Supporting Information

Ligand-Controlled Rh(I) -Catalyzed Intramolecular Alkyne Sila-Cyclization: Divergent Catalysis and Mechanistic Studies

Wei-Ke Zhu[a‡], Jia-Wei Si [a‡], Sui-Fang Peng[a], Li Li[a], Fei Ye[a], Zheng Xu*[a], and Li-Wen Xu*[a,b]

[a] Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, and Key Laboratory of Organosilicon Material Technology of Zhejiang Province, College of Material, Chemistry and Chemical Engineering, Hangzhou Normal University, Hangzhou 311121, P. R. China. Email: liwenxu@hznu.edu.cn

[b] State Key Laboratory for Oxo Synthesis and Selective Oxidation, Suzhou Research Institute (SRI), Lanzhou Institute of Chemical Physics (LICP), Chinese Academy of Sciences (CAS), No.18. Tianshuizhong road, Lanzhou city, 730000, P. R. China

[c] Deqing Third People's Hospital and The Affiliated Hospital of Hangzhou Normal University, Hangzhou Normal University, Hangzhou, 310015, China.

‡ These authors contributed equally to this work

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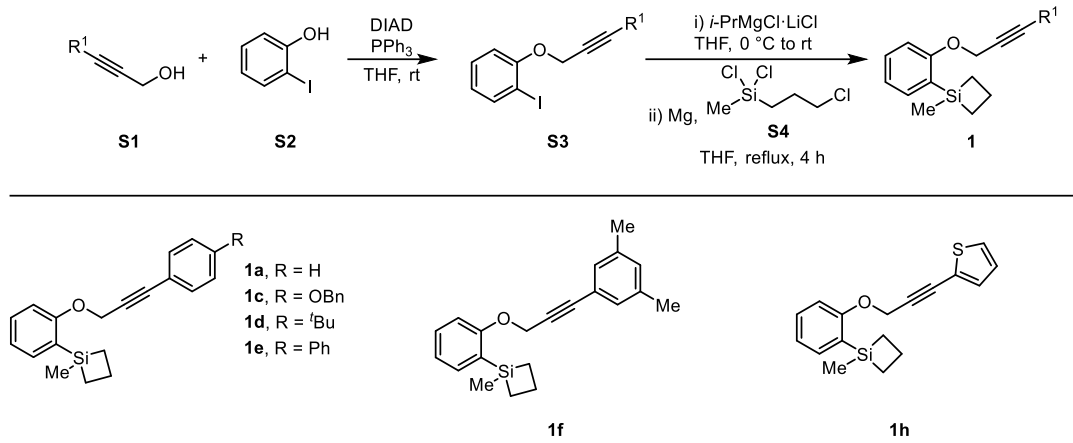
1. General Information

Unless specifically stated, all reagents were commercially obtained and where appropriate, purified prior to use. For example, dichloromethane (DCM),acetonitrile (MeCN) was freshly distilled from CaH_2; Toluene, tetrahydrofuran (THF) and 1, 4-dioxane were dried and distilled from metal sodium and benzophenone. Other commercially available reagents and solvents were used directly without purification. Reactions were monitored by thin layer chromatography (TLC) using silica gel plates. Flash column chromatography was performed over silica (200-300 mesh). ^{1}H, ^{13}C, ^{19}F, NMR spectra were recorded on a Bruker 400 MHz or 500 MHz spectrometer in $CDCl_3$ or C_7D_8 (Toluene-D8). The chemical shifts (δ) were quoted in parts per million (ppm) referenced to TMS (0.00 ppm for ^{1}H NMR) and $CDCl_3$ (77.16 ppm for ^{13}C NMR). Multiplicities were given as: s (singlet); d (doublet); dd (doublets of doublet); t (triplet); q (quartet); td (triplet of doublets) or m (multiplets). Coupling constants, *J*, were reported in Hertz unit (Hz). High resolution mass spectra (HRMS) of the products were obtained on a Bruker Daltonics micro TOF-spectrometer. HPLC was carried out with a Agilent 1260 infinity, Waters AcQuity HPLC or Waters AcQuity UPLC using a chiralcel OD column, a chiralcel OX column, a chiralcel AD column, a chiralcel OJ column, a chiralcel Phenomenex column.

2. General Procedures for the Synthesis of Silacyclobutanes

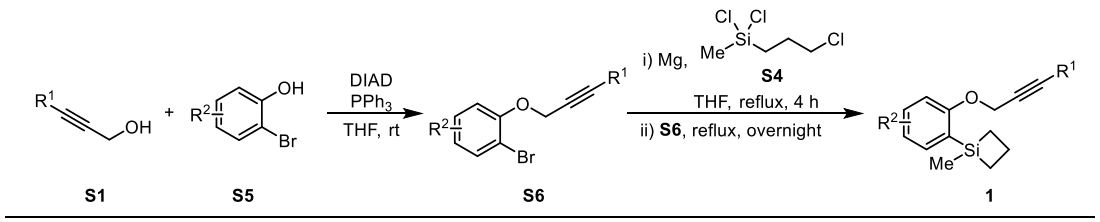
Procedure A

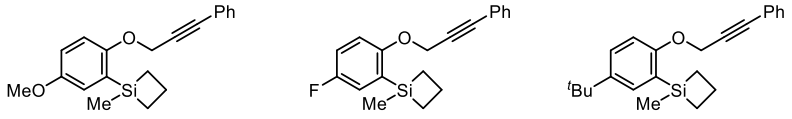


Step I: Following a modified literature procedure[1]. To a flame-dried flask equipped with a magnetic stir bar and a rubber septum was added 2-iodophenol **S2** (1.0 equiv), PPh_3 (1.1 equiv), propargyl alcohol derivative **S1** (1.0 equiv) and THF (0.5 M). With stirring, DIAD (1.1 equiv) was added dropwise, and then the reaction mixture was stirred overnight at room temperature. Upon completion, the reaction mixture was concentrated under vacuum and directly purified via flash chromatography on silica gel to afford **S3**.

Step II: Following a modified literature procedure[2,3]. *i*-PrMgCl·LiCl (1.3 M in THF, 1.3 equiv) was added dropwise to a solution of iodoaryls **S3** (1.0 equiv), in anhydrous THF under N_2 at 0 °C, and the reaction mixture was stirred at 0 °C for 1 h. Magnesium (1.5 equiv), 5 mL solution of **S4** (1.0 equiv) in THF, and a grain of I_2 in dry THF were heated to initiate the Grignard reaction. The remaining **S4** solution was added dropwise over a period of 1 h, and the resulting solution was refluxed for additional 4 h, and then reaction mixture was cooled to room temperature. To a solution of Grignard reagent derived from **S3** was drowpised 1-chloro-1-methylsiletane at 0 °C, the reaction mixture was allowed to warm to room temperature and stirred overnight. To the mixture was added aq. NH_4Cl and the mixture was extracted with EtOAc (× 3), the combined EtOAc solution was washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash chromatography on silica gel to afford **1**.

Procedure B

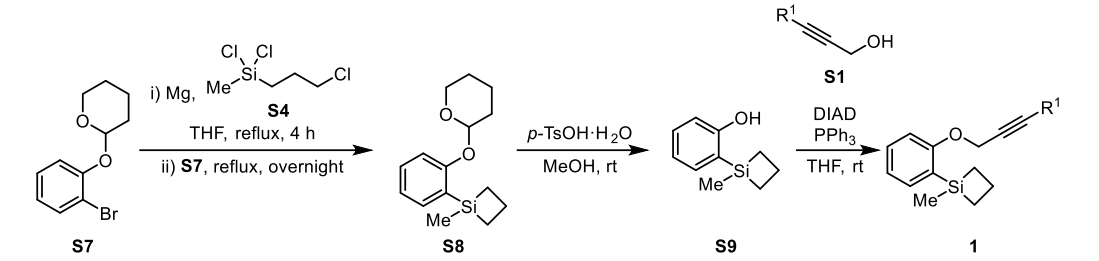


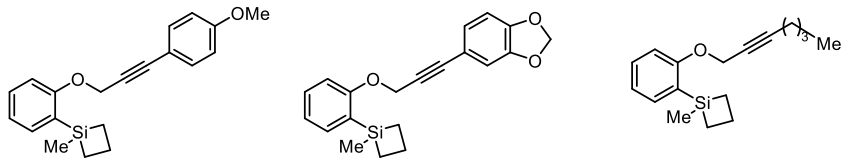


Step I: Following a modified literature procedure[1]. To a flame-dried flask equipped with a magnetic stir bar and a rubber septum was added 2-bromophenol derivative **S5** (1.0 equiv), PPh_3 (1.1 equiv), propargyl alcohol derivative **S1** (1.0 equiv) and THF (0.5 M). With stirring, DIAD (1.1 equiv) was added dropwise, and then the reaction mixture was stirred overnight at room temperature. Upon completion, the reaction mixture was concentrated under vacuum and directly purified via flash chromatography on silica gel to afford **S6**.

Step II: Following a modified literature procedure[3]. Magnesium (3.0 equiv), 5 mL solution of **S4** (1.0 equiv) in THF, and a grain of I_2 in dry THF were heated to initiate the Grignard reaction. The remaining **S4** solution was added dropwise over a period of 1 h, and the resulting solution was refluxed for additional 4 h. **S6** (1.5 equiv) was dissolved in THF and then added dropwise over a period of 3 h, followed by refluxing (by oil bath) the resulting solution overnight. The reaction was allowed to cool to room temperature before quenching with aq. NH_4Cl. The mixture was extracted with EtOAc (× 3). The combined organic layers were then dried over Na_2SO_4 and concentrated under reduced vacuum. The crude product was purified by silica gel flash column chromatography to afford **1**.

Procedure C





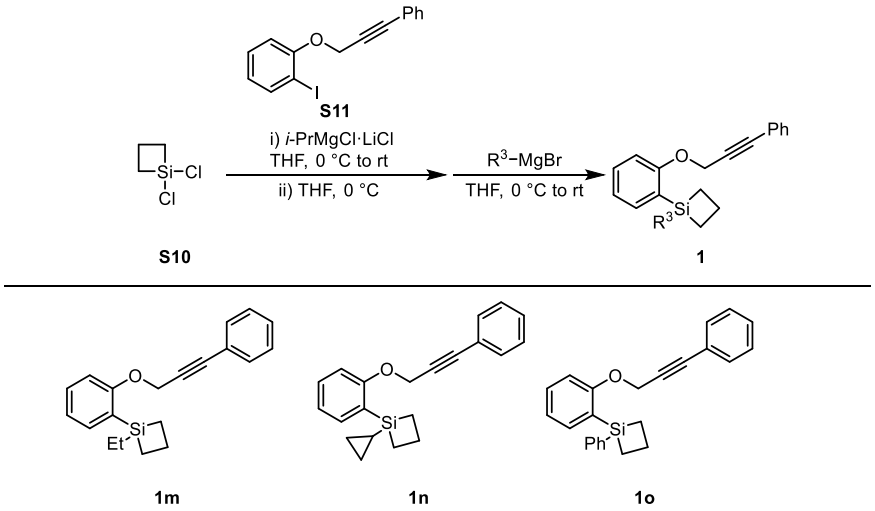
Step I: Following a modified literature procedure[3]. Magnesium (3.0 equiv), 5 mL solution of **S4** (1.0 equiv) in THF, and a grain of I_2 in dry THF were heated to initiate the Grignard reaction. The remaining **S4** solution was added dropwise over a period of 1 h, and the resulting solution was refluxed for additional 4 h. **S7** (1.5 equiv) was dissolved in THF and then added dropwise over a period of 3 h, followed by refluxing (by oil bath) the resulting solution overnight. The reaction was allowed to cool to room temperature before quenching with aq. NH_4Cl. The mixture was extracted with EtOAc (× 3). The combined organic layers were then dried over Na_2SO_4 and concentrated under reduced vacuum. The crude product was purified by silica gel flash column chromatography to afford **S8**.

Step II: To a solution of **S8** (1.0 equiv) in MeOH (0.5 M) was added *p*-toluenesulfonic acid hydrate (10 mol%). After stirring for 40 min at room temperature, the reaction mixture was extracted with EtOAc (× 3), washed with brine and dried over Na_2SO_4. The crude product was purified by silica gel flash column chromatography to afford **S9**.

Step III: Following a modified literature procedure[1]. To a flame-dried flask equipped with a magnetic stir bar and a rubber septum was added 2-(1-methylsiletan-1-yl)phenol **S9** (1.0 equiv), PPh_3 (1.1 equiv), propargyl alcohol derivative **S1** (1.0 equiv) and THF (0.5 M). With stirring, DIAD (1.1 equiv) was added dropwise, and then the reaction mixture was stirred

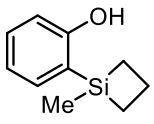
overnight at room temperature. Upon completion, the reaction mixture was concentrated under vacuum and directly purified via flash chromatography on silica gel to afford **1**.

Procedure D



Step I: Following a modified literature procedure[2,3]. *i*-PrMgCl·LiCl (1.3 M in THF, 1.3 equiv) was added dropwise to a solution of iodoaryls **S11** (1.0 equiv), in anhydrous THF under N_2 at 0 °C, and the reaction mixture was stirred at 0 °C for 1 h. To a solution of the **S10** (1.0 equiv) in THF was dropwised Grignard reagent derived from **S11** at 0 °C, the reaction mixture was stirred at this temperature for 8 h. The Grignard reagent (R-MgBr) (1.0 equiv) was added at 0 ℃. The resulting mixture was stirred at room temperature for another 8 h before quenching with aq. NH_4Cl. The mixture was extracted with EtOAc (× 3). The combined organic layers were then dried over Na_2SO_4 and concentrated under reduced vacuum. The residue was purified by silica gel flash column chromatography to afford **1**.

2-(1-methylsiletan-1-yl)phenol (S9)



S9

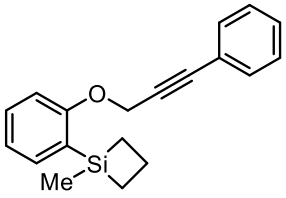
$C_{10}H_{14}OSi$

M = 178.31 g/mol

Following the **step II of procedure A**, **S9** was obtained as a colorless oil (R_f = 0.4, petroleum ether/ethyl acetate = 10:1) in 78% yield (2.49 g, 14.0 mmol). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.51 (d, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.03 (t, *J* = 7.3 Hz, 1H), 6.76 (d, *J* = 8.1 Hz,

1H), 4.99 (s, 1H), 2.32-2.16 (m, 2H), 1.49-1.36 (m, 2H), 1.30-1.20 (m, 2H), 0.60 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.2, 135.3, 131.4, 124.3, 120.8, 114.6, 18.5, 14.3, -0.6. **HRMS (ESI, *m/z*)** calcd for $C_{10}H_{15}OSi$ $[M+H]^+$: 179.0887, found: 179.0888.

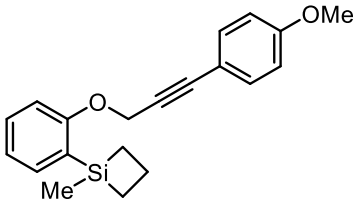
1-methyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)siletane (1a)



1a
$C_{19}H_{20}OSi$
M = 292.45 g/mol

Following the **procedure A**, **1a** was obtained as a colorless oil (R_f = 0.3, petroleum ether) in 59% yield (3.44 g, 11.8 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.50 (dd, J = 7.6, 2.0 Hz, 1H), 7.44-7.36 (m, 3H), 7.33-7.25 (m, 3H), 7.03 (m, 2H), 4.91 (s, 2H), 2.22-2.08 (m, 2H), 1.48-1.30 (m, 2H), 1.24-1.08 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.5, 135.2, 131.9, 131.3, 128.7, 128.4, 127.6, 122.6, 121.4, 111.3, 86.9, 84.3, 56.8, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{19}H_{20}NaOSi$ $[M+Na]^+$: 315.1176, found: 315.1178.

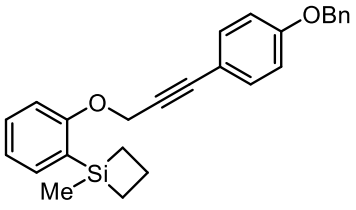
1-(2-((3-(4-methoxyphenyl)prop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1b)



1b
$C_{20}H_{22}O_2Si$
M = 322.48 g/mol

Following the **procedure C**, **1b** was obtained as a pale yellow oil (R_f = 0.4, petroleum ether/ethyl acetate = 50:1) in 40% yield (0.13 g, 0.4 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (dd, J = 7.2, 1.6 Hz, 1H), 7.44-7.32 (m, 3H), 7.08-7.00 (m, 2H), 6.82 (m, 2H), 4.90 (s, 2H), 3.79 (s, 3H), 2.22-2.09 (m, 2H), 1.42-1.30 (m, 2H), 1.21-1.10 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 159.9, 135.2, 133.4, 131.2, 127.5, 121.4, 114.6, 114.0, 111.4, 86.9, 83.0, 56.9, 55.4, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{22}NaO_2Si$ $[M+Na]^+$: 345.1281, found: 345.1278.

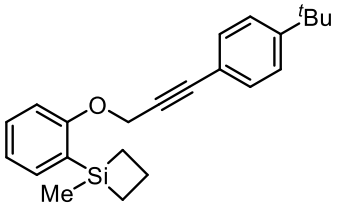
1-(2-((3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1c)



1c
$C_{26}H_{26}O_2Si$
M = 398.58 g/mol

Following the **procedure A**, **1c** was obtained as a white solid (R_f = 0.4, petroleum ether/ethyl acetate = 50:1) in 37% yield (1.0 g, 2.5 mmol). **M.P.** 42-44 ℃.**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (dd, *J* = 7.3, 2.0 Hz, 1H), 7.41-7.27 (m, 8H), 7.04-6.98 (m, 2H), 6.87 (d, *J* = 8.6 Hz, 2H), 5.01 (s, 2H), 4.87 (s, 2H), 2.23-2.04 (m, 2H), 1.42-1.29 (m, 2H), 1.23-1.10 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 159.1, 136.6, 135.1, 133.4, 131.2, 128.7, 128.2, 127.6, 127.5, 121.4, 114.92, 114.89, 111.3, 86.9, 83.0, 70.1, 56.8, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{26}H_{26}NaO_2Si$ $[M+Na]^+$: 421.1594, found: 421.1594.

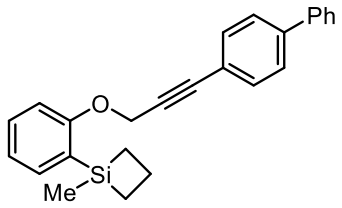
1-(2-((3-(4-(*tert*-butyl)phenyl)prop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1d)



1d
$C_{23}H_{28}OSi$
M = 348.56 g/mol

Following the **procedure A**, **1d** was obtained as a colorless oil (R_f = 0.3, petroleum ether) in 16% yield (0.47 g, 1.3 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (dd, *J* = 7.1, 1.8 Hz, 1H), 7.43-7.29 (m, 5H), 7.07-7.00 (m, 2H), 4.91 (s, 2H), 2.22-2.08 (m, 2H), 1.41-1.32 (m, 2H), 1.29 (s, 9H), 1.21-1.10 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 152.0, 135.2, 131.6, 131.2, 127.6, 125.4, 121.4, 119.6, 111.4, 87.1, 83.6, 56.9, 34.9, 31.3, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{23}H_{28}NaOSi$ $[M+Na]^+$: 371.1802, found: 371.1796.

1-(2-((3-([1,1'-biphenyl]-4-yl)prop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1e)



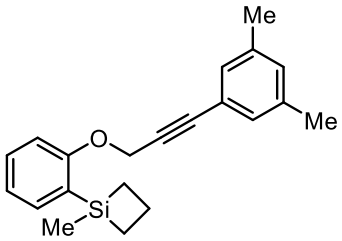
1e

$C_{25}H_{24}OSi$

M = 368.55 g/mol

Following the **procedure A**, **1e** was obtained as a white solid (R_f = 0.2, petroleum ether) in 61% yield (1.5 g, 4.1 mmol). **M.P.** 63-65 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.60-7.30 (m, 11H), 7.09-7.01 (m, 2H), 4.94 (s, 2H), 2.22-2.10 (m, 2H), 1.42-1.33 (m, 2H), 1.23-1.11 (m, 2H), 0.56 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 141.5, 140.4, 135.2, 132.3, 131.3, 129.0, 127.8, 127.6, 127.2, 127.1, 121.5, 121.4, 111.4, 86.8, 85.0, 56.8, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{25}H_{24}NaOSi$ $[M+Na]^+$: 391.1489, found: 391.1489.

1-(2-((3-(3,5-dimethylphenyl)prop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1f)



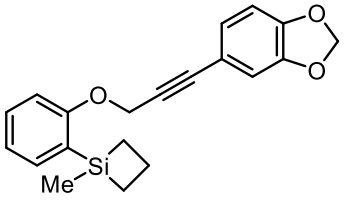
1f

$C_{21}H_{24}OSi$

M = 320.51 g/mol

Following the **procedure A**, **1f** was obtained as a pale yellow oil (R_f = 0.3, petroleum ether) in 13% yield (0.34 g, 1.1 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.50 (dd, J = 7.1, 1.7 Hz, 1H),7.43-7.36 (m, 1H), 7.08-7.00 (m, 4H), 6.94 (s, 1H), 4.90 (s, 2H), 2.26 (s, 6H), 2.22-2.08 (m, 2H), 1.43-1.31 (m, 2H), 1.21-1.09 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 138.0, 135.2, 131.3, 130.6, 129.5, 127.5, 122.2, 121.4, 111.3, 87.3, 83.6, 56.8, 21.2, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{21}H_{24}NaOSi$ $[M+Na]^+$: 343.1489, found: 343.1489.

1-(2-((3-(benzo[*d*][1,3]dioxol-5-yl)prop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1g)



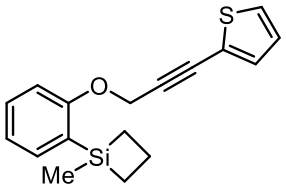
1g

$C_{20}H_{20}O_3Si$

M = 336.46 g/mol

Following the **procedure C**, **1g** was obtained as a colorless oil (R_f = 0.2, petroleum ether/ethyl acetate = 50:1) in 37% yield (0.25 g, 0.74 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.39 (td, *J* = 8.0, 2.0 Hz, 1H), 7.03 (dd, *J* = 7.8, 5.8 Hz, 2H), 6.94 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.86 (d, *J* = 1.6 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.95 (s, 2H), 4.89 (s, 2H), 2.22-2.08 (m, 1H), 1.43-1.29 (m, 2H), 1.23-1.09 (m, 2H), 0.54 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 148.2, 147.5, 135.2, 131.2, 127.6, 126.6, 121.4, 115.8, 111.9, 111.3, 108.5, 101.5, 86.8, 82.7, 56.8, 18.6, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{20}NaO_3Si$ $[M+Na]^+$: 359.1074, found: 359.1069.

1-methyl-1-(2-((3-(thiophen-2-yl)prop-2-yn-1-yl)oxy)phenyl)siletane (1h)



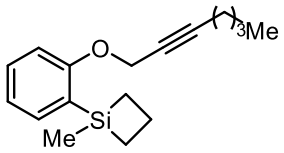
1h

$C_{17}H_{18}OSSi$

M = 298.48 g/mol

Following the **procedure A**, **1h** was obtained as a yellow oil (R_f = 0.3, petroleum ether) in 25% yield (0.73 g,2.4 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.43 (dd, *J* = 7.1, 1.8 Hz, 1H), 7.33 (td, *J* = 7.8, 1.8 Hz, 1H), 7.18 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.14 (dd, *J* = 3.6, 1.0 Hz, 1H), 7.00-6.93 (m, 2H), 6.89 (dd, *J* = 5.1, 3.6 Hz, 1H), 4.86 (s, 2H), 2.15-1.99 (m, 2H), 1.33-1.23 (m, 2H), 1.14-1.04 (m, 2H), 0.47 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.5, 135.2, 132.8, 131.3, 127.7, 127.6, 127.1, 122.4, 121.5, 111.3, 88.3, 80.3, 56.8, 18.4, 14.5, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{17}H_{18}NaOSSi$ $[M+Na]^+$: 321.0740, found: 321.0750.

1-(2-(hept-2-yn-1-yloxy)phenyl)-1-methylsiletane (1i)



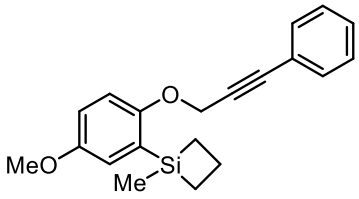
1i

$C_{17}H_{24}OSi$

M = 272.46 g/mol

Following the **procedure C**, **1i** was obtained as a colorless oil (R_f = 0.35, petroleum ether) in 22% yield (0.12 g, 0.44 mmol). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.48 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.37 (td, *J* = 7.8, 1.8 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 4.67 (s, 2H), 2.25-2.07 (m, 4H), 1.52-1.42 (m, 2H), 1.43-1.27 (m, 4H), 1.21-1.08 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H), 0.52 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 162.6, 135.1, 131.2, 127.4, 121.2, 111.3, 88.0, 75.3, 56.6, 30.6, 21.9, 18.6, 18.3, 14.5, 13.7, -0.5. **HRMS (ESI, *m/z*):** calcd for $C_{17}H_{24}NaOSi$ $[M+Na]^+$: 295.1489, found: 295.1485.

1-(5-methoxy-2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1j)



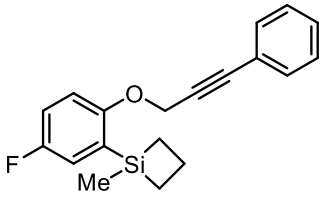
1j

$C_{20}H_{22}O_2Si$

M = 322.48 g/mol

Following the **procedure B**, **1j** was obtained as a yellow oil (R_f = 0.4, petroleum ether/ethyl acetate = 50:1) in 14% yield (0.45 g, 1.4 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.45-7.37 (m, 2H), 7.33-7.25 (m, 3H), 7.05 (d, *J* = 3.2 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.90 (dd, *J* = 8.9, 3.1 Hz, 1H), 4.86 (s, 2H), 3.79 (s, 3H), 2.24-2.09 (m, 2H), 1.42-1.30 (m, 2H), 1.23-1.11 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 156.7, 154.3, 131.9, 129.2, 128.7, 128.4, 122.6, 120.7, 115.4, 112.9, 86.8, 84.6, 57.6, 55.9, 18.3, 14.6, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{22}NaO_2Si$ $[M+Na]^+$: 345.1281, found: 345.1276.

1-(5-fluoro-2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1k)



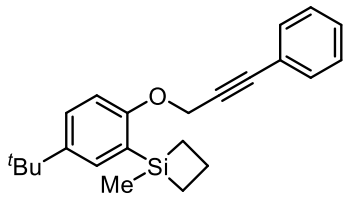
1k

$C_{19}H_{19}FOSi$

M = 310.44 g/mol

Following the **procedure B**, **1k** was obtained as a pale yellow oil (R_f = 0.3, petroleum ether) in 14% yield (0.43 g, 1.4 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.41 (dd, J = 6.8, 2.4 Hz, 2H), 7.35-7.25 (m, 3H), 7.17 (dd, J = 8.0, 3.1 Hz, 1H), 7.05 (td, J = 8.4, 3.1 Hz, 1H), 6.98 (dd, J = 8.9, 3.9 Hz, 1H), 4.88 (s, 2H), 2.22-2.06 (m, 2H), 1.40-1.29 (m, 2H), 1.23-1.12 (m, 2H), 0.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.3 (d, J = 1.7 Hz), 157.8 (d, J = 240.0 Hz), 131.9, 130.1 (d, J = 4.0 Hz), 128.8, 128.4, 122.4, 121.2 (d, J = 20.9 Hz), 117.1 (d, J = 23.3 Hz), 112.7 (d, J = 7.1 Hz), 87.1, 84.1, 57.5, 18.3, 14.4, -0.6. **^{19}F NMR (471 MHz, $CDCl_3$)** δ -123.6 (s). **HRMS (ESI, *m/z*):** calcd for $C_{19}H_{19}FNaOSi$ $[M+Na]^+$: 333.1081, found: 333.1068.

1-(5-(*tert*-butyl)-2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1-methylsiletane (1l)



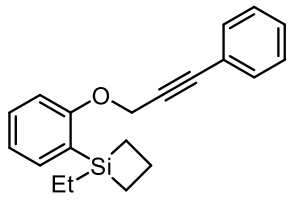
1l

$C_{23}H_{28}OSi$

M = 348.56 g/mol

Following the **procedure B**, **1l** was obtained as a pale yellow oil (R_f = 0.3, petroleum ether) in 14% yield (0.49 g, 1.4 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.60 (d, J = 2.5 Hz, 1H), 7.53-7.47 (m, 3H), 7.40-7.35 (m, 3H), 7.07 (d, J = 8.6 Hz, 1H), 4.97 (s, 2H), 2.32-2.19 (m, 2H), 1.54-1.43 (m, 2H), 1.41 (s, 9H), 1.32-1.19 (m, 2H), 0.65 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.5, 143.7, 132.0, 131.9, 128.7, 128.4, 128.0, 126.7, 122.6, 110.8, 86.8, 84.6, 56.9, 34.4, 31.7, 18.4, 14.6, -0.5. **HRMS (ESI, *m/z*)** calcd for $C_{23}H_{28}NaOSi$ $[M+Na]^+$: 371.1802, found: 371.1803.

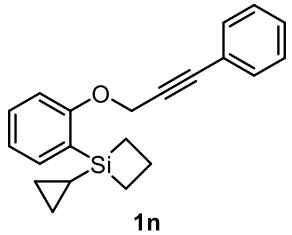
1-ethyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)siletane (1m)



1m
$C_{20}H_{22}OSi$
M = 306.48 g/mol

Following the **procedure D**, **1m** was obtained as a colorless oil (R_f = 0.3, petroleum ether) in 13% yield (0.39 g, 1.3 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.43-7.36 (m, 3H), 7.34-7.26 (m, 3H), 7.08-7.00 (m, 2H), 4.90 (s, 2H), 2.21-2.05 (m, 2H), 1.38-1.17 (m, 4H), 1.10-0.95 (m, 5H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.5, 135.5, 131.9, 131.1, 128.7, 128.4, 126.8, 122.6, 121.4, 111.2, 86.9, 84.3, 56.7, 18.6, 12.7, 7.7, 7.6. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{22}NaOSi$ $[M+Na]^+$: 329.1332, found: 329.1330.

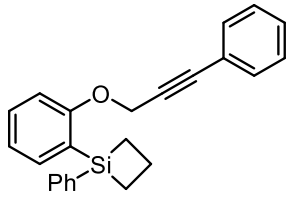
1-cyclopropyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)siletane (1n)



1n
$C_{21}H_{22}OSi$
M = 318.49 g/mol

Following the **procedure D**, **1n** was obtained as a colorless oil (R_f = 0.3, petroleum ether) in 25% yield (0.79 g, 2.5 mmol). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.54 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.44-7.37 (m, 3H), 7.34-7.26 (m, 3H), 7.03 (t, *J* = 7.2 Hz, 2H), 4.92 (s, 2H), 2.20-1.96 (m, 2H), 1.36-1.23 (m, 2H), 1.18-1.07 (m, 2H), 0.77-0.61 (m, 2H), 0.49-0.36 (m, 2H), 0.11-0.01 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.6, 135.6, 131.9, 131.3, 128.7, 128.4, 126.4 122.6, 121.4, 111.2, 86.9, 84.3, 77.5, 18.4, 12.5, 2.0, -5.0. **HRMS (ESI, *m/z*)** calcd for $C_{21}H_{22}NaOSi$ $[M+Na]^+$: 341.1332, found: 341.1332.

1-phenyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)siletane (1o)



1o

$C_{24}H_{22}OSi$

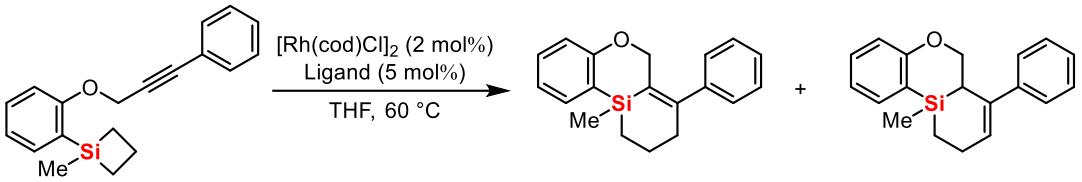
M = 354.52 g/mol

Following the **procedure D**, **1o** was obtained as a white solid (R_f = 0.2, petroleum ether) in 27% yield (0.95 g, 2.7 mmol). **M.P.** 78-80 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.70-7.64 (m, 2H), 7.49 (dd, *J* = 7.1, 1.8 Hz, 1H), 7.45-7.37 (m, 3H), 7.37-7.27 (m, 6H), 7.09-7.01 (m, 2H), 4.84 (s, 2H), 2.39-2.09 (m, 2H), 1.67-1.37 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.7, 137.6, 136.0, 134.4, 131.9, 131.7, 129.4, 128.7, 128.4, 127.8, 125.5, 122.6, 121.6, 111.5, 87.0, 84.2, 56.7, 18.6, 14.2. **HRMS (ESI, *m/z*)** calcd for $C_{24}H_{22}NaOSi$ $[M+Na]^+$: 377.1332, found: 377.1332.

3. Rhodium-Catalyzed Ring Expansion of Silacyclobutanes

3.1 Optimization of reaction conditions for the synthesis of silacycle 3a by Rh catalysis

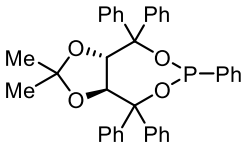
Table S1. Evaluation of ligand in the reaction[a]



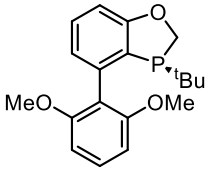
1a **3a** **4a**

Entry	Ligand	*Yield of* 3a+4a (%)[b]	3a:4a (%)[c]
1	L1	83	>99:1
2	L2	trace	-
3	L3	trace	-
4	L4	trace	-
5	L5	trace	-
6	L6	trace	-
7	L7	38	2:1
8	L8	18	10:1
9	L9	24	1:4
10	L10	43	10:1
11	L11	30	1:1
12	L12	25	1:10
13	L13	41	>25:1
14	L14	39	>25:1
15	L15	23	19:1
16	L16	28	10:1

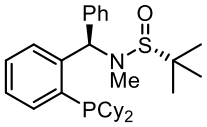
[a] All the reactions were carried out by using **1a** (0.1 mmol), $[Rh(cod)Cl]_2$ (2 mol%), Ligand (5 mol%) in THF (0.1 M) for 12 h under an N_2 atmosphere. [b] Isolated yield. [c] Determined by ^1H NMR analysis.



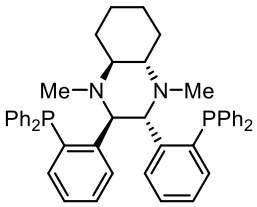
L1



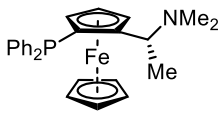
L2



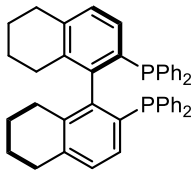
L3



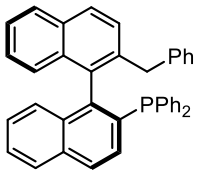
L4



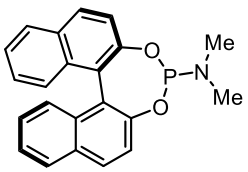
L5



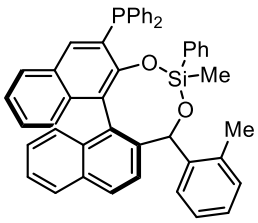
L6



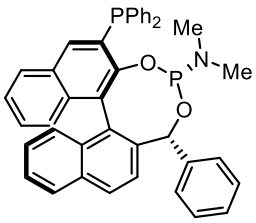
L7



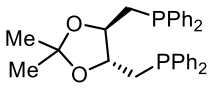
L8



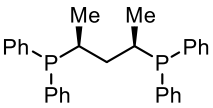
L9



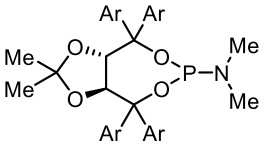
L10



L11

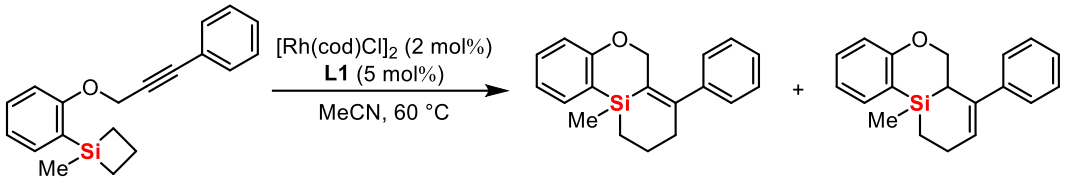


L12



L13, Ar = Ph
L14, Ar = 3,5-(^{t}Bu)$_2$C$_6$H$_3$
L15, Ar = 4-OMeC$_6$H$_4$
L16, Ar = 4-CF$_3$C$_6$H$_4$

Table S2. Evaluation of other conditions in the reaction[a]

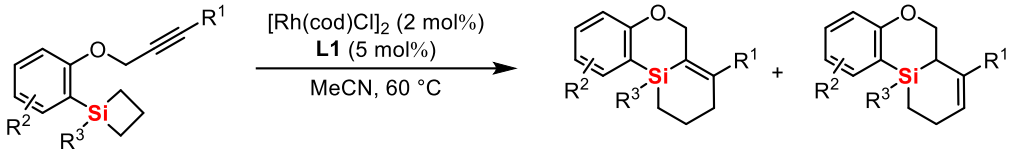


1a **3a** **4a**

Entry	variation from "standard conditions"[a]	*Yield of* 3a+4a (%)[b]	3a:4a (%)[c]
1	none	93	>99:1
2	$[Rh(OAc)_2]_2$ *instead of* $[Rh(cod)Cl]_2$	trace	-
3	$Rh(cod)BF_4$ *instead of* $[Rh(cod)Cl]_2$	trace	-
4	$[Rh(cod)OH]_2$ *instead of* $[Rh(cod)Cl]_2$	trace	-
5	THF *instead of* MeCN	83	>99:1
6	toluene *instead of* MeCN	83	>50:1
7	DCE *instead of* MeCN	68	>99:1
8	1,4-dioxane *instead of* MeCN	81	>15:1
9	40 °C *instead of* 60 °C	27	>99:1
10	Room temperature *instead of* 60 °C	trace	-

[a] All the reactions were carried out by using **1a** (0.1 mmol), $[Rh(cod)Cl]_2$ (2 mol%), **L1** (5 mol%) in solvent (0.1 M) for 12 h under an N_2 atmosphere, and for entries 2-4, with the solvent is THF. [b] Isolated yield. [c] Determined by crude ^1H NMR analysis.

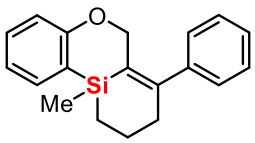
3.2 General Procedure IV for the Synthesis of Product 3



1 3 4

To a flame-dried Schlenk tube equipped with a septum and a magnetic stir bar, $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol, 2.0 mol%) and **L1** (2.9 mg, 0.005 mmol, 5.0 mol%) were added. The tube was evacuated under high vacuum and backfilled with nitrogen gas (3 times). MeCN (1.0 mL) was added to the tube, and then silacyclobutanes **1** (SCBs) (0.1 mmol, 1.0 equiv, 0.1 M) was successively added dropwise. The reaction tube was stirred at 60 ℃ for 6 h. After removing the solvent under vacuum, the residues were purified by flash chromatography on silica gel to yield the target product **3**.

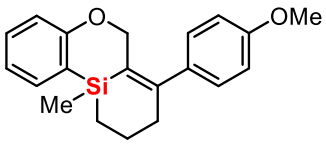
11-methyl-7-phenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3a)



3a
$C_{19}H_{20}OSi$
M = 292.45 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1a** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 93% yield (27.1 mg) as colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.39-7.33 (m, 3H), 7.30-7.25 (m, 2H), 7.22-7.17 (m, 2H), 6.97 (td, *J* = 7.2, 1.0 Hz, 1H), 6.86 (d, *J* = 8.3 Hz, 1H), 4.69 (d, *J* = 12.0 Hz, 1H), 4.49 (dt, *J* = 12.0, 1.6 Hz, 1H), 2.64-2.53 (m, 1H), 2.48-2.36 (m, 1H), 2.22-2.10 (m, 1H), 1.99-1.80 (m, 1H), 1.15-1.06 (m, 1H), 0.75 (td, *J* = 13.6, 3.6 Hz, 1H), 0.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 163.9, 155.4, 141.8, 134.9, 131.1, 128.3, 127.8, 127.3, 127.2, 121.9, 121.0, 118.2, 68.8, 37.1, 20.8, 9.3, -2.4. **HRMS (ESI, *m/z*)** calcd for $C_{19}H_{20}NaOSi$ $[M+Na]^+$: 315.1176, found: 315.1178.

7-(4-methoxyphenyl)-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3b)



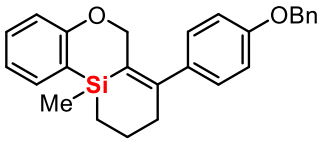
3b

$C_{20}H_{22}O_2Si$

M = 322.48 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1b** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 97% yield (31.3 mg) as pale yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.29 (dd, *J* = 7.2, 1.8 Hz, 1H), 7.23-7.17 (m, 1H), 7.10-7.05 (m, 2H), 6.89 (td, *J* = 7.2, 1.0 Hz, 1H), 6.84-6.76 (m, 3H), 4.66 (d, *J* = 11.9 Hz, 1H), 4.42 (dt, *J* = 11.9, 1.5 Hz, 1H), 3.74 (s, 3H), 2.57-2.46 (m, 1H), 2.37-2.26 (m, 1H), 2.13-2.02 (m, 1H), 1.87-1.73 (m, 1H), 1.05-0.96 (m, 1H), 0.65 (td, *J* = 13.6, 3.6 Hz, 1H), 0.37 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 163.9, 158.8, 155.0, 134.9, 134.1, 131.1, 129.0, 126.6, 121.9, 121.0, 118.2, 113.6, 68.8, 55.4, 37.2, 20.8, 9.3, -2.4. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{22}NaO_2Si$ $[M+Na]^+$: 345.1281, found: 345.1285.

