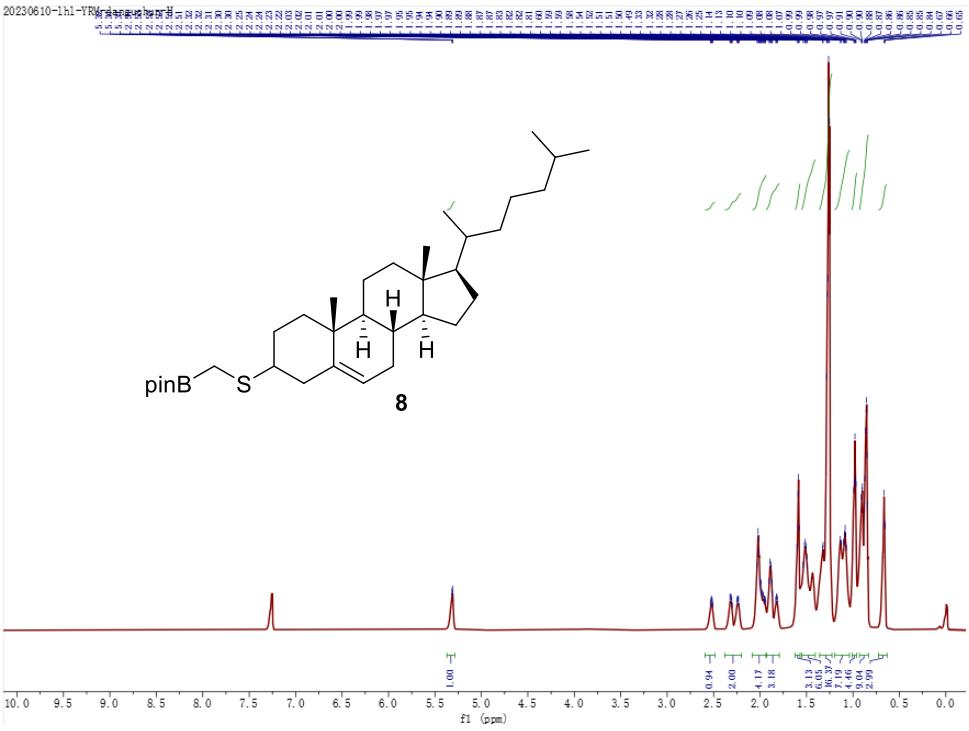



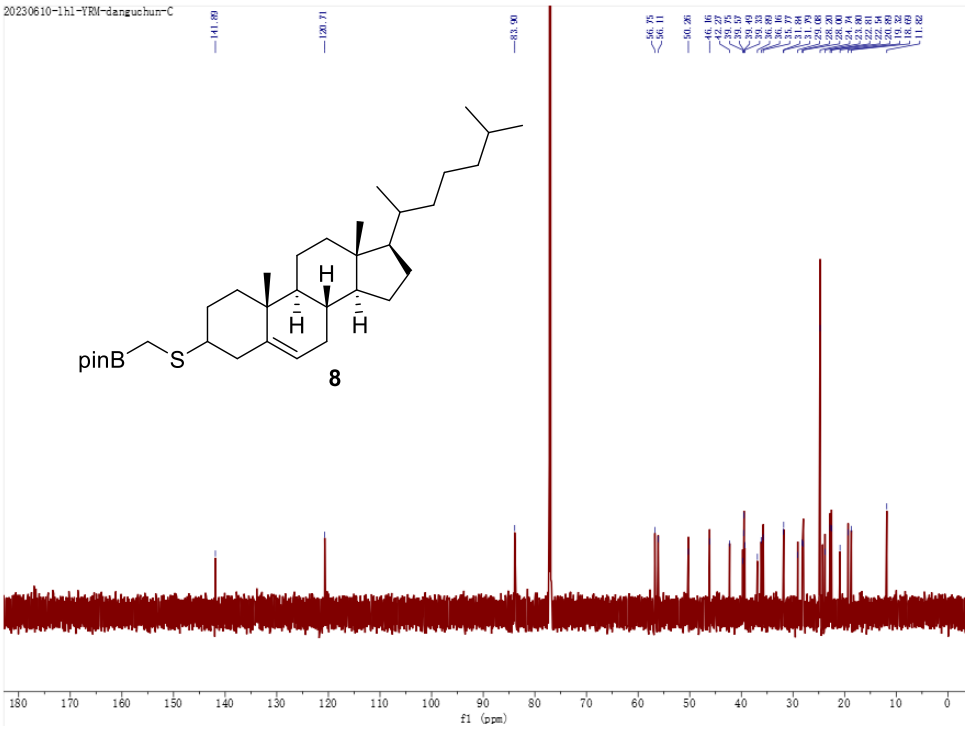
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **4f-3**