7-(4-(benzyloxy)phenyl)-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxa siline (3c)



3c

$C_{26}H_{26}O_2Si$

M = 398.58 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1c** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 93% yield (37.0 mg) as white solid. **M.P.** 114-116 ℃. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.38-7.22 (m, 6H), 7.22-7.16 (m, 1H), 7.07 (d, *J* = 8.7 Hz, 2H), 6.91-6.85 (m, 3H), 6.78 (d, *J* = 8.4 Hz, 1H), 4.98 (s, 2H), 4.67 (d, *J* = 11.9 Hz, 1H), 4.41 (d, *J* = 11.8 Hz, 1H), 2.56-2.45 (m, 1H), 2.38-2.24 (m, 1H), 2.12-2.01 (m, 1H), 1.87-1.71 (m, 1H), 1.05-0.94 (m, 1H), 0.64 (td, *J* = 13.6, 3.6 Hz, 1H), 0.36 (s, 3H). **^{13}C NMR**

(100 MHz, $CDCl_3$) δ 163.9, 158.1, 155.0, 137.1, 134.9, 134.4, 131.1, 129.1, 128.7, 128.1, 127.6, 126.7, 121.9, 121.0, 118.2, 114.5, 70.1, 68.8, 37.2, 20.8, 9.3, -2.4. **HRMS (ESI, *m/z*)** calcd for $C_{26}H_{26}NaO_2Si$ $[M+Na]^+$: 421.1594, found: 421.1592.

7-(4-(*tert*-butyl)phenyl)-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3d)

3d
$C_{23}H_{28}OSi$
M = 348.56 g/mol

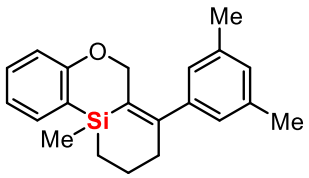
Following the **general procedure IV**, the reaction was carried out with SCBs **1d** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 88% yield (30.8 mg) as colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.40-7.33 (m, 3H), 7.32-7.22 (m, 1H), 7.17-7.10 (m, 2H), 6.96 (td, *J* = 7.2, 1.0 Hz, 1H), 6.86 (dd, *J* = 8.2, 1.0 Hz, 1H), 4.75 (d, *J* = 11.9 Hz, 1H), 4.49 (dt, *J* = 11.8, 1.5 Hz, 1H), 2.66-2.54 (m, 1H), 2.48-2.37 (m, 1H), 2.22-2.09 (m, 1H), 1.96-1.80 (m, 1H), 1.33 (s, 9H), 1.14-1.04 (m, 1H), 0.74 (td, *J* = 13.6, 3.6 Hz, 1H), 0.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 163.9, 155.5, 150.1, 138.8, 134.9, 131.1, 127.5, 126.8, 125.2, 121.9, 121.0, 118.2, 68.8, 37.1, 34.7, 31.5, 20.9, 9.3, -2.3. **HRMS (ESI, *m/z*)** calcd for $C_{23}H_{28}NaOSi$ $[M+Na]^+$: 371.1802, found: 371.1800.

7-([1,1'-biphenyl]-4-yl)-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3e)

3e
$C_{25}H_{24}OSi$
M = 368.55 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1e** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 82% yield (30.2 mg) as white solid. **M.P.** 101-103 ℃. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.63-7.57 (m, 4H), 7.48-7.42 (m, 2H), 7.40-7.34 (m, 2H), 7.31-7.26 (m, 3H), 6.98 (td, *J* = 7.2, 1.0 Hz, 1H), 6.87 (dd, *J* = 8.2, 1.0 Hz, 1H), 4.78 (d, *J* = 11.9 Hz, 1H), 4.53 (dt, *J* = 11.9, 1.5 Hz, 1H), 2.69-2.59 (m, 1H), 2.52-2.41 (m, 1H), 2.25-2.13 (m, 1H), 1.98-1.84 (m, 1H), 1.17-1.07 (m, 1H), 0.76 (td, *J* = 13.6, 3.6 Hz, 1H), 0.47 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 163.9, 155.0, 140.9, 140.7, 140.1, 134.9, 131.2, 128.9, 128.3, 127.5, 127.4, 127.2, 127.1, 121.9, 121.1, 118.2, 68.8, 37.1, 20.9, 9.3, -2.4. **HRMS (ESI, *m/z*)** calcd for $C_{25}H_{24}NaOSi$ $[M+Na]^+$: 391.1489, found: 391.1493.

7-(3,5-dimethylphenyl)-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3f)

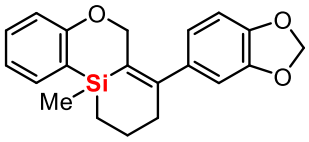


3f
$C_{21}H_{24}OSi$
M = 320.51 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1f** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 87% yield (27.8 mg) as pale yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.29 (dd, *J* = 7.2, 1.8 Hz, 1H), 7.22-7.16 (m, 1H), 6.89 (td, *J* = 7.2, 1.0 Hz, 1H), 6.84 (s, 1H), 6.78 (dd, *J* = 8.3, 1.0 Hz, 1H), 6.72 (s, 2H), 4.65 (d, *J* = 12.0 Hz, 1H), 4.42 (dt, *J* = 11.9, 1.6 Hz, 1H), 2.52-2.42 (m, 1H), 2.40-2.28 (m, 1H), 2.24 (s, 6H), 2.12-2.01 (m, 1H), 1.87-1.72 (m, 1H), 1.05-0.97 (m, 1H), 0.66 (td, *J* = 13.6, 3.6 Hz, 1H), 0.36 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 164.0, 155.7, 141.9, 137.7, 134.8, 131.1, 128.9, 126.7, 125.5, 122.0, 121.0, 118.3, 69.0, 37.2, 21.5, 20.9, 9.3, -2.3. **HRMS (ESI, *m/z*)** calcd for $C_{21}H_{24}NaOSi$ $[M+Na]^+$: 343.1489, found: 343.1492.

7-(benzo[*d*][1,3]dioxol-5-yl)-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]

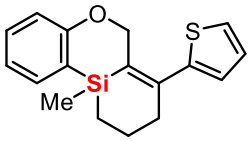
oxasiline (3g)



3g
$C_{20}H_{20}O_3Si$
M = 336.46 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1g** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 95% yield (31.8 mg) as pale yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.28 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.22-7.17 (m, 1H), 6.89 (td, *J* = 7.3, 1.0 Hz, 1H), 6.78 (dd, *J* = 8.3, 1.0 Hz, 1H), 6.72 (d, *J* = 7.9 Hz, 1H), 6.63 (d, *J* = 1.6 Hz, 1H), 6.59 (dd, *J* = 8.0, 1.7 Hz, 1H), 5.89-5.86 (m, 2H), 4.67 (d, *J* = 11.9 Hz, 1H), 4.40 (dt, *J* = 11.9, 1.5 Hz, 1H), 2.52-2.41 (m, 1H), 2.35-2.24 (m, 1H), 2.11-2.00 (m, 1H), 1.85-1.71 (m, 1H), 1.05-0.95 (m, 1H), 0.64 (td, *J* = 13.6, 3.6 Hz, 1H), 0.36 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 163.9, 154.9, 147.5, 146.7, 135.7, 134.8, 131.1, 127.2, 121.8, 121.2, 121.0, 118.2, 108.5, 108.2, 101.1, 68.7, 37.2, 20.8, 9.3, -2.4. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{20}NaO_3Si$ $[M+Na]^+$: 359.1074, found: 359.1077.

11-methyl-7-(thiophen-2-yl)-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3h)

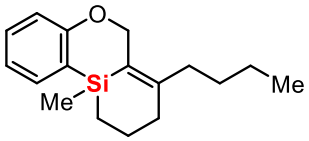


3h
$C_{17}H_{18}OSSi$
M = 298.48 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1h** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 87% yield (25.8 mg) as yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.36 (dd, *J* = 7.3, 1.8 Hz, 1H), 7.34-7.25 (m, 2H), 7.06-6.95 (m, 3H), 6.91 (dd, *J* = 8.3, 1.1 Hz, 1H), 5.06 (d, *J* = 12.6 Hz, 1H), 4.71 (dt, *J* = 12.6, 1.8 Hz, 1H), 2.74-2.62

(m, 1H), 2.58-2.45 (m, 1H), 2.24-2.10 (m, 1H), 1.98-1.82 (m, 1H), 1.15-1.04 (m, 1H), 0.76 (td, *J* = 13.6, 3.6 Hz, 1H), 0.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 163.8, 145.5, 143.1, 134.4, 131.2, 130.2, 126.9, 126.2, 125.1, 123.2, 121.6, 118.4, 69.9, 37.8, 20.8, 8.8, -2.5. **HRMS (ESI, *m/z*)** calcd for $C_{17}H_{18}NaOSSi$ $[M+Na]^+$: 321.0740, found: 321.0748.

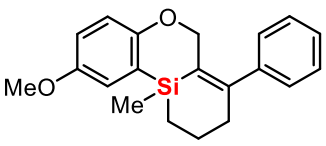
7-butyl-11-methyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3i)



3i
$C_{17}H_{24}OSi$
M = 272.46 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1i** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 83% yield (22.5 mg) as colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.33 (dd, *J* = 7.2, 1.8 Hz, 1H), 7.29-7.23 (m, 1H), 6.95 (td, *J* = 7.2, 1.0 Hz, 1H), 6.86 (dd, *J* = 8.2, 1.0 Hz, 1H), 4.99 (d, *J* = 12.3 Hz, 1H), 4.51 (d, *J* = 12.3 Hz, 1H), 2.34-2.21 (m, 2H), 2.18-1.94 (m, 3H), 1.81-1.66 (m, 1H), 1.48-1.27 (m, 4H), 1.04-0.93 (m, 1H), 0.91 (t, *J* = 6.9 Hz, 3H), 0.68-0.59 (m, 1H), 0.36 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 163.9, 155.8, 134.6, 130.9, 124.5, 123.0, 121.1, 118.2, 68.2, 35.1, 33.5, 31.4, 23.0, 20.8, 14.2, 9.4, -2.2. **HRMS (ESI, *m/z*)** calcd for $C_{17}H_{24}NaOSi$ $[M+Na]^+$: 295.1489, found: 295.1485.

2-methoxy-11-methyl-7-phenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3j)

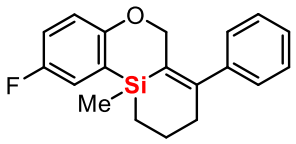


3j
$C_{20}H_{22}O_2Si$
M = 322.48 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1j** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃

for 6 h. The title compound was obtained in 84% yield (27.2 mg) as colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.37-7.31 (m, 2H), 7.29-7.26 (m, 1H), 7.21-7.15 (m, 2H), 6.89-6.79 (m, 3H), 4.61 (d, *J* = 12.2 Hz, 1H), 4.49 (dt, *J* = 12.1, 1.6 Hz, 1H), 3.78 (s, 3H), 2.62-2.51 (m, 1H), 2.49-2.37 (m, 1H), 2.21-2.10 (m, 1H), 1.96-1.81 (m, 1H), 1.16-1.04 (m, 1H), 0.83-0.73 (m, 1H), 0.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 157.9, 154.8, 154.0, 142.0, 128.3, 127.8, 127.7, 127.2, 123.6, 119.2, 118.5, 117.1, 69.5, 55.9, 37.1, 20.8, 9.1, -2.4. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{22}NaO_2Si$ $[M+Na]^+$: 345.1281, found: 345.1277.

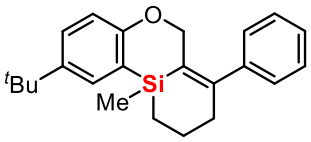
2-fluoro-11-methyl-7-phenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3k)



3k
$C_{19}H_{19}FOSi$
M = 310.44 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1k** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 78% yield (24.2 mg) as white solid. **M.P.** 89-91 ℃. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.36 (t, *J* = 7.3 Hz, 2H), 7.29 (d, *J* = 7.1 Hz, 1H), 7.18 (d, *J* = 7.0 Hz, 2H), 7.02 (dd, *J* = 7.9, 3.1 Hz, 1H), 6.95 (td, *J* = 8.6, 3.1 Hz, 1H), 6.80 (dd, *J* = 9.0, 4.3 Hz, 1H), 4.64 (d, *J* = 12.0 Hz, 1H), 4.48 (dt, *J* = 12.2, 1.6 Hz, 1H), 2.64-2.53 (m, 1H), 2.50-2.37 (m, 1H), 2.23-2.12 (m, 1H), 1.98-1.81 (m, 1H), 1.17-1.05 (m, 1H), 0.76 (td, *J* = 13.6, 3.6 Hz, 1H), 0.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 159.8, 157.6 (d, *J* = 240.1 Hz), 155.6, 141.8, 128.4, 127.7, 127.3, 126.9, 124.0 (d, *J* = 4.1 Hz), 119.7 (d, *J* = 3.5 Hz), 119.6 (d, *J* = 9.2 Hz), 117.9 (d, *J* = 22.9 Hz), 69.4, 37.1, 20.8, 9.0, -2.5. **^{19}F NMR (471 MHz, $CDCl_3$)** ***δ*** -123.9 (s). **HRMS (ESI, *m/z*)** calcd for $C_{19}H_{19}NaFOSi$ $[M+Na]^+$: 333.1081, found: 333.1081.

2-(*tert*-butyl)-11-methyl-7-phenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3l)



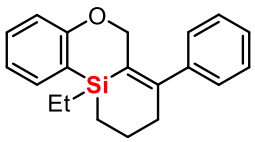
3l

$C_{23}H_{28}OSi$

M = 348.56 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1l** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 76% yield (26.5 mg) as yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$) *δ*** 7.37-7.31 (m, 4H), 7.30-7.26 (m, 1H), 7.21-7.16 (m, 2H), 6.82 (dd, *J* = 7.8, 1.1 Hz, 1H), 4.66 (d, *J* = 11.9 Hz, 1H), 4.48 (dt, *J* = 11.9, 1.6 Hz, 1H), 2.65-2.54 (m, 1H), 2.47-2.35 (m, 1H), 2.24-2.12 (m, 1H), 1.97-1.83 (m, 1H), 1.31 (s, 9H), 1.17-1.07 (m, 1H), 0.77 (td, *J* = 13.7, 3.6 Hz, 1H), 0.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) *δ*** 161.8, 155.2, 143.3, 141.9, 130.9, 128.6, 128.3, 127.8, 127.5, 127.2, 121.1, 117.7, 68.8, 37.1, 34.3, 31., 20.9, 9.4, -2.2. **HRMS (ESI, *m/z*)** calcd for $C_{23}H_{28}NaOSi$ $[M+Na]^+$: 371.1802, found: 371.1799.

11-ethyl-7-phenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3m)



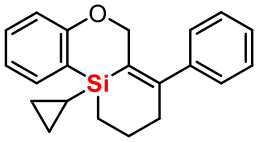
3m

$C_{20}H_{22}OSi$

M = 306.48 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1m** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 82% yield (25.1 mg) as yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$) *δ*** 7.39-7.32 (m, 3H), 7.31-7.25 (m, 2H), 7.21-7.17 (m, 2H), 6.97 (td, *J* = 7.2, 1.1 Hz, 1H), 6.86 (dd, *J* = 8.3, 1.0 Hz, 1H), 4.70 (d, *J* = 12.0 Hz, 1H), 4.52 (dt, *J* = 12.0, 1.6 Hz, 1H), 2.63-2.51 (m, 1H), 2.48-2.35 (m, 1H), 2.16-2.03 (m, 1H), 1.98-1.84 (m, 1H), 1.19-1.08 (m, 4H), 1.02-0.94 (m, 2H), 0.81-0.68 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$) *δ*** 164.1, 155.8, 142.0, 135.1, 131.1, 128.3, 127.8, 127.2, 126.9, 121.1, 120.9, 118.2, 77.5, 77.2, 76.8, 69.4, 37.1, 21.3, 8.2, 7.7, 6.6. **HRMS (ESI, *m/z*)** calcd for $C_{20}H_{22}NaOSi$ $[M+Na]^+$: 329.1332, found: 329.1333.

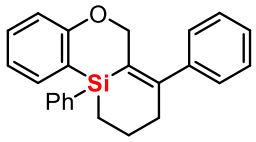
11-cyclopropyl-7-phenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3n)



3n
$C_{21}H_{22}OSi$
M = 318.49 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1n** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 82% yield (26.0 mg) as yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.38-7.26 (m, 5H), 7.22-7.17 (m, 2H), 6.95 (td, *J* = 7.2, 1.0 Hz, 1H), 6.85 (dd, *J* = 8.2, 1.0 Hz, 1H), 4.70 (d, *J* = 12.0 Hz, 1H), 4.58 (dt, *J* = 12.1, 1.6 Hz, 1H), 2.63-2.52 (m, 1H), 2.46-2.35 (m, 1H), 2.19-2.07 (m, 1H), 2.02-1.88 (m, 1H), 1.18-1.06 (m, 1H), 0.80-0.63 (m, 3H), 0.49-0.36 (m, 2H), -0.02--0.13 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** ***δ*** 164.1, 155.7, 141.9, 135.2, 131.2, 128.3, 127.8, 127.3, 126.8, 120.8, 119.9, 118.3, 69.3, 37.1, 21.4, 7.6, 2.1, 1.7, -6.2. **HRMS (ESI, *m/z*)** calcd for $C_{21}H_{22}NaOSi$ $[M+Na]^+$: 341.1332, found: 341.1330.

7,11-diphenyl-8,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (3o)



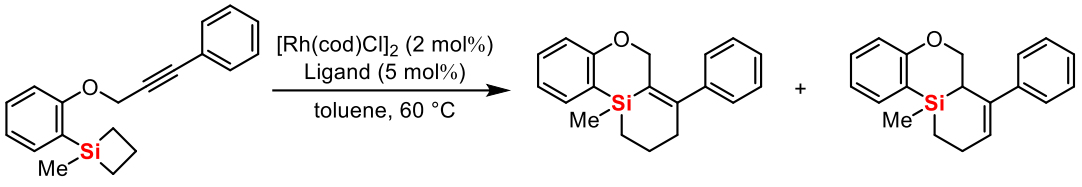
3o
$C_{24}H_{22}OSi$
M = 354.52 g/mol

Following the **general procedure IV**, the reaction was carried out with SCBs **1o** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **L1** (2.9 mg, 0.005 mmol) and MeCN (1.0 mL) at 60 ℃ for 6 h. The title compound was obtained in 86% yield (30.3 mg) as yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** ***δ*** 7.73-7.68 (m, 2H), 7.45 (dd, *J* = 7.2, 1.8 Hz, 1H), 7.41-7.27 (m, 7H), 7.23-7.20 (m, 2H), 6.99 (td, *J* = 7.3, 1.1 Hz, 1H), 6.90 (dd, *J* = 8.4, 1.0 Hz, 1H), 4.75 (d, *J* = 12.1 Hz, 1H), 4.59 (dt, *J* = 12.0, 1.5 Hz, 1H), 2.72-2.61 (m, 1H), 2.59-2.45 (m, 1H), 2.25-2.14 (m, 1H), 2.13-1.93 (m, 1H), 1.53-1.46 (m, 1H), 1.08-0.91 (m, 1H). **^{13}C NMR (100 MHz,**

$CDCl_3$) δ 164.3, 156.6, 141.8, 136.1, 135.5, 135.1, 131.5, 129.7, 128.4, 128.2, 127.8, 127.4, 125.9, 121.2, 119.8, 118.4, 69.0, 37.1, 21.4, 8.5. **HRMS (ESI, *m/z*)** calcd for $C_{24}H_{22}NaOSi$ $[M+Na]^+$: 377.1332, found: 377.1334.

4.5 Optimization of reaction conditions for the synthesis of silacycle 4a by Rh catalysis

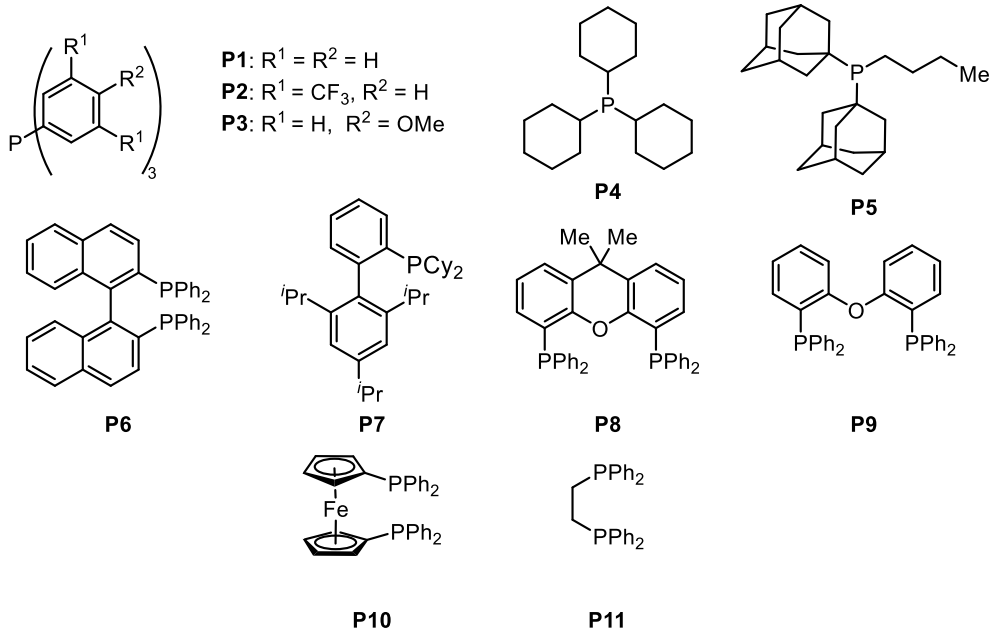
Table S3. Evaluation of ligand in the reaction[a]



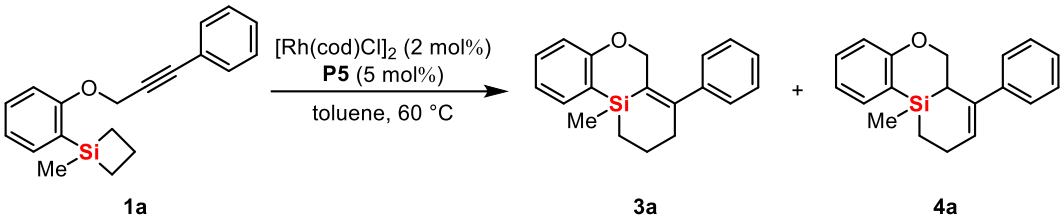
1a **3a** **4a**

Entry	Ligand	*Yield of* 3a+4a (%)[b]	3a:4a (%)[c]
1	P1	75	4:1
2	P2	37	1:3
3	P3	54	2:1
4	P4	31	1:2
5	P5	53	1:10
6	P6	46	7:1
7	P7	trace	-
8	P8	trace	-
9	P9	trace	-
10	P10	62	2:3
11	P11	35	3:2

[a] All the reactions were carried out by using **1a** (0.1 mmol), $[Rh(cod)Cl]_2$ (2 mol%), Ligand (5 mol%) in toluene (0.1 M) for 12 h under an N_2 atmosphere. [b] Isolated yield. [c] Determined by ^1H NMR analysis.

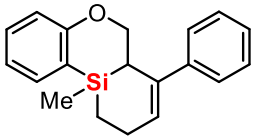


4.6 General Procedure VII for the Synthesis of Product 4a



To a flame-dried Schlenk tube equipped with a septum and a magnetic stir bar, $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol, 2.0 mol%) and **P5** (1.8 mg, 0.005 mmol, 5.0 mol%) were added. The tube was evacuated under high vacuum and backfilled with nitrogen gas (3 times). Toluene (1.0 mL) was added to the tube, and then silacyclobutanes **1a** (SCBs) (0.1 mmol, 1.0 equiv, 0.1 M) was successively added dropwise. The reaction tube was stirred at 60 °C for 12 h. After removing the solvent under vacuum, the residues were purified by flash chromatography on silica gel to yield the target product **4a**.

11-methyl-7-phenyl-6a,9,10,11-tetrahydro-6*H*-benzo[*b*]silino[1,2-*d*][1,4]oxasiline (4a)



4a

$C_{19}H_{20}OSi$

M = 292.45 g/mol

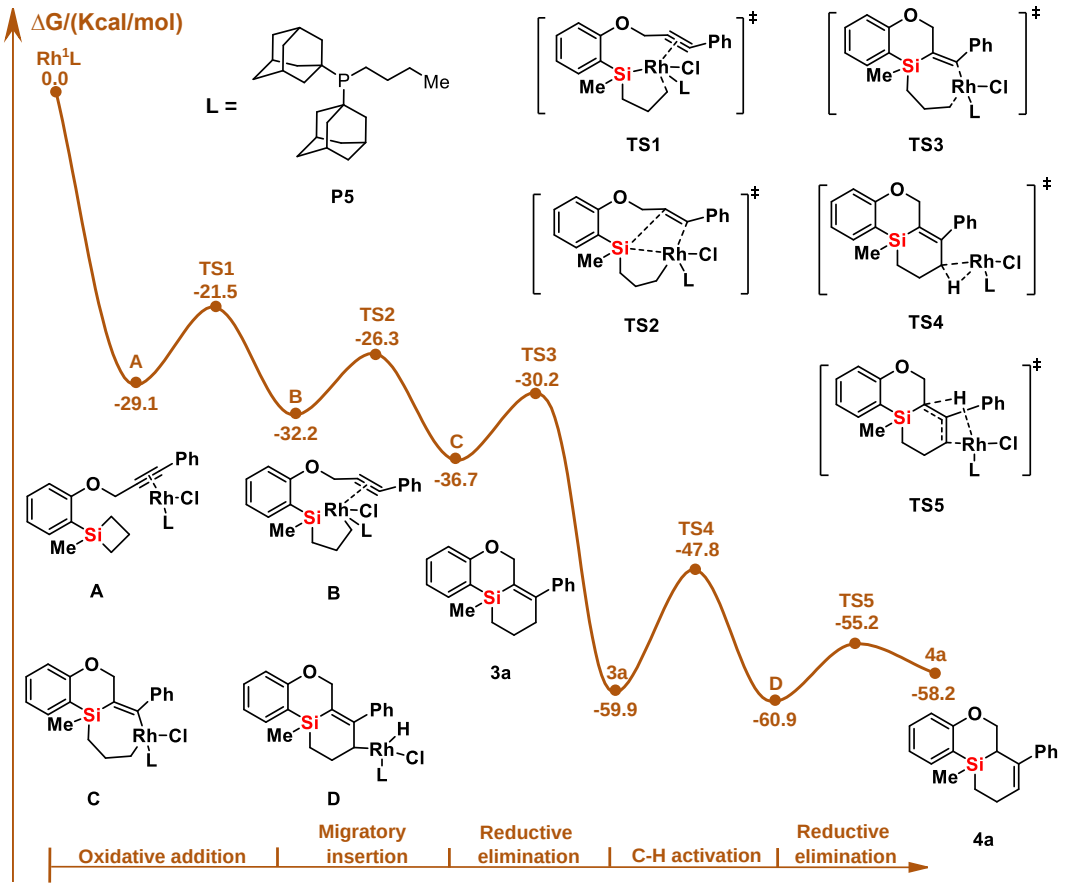
Following the **general procedure VII**, the reaction was carried out with SCBs **1a** (0.1 mmol), $[Rh(cod)Cl]_2$ (1.0 mg, 0.002 mmol), **P5** (1.8 mg, 0.005 mmol) and toluene (1.0 mL) at 60 ℃ for 12 h. The title compound was obtained in 53% yield (15.6 mg, **3a:4a** = 1:10) as pale yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.38-7.31 (m, 3H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.21-7.14 (m, 2H), 6.93 (td, *J* = 7.3, 1.0 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 6.11 (dd, *J* = 6.2, 4.1 Hz, 1H), 4.19 (dd, *J* = 11.5, 4.6 Hz, 1H), 3.90 (dd, *J* = 11.6, 9.3 Hz, 2H), 2.46-2.32 (m, 2H), 2.25-2.09 (m, 1H), 1.05-0.94 (m, 1H), 0.88-0.74 (m, 1H), 0.31 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$) δ** 165.3, 143.6, 137.6, 135.1, 131.8, 131.1, 128.5, 126.9, 126.3, 121.6, 120.0, 117.7, 70.1, 25.0, 22.4, 8.8, -3.5. **HRMS (ESI, *m/z*)** calcd for $C_{19}H_{20}NaOSi$ $[M+Na]^+$: 315.1176, found: 315.1176.

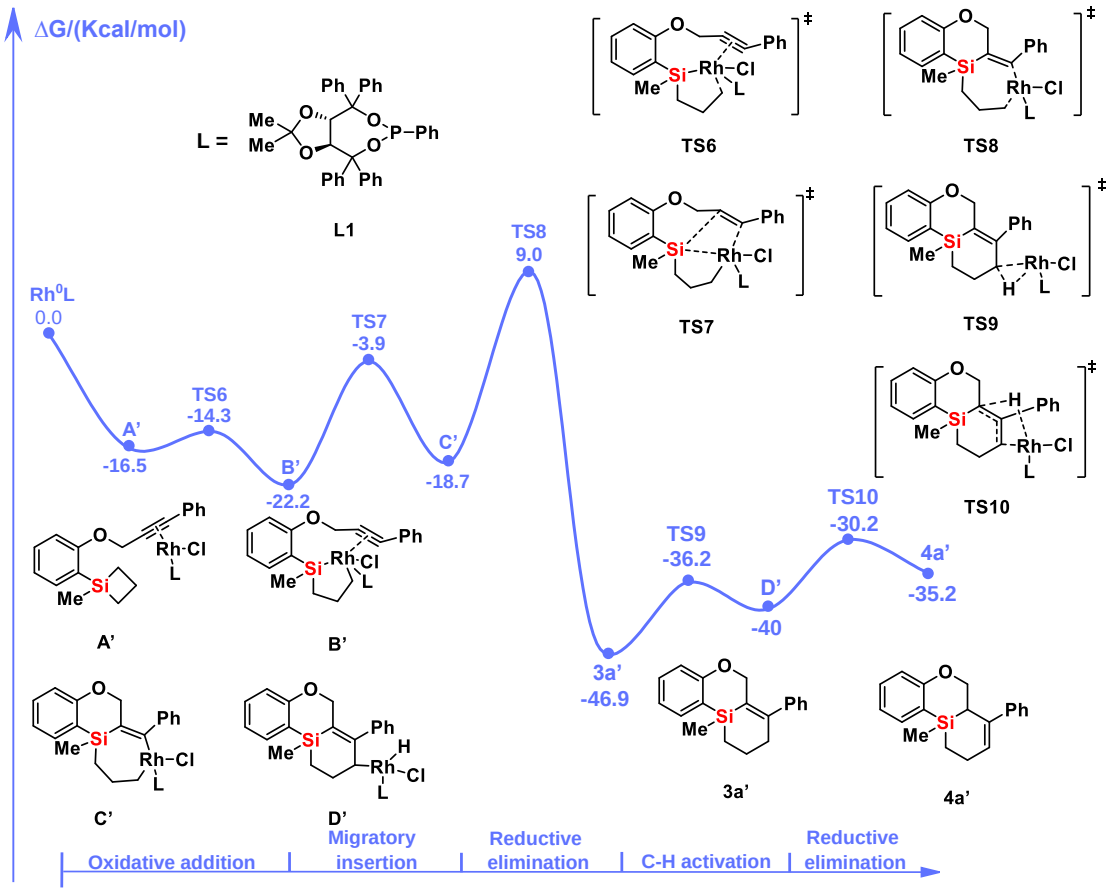
4. DFT Studies

4.1 Computational methods

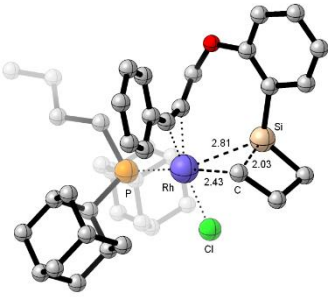
All calculations were performed with the Gaussian 16 suites of programs. Geometry optimization for all stationary points along the reaction paths without any symmetry constraints was conducted with the M06L functional. The standard 6-31G(d,p) basis was emplolyed for the C, H, O, P, and Si atoms, whereas the SDD valence basis set in combination with the corresponding effective core potential were used for the Rh atom. The connectivity of the stationary points was verified by IRC runs or the vibrational mode of the imaginary frequencies. Optimized structures are illustrated using CYL view.

4.2 Energy profiles and energy parameters of Rh-catalyzed Intramolecular reaction of 1a.

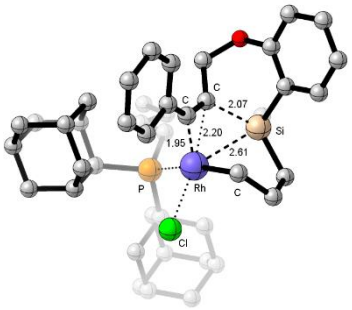




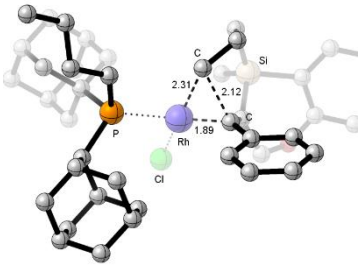
L = P5



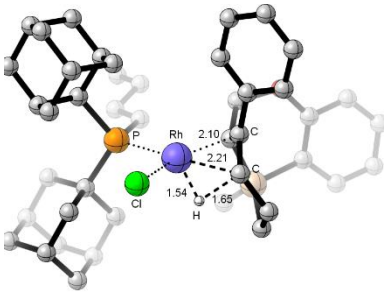
TS1



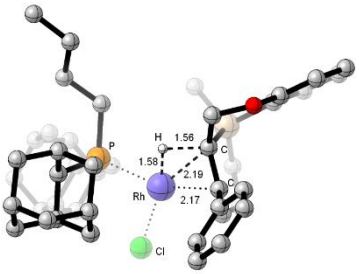
TS2



TS3

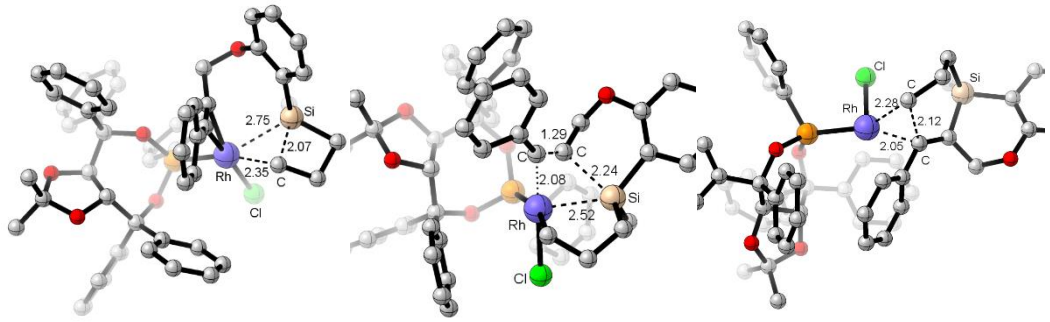


TS4

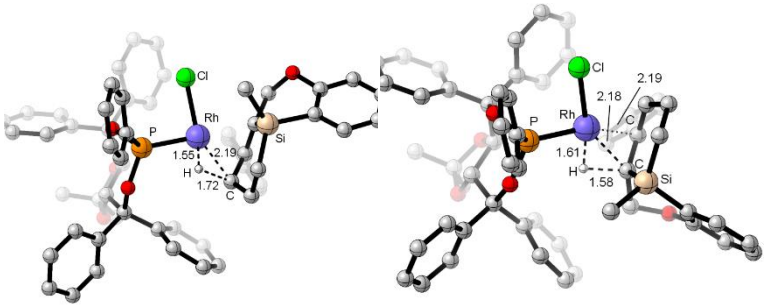


TS5

L = L1



TS6 TS7 TS8



TS9 TS10

Table S4 Energy Parameters (in kcal/mol) for Rh-**P5**-catalyzed Intramolecular reaction of **1a** calculated at M06L/6-31G(d,p)-SDD(Rh) level of theory.[a].

Structures[a]	ΔE[b]	ΔH[b]	ΔG[b]	ΔS[b][c]
Rh^0L	0.0	0.0	0.0	0.0
A	-47.0	-47.3	-29.1	-60.9
TS1	-41.6	-42.7	-21.5	-71.2
B	-52.5	-53.5	-32.2	-71.5
TS2	-46.7	-48.0	-26.3	-72.7
C	-55.9	-56.8	-36.7	-67.5
TS3	-50.3	-51.5	-30.2	-71.4
3a	-80.9	-82.3	-59.9	-75.0
TS4	-68.7	-70.2	-47.8	-74.9
D	-82.1	-83.4	-60.9	-75.3
TS5	-76.7	-78.2	-55.2	-77.1
4a	-78.6	-80.0	-58.2	-73.2

[a] Relative activation energy and reaction parameters were calculated based on those of **Rh^0L**. [b] Parameters for all the transition state (TSs) should read as those with double dagger like $\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$, and $\Delta G^{\neq}$. [c] in $cal.mol^{-1}.K^{-1}$.

Table S5 Electronic energies, enthalpies, free energies and imaginary frequencies calculated at M06L/6-31G(d,p)-SDD(Rh) level of theory.

Structures	ΔE	ΔH	ΔG
Rh^0L	-1849.872271	-1849.845477	-1849.928675
R	-1100.501899	-1100.48008	-1100.556702
A	-2950.44901	-2950.400857	-2950.531721
TS1	-2950.440399	-2950.393643	-2950.519638
B	-2950.457879	-2950.410756	-2950.536618
TS2	-2950.448641	-2950.401975	-2950.52725
C	-2950.463288	-2950.416071	-2950.54383
TS3	-2950.454278	-2950.407649	-2950.533563
3a	-2950.503101	-2950.456674	-2950.580854
TS4	-2950.483669	-2950.43738	-2950.5616
D	-2950.504967	-2950.458435	-2950.582488
TS5	-2950.496379	-2950.450208	-2950.573408
4a	-2950.499496	-2950.453036	-2950.578089

Table S6 Energy Parameters (in kcal/mol) for Rh-**L1**-catalyzed Intramolecular reaction of **1a** calculated at M06L/6-31G(d,p)-SDD(Rh) level of theory.[a].

Structures[a]	ΔE[b]	ΔH[b]	ΔG[b]	ΔS[b][c]
Rh^0L	0.0	0.0	0.0	0.0
A'	-35.7	-35.4	-16.5	-63.3
TS6	-34.9	-35.3	-14.3	-70.3
B'	-42.4	-42.4	-22.2	-67.6
TS7	-24.6	-24.9	-3.9	-70.3
C'	-39.3	-39.5	-18.7	-69.9
TS8	-11.5	-12.1	9.0	-70.7
3a	-67.7	-68.2	-46.9	-71.4

TS9	-56.5	-57.0	-36.2	-69.7
D'	-59.8	-60.1	-40.0	-67.5
TS10	-51.4	-52.0	-30.2	-73.3
4a'	-55.1	-55.5	-35.2	-68.0

[a] Relative activation energy and reaction parameters were calculated based on those of **Rh^0L**. [b] Parameters for all the transition state (TSs) should read as those with double dagger like $\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$, and $\Delta G^{\neq}$. [c] in $cal.mol^{-1}.K^{-1}$.

Table S7 Electronic energies, enthalpies, free energies and imaginary frequencies calculated at M06L/6-31G(d,p)-SDD(Rh) level of theory.

Structures	ΔE	ΔH	ΔG
Rh^0L	-2642.560583	-2642.521289	-2642.632265
R	-1100.501899	-1100.48008	-1100.556702
A'	-3743.119342	-3743.058755	-3743.215332
TS6	-3743.118116	-3743.05854	-3743.211814
B'	-3743.130037	-3743.069821	-3743.224366
TS7	-3743.101612	-3743.041972	-3743.195247
C'	-3743.125137	-3743.0653	-3743.218756
TS8	-3743.080829	-3743.021543	-3743.17461
3a'	-3743.17039	-3743.111057	-3743.263781
TS9	-3743.152476	-3743.093072	-3743.246602
D'	-3743.157828	-3743.098092	-3743.252664
TS10	-3743.144351	-3743.085219	-3743.237039
4a'	-3743.150268	-3743.090711	-3743.245068

4.3 Cartesian Coordinates of the Stationary Points

L=P5

Rh-P5

C	-2.86595600	0.41805000	0.87898500
H	-2.50907100	1.12332800	1.64043000
H	-3.02619900	-0.54387000	1.37742400
C	-1.80424800	0.27276000	-0.24003100

C	-4.20272900	0.90702800	0.29033700
H	-4.93543200	0.99461700	1.10142600
C	-4.00472200	2.27608500	-0.38228300
H	-3.66839200	3.01445800	0.35593500
H	-4.95770900	2.63661700	-0.78868000
C	-1.62911600	1.66014500	-0.91335300
H	-0.87309900	1.60919600	-1.70334600
H	-1.25905800	2.38137200	-0.17273000
C	-2.96445400	2.14371700	-1.50738900
H	-2.80825700	3.11800900	-1.98489300
C	-3.45703000	1.12483200	-2.55137600
H	-4.39890200	1.46767300	-2.99697700
H	-2.72788500	1.03876700	-3.36717400
C	-2.31957300	-0.73400000	-1.29332400
H	-2.45174400	-1.72468600	-0.84592800
H	-1.59064200	-0.84457600	-2.10318600
C	-4.69899300	-0.11380100	-0.74967300
H	-4.86247000	-1.08885500	-0.27279200
H	-5.66312400	0.20776200	-1.16213900
C	-3.66050000	-0.24472100	-1.87840400
H	-4.01009100	-0.97310300	-2.62001500
P	-0.15597800	-0.18104000	0.54876200
C	0.82342400	-1.15850000	-0.71137500
H	0.18174000	-1.97870800	-1.05493400
C	2.09911300	-1.76999400	-0.07338700
C	1.24705600	-0.32176300	-1.94489500
H	1.83179800	-2.35301100	0.81385000
C	3.10490700	-0.66881600	0.31185400
C	2.76059600	-2.70922000	-1.10410400
H	0.36766600	0.13714400	-2.40499100

C	2.25683200	0.77158100	-1.55382300
C	1.90963200	-1.26450600	-2.97212500
H	3.98669600	-1.11708600	0.78425000
H	2.67442600	0.01467800	1.08192700
C	3.50868700	0.13915600	-0.92963800
H	2.06702000	-3.51573000	-1.37326400
H	3.64408400	-3.18099500	-0.65689000
C	3.16361800	-1.91048900	-2.35655900
H	1.80171400	1.50077100	-0.84096200
H	2.52366400	1.36665000	-2.43502600
H	1.19626200	-2.03772600	-3.28386100
H	2.18037700	-0.69612200	-3.87026100
H	4.21173200	0.92656200	-0.64136100
C	4.16238800	-0.80748000	-1.95880500
H	3.62701200	-2.58332800	-3.08778700
H	4.47104000	-0.24024000	-2.84522100
H	5.06854800	-1.25456600	-1.53251100
C	-0.50902900	-1.43250000	1.87448600
H	-1.14808900	-0.93037600	2.60808300
H	0.45194600	-1.58142600	2.38004700
C	-1.10667500	-2.78744800	1.47879800
H	-2.09800200	-2.64414100	1.03443400
H	-0.48937700	-3.25981800	0.70487300
C	-1.22679700	-3.74069600	2.67319000
H	-1.84159400	-3.26837200	3.45047100
H	-0.23321200	-3.88696500	3.11691600
C	-1.82707400	-5.09500300	2.29007300
H	-1.90152800	-5.75891200	3.15664300
H	-2.83336300	-4.97667000	1.87280900
H	-1.21314800	-5.59896500	1.53515900

Rh	1.10742500	1.55776200	1.20907500
Cl	2.42141600	3.37590800	1.90161200

R

C	4.24972000	-0.51115600	0.25849000
C	2.87707500	-0.25052000	0.20986300
C	2.02101600	-1.32844600	-0.08990700
C	2.51184600	-2.61261800	-0.33103400
C	3.89182200	-2.83257500	-0.27066100
C	4.76467900	-1.78991500	0.02264100
H	4.93213500	0.30257500	0.48632600
H	1.84918900	-3.43682700	-0.56557400
H	4.27615600	-3.83078300	-0.45817600
H	5.83452500	-1.96655600	0.06726600
C	3.46939900	2.81424600	0.32993500
C	1.59335100	2.31464400	-1.09603200
C	3.02761400	2.93353700	-1.16609400
H	4.53312600	2.62896300	0.49771700
H	3.19193300	3.71294200	0.89273700
H	1.28013000	1.73033700	-1.96332100
H	0.83753600	3.08514300	-0.90668000
H	3.67050800	2.30402600	-1.79034400
H	3.06898900	3.94973400	-1.57485200
C	1.01064400	1.45548500	2.01212000
H	0.17161300	0.77524100	1.84188300
H	1.54658800	1.12194200	2.90704600
H	0.61342200	2.45687800	2.20613000
C	-0.26305100	-2.03029600	-0.36418300
H	-0.09770800	-2.47217900	-1.35771700
H	-0.14027700	-2.83192500	0.37842900

C	-1.59894700	-1.46108500	-0.27521700
C	-2.71245200	-0.99158700	-0.19818500
C	-4.02363600	-0.43435400	-0.11257900
C	-4.51722200	0.38389200	-1.14513000
C	-4.83762800	-0.69394300	1.00504800
C	-5.79500700	0.92780200	-1.05757900
H	-3.88783400	0.58485700	-2.00522800
C	-6.11514800	-0.14791300	1.08330900
H	-4.45541600	-1.32291600	1.80174500
C	-6.59707400	0.66353600	0.05435500
H	-6.16661600	1.55921300	-1.85857700
H	-6.73604300	-0.35421200	1.94952100
H	-7.59366700	1.08896800	0.11912600
O	0.69026400	-0.99503000	-0.12640800
Si	2.14339900	1.45874400	0.50920300

A

C	-6.39303800	-0.75956000	-0.15459400
C	-5.06283400	-0.40434800	0.16482400
C	-4.82573900	-0.04430100	1.50817900
C	-5.86493500	-0.00714200	2.44658600
C	-7.16205400	-0.34973000	2.08474600
C	-7.42974300	-0.74439300	0.77382200
H	-6.62366300	-1.03692900	-1.17990800
H	-5.62081400	0.29052300	3.46081700
H	-7.95541100	-0.31764100	2.82567800
H	-8.43488900	-1.02319800	0.47355900
C	-4.82839100	0.03519100	-2.96254300
C	-2.96426400	1.11187000	-1.89325800
C	-3.58616000	0.91683700	-3.30771500

H	-5.71222700	0.65338500	-2.77496200
H	-5.08669800	-0.72100900	-3.70801800
H	-3.81791100	1.85166800	-3.83009100
H	-2.88005800	0.35493100	-3.92706800
C	-3.06435000	-2.11143400	-1.53556100
H	-2.46422900	-2.38670600	-0.66604300
H	-3.82142800	-2.88993900	-1.68528800
H	-2.39674000	-2.08866100	-2.40148400
C	-2.43182200	-0.37060600	1.66699400
H	-1.95119700	-0.68357500	2.60545300
H	-2.68893700	-1.27812100	1.11568300
C	-1.50911900	0.48796300	0.89599400
C	-1.00544900	1.62880700	0.64178500
C	-0.73394200	3.01838900	0.89382000
C	-0.74823400	3.51809700	2.21002900
C	-0.41640800	3.89052900	-0.16325100
C	-0.43989300	4.85307900	2.45827600
H	-1.00194800	2.84784700	3.02523600
C	-0.11493900	5.22490300	0.09094500
H	-0.39827900	3.49960700	-1.17459100
C	-0.11944700	5.70903000	1.40165200
H	-0.44928700	5.22740500	3.47761100
H	0.12930800	5.88797800	-0.73338600
H	0.12299300	6.74878600	1.59869400
O	-3.61113300	0.34870500	2.02757500
Si	-3.92823900	-0.44843400	-1.35601200
C	0.33105700	-2.91136400	0.29665200
H	-0.33304800	-2.51623200	-0.47553700
H	-0.10441500	-2.64402500	1.26873400
C	1.72584000	-2.25895400	0.14118000

C	0.43501500	-4.44176900	0.17485100
H	-0.56622700	-4.87413700	0.29139600
C	0.99689900	-4.79699300	-1.21306000
H	0.33089900	-4.41467300	-1.99529100
H	1.04948700	-5.88672700	-1.33040400
C	2.30396300	-2.64724600	-1.24157400
H	3.30537300	-2.21921500	-1.36409900
H	1.67294800	-2.24476600	-2.03547500
C	2.39786000	-4.17950200	-1.36907100
H	2.79840500	-4.42172000	-2.36045900
C	3.33269700	-4.72979800	-0.27974700
H	3.42612700	-5.81934200	-0.36950100
H	4.33946700	-4.30888800	-0.39889100
C	2.65752200	-2.82929500	1.23566600
H	2.26590000	-2.59663700	2.22873900
H	3.65678300	-2.38278600	1.16079400
C	1.36932500	-4.98602800	1.26902900
H	0.96719300	-4.74772800	2.26255400
H	1.43547900	-6.07899400	1.20220500
C	2.76667000	-4.36284200	1.10168300
H	3.43411000	-4.73396700	1.88922600
P	1.49291900	-0.38322600	0.26296000
C	3.12250900	0.33112200	-0.33642200
H	3.81682300	-0.50931400	-0.20638500
C	3.70434300	1.52513600	0.46070000
C	3.10436800	0.70712900	-1.84301200
H	3.71720900	1.29867800	1.52536800
C	2.89705000	2.80887800	0.21565100
C	5.16071300	1.73886000	-0.00497200
H	2.64719500	-0.09369900	-2.42618100

C	2.30592900	2.00271200	-2.07330000
C	4.55999500	0.92646900	-2.29921100
H	3.32329500	3.62726200	0.80938000
H	1.86348000	2.68271400	0.54755600
C	2.92664800	3.16254000	-1.28094100
H	5.75334900	0.83560800	0.19032600
H	5.61113800	2.55097000	0.57969800
C	5.19115500	2.08402500	-1.50340800
H	1.26289100	1.85402300	-1.77025200
H	2.29060900	2.22624600	-3.14640500
H	5.14444700	0.00757000	-2.15829000
H	4.57353800	1.15341900	-3.37216100
H	2.34727300	4.07792000	-1.44781500
C	4.38228300	3.37478000	-1.73790800
H	6.22871400	2.23308300	-1.82634000
H	4.40519500	3.64388900	-2.80134700
H	4.83670500	4.20692600	-1.18459600
C	1.34463200	-0.02877900	2.08997700
H	0.53645600	-0.69912900	2.40252300
H	0.92058100	0.97370300	2.15572300
C	2.53286000	-0.15847900	3.06848300
H	3.36662400	-0.71823200	2.63803200
H	2.92381400	0.83985600	3.29036600
C	2.11599500	-0.81347600	4.39110000
H	1.71336400	-1.81526400	4.18938400
H	1.29018100	-0.23800500	4.83001500
C	3.26952700	-0.91433000	5.39010700
H	2.94912200	-1.38156500	6.32629600
H	4.09096500	-1.51328300	4.98117400
H	3.67074500	0.07629600	5.63104900

Rh	-0.38372200	0.25592100	-0.78398100
Cl	0.03875400	-0.65330100	-2.94509600
H	-3.34683100	1.99660000	-1.37335300
H	-1.86922500	1.22784700	-1.93380900

TS1

C	-5.54887600	-1.53554900	-0.54620900
C	-4.27837200	-1.49735600	0.08374600
C	-4.32401000	-1.29284400	1.48686800
C	-5.54477400	-1.13971300	2.16534900
C	-6.75656200	-1.18717600	1.49686900
C	-6.76066800	-1.38918900	0.11777700
H	-5.58799800	-1.68425900	-1.61681700
H	-5.49862600	-0.98327500	3.23781000
H	-7.68464800	-1.06583400	2.04743900
H	-7.69192900	-1.42996500	-0.43810000
C	-3.48501400	-1.88715700	-2.98896200
C	-2.61786100	0.15564500	-2.01003300
C	-3.01528100	-0.45556200	-3.36884400
H	-4.54544300	-2.06733900	-3.17219900
H	-2.93136400	-2.66496700	-3.52355300
H	-3.78683300	0.14194700	-3.86765900
H	-2.14012300	-0.49373800	-4.01911800
C	-1.80200100	-3.23628700	-0.90536500
H	-1.24081100	-3.31474700	0.02280500
H	-2.50858000	-4.07606500	-0.95598700
H	-1.10061700	-3.32300100	-1.73876500
C	-1.93421800	-1.33812700	1.94415700
H	-1.34112300	-1.27576000	2.86358700
H	-1.76729400	-2.32415600	1.50838100

C	-1.55646200	-0.25651000	1.01539700
C	-1.62863000	0.96026400	0.65771400
C	-2.15196600	2.28950100	0.81413100
C	-2.88061300	2.60342500	1.97979800
C	-1.98084800	3.27845300	-0.16913500
C	-3.40660700	3.87900200	2.15508300
H	-3.03650800	1.82899900	2.72431500
C	-2.50920600	4.55346600	0.01389500
H	-1.43131800	3.03461600	-1.07000400
C	-3.21931400	4.85997900	1.17631000
H	-3.96820900	4.10977100	3.05543300
H	-2.36682200	5.30881700	-0.75307400
H	-3.62995700	5.85498300	1.31773600
O	-3.27881700	-1.20726500	2.37693100
Si	-2.85556000	-1.68968500	-1.19538100
C	1.53482100	-2.75655500	0.35080400
H	0.80536000	-2.69516000	-0.45682700
H	0.98220300	-2.68407400	1.29768600
C	2.52097500	-1.57466300	0.21924900
C	2.28285400	-4.09953600	0.28617800
H	1.55575800	-4.91456800	0.38677400
C	2.99916400	-4.20569800	-1.07170600
H	2.26646800	-4.15697000	-1.88561900
H	3.51524400	-5.17082300	-1.15172400
C	3.26905600	-1.70327700	-1.13119600
H	4.00009100	-0.89370400	-1.23547300
H	2.56153900	-1.62190900	-1.95650000
C	4.00947600	-3.05272300	-1.20583300
H	4.51499800	-3.11770300	-2.17664700
C	5.04443100	-3.13560200	-0.07249300

H	5.59434500	-4.08376700	-0.12389200
H	5.78189500	-2.32899600	-0.17522900
C	3.56506600	-1.67588900	1.35563600
H	3.07683900	-1.61123700	2.33087300
H	4.28408000	-0.85007500	1.29073100
C	3.31371700	-4.17496000	1.42527800
H	2.80769100	-4.11199400	2.39773300
H	3.84022500	-5.13705100	1.39815800
C	4.31959300	-3.01967200	1.27807700
H	5.04840200	-3.05698300	2.09725100
P	1.49438000	0.02256700	0.29289400
C	2.69074300	1.33435900	-0.32955700
H	3.67008100	0.87365600	-0.14851700
C	2.69871700	2.69817400	0.40350600
C	2.56405100	1.59800500	-1.85474900
H	2.76944400	2.54855600	1.47883500
C	1.43895300	3.51470800	0.08164700
C	3.94839700	3.47719300	-0.05949800
H	2.49714800	0.65420000	-2.39761600
C	1.30861800	2.43183000	-2.16504400
C	3.81057600	2.38149300	-2.31110400
H	1.46503000	4.46245100	0.63398500
H	0.54494300	2.97967300	0.41340300
C	1.36614300	3.78018500	-1.43198000
H	4.85579700	2.91276700	0.19163300
H	4.00272700	4.43001900	0.48226600
C	3.87985700	3.73222300	-1.57459900
H	0.41462300	1.87436500	-1.86193000
H	1.23347900	2.57816200	-3.24897200
H	4.71847200	1.79617000	-2.11460400

H	3.76222400	2.54382700	-3.39481900
H	0.46752500	4.36701700	-1.65776100
C	2.61628100	4.55703300	-1.88691100
H	4.77102400	4.28450900	-1.89677300
H	2.55757900	4.76184800	-2.96320800
H	2.66651300	5.52722900	-1.37596200
C	1.24204000	0.30708700	2.12167600
H	0.85821600	-0.66207200	2.46029000
H	0.39366700	0.98841300	2.19591400
C	2.36332000	0.76971800	3.07679700
H	3.35979800	0.60342500	2.66069800
H	2.27757900	1.84957500	3.23453600
C	2.26615600	0.08096100	4.44377300
H	2.35076000	-1.00593200	4.30990600
H	1.26676700	0.25817400	4.86307300
C	3.33522000	0.56235800	5.42584600
H	3.24609500	0.05925500	6.39354300
H	4.34098700	0.36573900	5.03790800
H	3.25326500	1.64077100	5.60100200
Rh	-0.55491100	-0.14256600	-0.77105700
Cl	0.35407600	-1.00933700	-2.81720100
H	-3.45156300	0.63906700	-1.48972100
H	-1.84637500	0.93141000	-2.10420600

B

C	-4.28568700	-2.90203800	-0.06332300
C	-3.08512600	-2.48067800	0.53242800
C	-3.14540000	-2.12191000	1.88783400
C	-4.32578700	-2.18415800	2.62558900
C	-5.50009000	-2.61439800	2.00549900

C	-5.48055700	-2.96797500	0.65603900
H	-4.28838600	-3.17982700	-1.11290800
H	-4.30991900	-1.89837800	3.67283900
H	-6.42340600	-2.66976400	2.57445900
H	-6.39159300	-3.29723900	0.16548700
C	-1.75496100	-3.06796900	-2.19182400
C	-2.45321700	-0.60864400	-2.20203300
C	-2.32756500	-1.89636300	-3.02729500
H	-2.39465600	-3.95875600	-2.20016200
H	-0.78225900	-3.37763300	-2.58957200
H	-3.32276100	-2.15618800	-3.41591700
H	-1.68586000	-1.71416000	-3.88938900
C	-0.25288600	-3.54655600	0.47346600
H	-0.72589100	-4.53658800	0.51000900
H	0.69356700	-3.64484700	-0.05879900
H	-0.06941000	-3.22578200	1.49845700
C	-1.83439700	-0.23807100	2.36786500
C	-1.77355400	0.15296500	0.94099100
C	-2.35616200	0.81892600	0.03867500
C	-3.44925100	1.63102000	-0.42951600
C	-4.71364900	1.45023900	0.16306000
C	-3.29370500	2.58997500	-1.44346500
C	-5.79158900	2.23374800	-0.23892300
H	-4.83693900	0.68132200	0.91924000
C	-4.37714600	3.36902500	-1.83956900
H	-2.32640400	2.71059500	-1.91605000
C	-5.62595700	3.19594400	-1.23819300
H	-6.76441900	2.08703100	0.22042100
H	-4.24864500	4.10964300	-2.62287600
H	-6.46925000	3.80310000	-1.55283400

O	-1.99789100	-1.65467200	2.52796800
Si	-1.45967300	-2.42242900	-0.44353400
C	2.81666200	-2.10066600	-0.89719200
H	2.00307700	-2.09533100	-1.62607000
H	2.50031900	-2.71379000	-0.04688300
C	3.09683000	-0.65546800	-0.42319300
C	4.08129200	-2.72960300	-1.51057200
H	3.84321900	-3.74932400	-1.83695900
C	4.53530400	-1.89009600	-2.71608600
H	3.74194600	-1.86150300	-3.47181300
H	5.41846600	-2.34481500	-3.18282600
C	3.60492000	0.17916500	-1.62504500
H	3.86692100	1.18922300	-1.29403200
H	2.82049000	0.26015800	-2.37756300
C	4.86123500	-0.46379300	-2.24308700
H	5.17598700	0.14589200	-3.09866700
C	5.98218800	-0.50374500	-1.19261100
H	6.89318700	-0.94232900	-1.61920000
H	6.23425100	0.51546100	-0.87170200
C	4.24108300	-0.70489200	0.62316800
H	3.95048600	-1.29901300	1.49375200
H	4.47727700	0.30336100	0.98462900
C	5.19693700	-2.76966800	-0.45240000
H	4.88293200	-3.38213600	0.40302500
H	6.09976000	-3.23495400	-0.86759800
C	5.51063400	-1.33599000	0.01043500
H	6.29352100	-1.35769500	0.77892300
P	1.47382100	0.05773600	0.32123500
C	1.99556200	1.86318300	0.55482900
H	3.08514100	1.80210900	0.65017700

C	1.49994900	2.67244900	1.77915700
C	1.68756600	2.69019200	-0.72758500
H	1.68086200	2.11519000	2.69708600
C	0.00793300	3.02263300	1.67414200
C	2.31690100	3.98270600	1.83695600
H	1.96219300	2.12766900	-1.61987300
C	0.19674100	3.03824400	-0.82232200
C	2.50103100	3.99785900	-0.66460500
H	-0.29400200	3.59409400	2.56128100
H	-0.59866200	2.11626600	1.65089200
C	-0.24937100	3.85009600	0.40240100
H	3.38551600	3.75514300	1.94113200
H	2.02246700	4.55474900	2.72603000
C	2.07157400	4.81647500	0.56703300
H	-0.39301300	2.11792600	-0.90572100
H	0.01768000	3.60331700	-1.74541800
H	3.57447600	3.77364600	-0.61651900
H	2.33491300	4.57772900	-1.58095100
H	-1.31775500	4.08176100	0.32314900
C	0.57049800	5.15346600	0.46327300
H	2.65511400	5.74380100	0.61661100
H	0.38264600	5.75828300	-0.43287300
H	0.26022500	5.75395400	1.32791200
C	1.46460200	-0.86046800	1.95548500
H	1.95728400	-1.80576700	1.71051400
H	0.43358600	-1.14319200	2.14924100
C	2.09456100	-0.29526900	3.23424900
H	3.02639800	0.23770600	3.01767500
H	1.41866800	0.43839200	3.68850200
C	2.37001400	-1.40281200	4.25818200

H	3.07298200	-2.12546700	3.82228100
H	1.44096200	-1.95704000	4.44575300
C	2.93106000	-0.86627800	5.57631800
H	3.12630700	-1.67483100	6.28746400
H	3.87238000	-0.32922000	5.41401600
H	2.22996300	-0.16890900	6.04849700
Rh	-0.76888000	-0.23006800	-0.89148000
Cl	0.46051700	-0.37858200	-2.93135900
H	-2.48279500	0.27999400	-2.83634500
H	-3.37288100	-0.63545400	-1.61327200
H	-0.92837100	0.02536900	2.91583600
H	-2.67998300	0.28655000	2.83502600

TS2

C	4.57520700	2.88983700	-0.27520400
C	3.57640600	2.35387400	0.55160800
C	3.96789400	1.90434300	1.82355700
C	5.28240100	2.00153600	2.27354400
C	6.24995700	2.55526000	1.43382500
C	5.89931500	2.99266600	0.15579500
H	4.31445600	3.23997500	-1.26923500
H	5.52740600	1.64713500	3.26944900
H	7.27717900	2.63668400	1.77660400
H	6.65243800	3.41692200	-0.50113300
C	1.56144000	3.20426000	-1.58238900
C	2.30144600	0.86238200	-2.21732900
C	1.98712500	2.26422000	-2.74181700
H	2.14481700	4.13312000	-1.54904300
H	0.51278000	3.50429900	-1.68557700
H	2.86493700	2.67220500	-3.26364800

H	1.18665300	2.19575800	-3.48294700
C	0.79008600	3.18155100	1.40639900
H	1.28880200	4.15000600	1.53366600
H	-0.23992000	3.37746000	1.10030800
H	0.79414300	2.68131700	2.37424500
C	2.33158200	0.21400000	2.25191900
C	2.02134300	0.13415700	0.79058600
C	2.19176100	-0.77375600	-0.12194400
C	2.89626800	-1.94157800	-0.57914300
C	3.91818900	-2.49788900	0.21627100
C	2.56544300	-2.55452800	-1.80121100
C	4.56834700	-3.65784500	-0.18984100
H	4.19571800	-2.01357400	1.14651400
C	3.22847500	-3.71006800	-2.20379100
H	1.78923400	-2.11603100	-2.41792900
C	4.22324900	-4.26938800	-1.39895000
H	5.34943400	-4.08352000	0.43265300
H	2.96500600	-4.17678400	-3.14776100
H	4.73363000	-5.17442300	-1.71393100
O	3.02002400	1.39339800	2.69094600
Si	1.75226900	2.26701800	0.06426700
C	-2.28060800	2.19312200	-0.99913500
H	-1.48064000	1.94092100	-1.70106200
H	-1.83406200	2.77913800	-0.18672900
C	-2.90306700	0.89282100	-0.42998500
C	-3.34615500	3.03938600	-1.71781600
H	-2.87174300	3.94710500	-2.11046900
C	-3.93990500	2.21909300	-2.87671700
H	-3.14913500	1.94798000	-3.58574700
H	-4.67956100	2.81870700	-3.42226500

C	-3.54546500	0.09190600	-1.58813300
H	-4.03229800	-0.80437600	-1.18723900
H	-2.77754900	-0.22681900	-2.29382200
C	-4.60074400	0.94756900	-2.31561100
H	-5.01957700	0.35710600	-3.13926400
C	-5.71625600	1.33327500	-1.33101300
H	-6.48589400	1.92914900	-1.83774900
H	-6.20819900	0.43062200	-0.94606000
C	-4.03498100	1.28824700	0.54663600
H	-3.63729900	1.86886000	1.38278600
H	-4.50624000	0.39005300	0.96301700
C	-4.45582700	3.41898600	-0.72281500
H	-4.03727400	4.01365000	0.09983900
H	-5.21287600	4.04070700	-1.21687300
C	-5.10489500	2.13716000	-0.17208600
H	-5.88580300	2.39988800	0.55241800
P	-1.47365900	-0.07570200	0.37878600
C	-2.13950900	-1.81527800	0.64966800
H	-3.20555100	-1.66385400	0.86824000
C	-1.52324100	-2.56385100	1.86266200
C	-2.03243000	-2.74637800	-0.58938800
H	-1.54936300	-1.93184600	2.74919400
C	-0.06916700	-2.98798600	1.59238600
C	-2.37656200	-3.82087700	2.13125900
H	-2.39960600	-2.23727100	-1.48053700
C	-0.57775700	-3.17171400	-0.83798100
C	-2.88577600	-4.00218600	-0.31882100
H	0.32889400	-3.49379300	2.48173700
H	0.55808800	-2.10993700	1.41261900
C	-0.01746800	-3.92555100	0.37490300

H	-3.41088300	-3.53010200	2.35575200
H	-1.98983100	-4.34244800	3.01615300
C	-2.33598100	-4.75347700	0.90813900
H	0.02483000	-2.28911800	-1.04613500
H	-0.53279500	-3.79901000	-1.73632300
H	-3.93417000	-3.72138800	-0.15258800
H	-2.86399400	-4.65474500	-1.20038400
H	1.01976900	-4.21906800	0.17860600
C	-0.87670200	-5.17479900	0.64485700
H	-2.94864800	-5.64240600	1.10219500
H	-0.83150900	-5.85225500	-0.21716700
H	-0.48488400	-5.72691900	1.50904300
C	-1.40701900	0.65889400	2.09541300
H	-1.38794100	1.73492200	1.90785800
H	-0.41285800	0.42603100	2.47766800
C	-2.45676000	0.35561100	3.18706700
H	-3.40071200	0.00841000	2.76055100
H	-2.10173200	-0.45965400	3.82517400
C	-2.72180900	1.57500700	4.07857800
H	-3.09284600	2.40327300	3.46041100
H	-1.77119600	1.91991400	4.50671100
C	-3.72118900	1.28245400	5.19894100
H	-3.89544900	2.16535700	5.82162600
H	-4.68720600	0.96563100	4.78995900
H	-3.35943600	0.47978500	5.85125500
Rh	0.71173200	0.31583600	-0.90454700
Cl	-0.36289200	-0.26641500	-2.95583100
H	2.31579100	0.11365100	-3.00922100
H	3.26868000	0.83694000	-1.70293900
H	1.42281000	0.18189300	2.85761700

H	2.93735800	-0.66555200	2.50717600

C

C	-7.35968300	-1.26803600	0.99734500
C	-6.04369300	-1.71251800	1.14690500
C	-5.08877300	-1.50587500	0.14331800
C	-5.49241200	-0.80715400	-1.01144000
C	-6.80012200	-0.35137700	-1.17423800
C	-7.73514600	-0.59248000	-0.16550300
H	-8.08872300	-1.44935900	1.78138300
H	-5.76014500	-2.23492800	2.05720900
H	-7.06768900	0.17317700	-2.08569500
H	-8.75732800	-0.24598400	-0.28749600
O	-4.59978400	-0.62583900	-2.04634600
C	-3.39335100	0.11972000	-1.78625400
H	-2.72495400	-0.12754400	-2.61386800
H	-3.62790700	1.19206800	-1.82426800
C	-2.69956100	-0.22221100	-0.46573400
C	-2.06363300	0.79906300	0.19524100
C	-0.71470200	-0.52302100	1.97384700
C	-2.64929400	-2.19291600	1.95514300
C	-2.05643900	-0.92360200	2.58587700
H	-0.35427000	0.37471300	2.48096100
H	-3.48166700	-2.57304200	2.56042400
H	-1.88772400	-2.98338200	1.94529400
H	-1.89902200	-1.09055300	3.66235800
Si	-3.25098200	-1.89792300	0.19917600
C	-2.78779200	-3.27152400	-0.99074600
H	-3.18982900	-3.06271500	-1.98531500
H	-1.69972700	-3.34253700	-1.07777400

H	-3.18461000	-4.23387100	-0.64911400
C	-2.43205300	2.08938200	0.70725900
C	-3.79769200	2.42739200	0.82687100
C	-1.45453100	3.00757800	1.12798700
C	-4.16351200	3.66921400	1.33337400
H	-4.54954200	1.70441000	0.52651700
C	-1.82510100	4.24671100	1.63554400
H	-0.41633500	2.72017200	1.04038500
C	-3.17988000	4.57981800	1.73428000
H	-5.21355600	3.92907800	1.42317600
H	-1.06444400	4.95288700	1.95350300
H	-3.47073000	5.54830500	2.13002800
H	-0.00120000	-1.33213500	2.16244600
H	-2.77974000	-0.10059400	2.52011500
C	1.80434000	-2.71649300	0.36799700
H	0.84345700	-2.60638200	-0.14830600
H	1.60604700	-2.62995600	1.44375300
C	2.76975900	-1.59248800	-0.08604500
C	2.40211200	-4.10207900	0.06613400
H	1.69614300	-4.87256800	0.39945300
C	2.63774300	-4.23067700	-1.44872600
H	1.68862700	-4.12131600	-1.98630500
H	3.03602400	-5.22564600	-1.68472700
C	3.03607600	-1.75103000	-1.60385500
H	3.74606400	-0.98866500	-1.94334600
H	2.11066900	-1.61101300	-2.16274400
C	3.62559500	-3.14236200	-1.90384400
H	3.78934600	-3.22390600	-2.98492200
C	4.96072600	-3.30765300	-1.16010500
H	5.40298900	-4.28796300	-1.37833700

H	5.67719500	-2.54793300	-1.49852600
C	4.11219400	-1.77804400	0.65668400
H	3.96679600	-1.69329200	1.73689200
H	4.82254200	-0.99773100	0.35679200
C	3.73621300	-4.25870300	0.81656800
H	3.57157200	-4.18101900	1.89935000
H	4.16360500	-5.25103500	0.62610900
C	4.71449600	-3.16580500	0.35077400
H	5.66270500	-3.26245100	0.89423700
P	1.90149100	0.06417300	0.28148200
C	2.88276300	1.31745100	-0.74032400
H	3.80361900	0.77706400	-0.98780600
C	3.31666800	2.63265900	-0.04747100
C	2.16204000	1.67770500	-2.06605000
H	3.83287000	2.41627800	0.88497500
C	2.10989000	3.54107000	0.22590700
C	4.30156600	3.37254800	-0.97818300
H	1.81248200	0.77073100	-2.55984800
C	0.95083100	2.58460400	-1.78541300
C	3.14914700	2.42467600	-2.98244500
H	2.44504600	4.45856700	0.72662200
H	1.42151600	3.04068600	0.91490000
C	1.40394300	3.88368400	-1.09900300
H	5.18304500	2.74545800	-1.16355600
H	4.65512500	4.28308200	-0.47736900
C	3.61181600	3.72672300	-2.30544900
H	0.22508900	2.04960900	-1.16430100
H	0.44266800	2.80906700	-2.73060100
H	4.01505200	1.78776600	-3.20623400
H	2.65918700	2.64600200	-3.93851500

H	0.53297500	4.51973900	-0.89776000
C	2.39272000	4.62630400	-2.01918400
H	4.31614900	4.25720200	-2.95786800
H	1.89572000	4.89458000	-2.95961300
H	2.72053500	5.56270800	-1.54888600
C	2.28194200	0.38895100	2.08195800
H	1.94352700	-0.52798900	2.57407700
H	1.56476800	1.15146400	2.39609400
C	3.68241800	0.75677800	2.62111600
H	4.47625200	0.50174000	1.91545500
H	3.74115200	1.84073700	2.76383500
C	3.97155900	0.08225700	3.96776800
H	3.92018400	-1.00791400	3.84513400
H	3.17697000	0.34474700	4.67874600
C	5.33435500	0.47131600	4.54303400
H	5.51985900	-0.02069400	5.50278100
H	6.14347600	0.18850200	3.86029900
H	5.40090800	1.55314800	4.70385000
Rh	-0.52380400	-0.23427900	-0.12984400
Cl	-0.16078000	-0.83878500	-2.45332600

TS3

C	-7.22310000	-2.15140000	1.19330000
C	-5.85570000	-2.21930000	1.47030000
C	-4.90540000	-1.85190000	0.51040000
C	-5.36880000	-1.39310000	-0.73650000
C	-6.72950000	-1.32100000	-1.03010000
C	-7.65470000	-1.70780000	-0.05870000
H	-7.94800000	-2.44660000	1.94600000
H	-5.52750000	-2.57040000	2.44620000

H	-7.04310000	-0.97130000	-2.00820000
H	-8.71710000	-1.65660000	-0.27930000
O	-4.45720000	-1.07710000	-1.72360000
C	-3.55130000	0.02250000	-1.46690000
H	-2.88910000	0.01980000	-2.33520000
H	-4.13070000	0.95470000	-1.45990000
C	-2.76400000	-0.13250000	-0.18050000
C	-2.27380000	0.98240000	0.52340000
C	-1.47410000	0.73060000	2.31130000
C	-2.45900000	-1.62710000	2.44540000
C	-2.29540000	-0.27200000	3.14790000
H	-1.07780000	1.53420000	2.93240000
H	-3.10940000	-2.18880000	3.12580000
H	-1.45970000	-2.07290000	2.52840000
H	-1.80890000	-0.39810000	4.12280000
Si	-3.03760000	-1.79250000	0.65310000
C	-2.25070000	-3.24930000	-0.22900000
H	-2.48090000	-3.19800000	-1.29630000
H	-1.16470000	-3.22740000	-0.11460000
H	-2.63190000	-4.19750000	0.16570000
C	-2.44240000	2.39530000	0.09020000
C	-2.81390000	3.37730000	1.02120000
C	-2.22610000	2.78520000	-1.24200000
C	-2.96100000	4.70920000	0.63540000
H	-3.00560000	3.09720000	2.05270000
C	-2.37440000	4.11490000	-1.62720000
H	-1.88540000	2.05070000	-1.96240000
C	-2.74250000	5.08320000	-0.69080000
H	-3.24920000	5.45350000	1.37170000
H	-2.18480000	4.39730000	-2.65820000

H	-2.85120000	6.12080000	-0.99110000
H	-0.75060000	-0.05140000	2.43760000
H	-3.27550000	0.17950000	3.34020000
C	2.39730000	-1.73340000	0.41330000
H	1.49550000	-1.60770000	-0.18980000
H	2.07970000	-2.04680000	1.41690000
C	3.15000000	-0.38130000	0.49640000
C	3.29880000	-2.81410000	-0.20890000
H	2.73980000	-3.75650000	-0.25460000
C	3.69500000	-2.37650000	-1.63030000
H	2.79650000	-2.24720000	-2.24450000
H	4.31030000	-3.15070000	-2.10610000
C	3.59210000	0.03950000	-0.92630000
H	4.16730000	0.97060000	-0.87120000
H	2.71550000	0.21940000	-1.55080000
C	4.47620000	-1.05280000	-1.55770000
H	4.75510000	-0.73380000	-2.56900000
C	5.74050000	-1.24180000	-0.70370000
H	6.39340000	-2.00330000	-1.14840000
H	6.31400000	-0.30650000	-0.66700000
C	4.42470000	-0.58630000	1.34720000
H	4.16210000	-0.90560000	2.35890000
H	4.98430000	0.35350000	1.43090000
C	4.56030000	-2.99760000	0.65130000
H	4.28350000	-3.32240000	1.66300000
H	5.20090000	-3.78030000	0.22600000
C	5.32900000	-1.66620000	0.71560000
H	6.22130000	-1.78340000	1.34310000
P	1.93030000	0.87830000	1.21690000
C	2.70950000	2.56490000	0.96760000

H	3.78930000	2.38050000	1.05890000
C	2.32730000	3.61570000	2.04470000
C	2.44840000	3.19630000	-0.43050000
H	2.46170000	3.19960000	3.04340000
C	0.87090000	4.08700000	1.88250000
C	3.27300000	4.82410000	1.88630000
H	2.64570000	2.46740000	-1.21760000
C	0.99670000	3.68340000	-0.56870000
C	3.39900000	4.40110000	-0.58570000
H	0.63080000	4.80030000	2.68150000
H	0.18420000	3.23990000	1.98100000
C	0.67790000	4.73450000	0.50190000
H	4.31350000	4.50460000	2.02820000
H	3.05460000	5.56400000	2.66700000
C	3.09010000	5.45520000	0.49490000
H	0.31480000	2.83620000	-0.47460000
H	0.85250000	4.10070000	-1.57270000
H	4.44460000	4.07510000	-0.50770000
H	3.27270000	4.83860000	-1.58370000
H	-0.36070000	5.06460000	0.39450000
C	1.63210000	5.93320000	0.35020000
H	3.77270000	6.30680000	0.38480000
H	1.48590000	6.40350000	-0.63050000
H	1.41230000	6.69590000	1.10870000
C	2.00640000	0.57290000	3.06490000
H	1.81590000	-0.50370000	3.14880000
H	1.11730000	1.05580000	3.47950000
C	3.23560000	0.95920000	3.91880000
H	4.12110000	1.12450000	3.30100000
H	3.04410000	1.91350000	4.42070000

C	3.55360000	-0.09090000	4.98980000
H	3.74840000	-1.05680000	4.50490000
H	2.66690000	-0.24160000	5.61970000
C	4.74980000	0.29710000	5.86070000
H	4.95780000	-0.46410000	6.61890000
H	5.65320000	0.41920000	5.25270000
H	4.56980000	1.24520000	6.37950000
Rh	-0.29760000	0.60840000	0.57730000
Cl	0.18950000	0.28800000	-1.69510000

3a

C	-7.75467700	0.41437500	0.05868100
C	-6.59626300	0.89111200	0.67821200
C	-5.36773600	0.24456800	0.49925100
C	-5.33807300	-0.87668000	-0.33970400
C	-6.47735700	-1.37092300	-0.96938200
C	-7.69373600	-0.71766500	-0.75755200
H	-8.70297600	0.92039100	0.21365900
H	-6.65422900	1.77122900	1.31403400
H	-6.40368500	-2.24943300	-1.60221500
H	-8.59412400	-1.09080000	-1.23689100
O	-4.13166900	-1.54006800	-0.49969500
C	-3.08357600	-0.78715200	-1.13647200
H	-2.27814200	-1.51878800	-1.21343500
H	-3.43017600	-0.52235800	-2.14394800
C	-2.64469700	0.47646600	-0.36962900
C	-2.07396100	1.64169700	-0.95635700
C	-2.30127900	3.04811000	-0.39329000
C	-3.65724300	2.46971400	1.70647700
C	-3.58956100	3.28313300	0.40581300

H	-2.32769600	3.73498400	-1.24526200
H	-4.55867000	2.72608400	2.27657800
H	-2.79124700	2.68494600	2.33810600
H	-3.65133900	4.35742500	0.62035000
Si	-3.68006600	0.65971800	1.22521800
C	-3.32120000	-0.58797000	2.58128900
H	-3.38508400	-1.60123000	2.17659700
H	-2.32959100	-0.42887200	3.00548600
H	-4.07429700	-0.48891300	3.37111700
C	-1.14186600	1.54294700	-2.10264100
C	-0.88405300	0.31157700	-2.78426700
C	-0.35258800	2.67161400	-2.50908900
C	0.04891500	0.25738400	-3.84468300
H	-1.52914200	-0.54009900	-2.67661600
C	0.56596300	2.58289500	-3.53118000
H	-0.47598900	3.61617900	-1.99801500
C	0.76638700	1.37068800	-4.22554400
H	0.17096000	-0.68169500	-4.37708100
H	1.13781200	3.46360400	-3.80847800
H	1.47347400	1.32082500	-5.04744300
H	-1.44050500	3.33660500	0.22095700
H	-4.45419000	3.04673000	-0.22863100
C	2.68852300	2.24802700	0.46582600
H	1.64436200	2.42717100	0.73092500
H	2.78613100	2.42676800	-0.61340200
C	3.05729000	0.77688500	0.78819400
C	3.60645400	3.21063900	1.24023300
H	3.32088300	4.24223800	1.00019600
C	3.43349700	2.96298600	2.74986900
H	2.38967400	3.13260400	3.03782700

H	4.05187000	3.66745100	3.32082800
C	2.93681500	0.53403700	2.31221000
H	3.24462700	-0.49217500	2.54626700
H	1.90154300	0.65675000	2.62890900
C	3.84008300	1.51592600	3.08268100
H	3.71353700	1.33641700	4.15711300
C	5.30621900	1.28334300	2.68453300
H	5.96706200	1.96239600	3.23817300
H	5.60846500	0.25934300	2.93996200
C	4.53654400	0.55353800	0.39580900
H	4.67902800	0.72785000	-0.67314900
H	4.83497000	-0.48072700	0.60636300
C	5.07124100	2.96921000	0.83759800
H	5.20273100	3.15550400	-0.23649600
H	5.73249600	3.66540500	1.36879500
C	5.45708700	1.51814600	1.17297800
H	6.49430900	1.33054800	0.86805900
P	1.83961700	-0.30815700	-0.17718000
C	1.98277500	-2.03475100	0.54212400
H	3.02744900	-2.10634300	0.87482800
C	1.74170000	-3.17905600	-0.47776200
C	1.06764100	-2.28700500	1.77314600
H	2.34419000	-3.02120700	-1.37173200
C	0.25783600	-3.27204800	-0.87670200
C	2.17975600	-4.50438700	0.17848400
H	1.16331100	-1.46874900	2.48887000
C	-0.41017500	-2.41294400	1.36605900
C	1.51046900	-3.61205600	2.42782500
H	0.13175800	-4.06640300	-1.62360000
H	-0.06434500	-2.33175300	-1.34217400

C	-0.60060100	-3.56008000	0.36713800
H	3.24453400	-4.45587100	0.44035000
H	2.06251200	-5.32518500	-0.54062700
C	1.33056600	-4.77478500	1.43241900
H	-0.76394200	-1.47082000	0.92550600
H	-1.01568100	-2.57768500	2.26378000
H	2.55890200	-3.54710000	2.74715000
H	0.91098700	-3.79210700	3.32856100
H	-1.65765300	-3.62703500	0.08174400
C	-0.15007900	-4.88188400	1.01779300
H	1.65223600	-5.71335200	1.89998000
H	-0.77295000	-5.09427800	1.89544800
H	-0.28312900	-5.71727800	0.31820600
C	2.58029800	-0.42390400	-1.87821500
H	2.69616000	0.62254400	-2.18125300
H	1.77201700	-0.79687000	-2.50509600
C	3.87452300	-1.21135300	-2.18607900
H	4.45403500	-1.42705800	-1.28583100
H	3.61159200	-2.18722500	-2.60826200
C	4.76315100	-0.48123400	-3.20023800
H	5.04170900	0.50191500	-2.79825800
H	4.17765800	-0.28099700	-4.10758500
C	6.02556800	-1.26737100	-3.55696000
H	6.64224900	-0.72915200	-4.28346500
H	6.63871400	-1.44821700	-2.66696800
H	5.77490000	-2.24272800	-3.98887900
Rh	-0.39862100	0.46620700	-0.29163000
Cl	-0.40268200	1.17303000	1.98660300