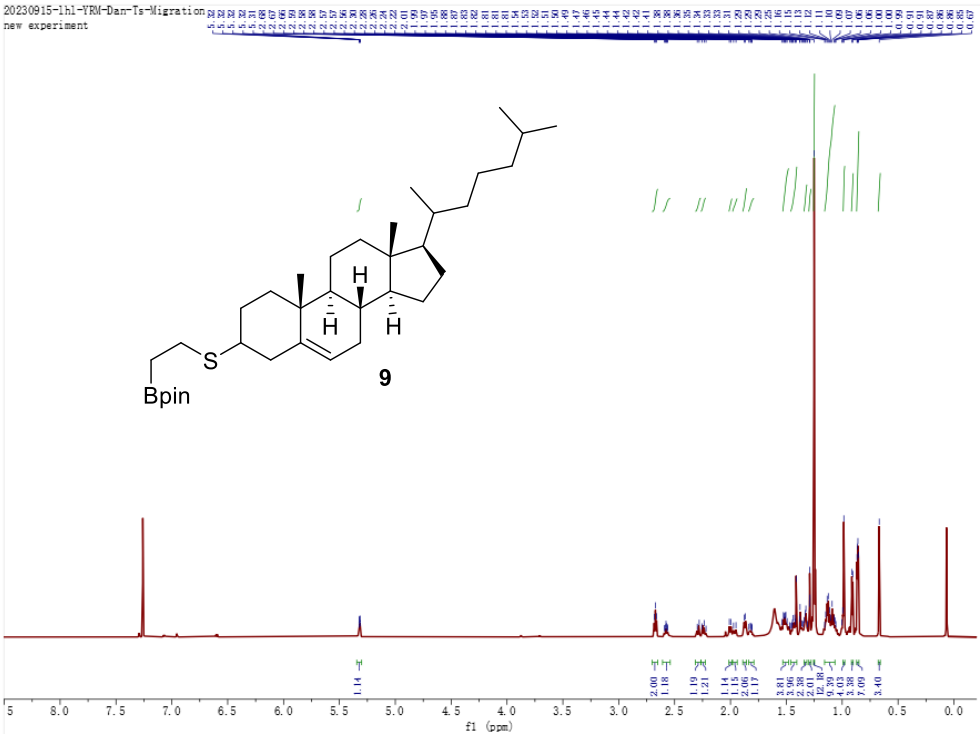



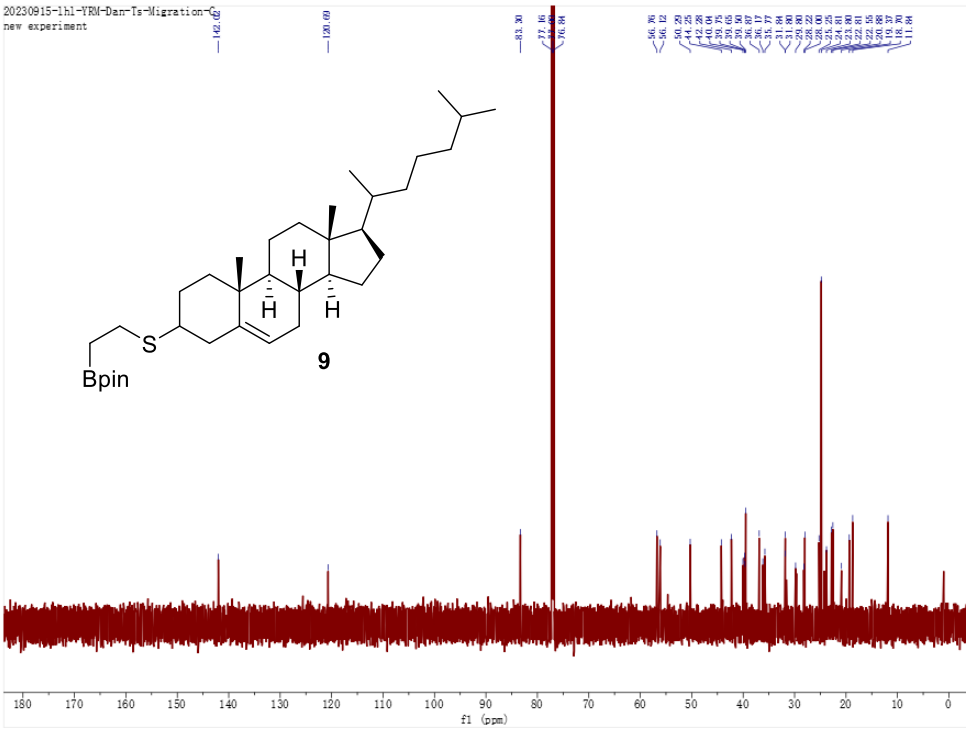
$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **8**



$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **9**



$^{1}$H NMR (800 MHz, $CDCl_3$) and $^{13}$C NMR (201MHz, $CDCl_3$) for **1i-*d***