TS4

C	-6.08600000	-2.77140000	-0.67230000
C	-5.38190000	-1.66000000	-0.17270000
C	-6.10090000	-0.73660000	0.61350000
C	-7.47040000	-0.91350000	0.85820000
C	-8.13540000	-2.01490000	0.33300000
C	-7.44390000	-2.95810000	-0.43420000
H	-5.55350000	-3.49870000	-1.28230000
H	-7.98530000	-0.17590000	1.46490000
H	-9.19590000	-2.14320000	0.53020000
H	-7.96090000	-3.82110000	-0.84230000
C	-3.19800000	-1.12160000	-2.43820000
C	-2.04680000	1.09130000	-1.78360000
C	-3.00620000	0.37530000	-2.75730000
H	-3.97570000	-1.55510000	-3.07620000
H	-2.27070000	-1.66730000	-2.65650000
H	-3.97530000	0.88970000	-2.73660000
H	-2.60900000	0.48760000	-3.77410000
C	-2.49800000	-2.71350000	0.13260000
H	-2.46130000	-2.66130000	1.22560000
H	-2.90000000	-3.69630000	-0.13920000
H	-1.48250000	-2.65410000	-0.27010000
C	-4.15870000	0.46780000	1.45820000
C	-3.32340000	0.31330000	0.21200000
C	-2.60410000	1.29780000	-0.38030000
C	-2.29390000	2.59560000	0.27760000
C	-1.85520000	2.64190000	1.61350000
C	-2.38840000	3.81320000	-0.41890000
C	-1.53140000	3.84870000	2.23180000
H	-1.74080000	1.71360000	2.16030000
C	-2.06950000	5.02250000	0.19700000

H	-2.73830000	3.81430000	-1.44600000
C	-1.63680000	5.04700000	1.52490000
H	-1.19100000	3.85050000	3.26310000
H	-2.16520000	5.95000000	-0.35970000
H	-1.38390000	5.98890000	2.00180000
O	-5.56820000	0.40040000	1.16310000
Si	-3.58540000	-1.35370000	-0.59980000
C	1.90020000	-2.85230000	-1.84880000
H	0.87370000	-2.63000000	-2.15480000
H	1.85340000	-3.40870000	-0.90590000
C	2.68720000	-1.53240000	-1.64800000
C	2.59310000	-3.73010000	-2.90830000
H	2.01250000	-4.65190000	-3.03370000
C	2.66380000	-2.97460000	-4.24640000
H	1.65280000	-2.73880000	-4.59820000
H	3.13700000	-3.60560000	-5.00940000
C	2.76530000	-0.79480000	-3.00990000
H	3.30700000	0.15090000	-2.89960000
H	1.75380000	-0.54260000	-3.33970000
C	3.46880000	-1.67760000	-4.05540000
H	3.51780000	-1.12960000	-5.00390000
C	4.89180000	-2.01330000	-3.57510000
H	5.41070000	-2.62510000	-4.32330000
H	5.47580000	-1.09170000	-3.45160000
C	4.12200000	-1.88740000	-1.18190000
H	4.09460000	-2.41960000	-0.22540000
H	4.71790000	-0.98340000	-1.02660000
C	4.01520000	-4.07290000	-2.43180000
H	3.97310000	-4.63340000	-1.48890000
H	4.51700000	-4.71570000	-3.16600000

C	4.81530000	-2.77280000	-2.23890000
H	5.82760000	-3.00870000	-1.88790000
P	1.75810000	-0.43170000	-0.43110000
C	3.01300000	0.64330000	0.44340000
H	3.70070000	-0.05950000	0.93050000
C	2.33120000	1.49600000	1.54060000
C	3.84550000	1.58390000	-0.46470000
H	1.70590000	0.86870000	2.17700000
C	1.47200000	2.60930000	0.91930000
C	3.42490000	2.15370000	2.40630000
H	4.31820000	1.01240000	-1.26710000
C	2.96840000	2.68990000	-1.07770000
C	4.94420000	2.23230000	0.40380000
H	0.96560000	3.16830000	1.71400000
H	0.62840000	2.17480000	0.33020000
C	2.32640000	3.52850000	0.03860000
H	4.03470000	1.37710000	2.88470000
H	2.95410000	2.72890000	3.21090000
C	4.30300000	3.06460000	1.52980000
H	2.17980000	2.24240000	-1.70970000
H	3.57770000	3.32310000	-1.73390000
H	5.59340000	1.45530000	0.82720000
H	5.57690000	2.87220000	-0.22360000
H	1.69750000	4.31140000	-0.40060000
C	3.42650000	4.16880000	0.90900000
H	5.08920000	3.52020000	2.14340000
H	4.04110000	4.84020000	0.29710000
H	2.97190000	4.77860000	1.69950000
C	1.09280000	-1.53750000	0.89690000
H	0.48830000	-2.28210000	0.37410000

H	0.37450000	-0.92850000	1.45080000
C	2.05680000	-2.21340000	1.87750000
H	2.86220000	-2.73080000	1.34600000
H	2.53910000	-1.45370000	2.50570000
C	1.32700000	-3.22580000	2.76940000
H	0.95540000	-4.04650000	2.14300000
H	0.43470000	-2.75300000	3.19690000
C	2.20690000	-3.77910000	3.89120000
H	1.66750000	-4.51120000	4.49990000
H	3.09900000	-4.27120000	3.48790000
H	2.54540000	-2.97650000	4.55680000
Rh	0.21220000	0.87230000	-1.24320000
Cl	0.81830000	1.82410000	-3.21040000
H	-0.91710000	-0.29130000	-1.41800000
H	-1.76890000	2.06260000	-2.20010000
H	-4.04510000	1.43840000	1.94200000
H	-3.92550000	-0.31740000	2.19430000

D

C	-5.39062000	-2.81309500	-0.02599800
C	-4.39580400	-1.89089200	0.34904500
C	-4.78495900	-0.82087700	1.18386900
C	-6.11801200	-0.68242600	1.59794800
C	-7.07222700	-1.61054500	1.20069600
C	-6.71359100	-2.68985800	0.38631700
H	-5.11636000	-3.64427900	-0.67291000
H	-6.37525100	0.15831500	2.23365500
H	-8.10057600	-1.49376400	1.53055200
H	-7.45762100	-3.41666100	0.07584100
C	-2.47797600	-2.23546400	-2.16037500

C	-2.23296600	0.38420000	-2.27864000
C	-2.57088800	-0.92221200	-2.96920900
H	-3.20876900	-2.95861800	-2.53940900
H	-1.49362900	-2.69234200	-2.32202100
H	-3.60481400	-0.80294400	-3.32670400
H	-1.95084300	-0.99144000	-3.86899400
C	-1.72910300	-3.37004800	0.61312700
H	-1.71288900	-3.19613000	1.69377300
H	-2.25737700	-4.31648700	0.44993600
H	-0.70219700	-3.49450800	0.26385900
C	-2.52230900	0.02235800	1.52859400
C	-2.09607000	-0.24843500	0.09552900
C	-2.43057900	0.72423800	-0.92363800
C	-2.76996500	2.14195200	-0.60252400
C	-2.07339800	2.89639900	0.35211800
C	-3.83411300	2.74783100	-1.28602300
C	-2.42634400	4.21795400	0.61449100
H	-1.23254600	2.45596300	0.87229500
C	-4.19691400	4.06614200	-1.01710300
H	-4.38586200	2.16986900	-2.02047100
C	-3.49277700	4.80669900	-0.06641800
H	-1.86531900	4.78828200	1.34888500
H	-5.02888200	4.51523800	-1.55091100
H	-3.77208600	5.83505700	0.14140200
O	-3.95167900	0.16414800	1.64392300
Si	-2.63825300	-1.99228200	-0.29987200
C	1.90946300	-2.85563900	-0.25851000
H	1.04158000	-2.74262200	-0.91782000
H	1.53216800	-3.11225100	0.73753700
C	2.69536300	-1.52214700	-0.21098400

C	2.80481600	-3.99709000	-0.77492500
H	2.21812300	-4.92377800	-0.79226200
C	3.29574700	-3.66169600	-2.19353800
H	2.44118200	-3.55782900	-2.87351600
H	3.91932300	-4.47856900	-2.57806500
C	3.19433100	-1.21247200	-1.64443700
H	3.74879900	-0.27067800	-1.66191300
H	2.34250100	-1.07285500	-2.31291600
C	4.09751500	-2.34962300	-2.15495200
H	4.43938000	-2.09638700	-3.16516500
C	5.30829900	-2.51124600	-1.21977300
H	5.97041400	-3.30525500	-1.58751400
H	5.89592300	-1.58449900	-1.20147700
C	3.91739300	-1.71275700	0.72370400
H	3.59497700	-1.95323500	1.73808900
H	4.50366800	-0.79293300	0.78762700
C	4.01239700	-4.16306600	0.16403700
H	3.67217900	-4.42296400	1.17498600
H	4.64858000	-4.98655200	-0.18322300
C	4.81559600	-2.85128600	0.19725300
H	5.67288000	-2.96021700	0.87285800
P	1.50707400	-0.16753100	0.34614800
C	2.53396500	1.26520500	1.00273000
H	2.91758000	0.87471300	1.95371100
C	1.63442400	2.48813200	1.32485200
C	3.76238000	1.76570600	0.20013600
H	0.73460000	2.15932000	1.85984100
C	1.23308300	3.22881300	0.03595600
C	2.42744200	3.44969300	2.23245600
H	4.40584600	0.92563800	-0.06700100

C	3.35325100	2.51670300	-1.07524300
C	4.55659900	2.71944800	1.11947700
H	0.57347800	4.06768000	0.28398500
H	0.66437600	2.57316400	-0.63570600
C	2.48333000	3.72806700	-0.70396800
H	2.70214000	2.94361900	3.16686300
H	1.79584600	4.30545000	2.50238200
C	3.68925200	3.93497400	1.49519800
H	2.80262600	1.86628500	-1.75856800
H	4.25810400	2.85083500	-1.59874600
H	4.88191900	2.19075800	2.02517800
H	5.46286000	3.05238200	0.59883200
H	2.17648200	4.25054000	-1.61638600
C	3.27357500	4.68083900	0.21240800
H	4.25949500	4.60682700	2.14812100
H	4.16370300	5.05233000	-0.31051300
H	2.66241900	5.55566400	0.46923900
C	0.73476500	-0.76685700	1.93502900
H	0.01604600	-1.52943600	1.63185600
H	0.12831400	0.08849100	2.25043000
C	1.55039100	-1.26591700	3.13145000
H	1.98448000	-2.24617000	2.90808100
H	2.39138100	-0.59593300	3.34740200
C	0.67646500	-1.39015100	4.38628000
H	-0.17826600	-2.04332700	4.16491200
H	0.25324800	-0.40607900	4.62803200
C	1.44339800	-1.93480700	5.59269700
H	0.80036200	-2.01062600	6.47483700
H	1.84580800	-2.93274100	5.38593800
H	2.28732300	-1.28455700	5.84901500

Rh	-0.30335900	0.30758800	-1.07265700
Cl	0.85777600	0.95396100	-3.07750300
H	-0.23567200	-1.15400300	-1.39149600
H	-2.22606800	1.22601400	-2.96645800
H	-2.14051400	0.94911400	1.95389900
H	-2.20049200	-0.79841900	2.18323600

TS5

C	-5.26399000	-3.11021500	0.51589900
C	-4.41081900	-2.00326200	0.68485600
C	-4.96807400	-0.84034000	1.25189000
C	-6.31942100	-0.79091900	1.61864300
C	-7.13117500	-1.90298300	1.43121900
C	-6.60630200	-3.07576900	0.87896600
H	-4.86050200	-4.01972600	0.07547800
H	-6.70598500	0.12686700	2.04902400
H	-8.17717600	-1.85548000	1.71937700
H	-7.23881400	-3.94528400	0.73139800
C	-2.27479500	-2.67628600	-1.58141800
C	-2.12065200	-0.16082700	-2.30247800
C	-2.43961800	-1.59613400	-2.66588900
H	-2.88377300	-3.55371700	-1.82796600
H	-1.23065000	-3.00913100	-1.56544600
H	-3.48131900	-1.59373800	-3.02131300
H	-1.82543500	-1.84997900	-3.53577000
C	-1.61298600	-3.00506500	1.40804100
H	-1.59235600	-2.51715700	2.38696800
H	-2.06839600	-3.99220500	1.54592300
H	-0.58620800	-3.15079200	1.06291100
C	-2.86113700	0.40264400	1.43922200

C	-2.27904700	-0.17983200	0.15245500
C	-2.41901200	0.55072200	-1.12629500
C	-2.66700800	2.02571800	-1.20779600
C	-1.83646900	2.83248200	-2.00548300
C	-3.74623200	2.62556200	-0.54285300
C	-2.06140300	4.20222800	-2.10749800
H	-0.99793100	2.38312200	-2.52611200
C	-3.96702900	4.00069400	-0.64743000
H	-4.42001900	2.01719000	0.04817600
C	-3.12447300	4.79576800	-1.42198200
H	-1.39821000	4.80730000	-2.71850900
H	-4.80700100	4.44626200	-0.12242700
H	-3.29549700	5.86546200	-1.49690200
O	-4.29035400	0.33755100	1.46790100
Si	-2.61739200	-2.03410000	0.14557400
C	1.99622300	-2.64567600	-0.88644000
H	1.36308800	-2.23353600	-1.67539600
H	1.33310100	-3.08954000	-0.13179100
C	2.82756800	-1.50740500	-0.24159300
C	2.92758200	-3.72886400	-1.46057300
H	2.31482900	-4.51783900	-1.91370700
C	3.83419000	-3.09656700	-2.53195600
H	3.22191700	-2.67263600	-3.33601600
H	4.48042500	-3.86318700	-2.97818100
C	3.77426300	-0.90099700	-1.30621500
H	4.39429100	-0.12221500	-0.84749000
H	3.18790000	-0.44289700	-2.10373200
C	4.69158400	-1.99175300	-1.88905700
H	5.33513900	-1.53551200	-2.65074800
C	5.55537200	-2.58655700	-0.76535400

H	6.23217900	-3.35196800	-1.16567100
H	6.18194300	-1.80425000	-0.31758300
C	3.69460600	-2.12595600	0.87814900
H	3.05427700	-2.59766800	1.62760100
H	4.28133400	-1.35111900	1.38594300
C	3.79174900	-4.32251700	-0.33499600
H	3.15256400	-4.79050500	0.42528700
H	4.44702600	-5.10763400	-0.73264400
C	4.63633600	-3.20398000	0.30099400
H	5.23926500	-3.61520200	1.12020800
P	1.60105000	-0.20533100	0.38383500
C	2.58423600	1.36555400	0.68489100
H	3.56763300	0.99918700	1.01177500
C	2.03117200	2.27105300	1.82208400
C	2.80366000	2.25745400	-0.56941200
H	1.82480600	1.68394300	2.71712000
C	0.74636100	3.00545600	1.39652100
C	3.11962500	3.30925100	2.16624900
H	3.12528000	1.64902500	-1.41514400
C	1.51665600	2.99932000	-0.96525800
C	3.89350800	3.29247500	-0.22354600
H	0.38116700	3.60653200	2.23933800
H	-0.04174300	2.28781400	1.13978800
C	1.03519600	3.89885300	0.17925900
H	4.03101700	2.79684200	2.50122200
H	2.77694600	3.93394800	3.00106700
C	3.41793300	4.18655700	0.93792900
H	0.74135100	2.27441800	-1.21720400
H	1.70885200	3.58991100	-1.86937600
H	4.82909200	2.78548900	0.04786100

H	4.10620400	3.90716300	-1.10683900
H	0.11642500	4.41432400	-0.12157400
C	2.12867800	4.92502500	0.52823800
H	4.19951600	4.91468200	1.18731500
H	2.32455900	5.56986300	-0.33772200
H	1.79488100	5.57682200	1.34626500
C	1.13752800	-0.72394800	2.12075700
H	0.66830000	-1.70525600	2.02637700
H	0.32024100	-0.03875700	2.37127300
C	2.15263800	-0.72851200	3.28220500
H	2.61998600	-1.71222800	3.37132400
H	2.97286200	-0.02622500	3.10214800
C	1.48187200	-0.38455700	4.61795900
H	0.65801500	-1.08838800	4.79744100
H	1.02137500	0.61025300	4.54638600
C	2.45759700	-0.41550300	5.79541100
H	1.95832500	-0.16578800	6.73664600
H	2.90822200	-1.40771400	5.90887900
H	3.27196200	0.30271300	5.64808500
Rh	-0.34601800	-0.00811800	-0.91736500
Cl	0.89729000	0.11818100	-2.97175300
H	-0.91338600	0.15033700	0.58741300
H	-2.01892400	0.46372500	-3.18529100
H	-2.63480100	1.46385500	1.56104100
H	-2.45965200	-0.14096700	2.30608700

4a

C	-5.42499900	-3.03061400	0.44659600
C	-4.52043400	-1.97062900	0.64806000
C	-5.03804000	-0.77012500	1.17164200

C	-6.40132600	-0.63954500	1.46757500
C	-7.26381900	-1.70713000	1.25182800
C	-6.77940000	-2.91545900	0.74024500
H	-5.05170700	-3.96686500	0.03701800
H	-6.75663900	0.30475300	1.86622200
H	-8.31863800	-1.59689200	1.48535000
H	-7.45217000	-3.74984100	0.57023000
C	-2.28878700	-2.79818600	-1.47669400
C	-2.10074300	-0.32003200	-2.29301300
C	-2.45265100	-1.76071700	-2.59983200
H	-2.85736300	-3.70532500	-1.71249900
H	-1.23371500	-3.09012000	-1.41216300
H	-3.49926300	-1.75939900	-2.94135500
H	-1.85496700	-2.06111600	-3.46695600
C	-1.78103200	-3.05715700	1.54683200
H	-1.76227900	-2.52554200	2.50319800
H	-2.27203700	-4.02117800	1.71959200
H	-0.75096400	-3.25612900	1.23656000
C	-2.88004000	0.37246100	1.43766700
C	-2.24325000	-0.26997000	0.19836900
C	-2.33127000	0.43900800	-1.13317200
C	-2.56711700	1.91465000	-1.26657400
C	-1.74716100	2.67240300	-2.12344300
C	-3.62404800	2.56515500	-0.61222300
C	-1.95776600	4.03776400	-2.29037300
H	-0.92621000	2.18838900	-2.64052200
C	-3.82783900	3.93695200	-0.77876800
H	-4.30269400	2.00017800	0.01370400
C	-2.99437200	4.68178700	-1.61026000
H	-1.30071500	4.60056200	-2.94678900

H	-4.65094100	4.41828900	-0.25844100
H	-3.15263400	5.74892900	-1.73402300
O	-4.30753700	0.37066700	1.40805400
Si	-2.71086400	-2.10634100	0.21078400
C	2.20428900	-2.61244900	-0.86408000
H	1.55788800	-2.24634600	-1.66561700
H	1.55650000	-3.08806800	-0.11442600
C	2.95767500	-1.42004900	-0.22003700
C	3.20782700	-3.64173100	-1.41581500
H	2.65112400	-4.47234700	-1.86679400
C	4.08406500	-2.96389900	-2.48481000
H	3.45458100	-2.58723700	-3.29914400
H	4.78149500	-3.69260900	-2.91728800
C	3.87708800	-0.76447800	-1.27904300
H	4.44672800	0.04906600	-0.81563000
H	3.27353900	-0.34057800	-2.08354500
C	4.86436500	-1.80156900	-1.84546100
H	5.48609500	-1.31352200	-2.60555700
C	5.75200400	-2.33064700	-0.70720700
H	6.47882400	-3.05666300	-1.09299700
H	6.32440400	-1.50644900	-0.26213500
C	3.84792100	-1.97271700	0.91503000
H	3.23045700	-2.47970100	1.66006600
H	4.37668200	-1.15790100	1.42456100
C	4.09580100	-4.16856200	-0.27539300
H	3.47926700	-4.66838000	0.48336300
H	4.80266900	-4.91518400	-0.65865000
C	4.86265500	-2.99350900	0.35735700
H	5.48232900	-3.35885600	1.18577800
P	1.64187300	-0.19356800	0.36219800

C	2.52469600	1.41067000	0.77233700
H	3.49589700	1.08779600	1.17353600
C	1.82301900	2.25141600	1.87619500
C	2.80079900	2.34833200	-0.43688300
H	1.57378400	1.62746500	2.73493300
C	0.53874600	2.91938200	1.35097800
C	2.81174900	3.34005800	2.34122400
H	3.23425500	1.78308800	-1.26281800
C	1.51359800	3.02769700	-0.93213600
C	3.79322800	3.43334100	0.03053900
H	0.05973300	3.47184600	2.16983900
H	-0.17441600	2.16267100	1.00236500
C	0.87977500	3.86364600	0.18675600
H	3.71879700	2.87162100	2.74533300
H	2.35969400	3.92088000	3.15542300
C	3.16447300	4.26623600	1.16435100
H	0.80925700	2.26973700	-1.27556100
H	1.75334300	3.65886200	-1.79677900
H	4.72905400	2.97252000	0.37392300
H	4.04719500	4.08382400	-0.81544200
H	-0.03788600	4.33375300	-0.18200800
C	1.87450100	4.94024200	0.65762900
H	3.87647700	5.03079400	1.49869400
H	2.10704800	5.62052000	-0.17138500
H	1.43098100	5.54759700	1.45755800
C	1.10465500	-0.79680000	2.05230500
H	0.70959100	-1.80374900	1.89690700
H	0.23018900	-0.17503600	2.27383400
C	2.04243400	-0.77533000	3.27704300
H	2.56826500	-1.72920100	3.36625800

H	2.82311600	-0.01533300	3.17079900
C	1.26842500	-0.52158400	4.57650000
H	0.48305900	-1.28238700	4.68082300
H	0.74926200	0.44404600	4.50543500
C	2.16860100	-0.53088900	5.81303200
H	1.59645200	-0.34558900	6.72728100
H	2.67514000	-1.49589200	5.92526900
H	2.94185400	0.24203000	5.73994900
Rh	-0.27253900	-0.09410100	-0.98781600
Cl	0.95821600	0.12113800	-3.00142500
H	-1.09854100	-0.23595100	0.55623500
H	-2.02288300	0.27378200	-3.19950000
H	-2.60961000	1.42524300	1.54001300
H	-2.53966300	-0.16124100	2.33629500

L=L1

Rh-L1

C	-1.20133205	-1.00938265	-0.32834506
C	-1.03538835	-0.52806500	1.10240348
C	-1.17227583	0.95620769	1.39154272
C	-0.37041260	1.94953381	0.55356773
H	-0.06011121	-0.87473949	1.38374782
H	-2.19647443	1.28737438	1.28382278
P	0.70228443	0.75871347	-1.26334169
O	0.91441470	1.54819954	0.21394187
O	0.02102456	-0.78092640	-1.06515487
C	2.34449321	0.62171075	-1.98642062
C	3.29739250	1.60799275	-1.70316023
C	2.66662817	-0.45835914	-2.80623141
C	4.58503802	1.51098249	-2.23316860

H	3.03516354	2.44002250	-1.08082932
C	3.95715236	-0.56272376	-3.33518747
H	1.92864668	-1.19976495	-3.02701776
C	4.91586672	0.42281747	-3.05100719
H	5.31287416	2.26591414	-2.01719213
H	4.20852592	-1.39300804	-3.95878157
H	5.90219239	0.33800602	-3.45063568
O	-0.80568832	0.92049666	2.73787045
O	-1.99738304	-0.97618943	1.99840993
C	-1.54560826	-0.25568904	3.18307905
C	-2.77714418	0.10145890	4.04879226
H	-3.27688768	-0.79873014	4.34594759
H	-2.45942952	0.63496611	4.92249154
H	-3.45437910	0.71313032	3.48796862
C	-0.55538464	-1.10290765	3.97681238
H	-0.26072256	-0.57760202	4.85817470
H	-1.01667278	-2.02564856	4.24762627
H	0.30344250	-1.29353118	3.36792939
Rh	-0.64916853	1.99265522	-2.65632082
Cl	-1.96453570	3.19479545	-4.01230733
C	-2.38630512	-0.74424146	-1.27146539
C	-2.55013712	-1.55010222	-2.40153891
C	-3.32243848	0.26388687	-0.98641691
C	-3.64206998	-1.34922789	-3.25338004
H	-1.83437311	-2.31355041	-2.61728704
C	-4.44278366	0.43242841	-1.81158255
H	-3.18925083	0.89526022	-0.13128511
C	-4.59690200	-0.36766521	-2.95221147
H	-3.74771626	-1.94551603	-4.13541383
H	-5.18140076	1.17006367	-1.57122430

H	-5.44215217	-0.22940195	-3.59264640
C	-1.01551102	-2.51838063	-0.17811693
C	0.21290848	-2.74055662	0.45033200
C	-1.87235853	-3.58409315	-0.46294586
C	0.58779746	-4.03768218	0.80791770
H	0.86218394	-1.91465671	0.66303235
C	-1.49305176	-4.88493589	-0.11734760
H	-2.81283884	-3.40341692	-0.94146019
C	-0.26470917	-5.11279291	0.51952606
H	1.52031947	-4.20824059	1.30141327
H	-2.14162963	-5.70465121	-0.33848558
H	0.02437334	-6.10697386	0.78451071
C	-1.05233813	3.18311702	-0.02145168
C	-2.40439224	3.58311055	0.07410067
C	-0.15969479	3.99916548	-0.75695358
C	-2.87766010	4.73306070	-0.57339210
H	-3.08777129	2.98871909	0.64650592
C	-0.63881036	5.18574134	-1.37209671
H	0.87232442	3.73702741	-0.83744242
C	-1.99720408	5.53425581	-1.29912602
H	-3.91660720	4.99120146	-0.52095509
H	0.03581914	5.82571125	-1.90152660
H	-2.35991531	6.41511306	-1.79199333
C	0.42333623	2.39271172	1.76708775
C	0.24441984	3.56667569	2.48218100
C	1.42841212	1.47723622	2.13526611
C	1.11288013	3.82281813	3.56653240
H	-0.52075592	4.25365098	2.21344023
C	2.26599967	1.71338954	3.21163862
H	1.54736213	0.56826348	1.57013571

C	2.11218389	2.89374758	3.93303882
H	1.00767678	4.72564333	4.12394358
H	3.01242762	0.99162518	3.48764284
H	2.76466831	3.09552163	4.75487781

A’

C	6.18152500	-0.17098400	0.87694900
C	5.20752200	0.68245100	0.32738300
C	4.68537800	1.67290200	1.17634100
C	5.11064700	1.81356300	2.49807000
C	6.07644600	0.94854500	3.01151500
C	6.61021700	-0.05211000	2.19874400
H	6.61177400	-0.95269500	0.25759600
H	4.68007000	2.60315700	3.10607900
H	6.41011300	1.05808800	4.03917000
H	7.36033100	-0.73252100	2.58989100
C	5.85483900	-0.58217200	-2.55067900
C	3.76112000	-1.33008000	-1.67500600
C	4.66899800	-1.52581100	-2.91704100
H	6.62837700	-1.11861400	-1.99220700
H	6.33180500	-0.07610800	-3.39360600
H	4.94575100	-2.56996500	-3.10433200
H	4.14119800	-1.15503800	-3.80097600
C	4.06340300	1.93753300	-2.34897900
H	3.35533600	2.51769100	-1.75994900
H	4.94105000	2.56639100	-2.54266900
H	3.60023200	1.66450100	-3.30038800
C	2.37084100	2.10504500	1.01534200
H	2.20387900	2.14602800	2.10166000
H	1.71441300	2.82932100	0.52958100

C	2.10961700	0.73517400	0.53630600
C	2.00156300	-0.51479800	0.71377300
C	2.17196200	-1.70006900	1.50500900
C	2.91977900	-1.63583600	2.69873300
C	1.60768300	-2.92058600	1.10621800
C	3.07291000	-2.77504900	3.48243300
H	3.38334100	-0.69726600	2.98491900
C	1.76360800	-4.05432100	1.89941200
H	1.04959000	-2.96083000	0.18033500
C	2.49140700	-3.98551800	3.08880600
H	3.65309200	-2.72302800	4.39910000
H	1.31596200	-4.99087300	1.58291000
H	2.61356200	-4.87129500	3.70494800
O	3.70931200	2.54145000	0.71097300
Si	4.64286000	0.39384600	-1.45313800
Rh	1.53726400	-0.07279000	-1.27841900
Cl	1.26233100	0.02316400	-3.64837500
H	4.11898100	-1.90938700	-0.81578200
H	2.72641300	-1.67405000	-1.84406400
C	-1.97203100	1.19260400	1.35378800
C	-3.06156800	0.19433500	0.85493300
C	-2.49925100	-1.20404000	0.57649600
C	-2.30864200	-1.45344400	-0.95372400
H	-3.51281400	0.60099200	-0.05406200
H	-1.53043400	-1.34836700	1.06481900
P	-0.48849500	0.66885800	-0.99446300
O	-1.74918800	-0.23453800	-1.50579600
O	-0.75773900	0.93834500	0.59781000
C	-0.89684100	2.22794600	-1.82976000
C	-2.21518100	2.66928400	-2.00089000

C	0.16706500	3.06213100	-2.19346500
C	-2.46369300	3.94068100	-2.50981900
H	-3.04396900	2.03371800	-1.71909800
C	-0.08555700	4.33597100	-2.70082600
H	1.18396500	2.69917800	-2.09689900
C	-1.39984100	4.77756600	-2.85425200
H	-3.48719100	4.28228100	-2.62516500
H	0.74380000	4.97608500	-2.98530600
H	-1.59714600	5.77061700	-3.24683600
O	-3.45267200	-2.08758800	1.13177200
O	-4.08069300	0.00553000	1.81663800
C	-4.27855200	-1.39307600	2.07037800
C	-3.84195900	-1.72632500	3.49169400
H	-4.40874200	-1.12853100	4.20940600
H	-4.01890800	-2.78626100	3.69415700
H	-2.78084500	-1.51042900	3.62395700
C	-5.72941200	-1.74271800	1.77840100
H	-5.89361100	-2.81463300	1.91658300
H	-6.38939800	-1.19559600	2.45652600
H	-5.96766200	-1.47943700	0.74631300
C	-1.59562600	0.90457100	2.80609300
C	-0.51400400	0.07134300	3.10983600
C	-2.36475500	1.42866000	3.85124800
C	-0.21261400	-0.24610800	4.43543500
H	0.10156400	-0.31611900	2.31253700
C	-2.06319300	1.11232600	5.17425600
H	-3.20132700	2.07986800	3.62784900
C	-0.98886200	0.27065700	5.47218700
H	0.63160500	-0.89686500	4.64321200
H	-2.66991700	1.52461000	5.97502500

H	-0.75757800	0.02598100	6.50464200
C	-2.39685000	2.64406900	1.16950500
C	-1.41254200	3.63722400	1.12067200
C	-3.74120200	3.01072500	1.06073200
C	-1.75987600	4.96825300	0.91724400
H	-0.37206700	3.35265400	1.21957100
C	-4.09093600	4.34985700	0.87045300
H	-4.51832800	2.25757700	1.13220600
C	-3.10327700	5.32889200	0.78474800
H	-0.98309600	5.72389500	0.85409900
H	-5.13849700	4.62223600	0.78289800
H	-3.37563400	6.36712600	0.62127600
C	-1.39532400	-2.64354700	-1.22338600
C	-1.40900100	-3.76548300	-0.38435500
C	-0.57336500	-2.64490800	-2.35475400
C	-0.61562500	-4.87487600	-0.68242000
H	-2.03478700	-3.77448000	0.50078600
C	0.24689000	-3.73953500	-2.62723600
H	-0.55233300	-1.78526000	-3.01114700
C	0.22448500	-4.86146400	-1.79647100
H	-0.64499200	-5.74300900	-0.03051000
H	0.89925100	-3.70681900	-3.49421600
H	0.85599000	-5.71725000	-2.01505100
C	-3.65377000	-1.63031700	-1.66715200
C	-4.16031600	-0.63999200	-2.51493500
C	-4.40436200	-2.79796200	-1.47181200
C	-5.40394700	-0.79880300	-3.13046600
H	-3.57071400	0.24346200	-2.71529600
C	-5.64624400	-2.95226200	-2.08239500
H	-4.01891900	-3.58688900	-0.84047000

C	-6.15627200	-1.94996800	-2.91035900
H	-5.77630600	-0.01931000	-3.78850800
H	-6.21441100	-3.86230800	-1.91433300
H	-7.12358100	-2.07365200	-3.38794800

TS6

C	-6.10523800	-0.19204800	-0.68121700
C	-5.09256000	0.69340800	-0.27078800
C	-4.66547800	1.64179400	-1.21634000
C	-5.21852800	1.71476800	-2.49498200
C	-6.22230400	0.82138700	-2.86790800
C	-6.66284900	-0.14055800	-1.95874800
H	-6.46551700	-0.94546500	0.01306500
H	-4.85379300	2.47389500	-3.17991400
H	-6.65594100	0.87762800	-3.86197400
H	-7.44062700	-0.84377800	-2.24018900
C	-5.52155300	-0.36862100	2.68698200
C	-3.57986200	-1.33006600	1.66427000
C	-4.42982300	-1.44130700	2.94549900
H	-6.41019700	-0.79873900	2.21519600
H	-5.84497300	0.18507600	3.57221700
H	-4.80985700	-2.45601600	3.11684100
H	-3.81198300	-1.16107000	3.80224000
C	-3.87571900	2.19489500	2.20466400
H	-3.28213700	2.79840400	1.52097500
H	-4.81338700	2.73004800	2.40563200
H	-3.33796600	2.05102300	3.14381600
C	-2.33942300	2.04000800	-1.21864300
H	-2.20780800	2.01458400	-2.31035600
H	-1.64560300	2.76884100	-0.79579900

C	-2.10268300	0.69321600	-0.67352000
C	-2.00471200	-0.56339500	-0.77679100
C	-2.16459900	-1.78681500	-1.50995800
C	-2.86967200	-1.77170300	-2.73114300
C	-1.63288100	-2.99409500	-1.03429800
C	-3.01322700	-2.94490800	-3.46465400
H	-3.30915400	-0.84160600	-3.07718900
C	-1.78080900	-4.16325600	-1.77604400
H	-1.10490700	-2.99859400	-0.09043600
C	-2.46573500	-4.14291100	-2.99222200
H	-3.56001000	-2.92945700	-4.40291000
H	-1.35897600	-5.08919000	-1.39882100
H	-2.58073500	-5.05606100	-3.56841600
O	-3.65334100	2.53512400	-0.89702600
Si	-4.36738900	0.53376200	1.47079600
Rh	-1.63026900	-0.02501600	1.22068200
Cl	-1.30336900	0.18100600	3.59033000
H	-4.07420500	-1.78936200	0.80064400
H	-2.60469100	-1.83615500	1.74499900
C	1.97357800	1.14384900	-1.39200300
C	3.04038200	0.14987000	-0.83787000
C	2.45804800	-1.23197900	-0.52041700
C	2.24045800	-1.42309800	1.01426600
H	3.47965700	0.58276200	0.06475800
H	1.49531400	-1.38337700	-1.01871200
P	0.43427900	0.71790800	0.94247800
O	1.67616700	-0.18387500	1.50927800
O	0.74116400	0.93083900	-0.65373100
C	0.86270700	2.29845600	1.72727400
C	2.18594100	2.71783600	1.91457800

C	-0.18974500	3.17037600	2.02735400
C	2.45027100	4.00352200	2.37769900
H	3.00680600	2.05313000	1.68125600
C	0.07802400	4.45825100	2.48937900
H	-1.21088400	2.82742700	1.91515200
C	1.39754800	4.87699900	2.66008000
H	3.47805800	4.32746800	2.50546700
H	-0.74381300	5.12754500	2.72444600
H	1.60759700	5.88085200	3.01701200
O	3.41022200	-2.14438000	-1.03010000
O	4.07496100	-0.08333300	-1.77344900
C	4.25947400	-1.49138900	-1.97772000
C	3.84208100	-1.86766900	-3.39413700
H	4.42786400	-1.30128700	-4.12198100
H	4.00962900	-2.93586000	-3.55755500
H	2.78604500	-1.64440900	-3.55170100
C	5.70142000	-1.84793400	-1.65162400
H	5.85448000	-2.92583900	-1.75058800
H	6.37792900	-1.33238800	-2.33815900
H	5.92786000	-1.55186400	-0.62585400
C	1.62444500	0.81082100	-2.84181800
C	0.54388000	-0.02602400	-3.13999200
C	2.41812600	1.29457300	-3.88803500
C	0.26774900	-0.38607000	-4.46020400
H	-0.09016800	-0.38267500	-2.34282400
C	2.14159600	0.93588400	-5.20573600
H	3.25439200	1.94776400	-3.66943600
C	1.06817600	0.09104100	-5.49757700
H	-0.57533300	-1.03970000	-4.66366500
H	2.76738300	1.31741100	-6.00708500

H	0.85654900	-0.18704300	-6.52578100
C	2.41737700	2.59464600	-1.24905400
C	1.44872900	3.60404500	-1.25319100
C	3.76522400	2.94467600	-1.12828500
C	1.81331900	4.93597700	-1.08970200
H	0.40592600	3.33255700	-1.36254200
C	4.13280100	4.28409600	-0.97842200
H	4.53163800	2.17801100	-1.15923100
C	3.15960400	5.28059500	-0.94506900
H	1.04744500	5.70491900	-1.06710800
H	5.18287100	4.54320000	-0.88107400
H	3.44544000	6.31964400	-0.81271600
C	1.32307100	-2.60255800	1.31631200
C	1.35162800	-3.75852400	0.52510900
C	0.48877100	-2.56142600	2.43779000
C	0.56059200	-4.85884000	0.86057600
H	1.98756100	-3.80112200	-0.35168900
C	-0.32864900	-3.64833900	2.74708900
H	0.45560200	-1.67436800	3.05620800
C	-0.29157900	-4.80396400	1.96421800
H	0.60142300	-5.75311200	0.24568000
H	-0.98976000	-3.58400100	3.60576200
H	-0.92034600	-5.65377400	2.21213800
C	3.57114600	-1.57841700	1.76081900
C	4.04877400	-0.57191000	2.60634000
C	4.33244100	-2.74557500	1.60705900
C	5.27562900	-0.71350800	3.25863700
H	3.44903800	0.31100400	2.77589700
C	5.55785500	-2.88256100	2.25413700
H	3.96854400	-3.54766400	0.97975700

C	6.03987200	-1.86374200	3.07866600
H	5.62526000	0.07886500	3.91377100
H	6.13482000	-3.79235700	2.11749700
H	6.99423500	-1.97407700	3.58474300

B’

C	6.17227200	-0.01675400	0.35291700
C	5.01698300	0.76547200	0.19108100
C	4.64318900	1.56769300	1.28030900
C	5.37691100	1.61781600	2.46288600
C	6.52671100	0.83639900	2.58645000
C	6.92035500	0.01245400	1.53176900
H	6.49685200	-0.66265800	-0.45684200
H	5.04189900	2.26594800	3.26679400
H	7.10828400	0.87014300	3.50297800
H	7.81051800	-0.60259100	1.62396400
C	4.89721000	-0.26545400	-2.71883100
C	3.38196600	-1.75045700	-1.37614100
C	4.21605900	-1.64826100	-2.65235800
H	5.97264400	-0.31336300	-2.51436200
H	4.78304100	0.19362700	-3.70480000
H	4.95222100	-2.46483800	-2.68477900
H	3.56187300	-1.77012700	-3.51800600
C	3.90091800	2.58633200	-1.97791800
H	3.55476500	3.25095700	-1.18512900
H	4.92195900	2.88768200	-2.24705800
H	3.26788600	2.68267800	-2.86222900
C	2.30458400	1.62846300	1.55658900
H	2.27506200	1.48969200	2.64752900
H	1.47191700	2.26892200	1.26398500

C	2.18164400	0.30483200	0.92189600
C	2.02718400	-0.94261500	0.93059700
C	1.97471700	-2.21114200	1.60165900
C	2.50701500	-2.32018400	2.90221100
C	1.36561500	-3.32708600	1.01186400
C	2.41235300	-3.52242100	3.59586600
H	2.99320700	-1.45839200	3.34799400
C	1.27558800	-4.52695100	1.71237300
H	0.96077500	-3.24153900	0.01371300
C	1.79445200	-4.62900700	3.00392200
H	2.82637600	-3.60065700	4.59674200
H	0.79664000	-5.38085400	1.24457800
H	1.72322000	-5.56598800	3.54784000
O	3.48974200	2.33882700	1.18068400
Si	4.00783200	0.78722400	-1.41757800
Rh	1.87582400	-0.26458200	-1.09519300
Cl	1.62607600	0.22453500	-3.42751600
H	4.01763500	-1.84332200	-0.48996600
H	2.70379100	-2.61221300	-1.39340600
C	-1.96022200	1.15059400	1.41456400
C	-3.04611900	0.25636100	0.73822500
C	-2.52404400	-1.13274800	0.35775400
C	-2.23160900	-1.23383300	-1.17399200
H	-3.40791900	0.77225400	-0.15514500
H	-1.59966800	-1.37158600	0.89317800
P	-0.31346700	0.78492400	-0.86390700
O	-1.58487700	0.00195500	-1.55668000
O	-0.70005400	0.90674500	0.73125100
C	-0.62504500	2.43864300	-1.54702100
C	-1.90207600	2.94187500	-1.82544300

C	0.49023700	3.27385300	-1.65970600
C	-2.05591500	4.27350000	-2.19989900
H	-2.77133600	2.30480500	-1.72945900
C	0.33458700	4.60727800	-2.03540700
H	1.47449600	2.87206500	-1.46078200
C	-0.93941600	5.10789900	-2.30246200
H	-3.04845300	4.66470100	-2.39918600
H	1.20717800	5.24690000	-2.12534700
H	-1.06566000	6.14685500	-2.59211300
O	-3.54933400	-2.02092400	0.75596600
O	-4.14350900	0.02301700	1.59964800
C	-4.41679200	-1.38151900	1.69697600
C	-4.10522000	-1.87271600	3.10535200
H	-4.69978300	-1.32004400	3.83659700
H	-4.34192600	-2.93720400	3.18698500
H	-3.04926500	-1.72399200	3.33487800
C	-5.85414600	-1.63109500	1.26757300
H	-6.07180500	-2.70231200	1.28391900
H	-6.54105200	-1.12245200	1.94889000
H	-6.00232700	-1.25608500	0.25340200
C	-1.71463400	0.70721900	2.85563900
C	-0.70556700	-0.21499900	3.15547500
C	-2.53767200	1.17269900	3.88727200
C	-0.53144200	-0.67635400	4.46157200
H	-0.04813000	-0.56109300	2.37182500
C	-2.36167300	0.71377700	5.19106300
H	-3.31891800	1.89040200	3.66724800
C	-1.36125500	-0.21600900	5.48332400
H	0.25423400	-1.39729900	4.66664600
H	-3.00931300	1.08284000	5.98078700

H	-1.22846100	-0.57336500	6.50016000
C	-2.32286800	2.62933900	1.33861700
C	-1.31295700	3.58855100	1.46780800
C	-3.64273200	3.05427700	1.15758000
C	-1.60467800	4.94454800	1.36757900
H	-0.29240700	3.26402700	1.62797100
C	-3.93866800	4.41671400	1.07239100
H	-4.44496400	2.32760000	1.09326100
C	-2.92132500	5.36417800	1.16294600
H	-0.80389400	5.67355700	1.44149800
H	-4.96760300	4.73251500	0.92810400
H	-3.15021300	6.42230400	1.08042300
C	-1.35580000	-2.43849100	-1.50030300
C	-1.52132600	-3.65563700	-0.82417600
C	-0.42590900	-2.35694500	-2.54123900
C	-0.77669800	-4.77362700	-1.20133600
H	-2.22717600	-3.72995000	-0.00494000
C	0.34985500	-3.46525300	-2.88439700
H	-0.29634600	-1.42848500	-3.07999100
C	0.17091000	-4.68066400	-2.22297600
H	-0.92576000	-5.71469500	-0.68016000
H	1.08897400	-3.36675100	-3.67303500
H	0.76458000	-5.54697500	-2.49822100
C	-3.52369500	-1.27669800	-2.00162400
C	-3.88925800	-0.20504400	-2.82296100
C	-4.35865700	-2.40201900	-1.95510000
C	-5.07795600	-0.24170500	-3.55511700
H	-3.23086900	0.64730000	-2.91036900
C	-5.54619800	-2.43462800	-2.68183800
H	-4.08364900	-3.25396100	-1.34921100

C	-5.91639800	-1.35119600	-3.48108800
H	-5.33942600	0.60055300	-4.18878000
H	-6.18115600	-3.31387800	-2.62686800
H	-6.84138700	-1.38006600	-4.04908700

TS7

C	-6.09708900	0.40322700	1.20635900
C	-4.77452200	0.71132400	0.80652400
C	-4.62750900	1.93277600	0.12294000
C	-5.72038500	2.75189200	-0.19183300
C	-7.00013400	2.39687000	0.20686000
C	-7.19013000	1.21682600	0.92945000
H	-6.27938900	-0.51569700	1.75370500
H	-5.52665700	3.67109600	-0.73487100
H	-7.84095700	3.04039800	-0.03421600
H	-8.18083200	0.92717700	1.26534500
C	-4.57150400	-2.26469100	1.08056400
C	-2.64609600	-2.86460100	-0.35081100
C	-3.65212100	-3.40883000	0.65096900
H	-5.29470000	-2.05038600	0.28483500
H	-5.15050700	-2.50428400	1.98121100
H	-4.23801300	-4.22686700	0.20362500
H	-3.12805400	-3.82001600	1.51508300
C	-3.14449800	-0.32462300	3.14673900
H	-2.51142500	0.55602700	3.27805200
H	-4.08783200	-0.14285300	3.67617300
H	-2.62577500	-1.17878200	3.58615600
C	-2.27440500	1.83084700	0.24636800
C	-2.12989400	0.44607800	-0.27945400
C	-1.94439000	-0.26757900	-1.32145200

C	-2.17869300	-0.46832200	-2.71969200
C	-2.99794900	0.45455800	-3.40395100
C	-1.60702200	-1.53745700	-3.42868700
C	-3.21422900	0.31401800	-4.77054900
H	-3.43846900	1.27451600	-2.84690000
C	-1.82796200	-1.66929200	-4.79662000
H	-1.00827700	-2.25754000	-2.88788300
C	-2.62716400	-0.74409100	-5.47237700
H	-3.84466400	1.02851600	-5.29149400
H	-1.38064000	-2.49823300	-5.33700700
H	-2.79968900	-0.85057800	-6.53901700
O	-3.42572300	2.44638400	-0.29899200
Si	-3.53550100	-0.67515700	1.33358100
Rh	-1.40507500	-1.34524100	0.43230900
Cl	-0.84870100	-2.83891900	2.23278000
H	-1.87743000	-3.59582000	-0.62932700
H	-3.15873200	-2.52607300	-1.25593800
H	-2.32292200	1.84255200	1.34117600
H	-1.42606800	2.43028800	-0.07180600
C	1.66335200	2.09613400	-0.16008700
C	2.66841300	1.06801700	-0.75350300
C	2.15099300	-0.32062500	-1.16662000
C	2.42192600	-1.41215500	-0.09457000
H	3.46725900	0.94489700	-0.01719000
H	1.06695900	-0.31035300	-1.33226000
P	0.49972600	-0.08145600	1.32117000
O	1.94860200	-0.85413600	1.16318400
O	0.77967200	1.47152600	0.80787500
C	0.58222500	0.22586000	3.11330400
C	1.11225400	-0.73377200	3.98379000

C	0.02665700	1.40524600	3.63015800
C	1.09702300	-0.50474300	5.35910300
H	1.52535800	-1.65005200	3.58301300
C	0.01266300	1.62730800	5.00613500
H	-0.36801600	2.15673300	2.95447100
C	0.54601400	0.67070600	5.87196200
H	1.51204100	-1.24949500	6.03131800
H	-0.41190700	2.54562300	5.40015100
H	0.53232800	0.84163700	6.94420800
O	2.80224700	-0.58851700	-2.39707800
O	3.19024000	1.61066100	-1.95671500
C	3.62613800	0.53564700	-2.77578100
C	3.33205400	0.88194500	-4.22586200
H	3.90500600	1.76392100	-4.52257500
H	3.61232000	0.04673900	-4.87239500
H	2.26894900	1.09267300	-4.35082200
C	5.10063700	0.23519400	-2.52612000
H	5.39939000	-0.66896600	-3.06091600
H	5.70523700	1.07460200	-2.88037300
H	5.29671500	0.08559700	-1.46439900
C	0.74081100	2.76328000	-1.18416200
C	0.19939100	4.01942600	-0.87313000
C	0.31367600	2.12979300	-2.35663100
C	-0.74126400	4.62410500	-1.70577600
H	0.51165400	4.52140500	0.03533500
C	-0.61783200	2.73816800	-3.19757400
H	0.69715200	1.16038000	-2.63718600
C	-1.15379800	3.98382100	-2.87375400
H	-1.15336400	5.59159500	-1.43641900
H	-0.93387300	2.22396600	-4.09819500

H	-1.88735400	4.44960700	-3.52452900
C	2.52692600	3.12404100	0.57891400
C	2.66311000	3.09597900	1.96785500
C	3.27240100	4.05140400	-0.16260300
C	3.51986000	3.99262700	2.61063200
H	2.09737300	2.38059100	2.54810100
C	4.12786800	4.94251700	0.48098500
H	3.18206700	4.06628100	-1.24225500
C	4.25359000	4.91885000	1.87193500
H	3.60809900	3.96234000	3.69268700
H	4.69676900	5.65762700	-0.10582200
H	4.91806300	5.61670000	2.37261100
C	1.70857500	-2.72052000	-0.41071100
C	1.14804100	-2.98425200	-1.66515600
C	1.69829800	-3.72457700	0.56326900
C	0.57066400	-4.22863600	-1.93113000
H	1.19660100	-2.24209600	-2.45164800
C	1.11419900	-4.95839200	0.30224100
H	2.13222800	-3.52262700	1.53506900
C	0.54566100	-5.21491400	-0.94741700
H	0.14383400	-4.42410200	-2.91048500
H	1.08887200	-5.71508600	1.07914900
H	0.08959000	-6.17866300	-1.15194000
C	3.91180800	-1.66592100	0.10632100
C	4.63210100	-1.01522500	1.11421700
C	4.58468400	-2.54079200	-0.75567900
C	6.00707500	-1.22201400	1.24351300
H	4.11289800	-0.35934600	1.80222600
C	5.95532000	-2.74804700	-0.62281200
H	4.03130000	-3.05306400	-1.53342000

C	6.67346100	-2.08504600	0.37428800
H	6.55328100	-0.70969800	2.02976000
H	6.46342300	-3.42815900	-1.29982600
H	7.74222300	-2.24666400	0.47729200

C'

C	-6.71172000	0.04900800	0.68133900
C	-5.31970900	0.24492300	0.74486400
C	-4.85325900	1.57612200	0.69235800
C	-5.74607600	2.64964800	0.56828200
C	-7.11459300	2.41407100	0.50526000
C	-7.60828600	1.10755100	0.56525900
H	-7.09819200	-0.96722300	0.71300500
H	-5.34212100	3.65597100	0.52795200
H	-7.79795200	3.25324600	0.41259800
H	-8.67638200	0.92030500	0.51755800
C	-4.47898800	-2.58835100	-0.39467100
C	-2.02306200	-3.07393600	-0.96264500
C	-3.32467600	-3.61725600	-0.39046900
H	-4.62420700	-2.18355400	-1.40476900
H	-5.42281400	-3.07346400	-0.11406800
H	-3.63303300	-4.49496400	-0.98036000
H	-3.14504100	-3.98119300	0.62667400
C	-3.90261600	-1.85020000	2.55600200
H	-3.76032800	-1.03560200	3.27231800
H	-4.79303800	-2.41084700	2.86260900
H	-3.02975400	-2.50845700	2.60629400
C	-2.52183300	1.01827400	1.12955300
C	-2.55785700	-0.25910000	0.30726700
C	-1.94495200	-0.37835900	-0.95100700

C	-2.25139900	-0.00593900	-2.29563300
C	-3.38337200	0.78533700	-2.58101800
C	-1.42706700	-0.44727200	-3.35101400
C	-3.68364600	1.11794400	-3.89755500
H	-4.00515200	1.13132000	-1.76448300
C	-1.73149900	-0.11104500	-4.66275100
H	-0.56697300	-1.05973500	-3.10716500
C	-2.86089800	0.67110100	-4.93543700
H	-4.55643300	1.72442400	-4.11774400
H	-1.09920300	-0.45449600	-5.47557600
H	-3.09975400	0.93178800	-5.96242700
O	-3.53036100	1.94652400	0.70231700
Si	-4.11045100	-1.19646800	0.80698400
Rh	-0.94712400	-1.57487500	0.10820700
Cl	-0.53934000	-3.33553500	1.79546700
H	-1.23919500	-3.83559500	-0.93314600
H	-2.16957900	-2.75794300	-2.00096100
H	-2.67158800	0.78390900	2.19079400
H	-1.58327100	1.55344000	1.01280000
C	1.47924300	2.15351400	0.21407300
C	2.69500900	1.41641000	-0.40085000
C	2.39470900	0.10136500	-1.14416500
C	2.70262500	-1.18299700	-0.32086700
H	3.40135700	1.23772500	0.41673500
H	1.33159800	0.04814200	-1.40179600
P	0.69028200	-0.35549700	1.31472200
O	2.20537400	-0.94030900	1.02019600
O	0.85921300	1.29261300	1.19922000
C	0.73892500	-0.41267500	3.13139100
C	1.37541800	-1.46900900	3.79404400

C	0.07333500	0.57522900	3.87064800
C	1.35831600	-1.52341200	5.18675700
H	1.87247200	-2.24034900	3.22095100
C	0.05498600	0.51104400	5.26325200
H	-0.40673800	1.40243500	3.36010500
C	0.69698500	-0.53874200	5.92233500
H	1.85531900	-2.34267600	5.69713500
H	-0.45566300	1.28266900	5.83154400
H	0.68124300	-0.58932600	7.00699400
O	3.14699300	0.18964900	-2.34636200
O	3.27643400	2.24863200	-1.39328700
C	3.91368400	1.41446300	-2.34991700
C	3.78866500	2.05649300	-3.72215500
H	4.32082100	3.01068900	-3.73481600
H	4.22611900	1.40101700	-4.47913800
H	2.74063700	2.23549200	-3.96612800
C	5.36804000	1.16449100	-1.96173300
H	5.82007600	0.43284500	-2.63413200
H	5.92300100	2.10406500	-2.03080500
H	5.44829300	0.78630600	-0.94329800
C	0.40215100	2.62945100	-0.76559100
C	-0.63683500	3.40432500	-0.22784500
C	0.38922500	2.36671100	-2.13848200
C	-1.66602200	3.88803000	-1.02923800
H	-0.62571200	3.63718900	0.83168200
C	-0.62953100	2.87141600	-2.94892400
H	1.16916200	1.78030200	-2.59800800
C	-1.66083200	3.62863000	-2.40050300
H	-2.46889800	4.46283000	-0.58085700
H	-0.62271200	2.64858200	-4.01056500

H	-2.45746000	4.00627400	-3.03337700
C	2.04096100	3.34341300	1.00233700
C	2.30014800	3.23742300	2.37162800
C	2.36503500	4.52926900	0.33252300
C	2.86423300	4.31042400	3.06450000
H	2.04777200	2.32322100	2.89429800
C	2.93348800	5.59555100	1.02552900
H	2.17332900	4.61033000	-0.73080500
C	3.18245000	5.49155200	2.39568200
H	3.05141400	4.21906800	4.13042400
H	3.17897200	6.51057200	0.49464800
H	3.61937300	6.32594000	2.93627000
C	2.03604300	-2.41029400	-0.93857200
C	1.58811100	-2.42552000	-2.26791000
C	1.98023200	-3.59220100	-0.19166000
C	1.08608600	-3.59989900	-2.83067900
H	1.67706100	-1.53761300	-2.88239300
C	1.46990500	-4.75981600	-0.74991200
H	2.31564300	-3.58476200	0.83746000
C	1.02282800	-4.76840200	-2.07244100
H	0.74565700	-3.59801600	-3.86179800
H	1.40356000	-5.65622800	-0.14321600
H	0.62424600	-5.67974500	-2.50740100
C	4.19862800	-1.42439600	-0.15765600
C	4.87639800	-1.00628800	0.99269700
C	4.91895700	-2.04381400	-1.18621900
C	6.25665400	-1.18808300	1.10240200
H	4.31947400	-0.55235100	1.80274400
C	6.29500300	-2.22568900	-1.07371200
H	4.39911300	-2.37802300	-2.07600200

C	6.97084700	-1.79325200	0.06905700
H	6.76991000	-0.85910400	2.00098900
H	6.84048900	-2.70695500	-1.87996300
H	8.04373800	-1.93570200	0.15625200

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C	-9.09010600	0.91816700	0.69320100
C	-7.86892000	0.39831200	1.11381000
C	-6.79526300	0.19072400	0.22855200
C	-7.00988700	0.51393100	-1.12504900
C	-8.22982700	1.04580900	-1.56252200
C	-9.26229400	1.25056800	-0.65407100
H	-9.89771900	1.06770100	1.40322800
H	-7.73622900	0.15517100	2.16633100
H	-8.34410600	1.28235600	-2.61532600
H	-10.20717800	1.66042800	-0.99948900
O	-6.05359200	0.36747100	-2.10092500
C	-5.10571400	-0.70587100	-1.94884400
H	-5.67079000	-1.64595400	-1.85061600
H	-4.56304000	-0.71983500	-2.89632300
C	-4.18593900	-0.51650100	-0.76311900
C	-2.87654700	-0.24273400	-0.92347300
C	-2.41515700	1.59163100	-0.13979900
C	-4.31076200	1.15604500	1.70601700
C	-3.69265000	2.04326400	0.60772400
H	-5.09655300	1.72819900	2.21440600
H	-3.57281400	0.86418900	2.45217700
H	-3.45671400	3.02558000	1.03805500
Si	-5.09851000	-0.33748300	0.85884500
C	-5.26185900	-1.90054400	1.89213900

H	-4.27361300	-2.24964400	2.19776100
H	-5.85872000	-1.71076600	2.79132900
H	-5.76217900	-2.68785400	1.31915800
C	-2.00552000	-0.50791600	-2.07263700
C	-0.89954000	0.33983300	-2.36519300
C	-2.06340100	-1.76919700	-2.73445000
C	0.11514300	-0.09148900	-3.24992900
H	-0.88445500	1.37460400	-2.06265300
C	-1.08279300	-2.15358300	-3.62303800
H	-2.89141900	-2.42940900	-2.50363400
C	0.03216000	-1.32310200	-3.86828600
H	0.93979100	0.57771500	-3.46069000
H	-1.15990400	-3.11262200	-4.12719300
H	0.80667200	-1.64575300	-4.55577700
H	-4.46553400	2.22170500	-0.15061200
Rh	-1.17488900	-0.11145200	0.09802600
Cl	-1.84604600	-0.95667300	2.17284600
C	2.96077300	1.53824400	-0.53443200
C	3.49692700	0.07097600	-0.63121600
C	2.45186900	-1.06060100	-0.69858400
C	2.19682600	-1.73898100	0.68259200
H	4.14535000	-0.07415800	0.23793300
H	1.50150800	-0.67255400	-1.07879200
P	0.90416500	0.53328800	1.16579700
O	1.95469600	-0.66177400	1.62958700
O	1.97632400	1.62033200	0.50471800
C	0.77555600	1.44739800	2.73315100
C	-0.46220700	1.90468700	3.19697400
C	1.94688700	1.76835100	3.43690700
C	-0.52951700	2.66799400	4.36399800

H	-1.36670700	1.64852300	2.66159600
C	1.87327000	2.52042000	4.60520500
H	2.90851600	1.44334900	3.05601200
C	0.63371900	2.97118300	5.07002500
H	-1.49301700	3.01769700	4.72176800
H	2.78066300	2.76208300	5.15053000
H	0.57865600	3.56134800	5.98010400
O	2.96510900	-1.98596400	-1.64020800
O	4.24157600	-0.10797400	-1.82701300
C	4.15231000	-1.46565700	-2.25009800
C	3.97340100	-1.47758000	-3.76051100
H	3.83020800	-2.50265900	-4.11117700
H	3.10001500	-0.87912100	-4.02513500
H	4.85513200	-1.05806600	-4.25206100
C	5.37713000	-2.24272000	-1.78058400
H	5.26131300	-3.30497800	-2.00781900
H	6.26919500	-1.86612200	-2.28889300
H	5.50961800	-2.13510900	-0.70348800
C	2.36427100	2.14174200	-1.81679500
C	3.06224000	2.15496000	-3.03495800
C	1.15181600	2.83765200	-1.74171600
C	2.52151100	2.78262100	-4.15666200
H	4.02600100	1.67467500	-3.10666400
C	0.61833900	3.47731500	-2.86170300
H	0.62354800	2.88038600	-0.79875600
C	1.29208000	3.43938700	-4.08080100
H	3.07251400	2.76581400	-5.09240000
H	-0.32763500	4.00418700	-2.77540600
H	0.87502300	3.92899800	-4.95534100
C	4.09569800	2.47058400	-0.06674000

C	3.78885300	3.56030800	0.75716200
C	5.42159900	2.27835300	-0.47163300
C	4.78952300	4.43602400	1.17347300
H	2.76732800	3.70592600	1.08513900
C	6.42108600	3.15898000	-0.05386300
H	5.67775800	1.44090700	-1.10901400
C	6.11111300	4.24036100	0.76919200
H	4.53425000	5.27193100	1.81817800
H	7.44597500	2.99199300	-0.37228300
H	6.89068100	4.92260700	1.09471500
C	0.98546400	-2.66275700	0.69677400
C	0.18481700	-2.90079500	-0.42345700
C	0.65788300	-3.27506200	1.91358400
C	-0.92353700	-3.75137700	-0.32240200
H	0.43770200	-2.47536600	-1.38592500
C	-0.44809900	-4.10829100	2.01219900
H	1.27089400	-3.07622100	2.78575200
C	-1.24449700	-4.35106500	0.88935700
H	-1.53186600	-3.93404000	-1.20003500
H	-0.69748500	-4.56220900	2.96605800
H	-2.11158300	-4.99990100	0.96475500
C	3.43746600	-2.47431800	1.16941300
C	4.34486200	-1.87204900	2.04619100
C	3.69741700	-3.76924400	0.70344400
C	5.50505900	-2.54598100	2.43428500
H	4.13028400	-0.88470100	2.43611800
C	4.85230100	-4.44190300	1.09402700
H	2.99253200	-4.24270300	0.03053100
C	5.76448400	-3.83005000	1.95672500
H	6.20045400	-2.06639300	3.11657400

H	5.04109800	-5.44509500	0.72376900
H	6.66514900	-4.35468700	2.26102700
H	-1.58236200	2.20967100	0.23191500
H	-2.52852900	1.87693400	-1.18637500

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C	7.20701500	-2.79349500	-1.94705600
C	5.81913500	-2.65269100	-1.87663200
C	5.20888100	-2.06843700	-0.75997200
C	6.03796500	-1.60231700	0.27634500
C	7.42449500	-1.73346900	0.22216500
C	8.00452700	-2.33861800	-0.89435000
H	7.66512600	-3.25815100	-2.81504700
H	5.20453600	-3.01250000	-2.69869200
H	8.02487500	-1.36891700	1.04920500
H	9.08397600	-2.44850600	-0.94443400
O	5.46445700	-1.06013000	1.41063500
C	4.69896200	0.15261400	1.23288200
H	4.31146000	0.37498700	2.22839700
H	5.38132700	0.95681900	0.92922500
C	3.56805000	0.00418600	0.23209500
C	3.05711500	1.10975500	-0.46935300
C	2.02037800	0.84655000	-1.53777600
C	2.38516400	-1.63550300	-2.04290000
C	2.36895200	-0.20710900	-2.60640000
H	2.77244100	-2.33501000	-2.79287800
H	1.35784200	-1.94838600	-1.82568000
H	1.65000000	-0.12618000	-3.43019300
Si	3.38714300	-1.74415100	-0.44622100
C	2.69783700	-3.02783400	0.73790900

H	2.93466500	-4.03602600	0.38012700
H	3.14364900	-2.90193100	1.72841600
H	1.61370300	-2.93141100	0.82787800
C	3.58006700	2.49296200	-0.33182200
C	3.89575800	3.23428500	-1.48028900
C	3.78000200	3.08263900	0.92595000
C	4.40854500	4.52659000	-1.37758400
H	3.75256900	2.79157900	-2.46160900
C	4.28858700	4.37568500	1.02771500
H	3.48208200	2.54150400	1.81758000
C	4.60646700	5.10284700	-0.12166200
H	4.65365700	5.08220100	-2.27789400
H	4.42523800	4.82074800	2.00883000
H	5.00247800	6.11049300	-0.03928100
H	3.35087000	0.05172200	-3.01982400
Rh	1.38929300	0.42586100	0.71271900
Cl	1.79799800	0.63155800	3.00102300
C	-2.40883200	-1.56813300	-0.80050200
C	-3.40326200	-0.37195100	-0.65846400
C	-2.72930600	0.96049200	-0.99556400
C	-2.34288800	1.75594200	0.29464100
H	-3.79728300	-0.35827000	0.36058700
H	-1.81345400	0.78915900	-1.56350600
P	-0.71217700	-0.30398000	1.07857700
O	-1.94980100	0.76756900	1.28055700
O	-1.11561200	-1.13347700	-0.29859500
C	-1.13054100	-1.40555000	2.46321200
C	-0.10044000	-2.15610000	3.04253500
C	-2.45346800	-1.60479100	2.88296600
C	-0.39512100	-3.11397200	4.01267900

H	0.92476500	-1.97383000	2.74796000
C	-2.74291500	-2.56067800	3.85127700
H	-3.25532700	-1.03045500	2.43851500
C	-1.71438400	-3.32121100	4.41304400
H	0.40921600	-3.69003100	4.45960200
H	-3.77144200	-2.72087200	4.15838700
H	-1.94347800	-4.07019300	5.16536200
O	-3.64741800	1.64510700	-1.82197800
O	-4.46960500	-0.48524300	-1.57842600
C	-4.75518600	0.79419900	-2.15301800
C	-4.81611500	0.62935800	-3.66382300
H	-3.86803900	0.22370700	-4.02307200
H	-5.62010000	-0.05972600	-3.93507300
H	-5.00269700	1.59528300	-4.14041300
C	-6.02699600	1.36476400	-1.53807100
H	-6.21089800	2.37229300	-1.91896400
H	-6.88053300	0.72872900	-1.78829600
H	-5.92599100	1.42064200	-0.45253500
H	1.01571500	0.45680400	-1.07131300
H	1.68912100	1.78797700	-1.97805700
C	-2.18433200	-1.87233800	-2.28231100
C	-1.14054400	-1.26831000	-2.98956100
C	-3.07128500	-2.70696200	-2.97195000
C	-0.98775100	-1.48652500	-4.35968000
H	-0.43848800	-0.63905600	-2.46137900
C	-2.92080200	-2.92433600	-4.33945700
H	-3.88318600	-3.18342500	-2.43614600
C	-1.87948700	-2.31299000	-5.04109300
H	-0.16709900	-1.01240000	-4.89035600
H	-3.61906900	-3.57402200	-4.85847600

H	-1.76219900	-2.48533500	-6.10667400
C	-2.87000200	-2.80293600	-0.03954700
C	-4.21720600	-3.01332200	0.26777900
C	-1.92177600	-3.75517300	0.35042600
C	-4.60565000	-4.14911200	0.98204400
H	-4.96556900	-2.29764200	-0.05561600
C	-2.30780500	-4.87879900	1.07365700
H	-0.87765900	-3.59089800	0.10996500
C	-3.65262200	-5.07737000	1.39638100
H	-5.65454600	-4.30056700	1.21915600
H	-1.55801700	-5.59472800	1.39528000
H	-3.95327800	-5.95192500	1.96531300
C	-1.20364400	2.73336300	0.03884000
C	-0.96275200	3.25778700	-1.23554500
C	-0.40369600	3.14624200	1.11253200
C	0.06948100	4.17975700	-1.43268700
H	-1.59041200	2.96717200	-2.07181600
C	0.62362700	4.06366000	0.91072700
H	-0.57689900	2.73577600	2.10025600
C	0.86719900	4.58143100	-0.36247500
H	0.24634500	4.58211900	-2.42603300
H	1.25229800	4.35297300	1.74478700
H	1.68582100	5.27531100	-0.51781800
C	-3.56144900	2.46437900	0.87832700
C	-4.26450100	1.92890000	1.96150800
C	-4.02211300	3.64817700	0.28831200
C	-5.42085200	2.55490600	2.43335000
H	-3.89432200	1.03703100	2.44900700
C	-5.17469800	4.27065800	0.75922600
H	-3.47843600	4.07773700	-0.54403500

C	-5.88376000	3.72297900	1.83064700
H	-5.95300000	2.12821700	3.27836600
H	-5.51964600	5.18655400	0.28880500
H	-6.78257200	4.20935800	2.19751000

TS9

C	8.32949800	1.25156100	0.13793700
C	7.06873300	1.60521900	-0.34837400
C	6.07644400	0.63931000	-0.55416500
C	6.37755200	-0.69763100	-0.23013200
C	7.63034500	-1.06609600	0.25832500
C	8.60744900	-0.08462100	0.43439900
H	9.09199100	2.01124600	0.28184000
H	6.85938500	2.64739100	-0.57893300
H	7.82400800	-2.10951100	0.48460000
H	9.58715800	-0.36492900	0.81059100
O	5.44678000	-1.68767700	-0.47232000
C	4.18693500	-1.61803700	0.23585100
H	3.57818700	-2.39676300	-0.23056300
H	4.36212900	-1.87802200	1.28766900
C	3.50565000	-0.27255100	0.12283000
C	2.67207500	0.21756800	1.13895000
C	2.03087800	1.50573200	0.91457400
C	3.61376700	2.60508700	-0.83858600
C	2.86589000	2.72265600	0.50181600
H	1.28186500	1.75104300	1.65379900
H	4.39479700	3.37171200	-0.90110500
H	2.91307900	2.80679200	-1.65851500
H	2.20970200	3.59839100	0.49384800
Si	4.31064000	0.87486700	-1.13674500

C	4.09806700	0.32936400	-2.91812600
H	4.38775800	-0.71917200	-3.02205500
H	3.05187900	0.41872100	-3.22301300
H	4.72244000	0.93522400	-3.58458100
C	2.31293100	-0.53763400	2.37081200
C	2.46490900	0.08918300	3.61509800
C	1.79941300	-1.84129500	2.32165900
C	2.11900700	-0.57400600	4.79165100
H	2.85332500	1.10209000	3.65545700
C	1.44298800	-2.49780800	3.49896900
H	1.64238000	-2.32001000	1.36067800
C	1.60197000	-1.86939600	4.73552500
H	2.24984900	-0.07911200	5.74963200
H	1.03566200	-3.50227600	3.44951700
H	1.32404500	-2.38588900	5.64938400
H	1.20596800	1.59237700	-0.58246600
H	3.58724200	2.88625500	1.31415000
Rh	1.32041000	0.04353700	-0.56213500
Cl	1.47152400	-2.00945200	-1.74159000
C	-2.35026300	1.76247000	0.49025000
C	-3.12030300	0.45393900	0.79423700
C	-2.34482500	-0.87701400	0.91413900
C	-2.34388100	-1.72514300	-0.38752200
H	-3.87102600	0.36049100	0.00364000
H	-1.29555700	-0.70778700	1.18747900
P	-0.76561100	0.36076800	-1.33710500
O	-1.84049000	-0.87237000	-1.45359200
O	-1.67766100	1.61640100	-0.78069200
C	-0.76470600	0.84333800	-3.08860900
C	-0.46583200	-0.13140700	-4.05178300

C	-0.96002200	2.17557700	-3.47578100
C	-0.38563900	0.22794500	-5.39567300
H	-0.27826300	-1.15298900	-3.74154300
C	-0.87436600	2.52620300	-4.82353700
H	-1.18720100	2.92604400	-2.72761500
C	-0.58910900	1.55438900	-5.78369200
H	-0.15693500	-0.52838600	-6.14025400
H	-1.03232800	3.55831700	-5.12214500
H	-0.52118100	1.83018500	-6.83183900
O	-3.00003600	-1.55587600	1.97781400
O	-3.75078100	0.58829500	2.05949500
C	-4.02937200	-0.71820600	2.54123600
C	-3.88157400	-0.72238900	4.05410500
H	-2.87083000	-0.42229500	4.33608600
H	-4.59712100	-0.02814100	4.50145600
H	-4.07373100	-1.72522300	4.44313800
C	-5.41410900	-1.17049000	2.08739500
H	-5.57277700	-2.21993000	2.34441000
H	-6.17406100	-0.56221000	2.58558000
H	-5.53038400	-1.06276100	1.00911300
C	-3.42533600	2.83318500	0.25012800
C	-3.90334300	3.08566200	-1.03929300
C	-3.99576900	3.50775900	1.33551700
C	-4.92439100	4.01593800	-1.24157900
H	-3.46933500	2.56090600	-1.88134800
C	-5.01925500	4.43069000	1.13142300
H	-3.63918200	3.30435900	2.33815200
C	-5.48489500	4.69191500	-0.15865800
H	-5.27968000	4.21004200	-2.24934800
H	-5.45196000	4.94823500	1.98237300

H	-6.27852900	5.41596800	-0.31691900
C	-1.36368200	2.24830900	1.55123800
C	-1.07273300	1.56814800	2.73620100
C	-0.76797000	3.49989500	1.33280600
C	-0.23050100	2.13919700	3.69448300
H	-1.50820400	0.60224400	2.93753500
C	0.07201200	4.07009400	2.28482800
H	-0.98904400	4.03425400	0.41493900
C	0.33745700	3.39292100	3.47853200
H	-0.01613800	1.58935000	4.60421700
H	0.51313300	5.04478700	2.09996500
H	0.98541400	3.83770700	4.22765200
C	-3.75970300	-2.11352200	-0.81236000
C	-4.48443900	-1.34200900	-1.72719800
C	-4.36003600	-3.24975500	-0.25583100
C	-5.79520500	-1.68819500	-2.06141600
H	-4.01408900	-0.48129600	-2.18692100
C	-5.66596900	-3.59664300	-0.59369300
H	-3.79989500	-3.85722500	0.44454100
C	-6.39149600	-2.81377000	-1.49362900
H	-6.34498700	-1.07909000	-2.77265200
H	-6.11760900	-4.48027000	-0.15276300
H	-7.40955700	-3.08457400	-1.75685100
C	-1.48178700	-2.97702400	-0.28756000
C	-1.30524900	-3.73398100	-1.45225400
C	-0.92143400	-3.42706600	0.90807200
C	-0.56856600	-4.91102900	-1.42901800
H	-1.74250500	-3.38184000	-2.38026600
C	-0.18246300	-4.61363700	0.93133100
H	-1.06942100	-2.87617000	1.82808000

C	0.00012600	-5.35484700	-0.23290100
H	-0.42805500	-5.47814600	-2.34385700
H	0.24412700	-4.96236800	1.86718900
H	0.57718600	-6.27435500	-0.21038500

D’

C	8.08964500	-1.64585000	-0.36040900
C	6.86855400	-1.80962200	0.29816200
C	6.01550500	-0.72237500	0.51967000
C	6.41113600	0.53976700	0.03333700
C	7.62523700	0.71798000	-0.62863500
C	8.46586700	-0.38077600	-0.81681200
H	8.74555100	-2.49754000	-0.51426600
H	6.58099200	-2.79737000	0.65131100
H	7.89716300	1.70897700	-0.97716900
H	9.41533900	-0.24789400	-1.32751500
O	5.62868400	1.64869900	0.28523600
C	4.28208100	1.67670800	-0.25561200
H	3.80449100	2.50818900	0.26920000
H	4.34675900	1.91370200	-1.32406200
C	3.51468800	0.39584000	-0.01271600
C	2.70647100	-0.20008500	-1.00295700
C	1.92550600	-1.36117000	-0.65539800
C	3.39362800	-2.34577100	1.29619600
C	2.50626900	-2.57827700	0.05306100
H	1.20841100	-1.64397500	-1.41434800
H	4.08989400	-3.18431600	1.41710800
H	2.76616300	-2.35008500	2.19682900
H	1.67608100	-3.24305300	0.31078200
Si	4.31126900	-0.69478700	1.29890300

C	4.35287000	0.07677300	3.00739400
H	4.88091300	1.03298400	2.96913700
H	3.33842700	0.26900700	3.36706800
H	4.86993700	-0.57845500	3.71721200
C	2.37613900	0.48023800	-2.28885100
C	2.51969100	-0.22879500	-3.48888400
C	1.88127700	1.79246700	-2.32665400
C	2.19273400	0.36463900	-4.70610000
H	2.88657200	-1.24940000	-3.45742200
C	1.52925300	2.37527400	-3.54486500
H	1.75097500	2.35275700	-1.40432100
C	1.68900000	1.66720700	-4.73615500
H	2.32351700	-0.19060800	-5.63036800
H	1.13666200	3.38628400	-3.56203400
H	1.42419500	2.12768800	-5.68317300
H	1.67298800	-0.58799600	1.70483400
H	3.09102400	-3.11943400	-0.70546900
Rh	1.29282200	0.31805700	0.57835800
Cl	1.52213200	2.32415300	1.87088500
C	-2.27436400	-1.85036700	-0.44767300
C	-3.12682000	-0.60043100	-0.78183100
C	-2.41724900	0.75453300	-0.98661400
C	-2.44319600	1.66738600	0.27043100
H	-3.85738400	-0.50595100	0.02727800
H	-1.36255500	0.61074400	-1.25398700
P	-0.75898700	-0.25996100	1.30897000
O	-1.96498100	0.85921300	1.38041300
O	-1.54066800	-1.61216200	0.77699600
C	-0.72671200	-0.70449800	3.07093700
C	-0.46268400	0.30949100	4.00335300

C	-0.86334000	-2.03210400	3.49627800
C	-0.36316400	-0.00709900	5.35663500
H	-0.30733000	1.32752100	3.66342700
C	-0.75620500	-2.33982100	4.85322200
H	-1.05779800	-2.81222600	2.77012500
C	-0.50974400	-1.32924300	5.78347500
H	-0.16090800	0.77908100	6.07750900
H	-0.86632000	-3.36900900	5.18177600
H	-0.42533700	-1.57163000	6.83867500
O	-3.09285000	1.33739600	-2.09059700
O	-3.78405800	-0.82804300	-2.01934700
C	-4.11265900	0.43706000	-2.57487700
C	-4.00049500	0.35107200	-4.08821500
H	-2.99290800	0.04829200	-4.37754400
H	-4.71497100	-0.38026800	-4.47376800
H	-4.21986800	1.32498500	-4.53238900
C	-5.49997500	0.87776800	-2.11790700
H	-5.69706100	1.90263500	-2.43886100
H	-6.25051400	0.21541000	-2.55794900
H	-5.59054700	0.83670300	-1.03278600
C	-3.28168800	-2.95726900	-0.10590000
C	-3.71741600	-3.13962100	1.21019400
C	-3.84450600	-3.73231600	-1.12600600
C	-4.68505500	-4.10149300	1.50462500
H	-3.29210100	-2.53497600	2.00157100
C	-4.81501200	-4.68752300	-0.83037600
H	-3.52369900	-3.58198100	-2.14986900
C	-5.23561800	-4.87960300	0.48686700
H	-5.00670500	-4.24018200	2.53262700
H	-5.24167500	-5.28386100	-1.63132600

H	-5.98744900	-5.62866600	0.71662500
C	-1.30522800	-2.32934100	-1.52662600
C	-1.04898900	-1.65551300	-2.72366300
C	-0.65102700	-3.54744000	-1.29040300
C	-0.17176500	-2.19462500	-3.66763200
H	-1.53239000	-0.71664800	-2.94369900
C	0.22773700	-4.08367900	-2.22680400
H	-0.84547700	-4.07764000	-0.36437300
C	0.46702000	-3.40900000	-3.42639200
H	0.01564300	-1.65024900	-4.58646400
H	0.72385500	-5.02720300	-2.02143900
H	1.14682500	-3.82635500	-4.16308500
C	-3.86509500	2.07701600	0.64584400
C	-4.60600600	1.35760000	1.58950400
C	-4.45537600	3.17803700	0.01297800
C	-5.92348500	1.71994700	1.87771500
H	-4.14369500	0.52590800	2.10692300
C	-5.76792500	3.54067200	0.30461100
H	-3.88274000	3.74522500	-0.71079000
C	-6.50990000	2.80914300	1.23404300
H	-6.48640100	1.15193500	2.61227000
H	-6.21209800	4.39622900	-0.19527300
H	-7.53331700	3.09213500	1.46108700
C	-1.57344200	2.90848500	0.12236500
C	-1.40452200	3.71930600	1.25107800
C	-1.00758100	3.30352700	-1.09167000
C	-0.67532800	4.89848900	1.17472400
H	-1.84291600	3.40830500	2.19294900
C	-0.27772900	4.49376800	-1.16778600
H	-1.15262200	2.71232500	-1.98753000

C	-0.10663400	5.29035900	-0.03895700
H	-0.53774400	5.50596900	2.06334700
H	0.14666300	4.80353400	-2.11796100
H	0.46402900	6.21181000	-0.10230500

TS10

C	-6.31428700	1.94226500	0.95005800
C	-5.23558800	1.34649500	0.27060600
C	-5.45717400	0.93863000	-1.05921100
C	-6.70854500	1.09971300	-1.66803300
C	-7.75301000	1.68392100	-0.96094500
C	-7.56031600	2.11646000	0.35512700
H	-6.17290900	2.26480300	1.97989300
H	-6.83346500	0.76495600	-2.69250000
H	-8.71981400	1.80823400	-1.44018500
H	-8.37405100	2.57608800	0.90728200
C	-3.75872500	-0.02247700	2.68627200
C	-2.97683200	-2.05937500	1.23969600
C	-3.80264100	-1.53566800	2.39801700
H	-4.63401100	0.26967100	3.27800300
H	-2.86988700	0.18624500	3.29114800
H	-4.83942500	-1.84176700	2.19097800
H	-3.48605400	-2.08354100	3.28934200
C	-2.65674700	2.60183300	1.40499000
H	-2.22239600	2.97344300	0.47194800
H	-3.32549500	3.37539600	1.79771000
H	-1.84816200	2.44424800	2.12176600
C	-3.12067300	0.53688800	-1.55361300
C	-2.78878400	-0.08159600	-0.20116100
C	-2.86041200	-1.54023600	-0.05555100

C	-2.62344400	-2.46343500	-1.20144100
C	-1.66992800	-2.20446200	-2.19896300
C	-3.37365900	-3.64374300	-1.28959200
C	-1.46908500	-3.09962000	-3.24508500
H	-1.04995700	-1.31944800	-2.12719600
C	-3.17105700	-4.54597700	-2.33424100
H	-4.12697700	-3.84902400	-0.53572800
C	-2.21752700	-4.27752700	-3.31627000
H	-0.71318800	-2.88706800	-3.99543600
H	-3.76165800	-5.45584000	-2.38156200
H	-2.05732600	-4.97842300	-4.12979400
O	-4.50812600	0.33626900	-1.84780900
Si	-3.59563700	0.99861000	1.12005800
Rh	-1.09181900	-0.76658800	0.98463000
Cl	-0.49040700	-1.86873400	3.03737500
H	-1.23761900	0.11303000	-0.35855200
H	-2.73132600	-3.11441200	1.33096900
H	-2.60164200	0.08912500	-2.39522600
H	-2.89487000	1.60734600	-1.54635000
C	1.62111000	1.93546700	-0.91979900
C	2.67598400	0.82725500	-1.17939700
C	2.21171500	-0.63853700	-1.08142500
C	2.57393300	-1.32377400	0.26501200
H	3.49236800	1.00878900	-0.47335500
H	1.12265900	-0.69726200	-1.17232800
P	0.77392900	0.46061100	1.33493900
O	2.18720500	-0.37777200	1.30636400
O	1.08375100	1.79322400	0.41127000
C	1.01658100	1.28196900	2.94012300
C	1.52660100	0.56158100	4.02853200

C	0.67049800	2.63163600	3.09768500
C	1.68728000	1.19220300	5.26121500
H	1.78560800	-0.48123800	3.90570600
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O	3.13667500	0.95080300	-2.51732100
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H	4.52335100	6.51873700	-0.91775200
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H	7.93182100	-1.97977500	0.68196600

4a'

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C	-5.49556500	1.19703500	0.17191300
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H	8.10127500	-1.64408300	0.82523600

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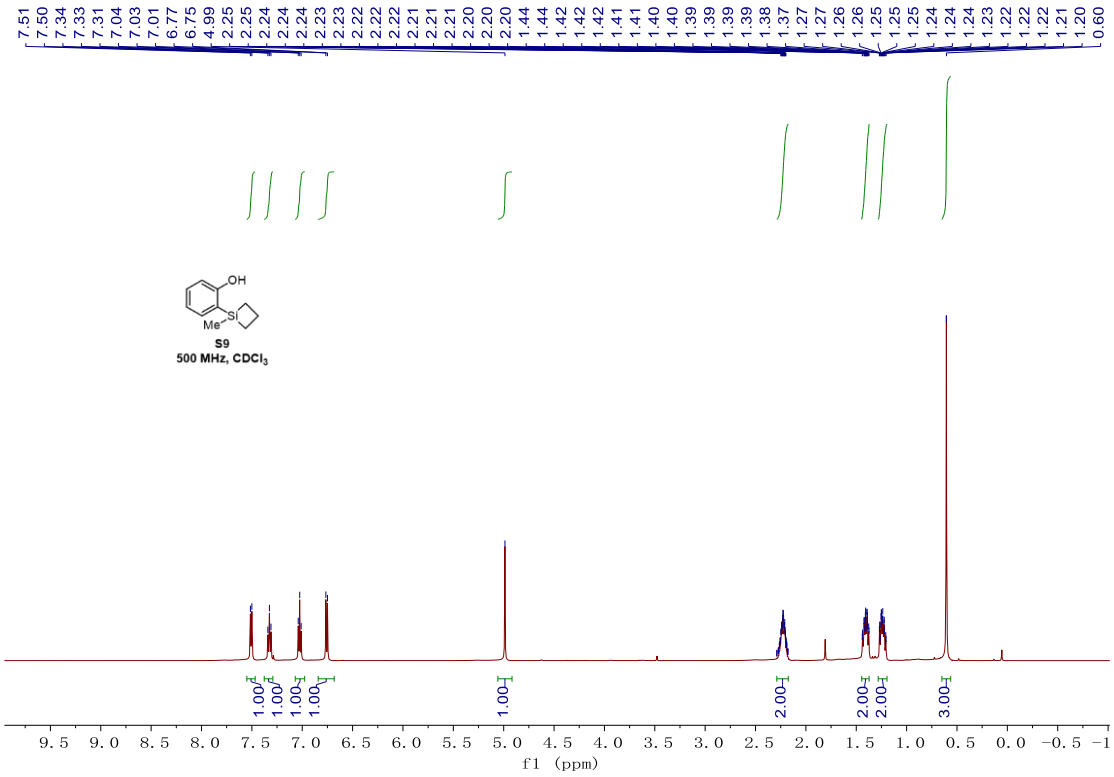
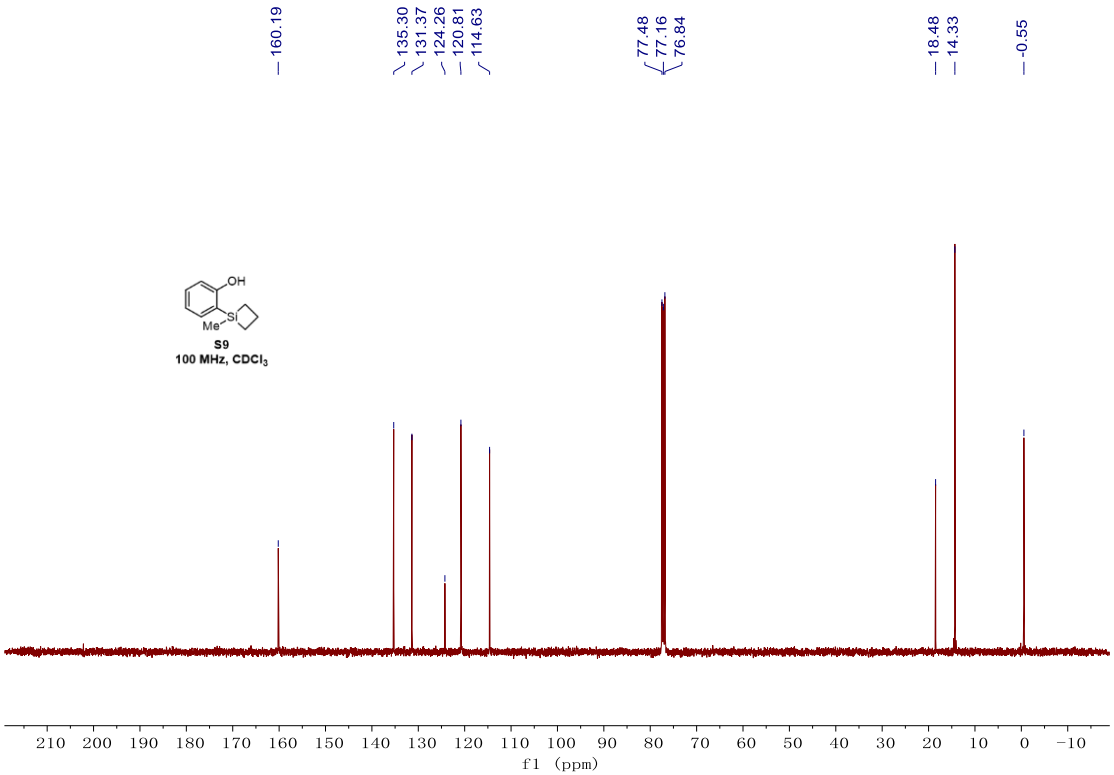
6. NMR Spectra

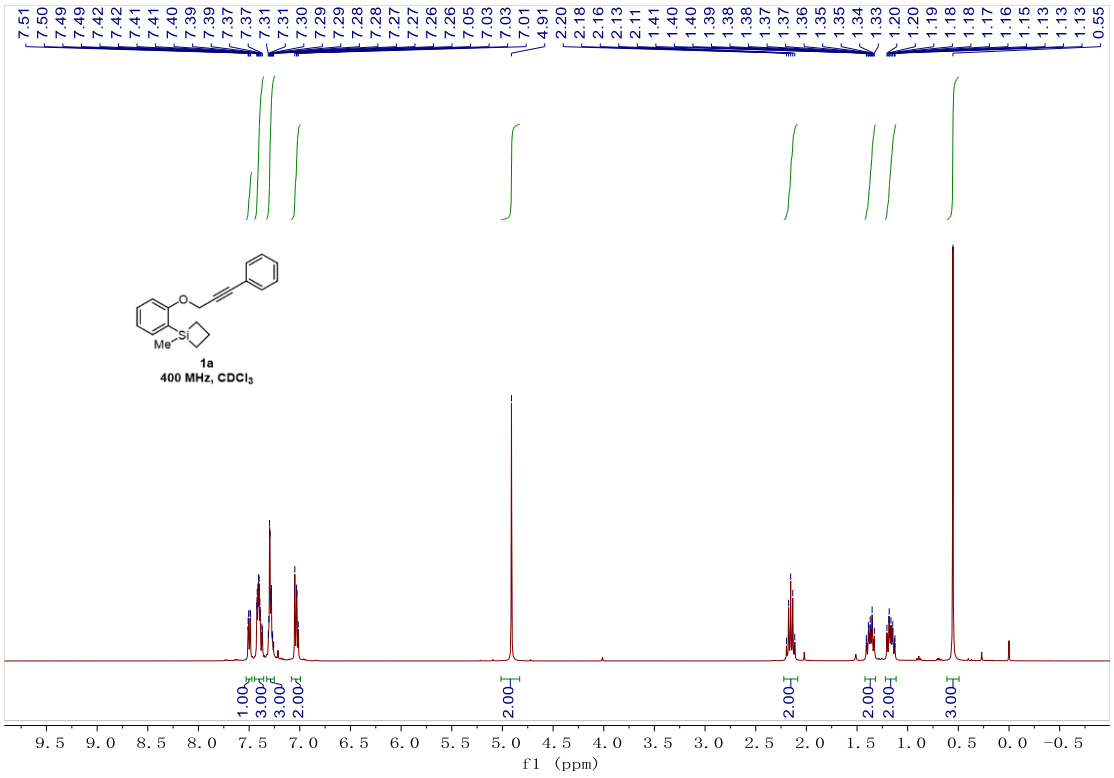
^{1}H NMR spectrum of S9



^{13}C NMR spectrum of S9



^{1}H NMR spectrum of 1a



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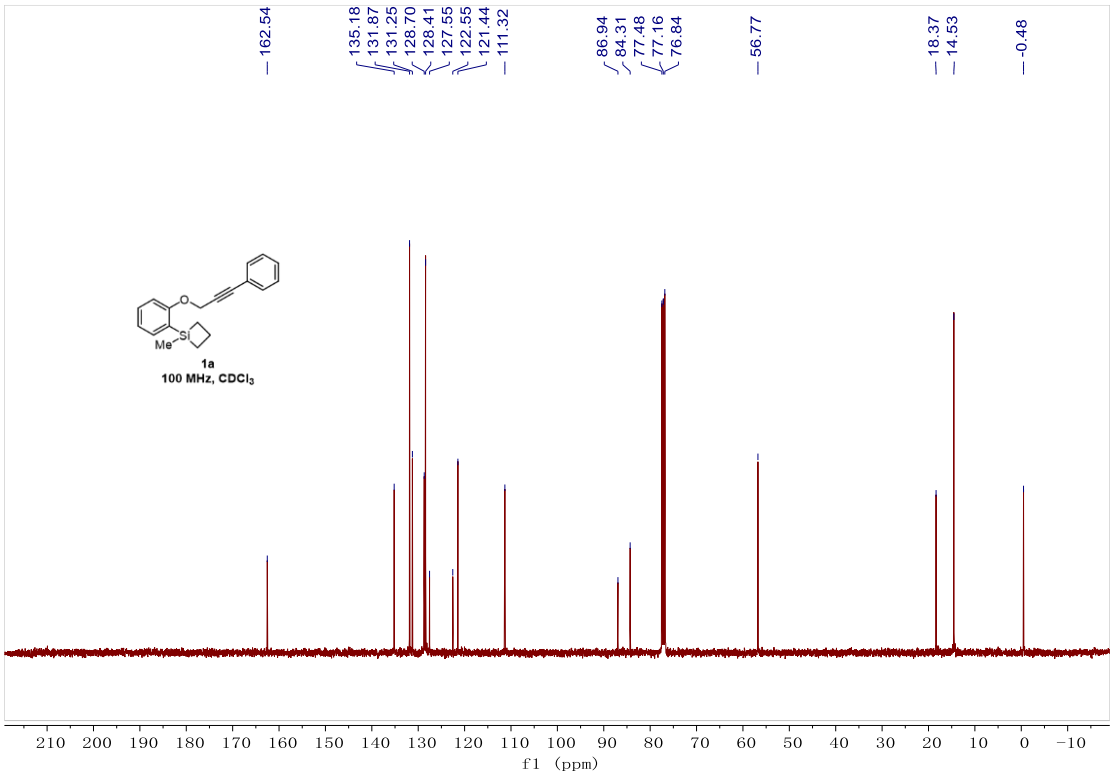
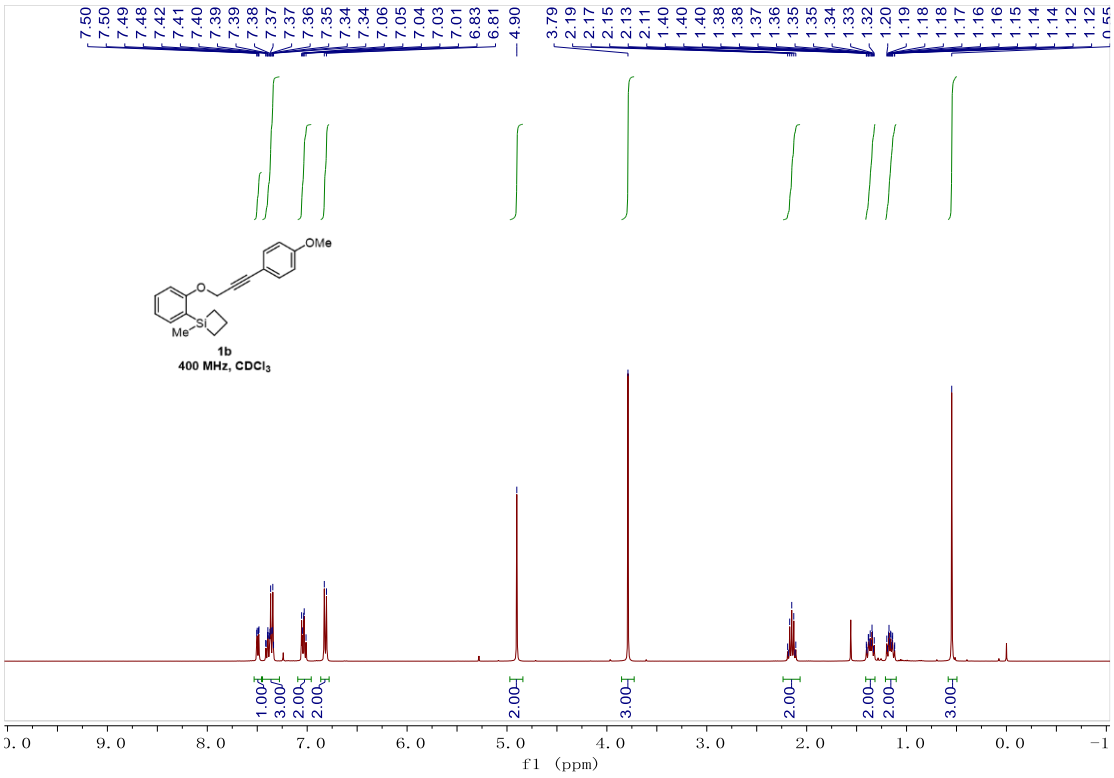
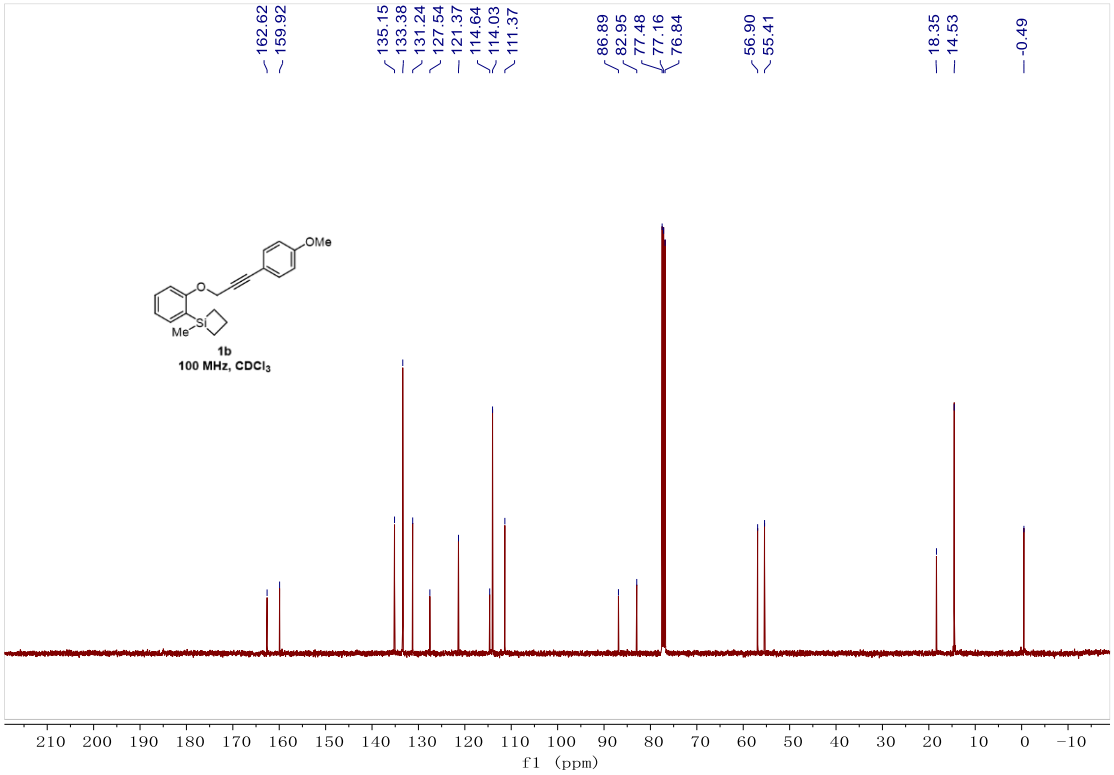


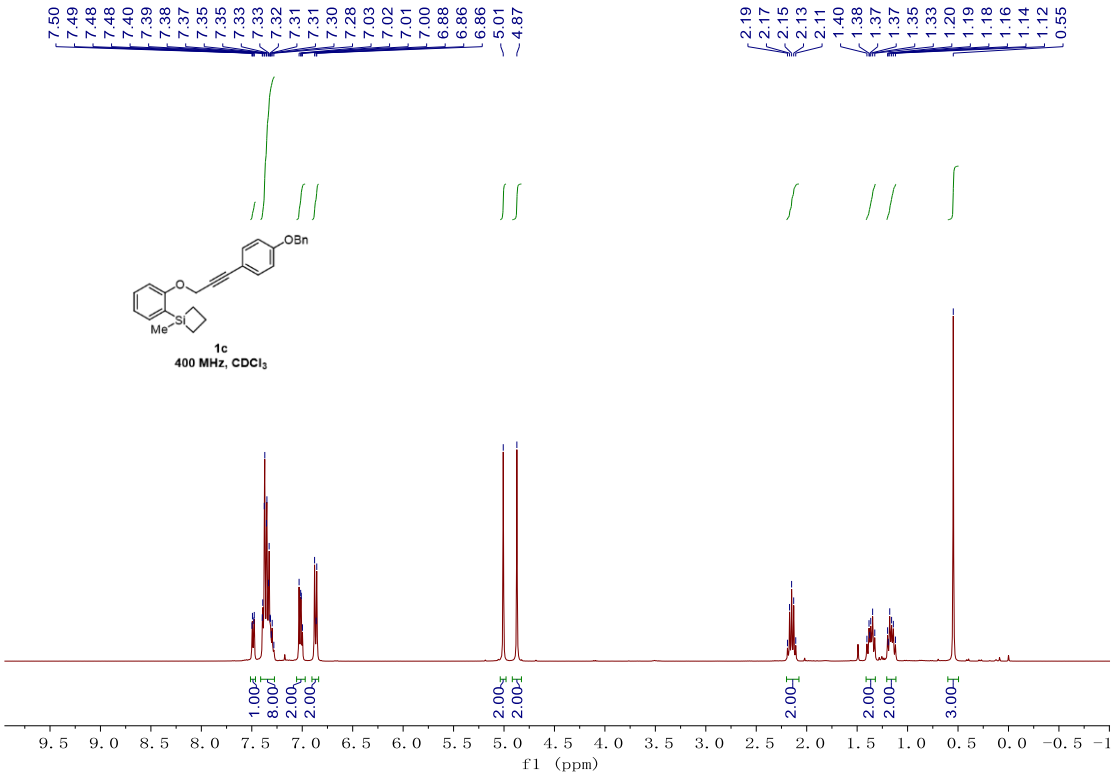
^{1}H NMR spectrum of 1b



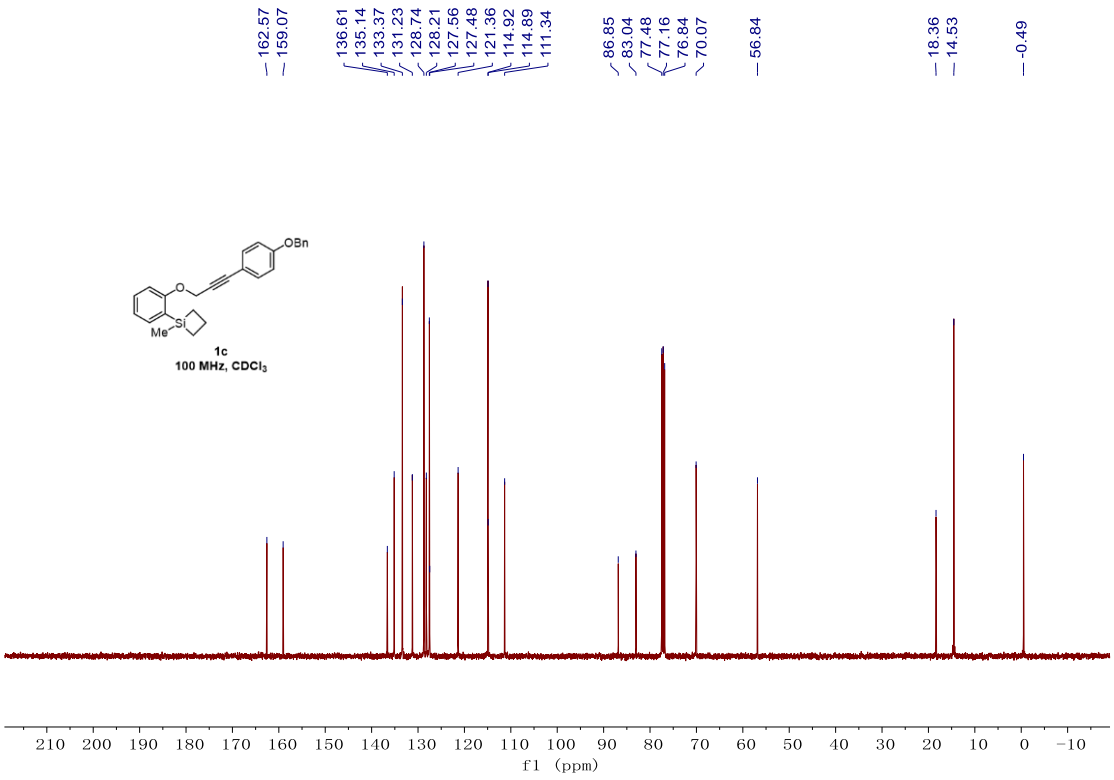
^{13}C NMR spectrum of 1b



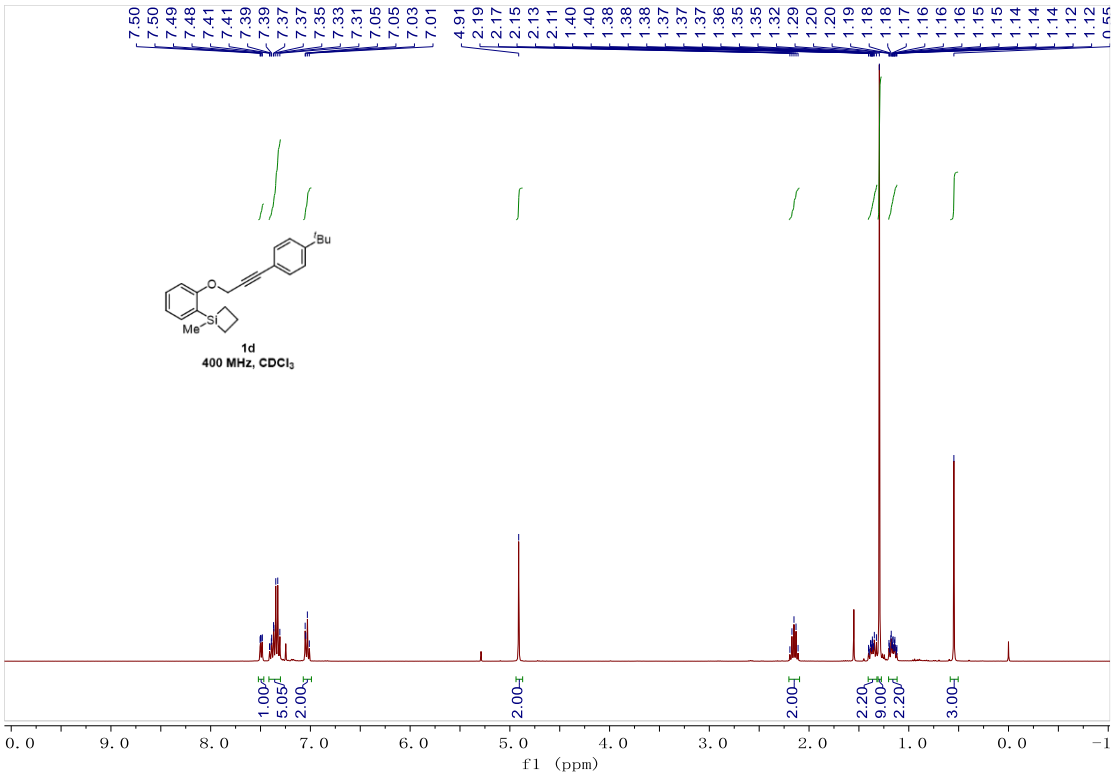
^{1}H NMR spectrum of 1c



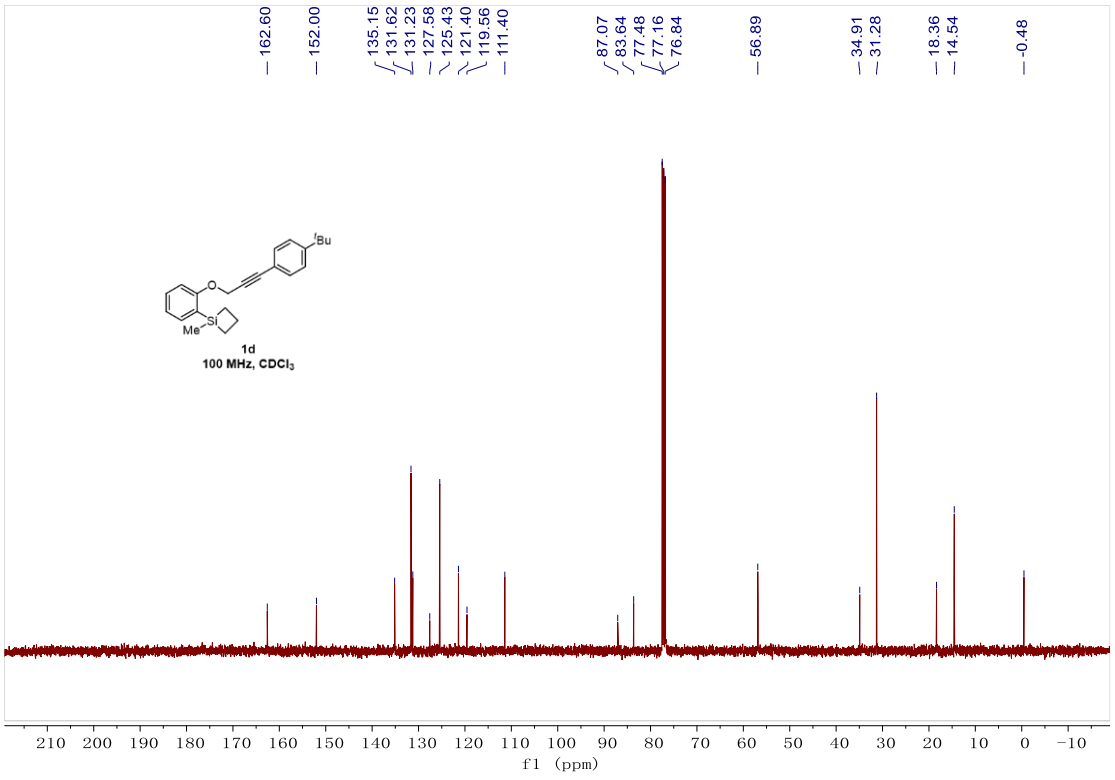
^{13}C NMR spectrum of 1c



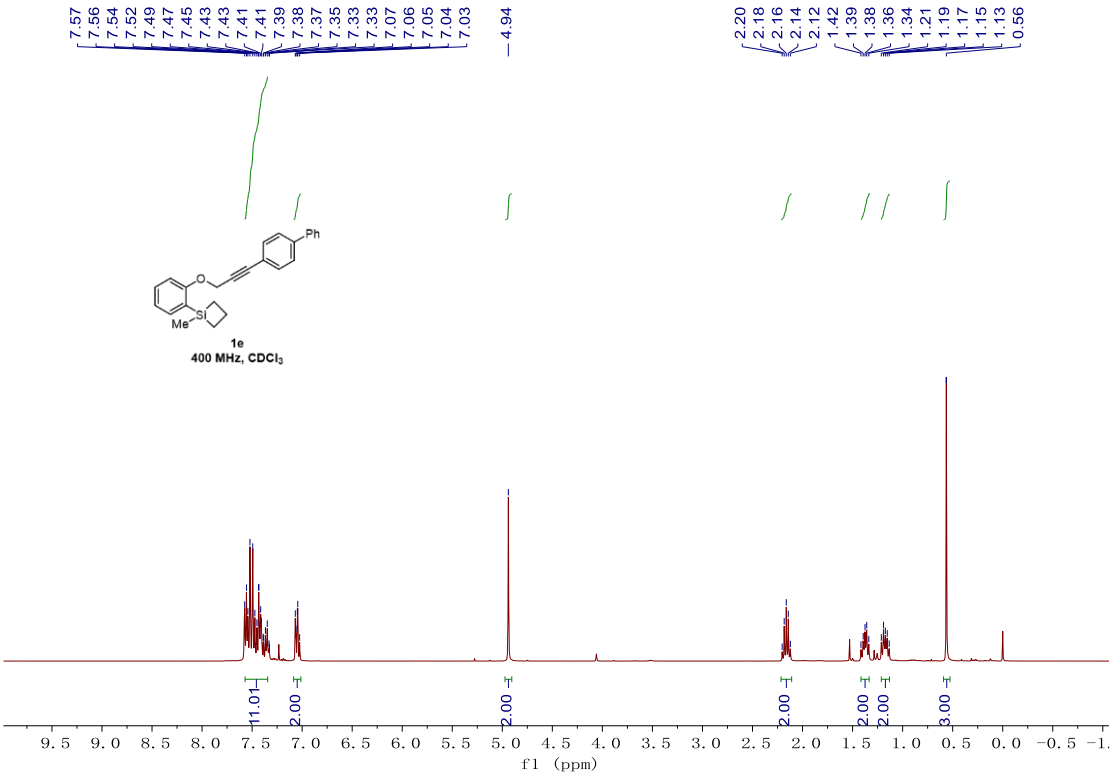
^{1}H NMR spectrum of 1d



^{13}C NMR spectrum of 1d



^{1}H NMR spectrum of 1e



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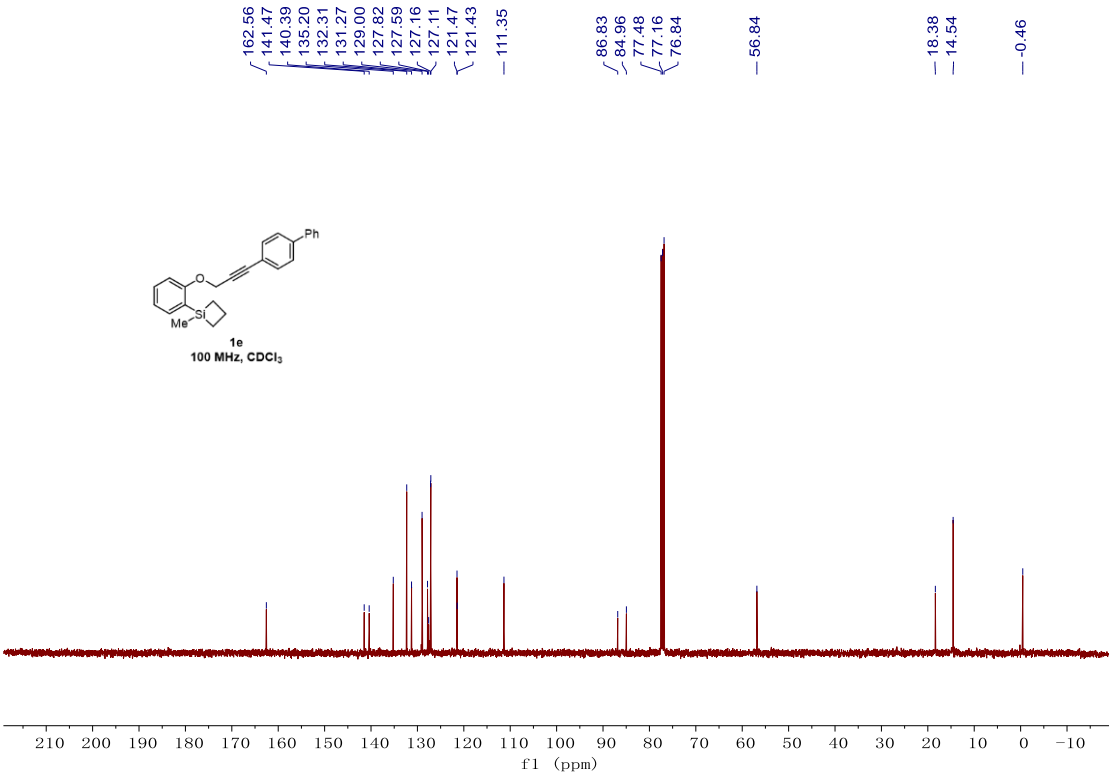
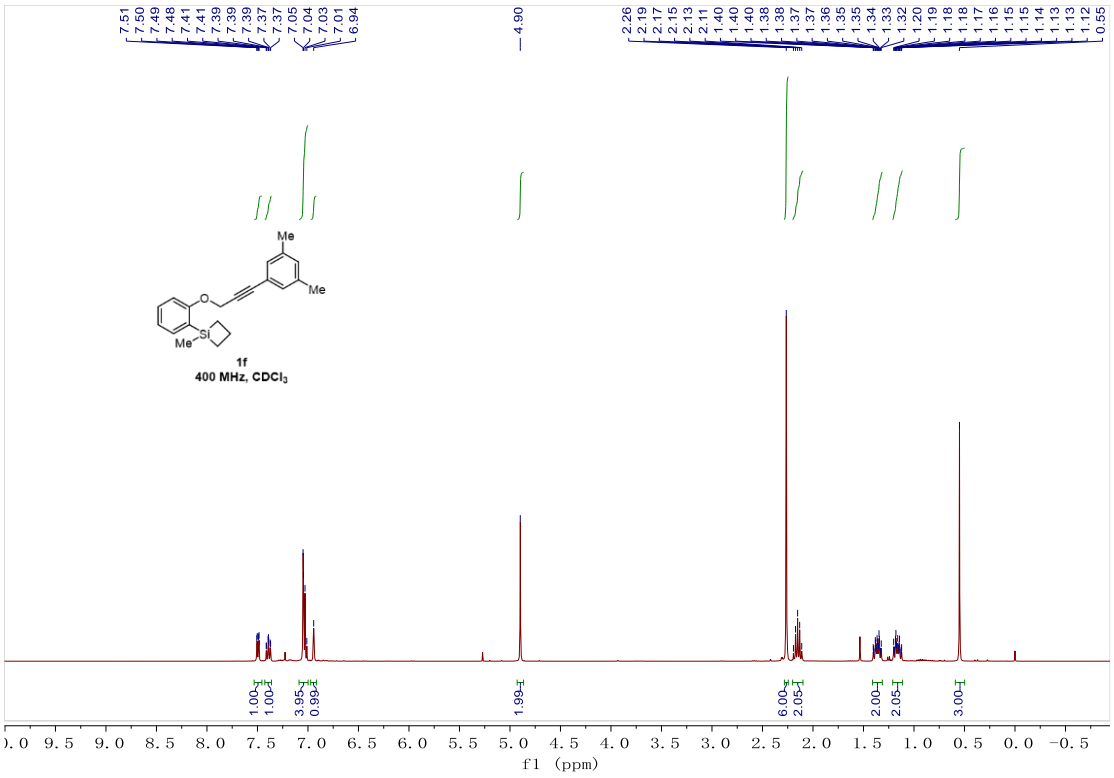
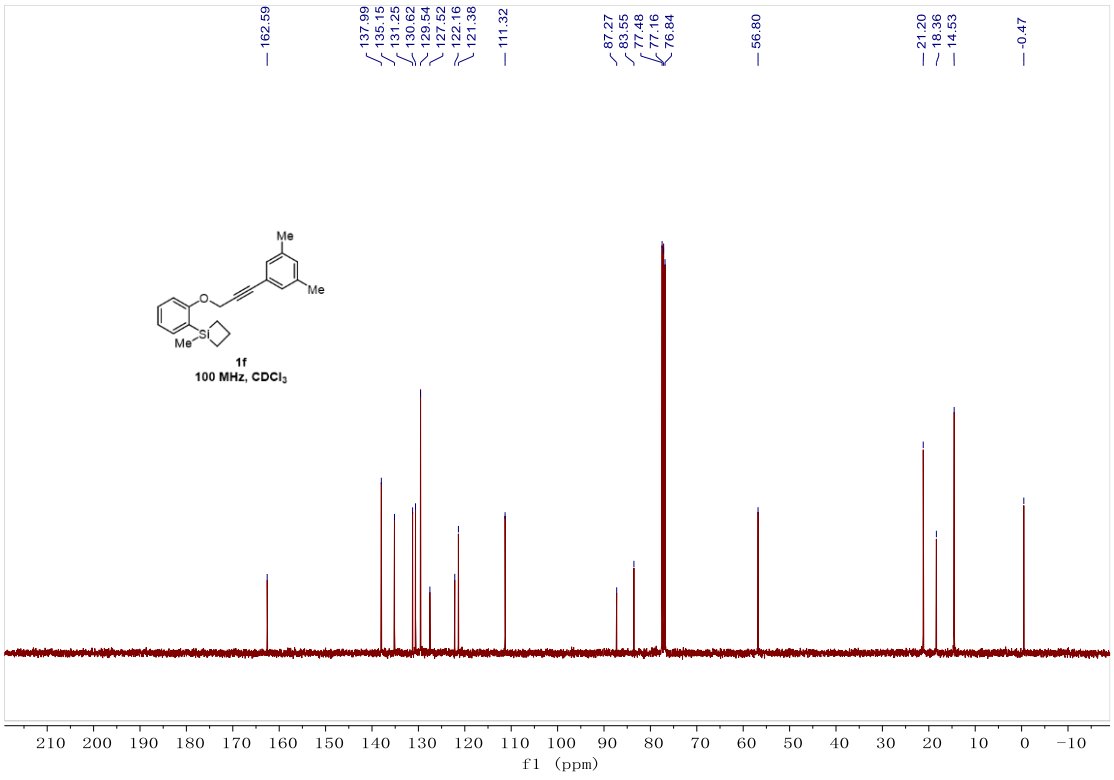


^{1}H NMR spectrum of 1f



^{13}C NMR spectrum of 1f



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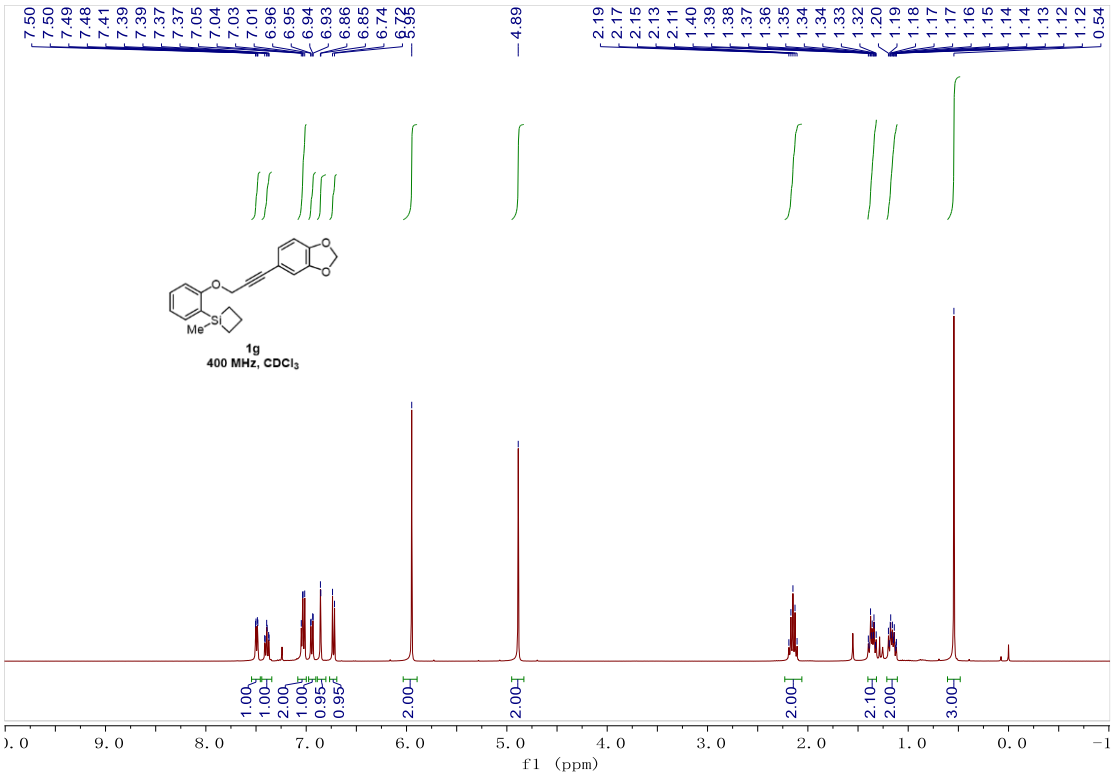

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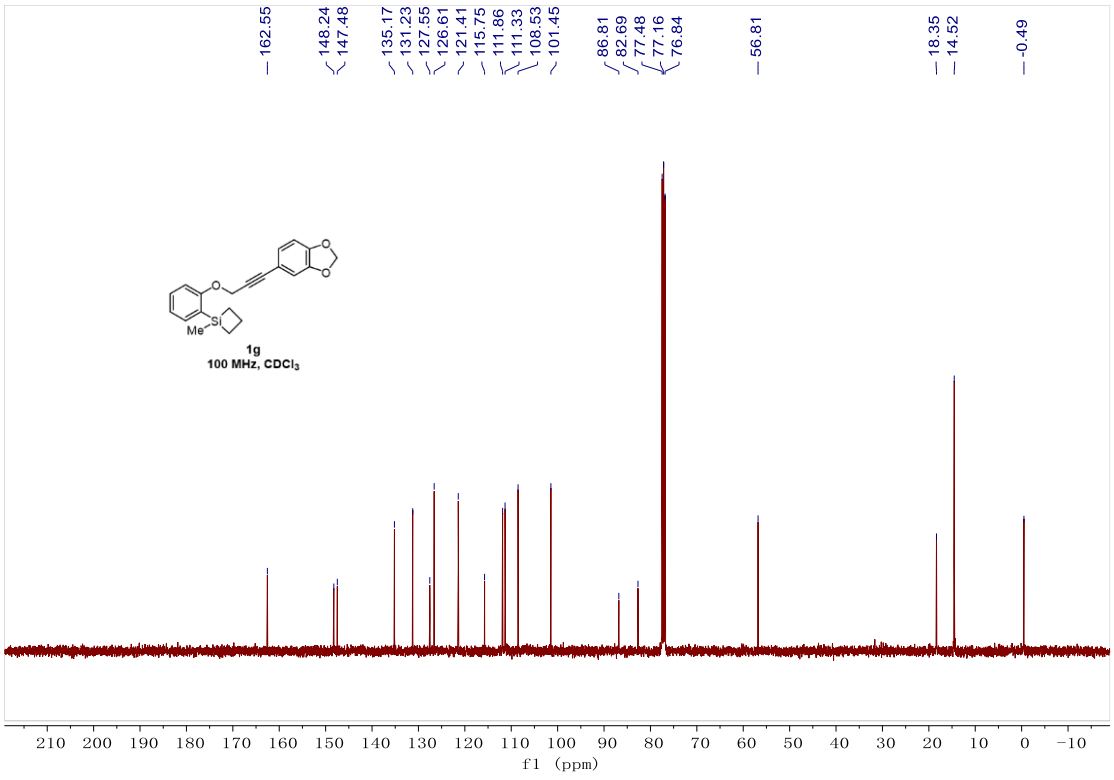

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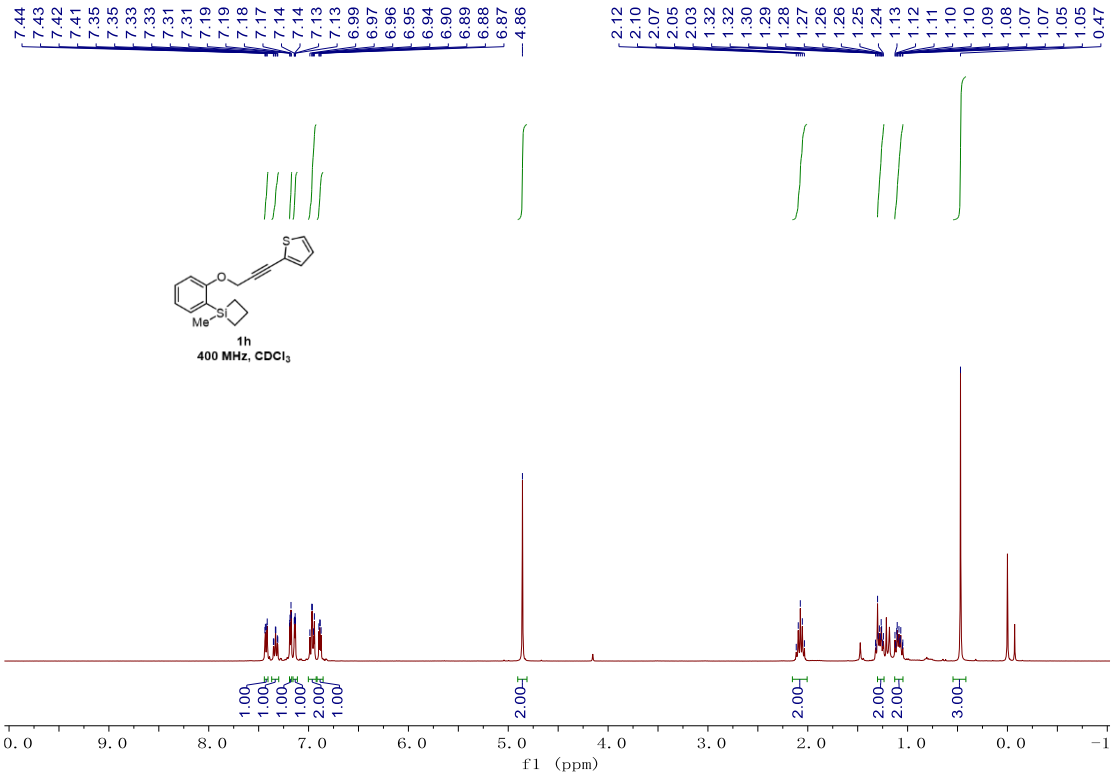

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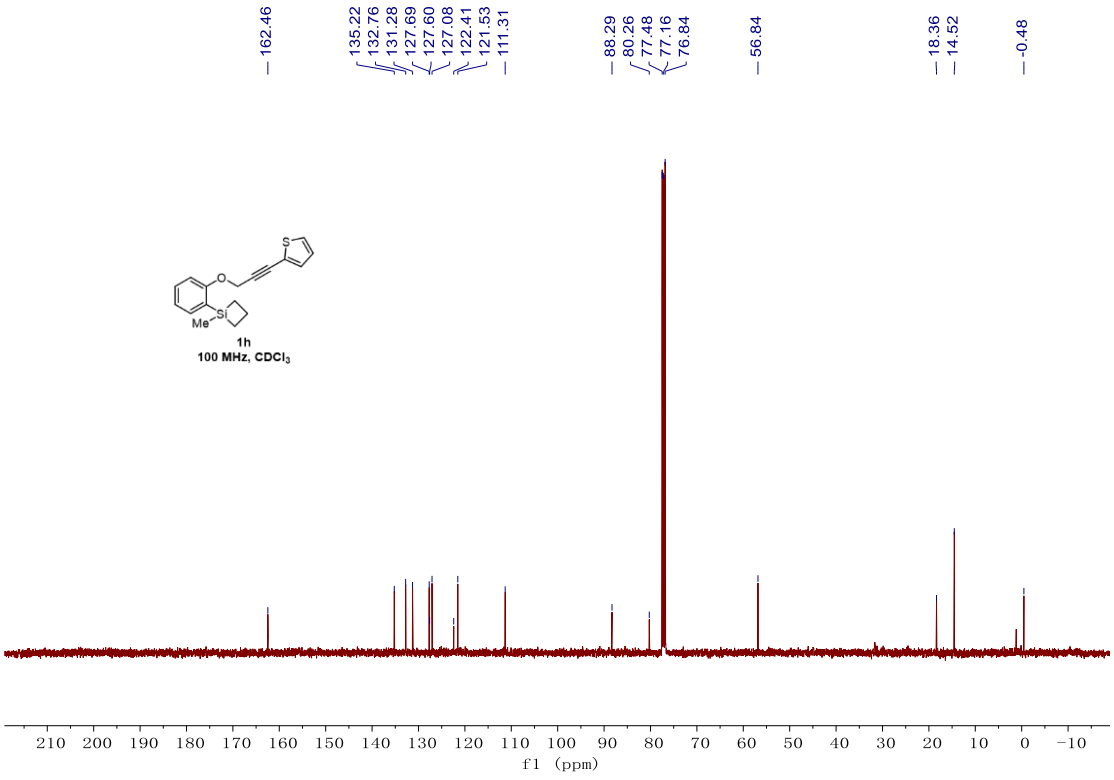
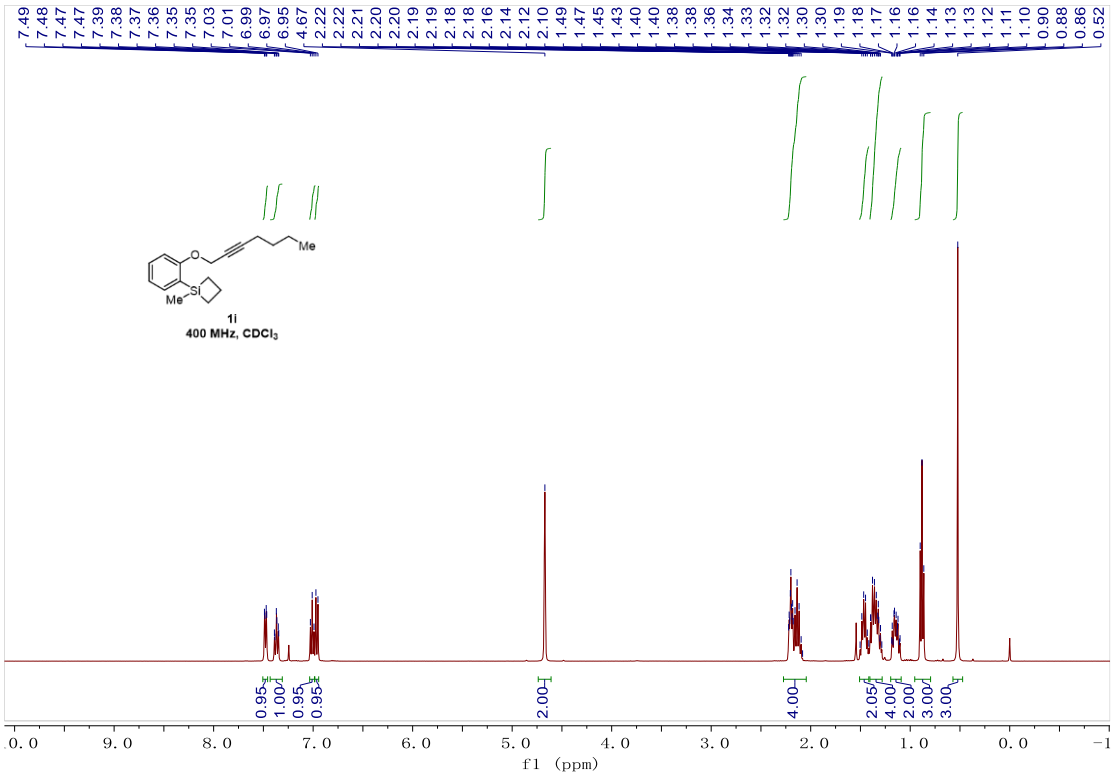


^{1}H NMR spectrum of 1i



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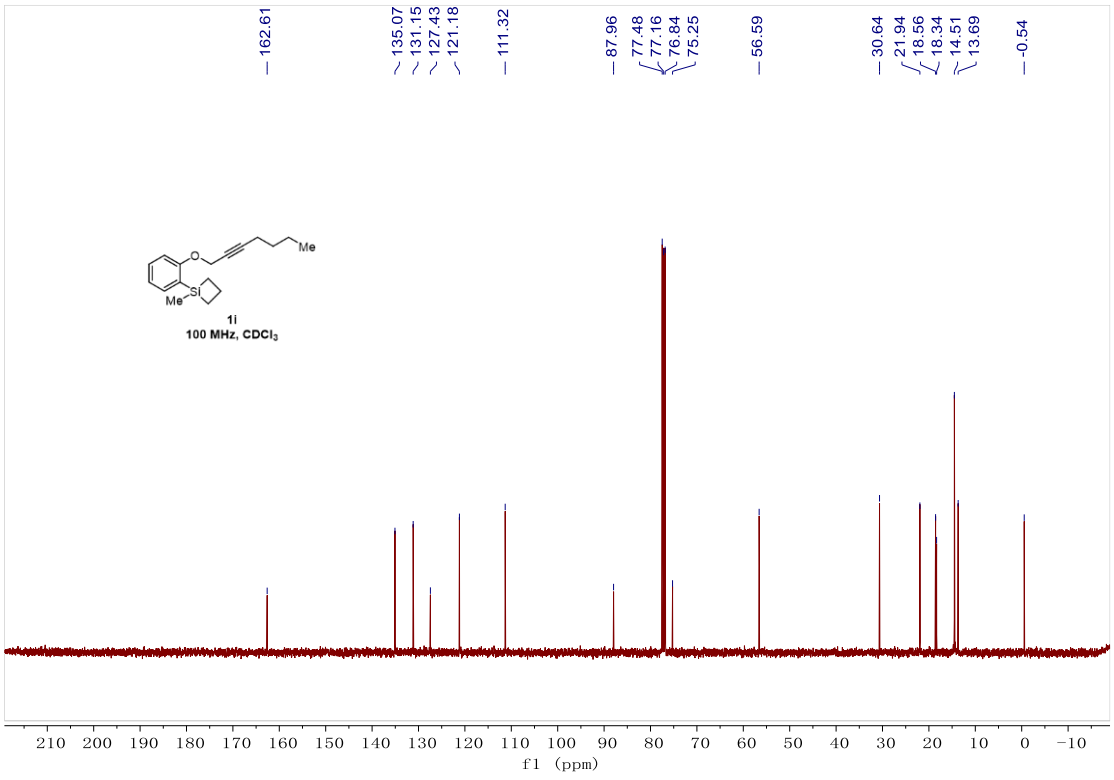

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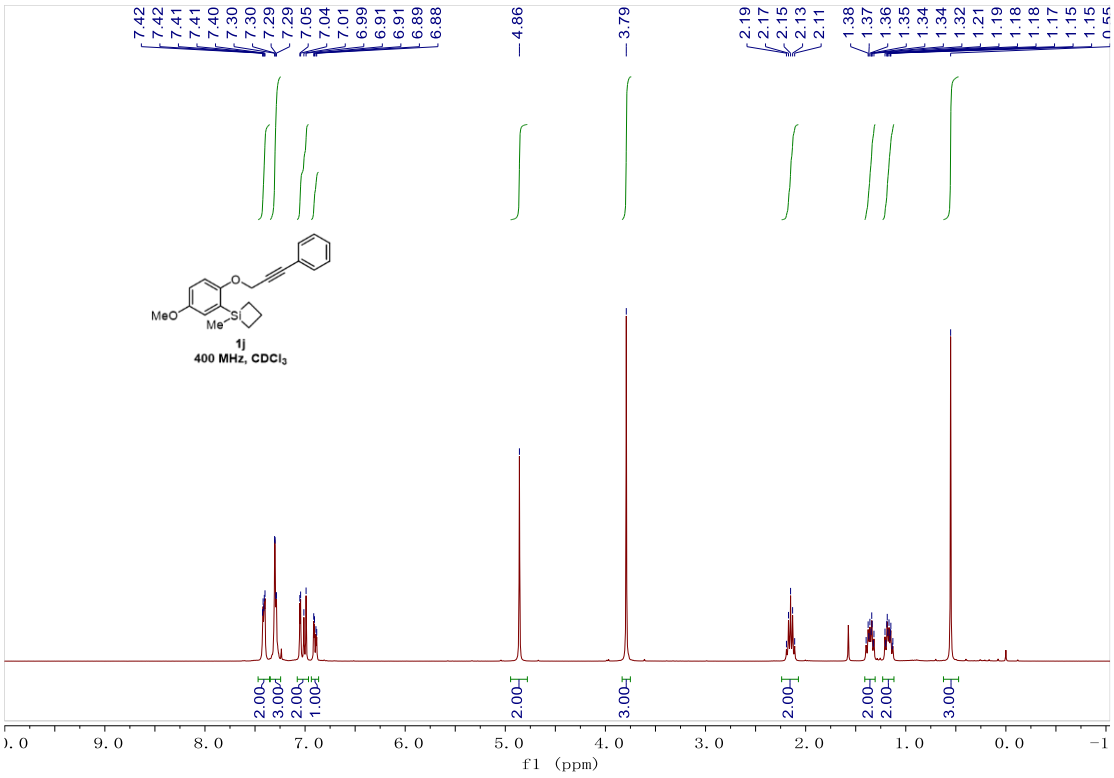

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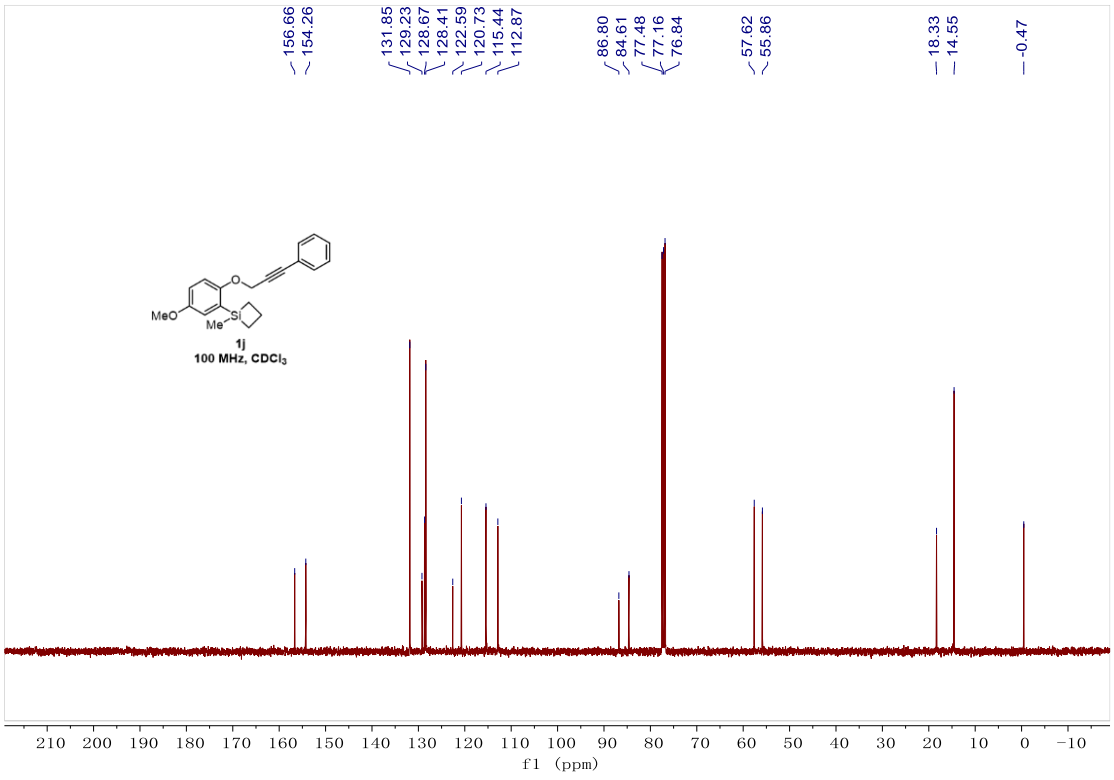
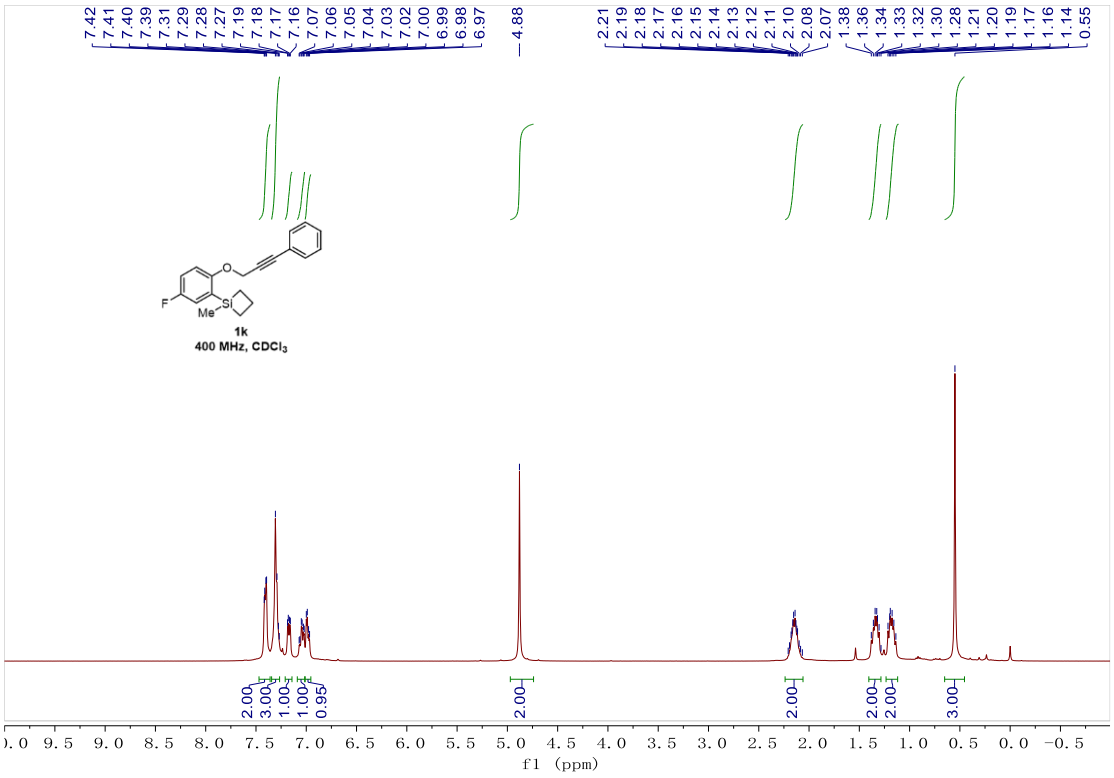


^{1}H NMR spectrum of 1k



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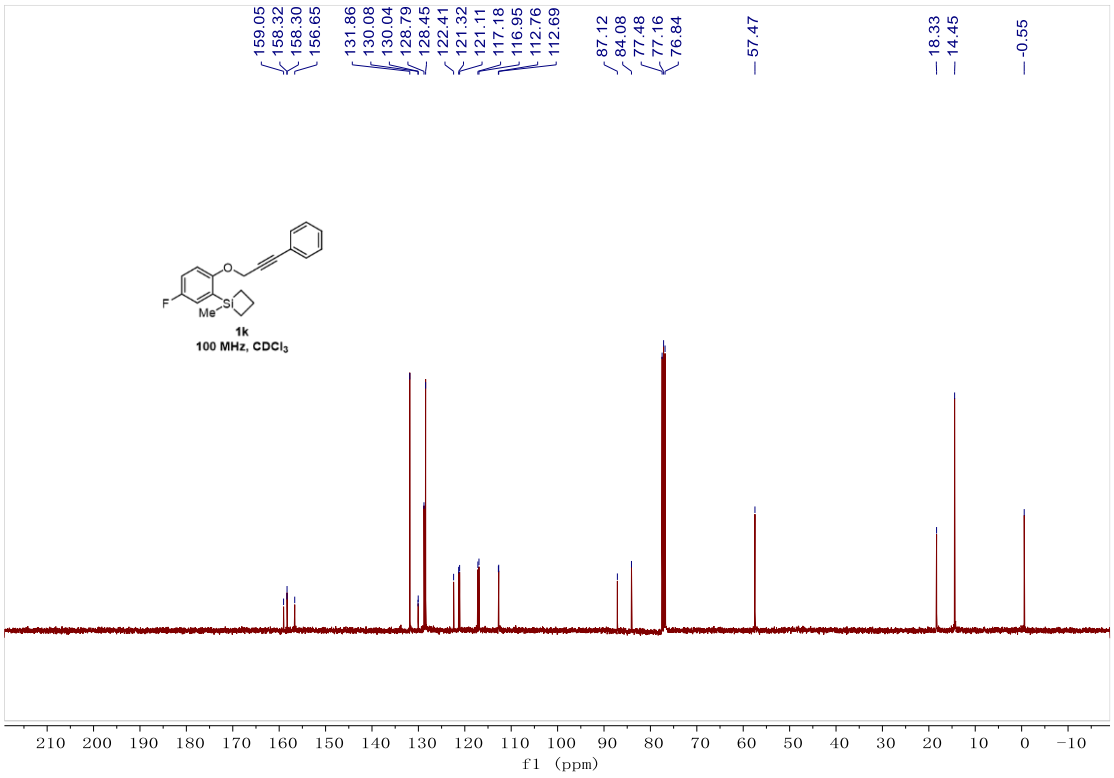
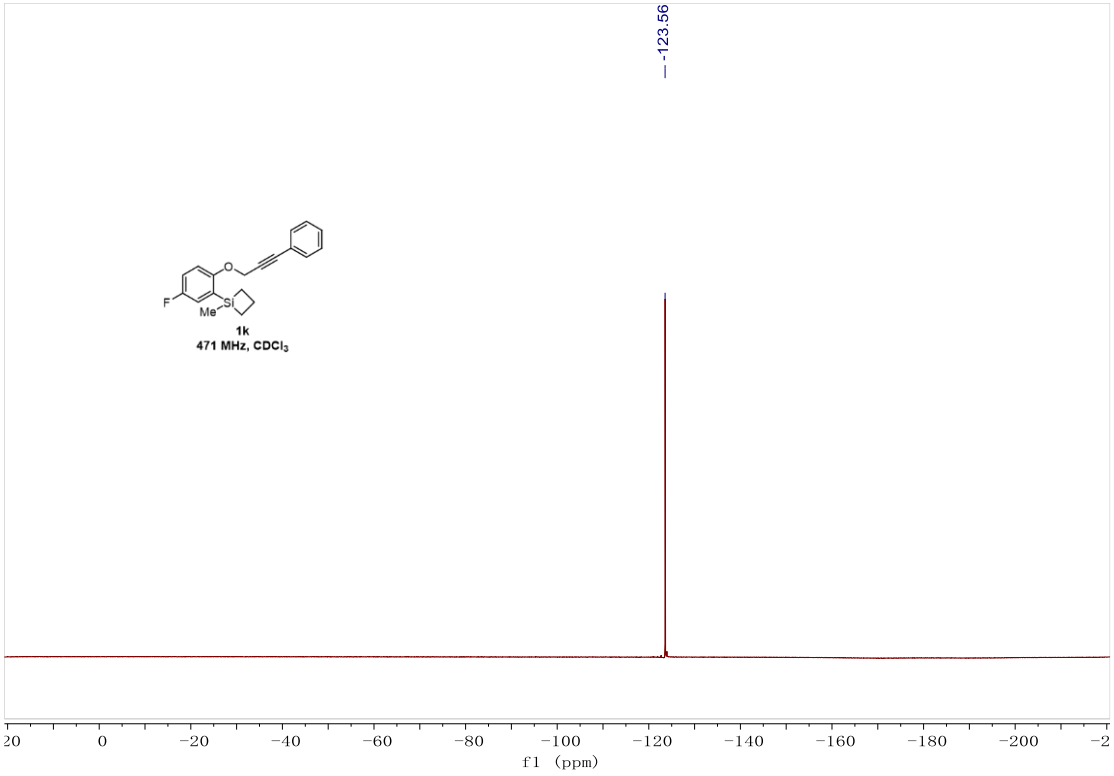
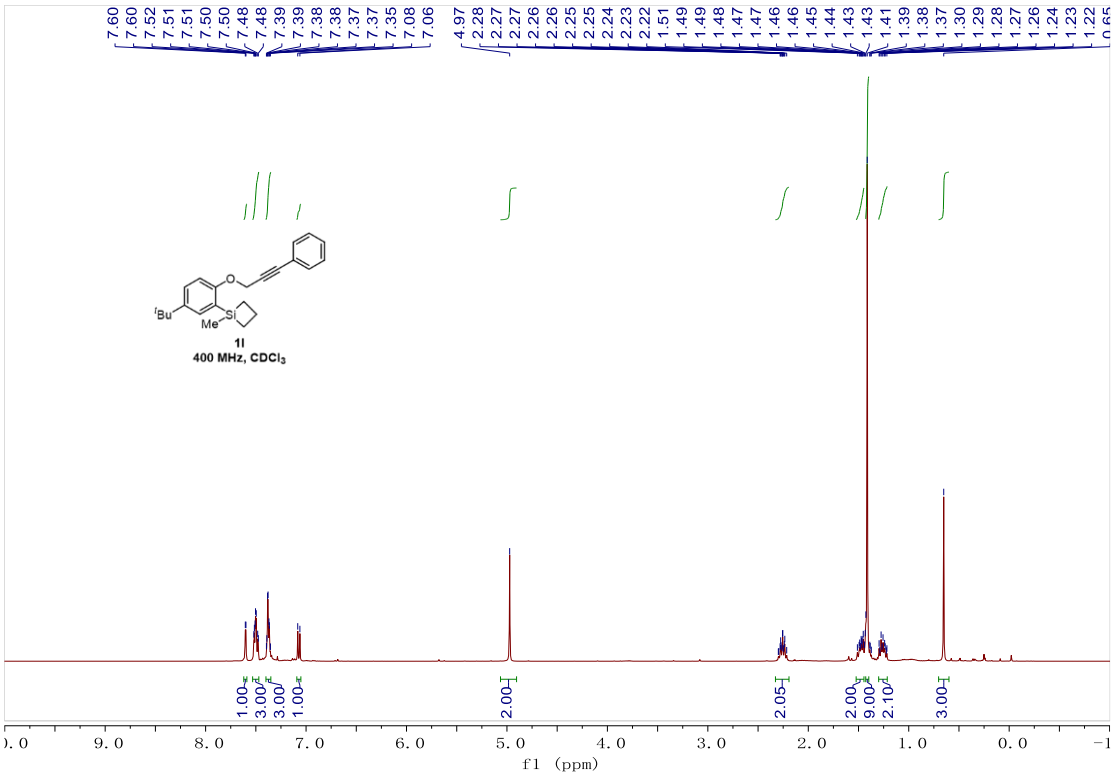


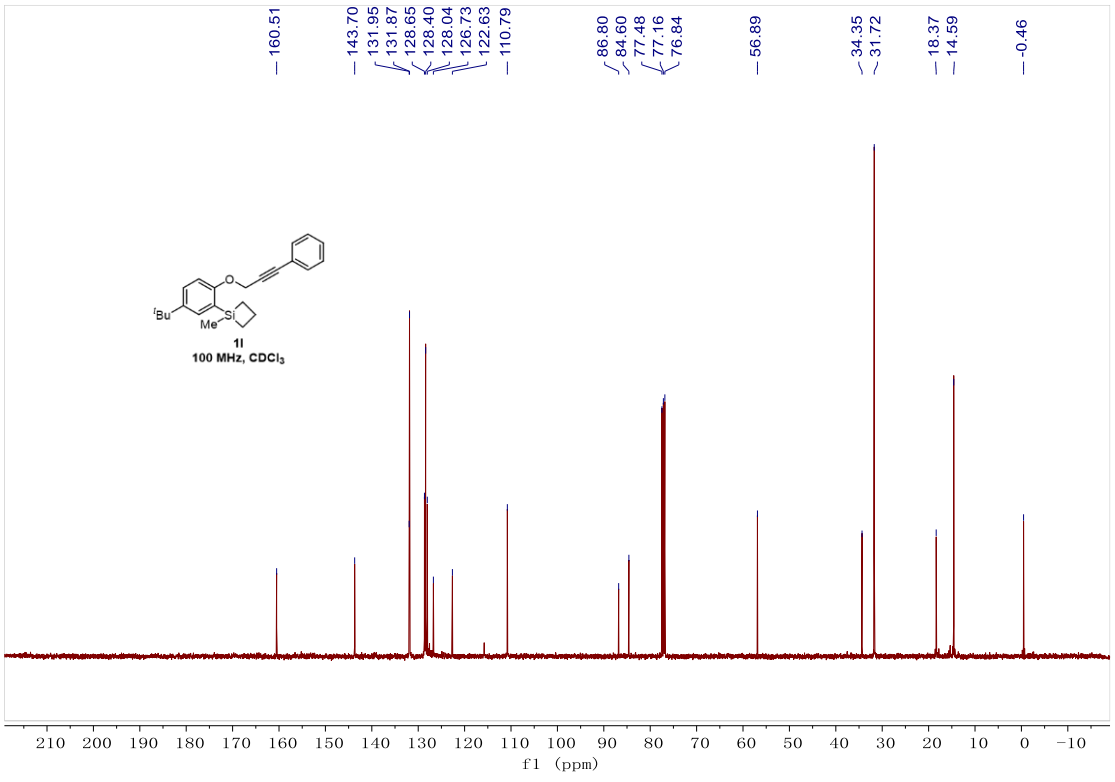
^{19}F NMR spectrum of 1k



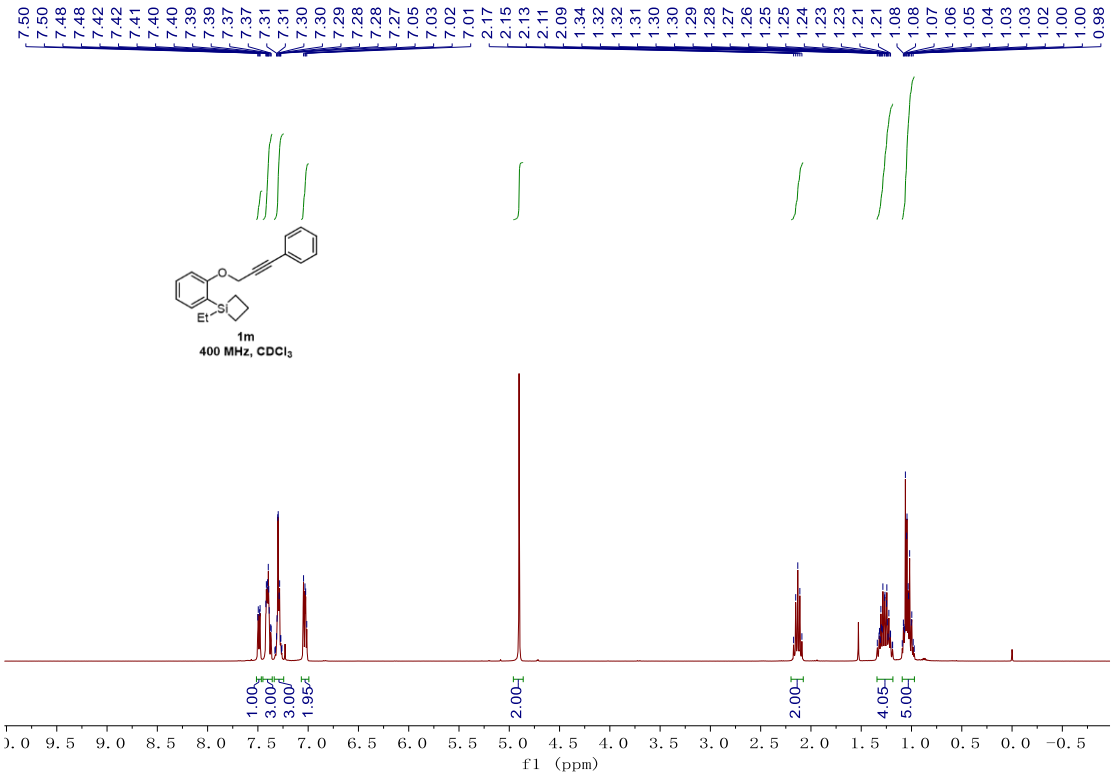
^{1}H NMR spectrum of 1l



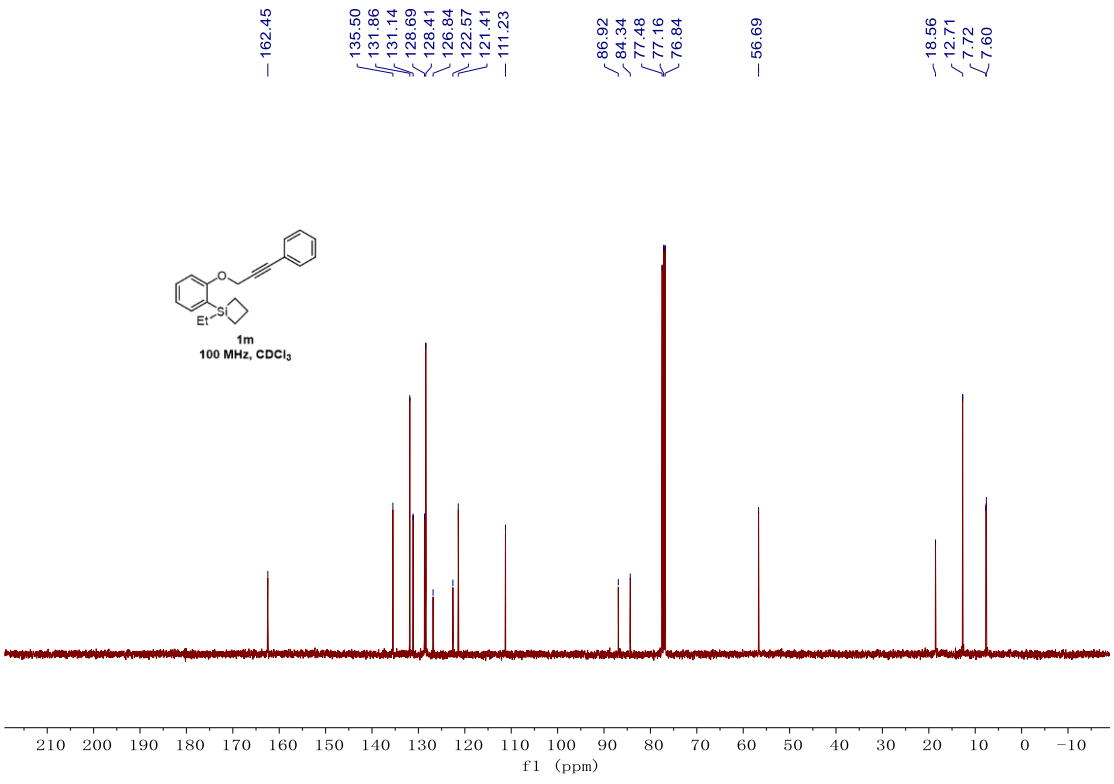
^{13}C NMR spectrum of 1l



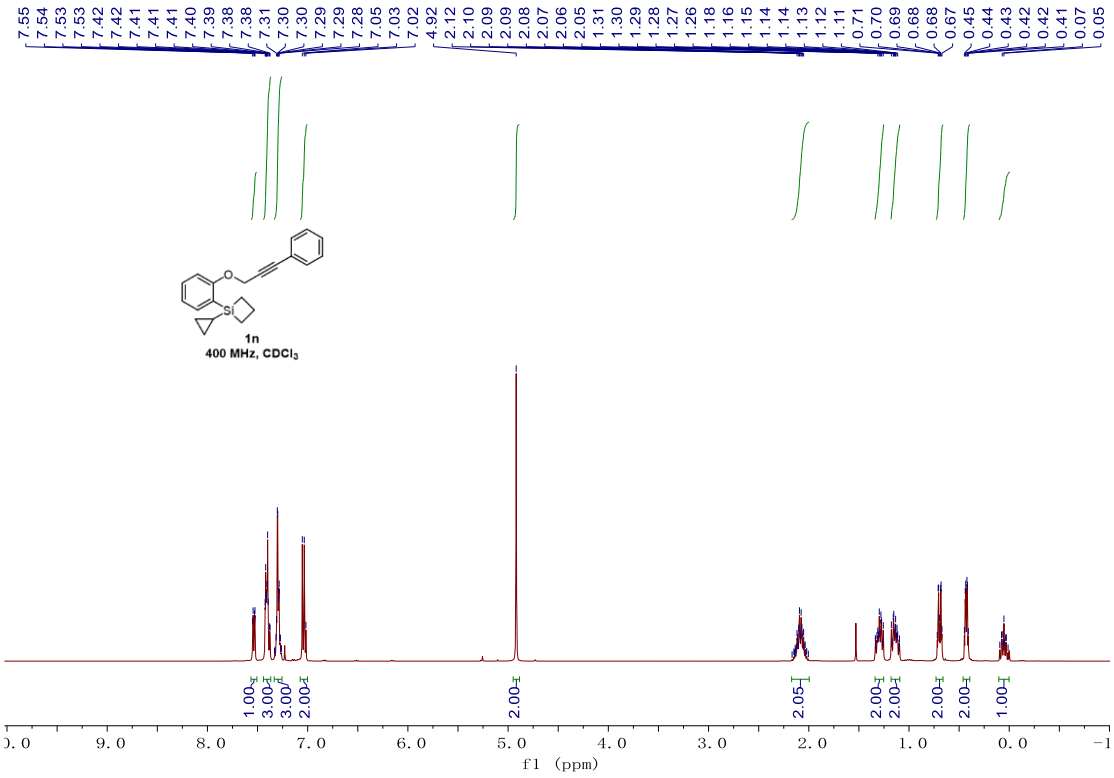
^{1}H NMR spectrum of 1m



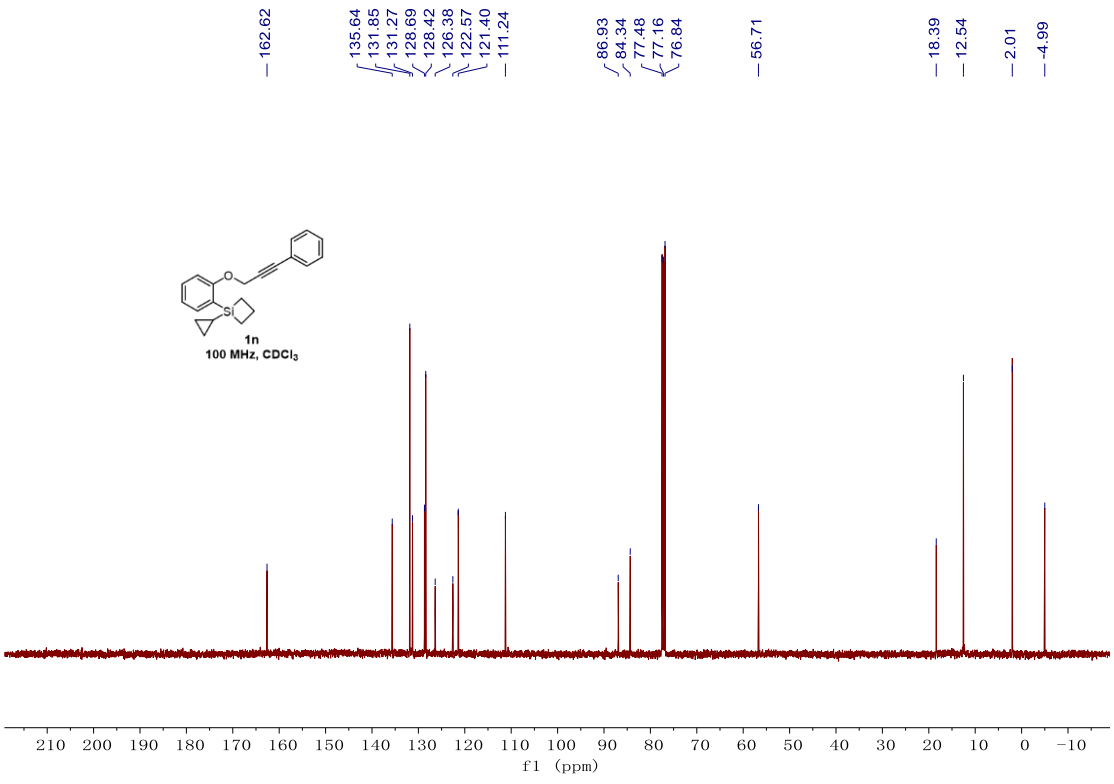
^{13}C NMR spectrum of 1m



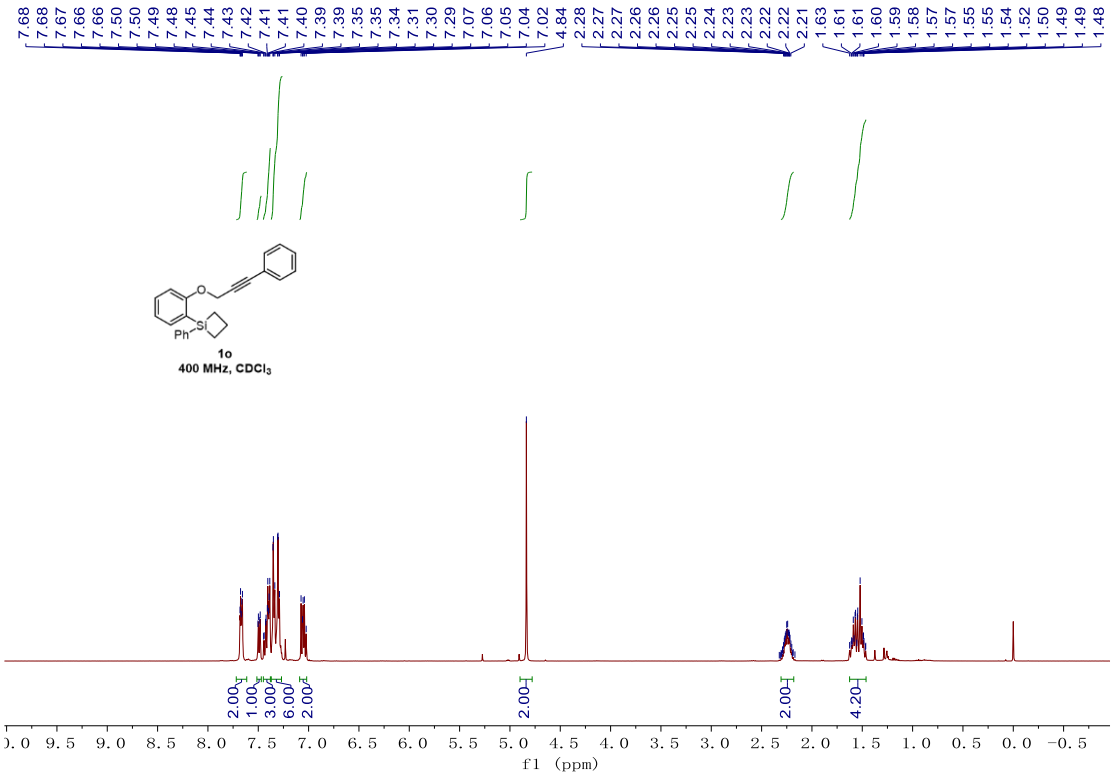
^{1}H NMR spectrum of 1n



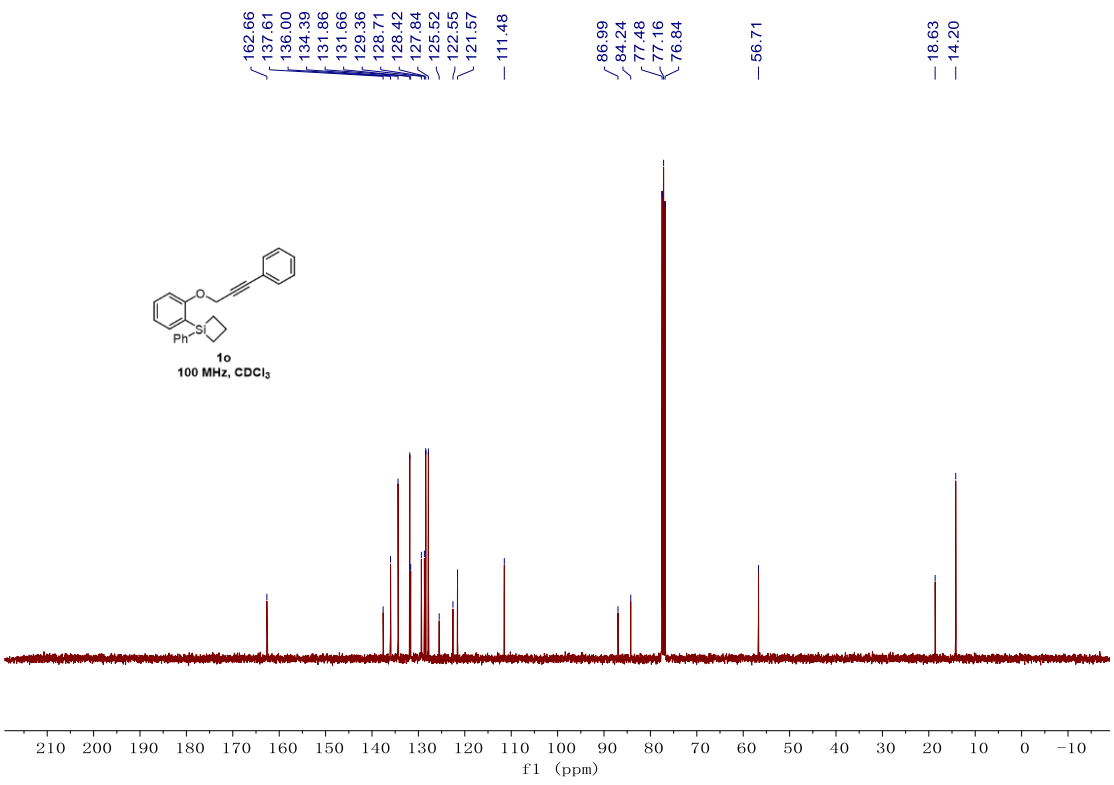
^{13}C NMR spectrum of 1n



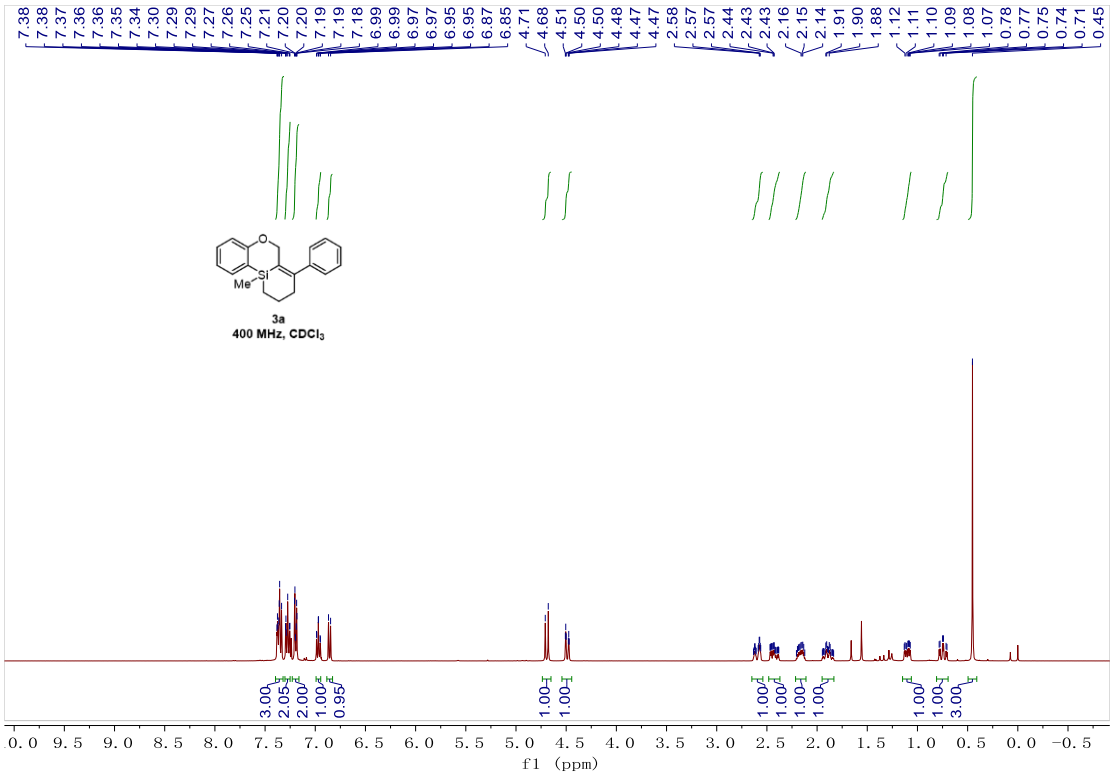
^{1}H NMR spectrum of 1o



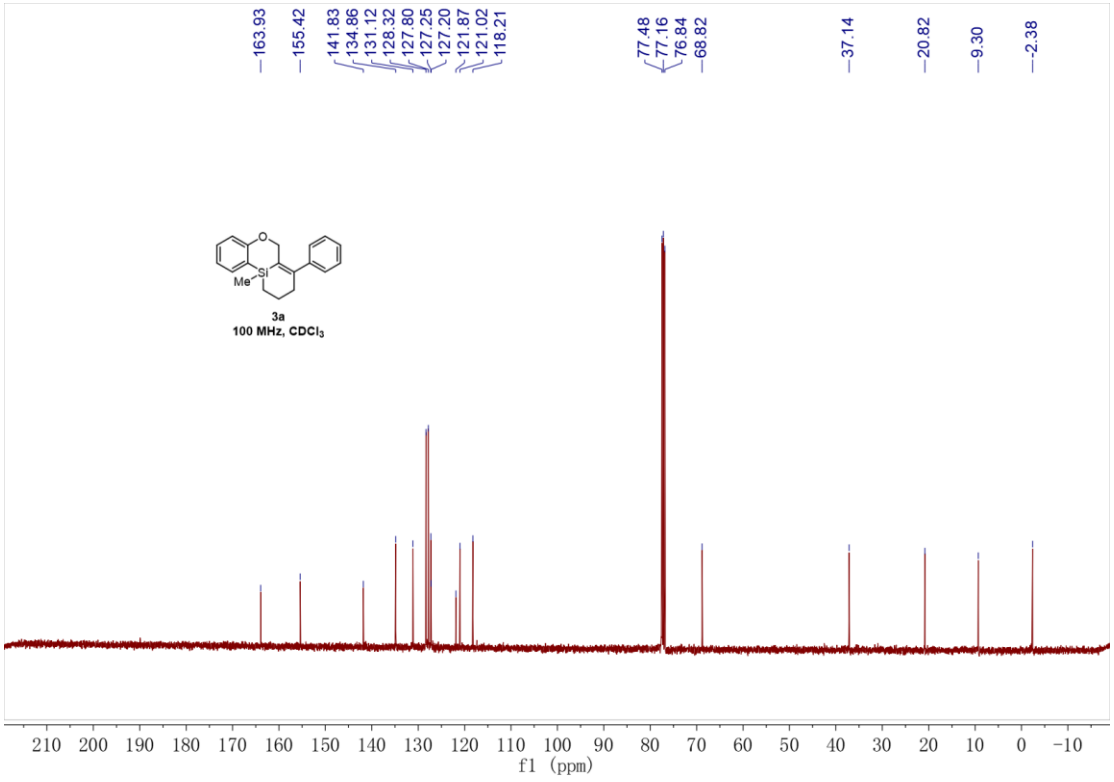
^{13}C NMR spectrum of 1o



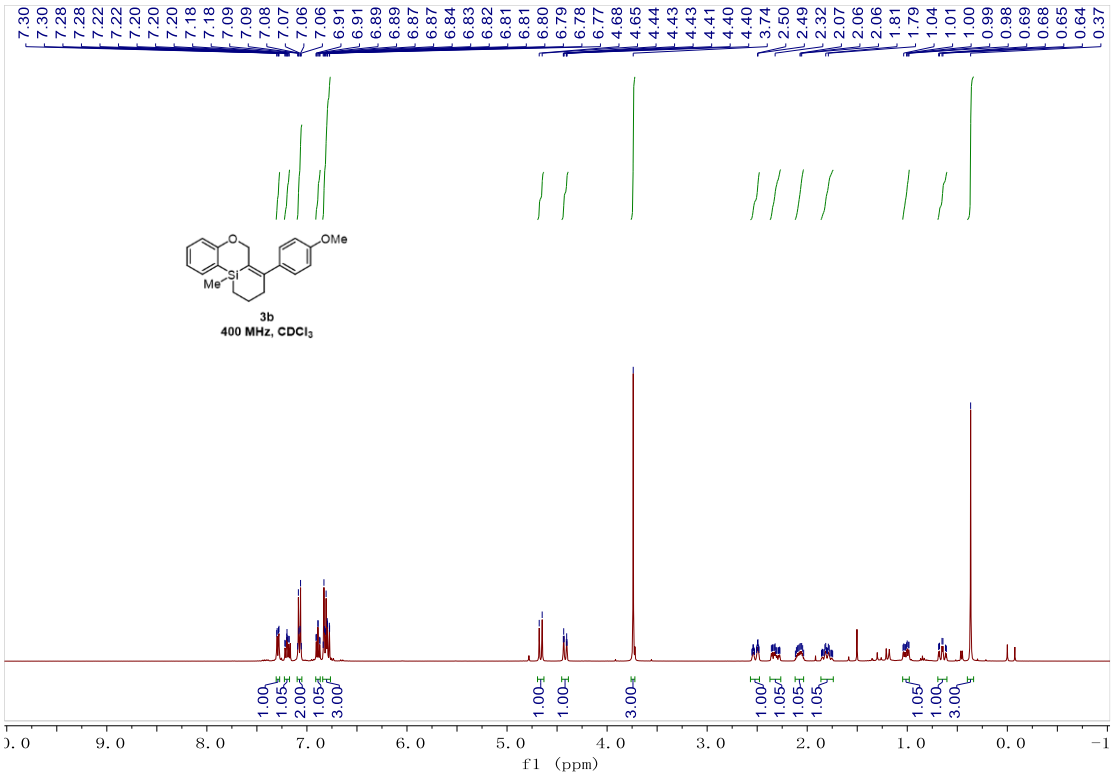
^{1}H NMR spectrum of 3a



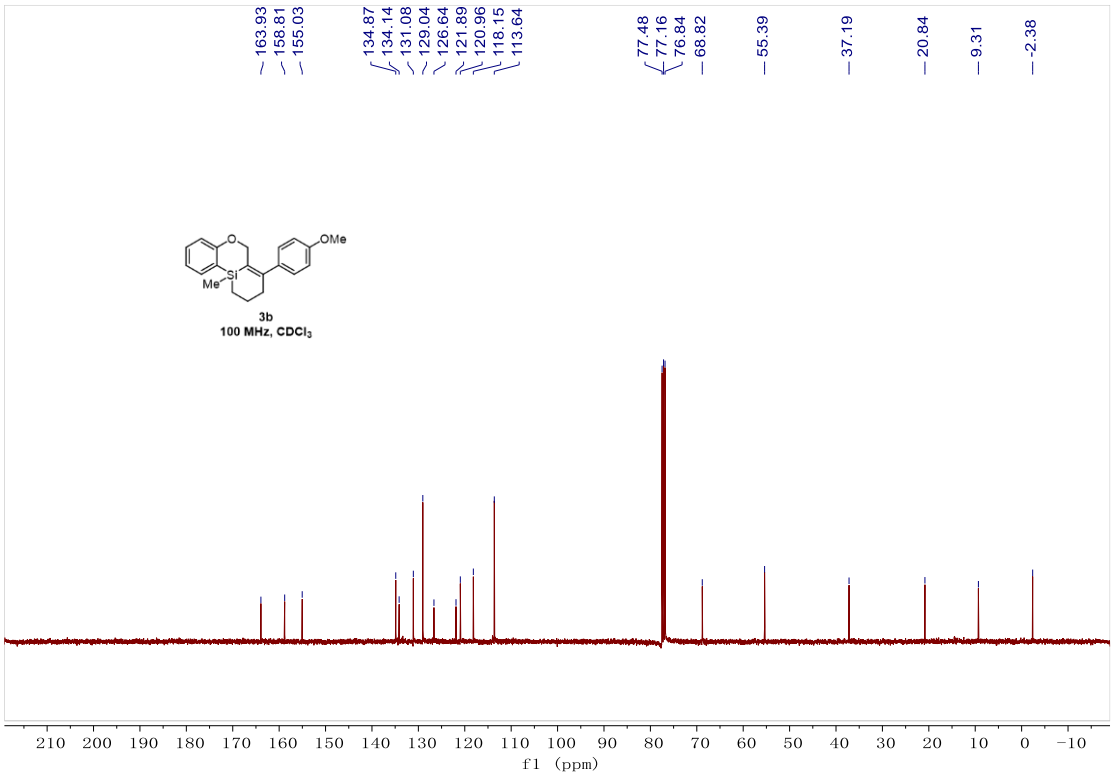
^{13}C NMR spectrum of 3a



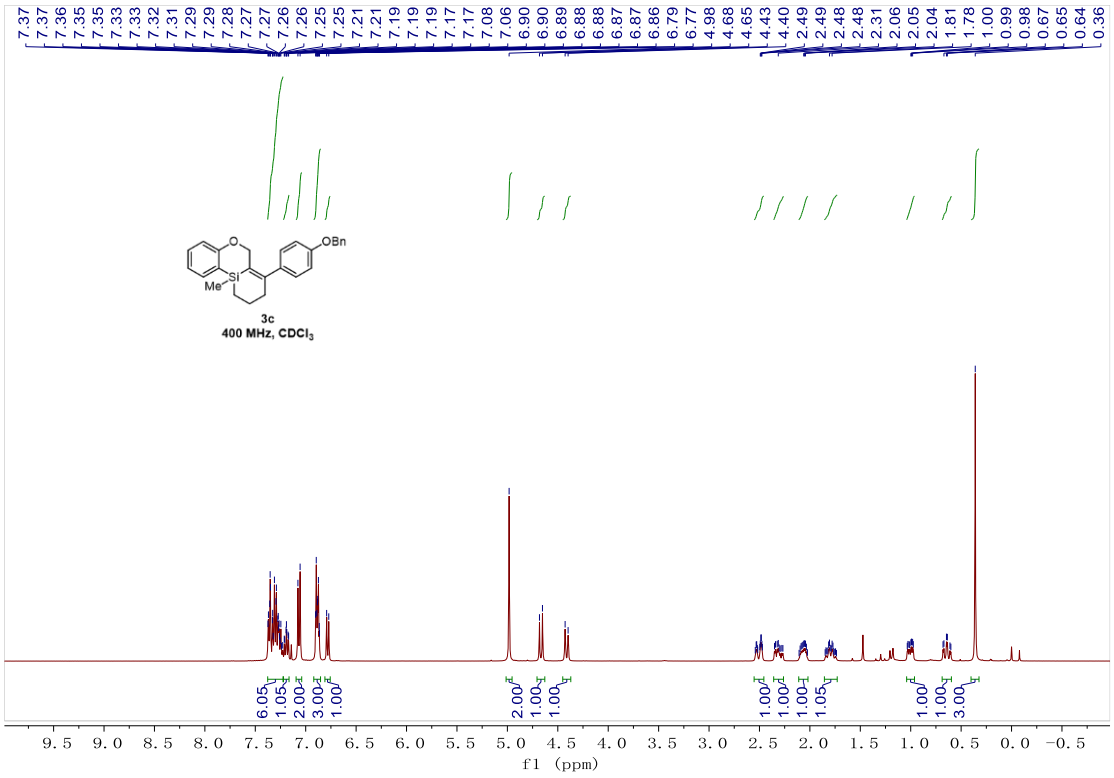
^{1}H NMR spectrum of 3b



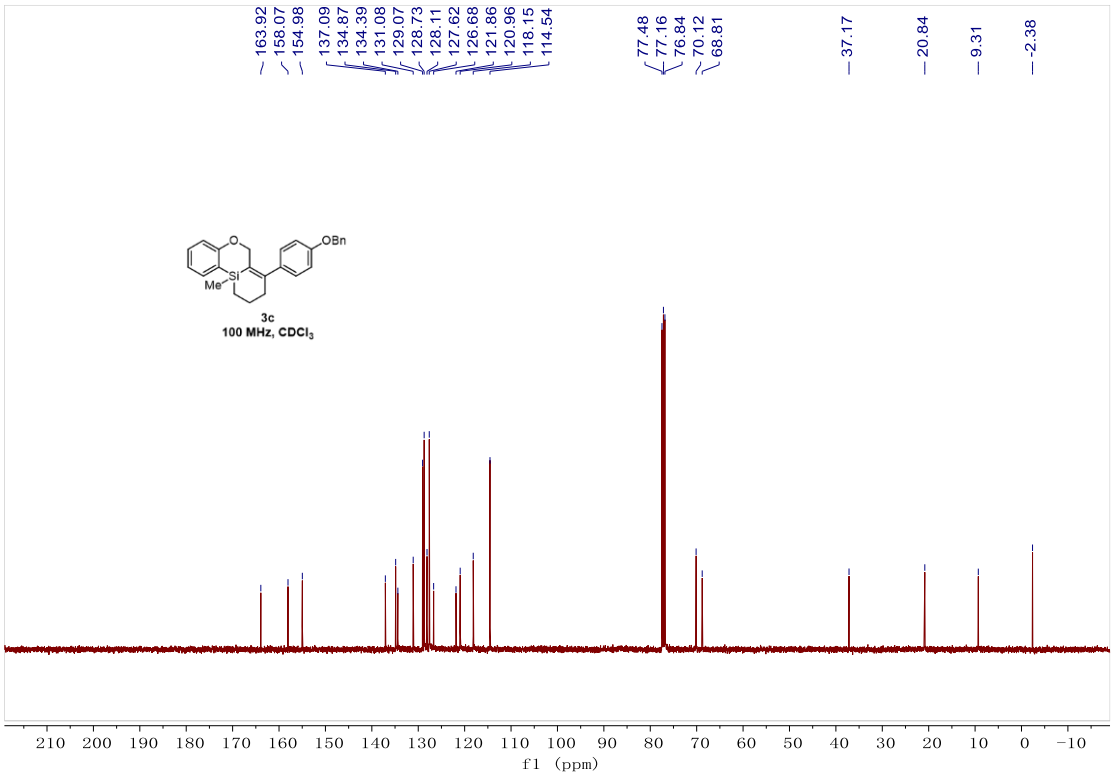
^{13}C NMR spectrum of 3b



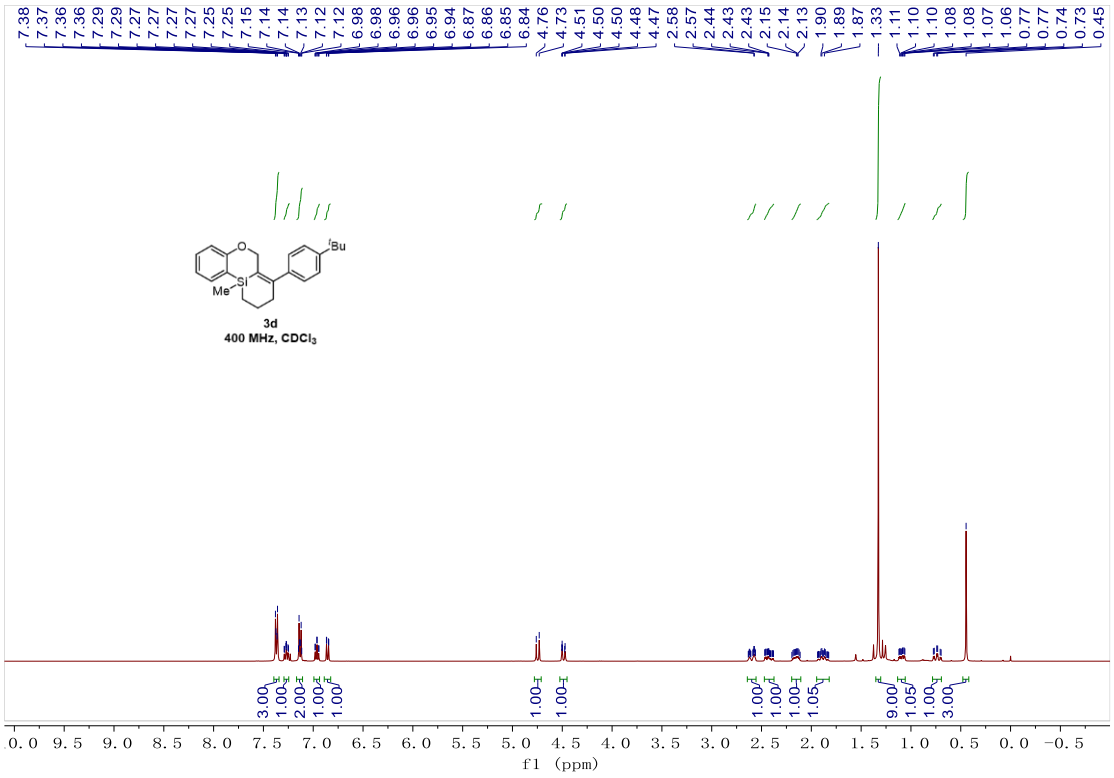
^{1}H NMR spectrum of 3c



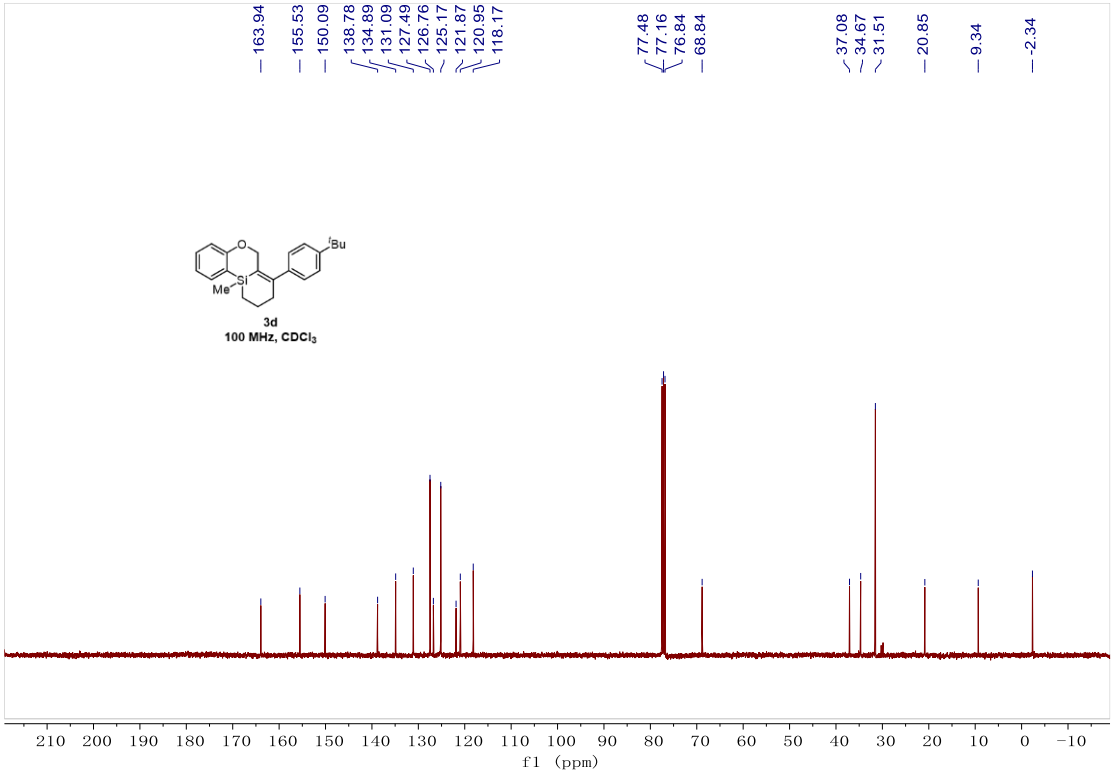
^{13}C NMR spectrum of 3c



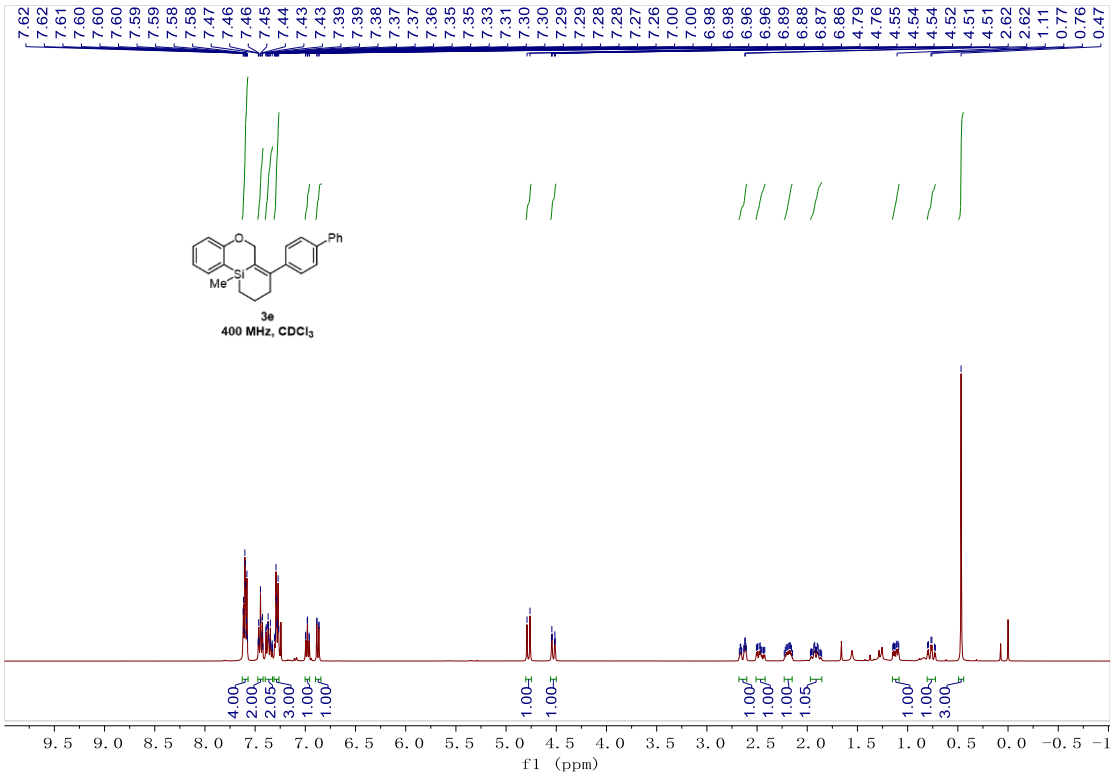
^{1}H NMR spectrum of 3d



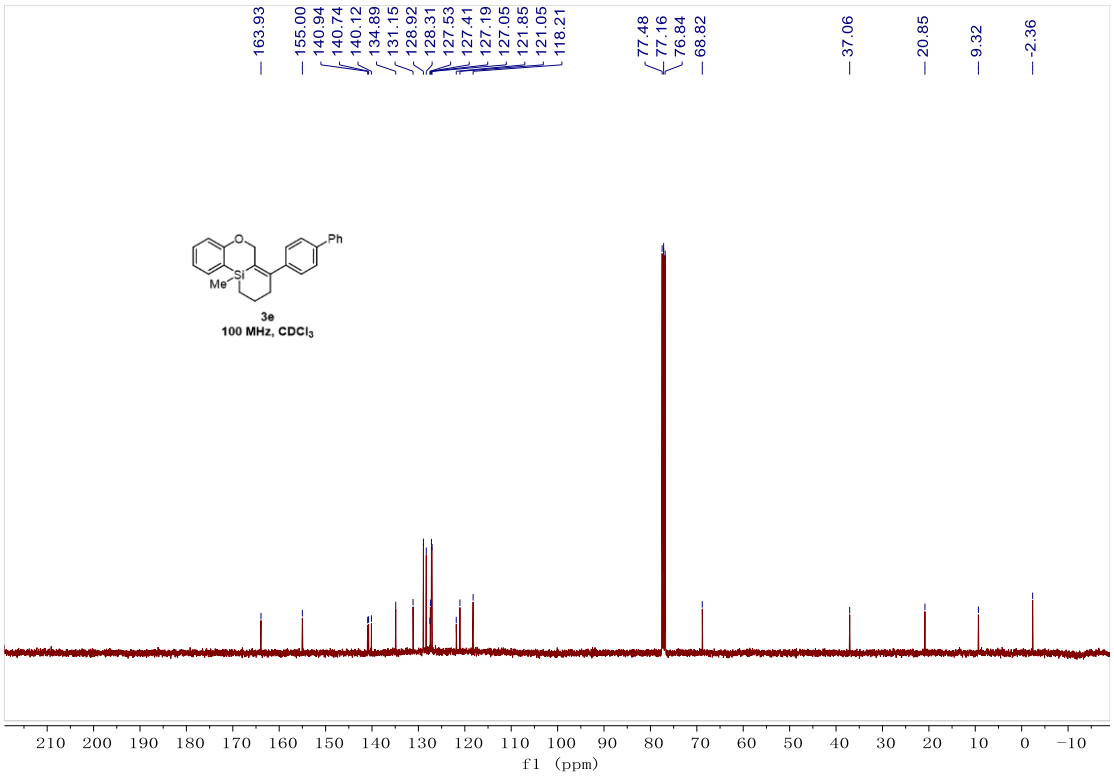
^{13}C NMR spectrum of 3d



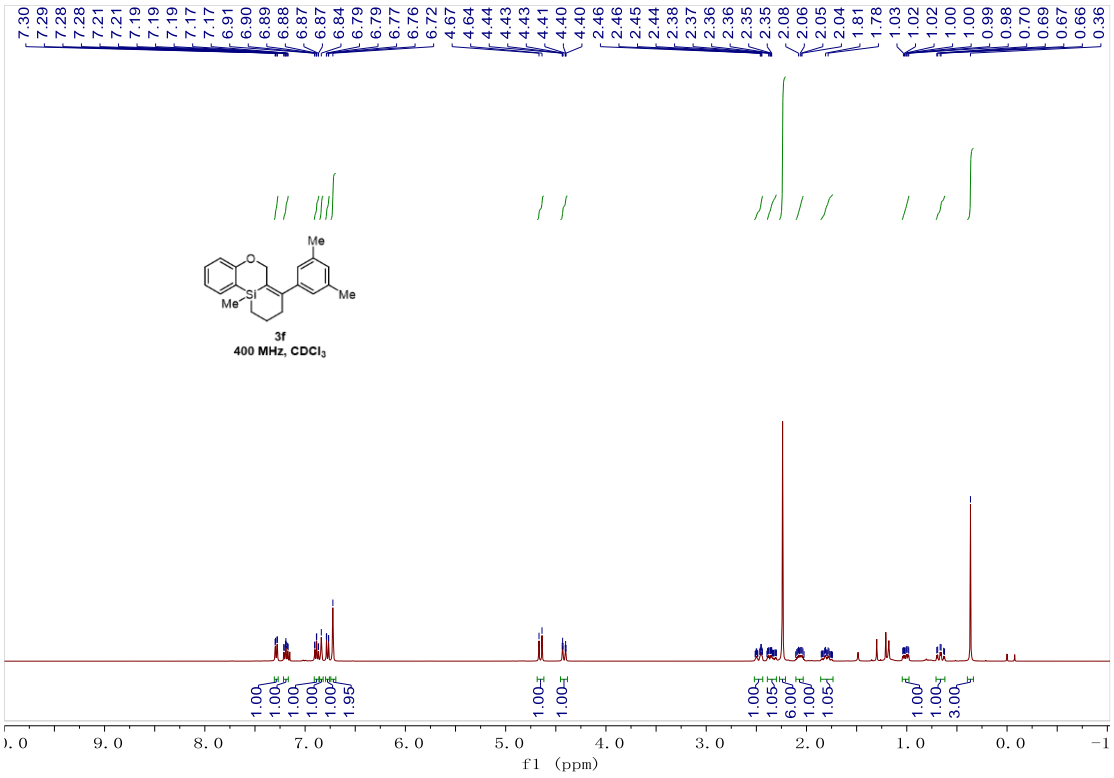
^{1}H NMR spectrum of 3e



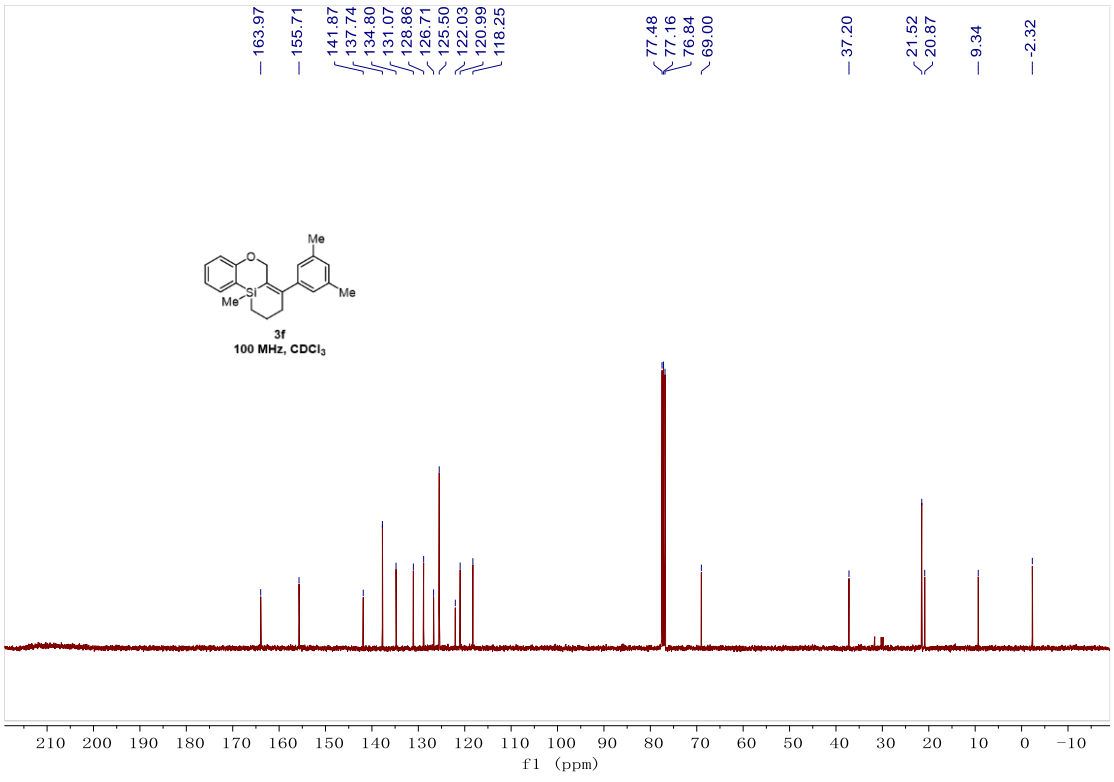
^{13}C NMR spectrum of 3e



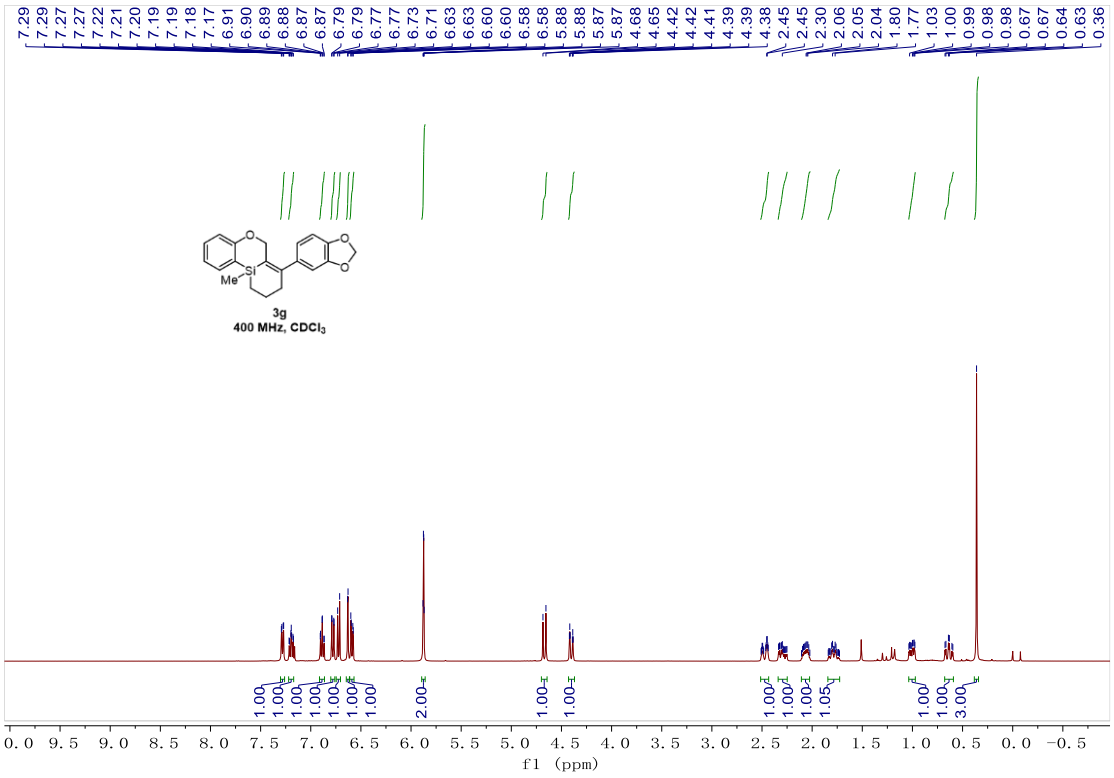
^{1}H NMR spectrum of 3f



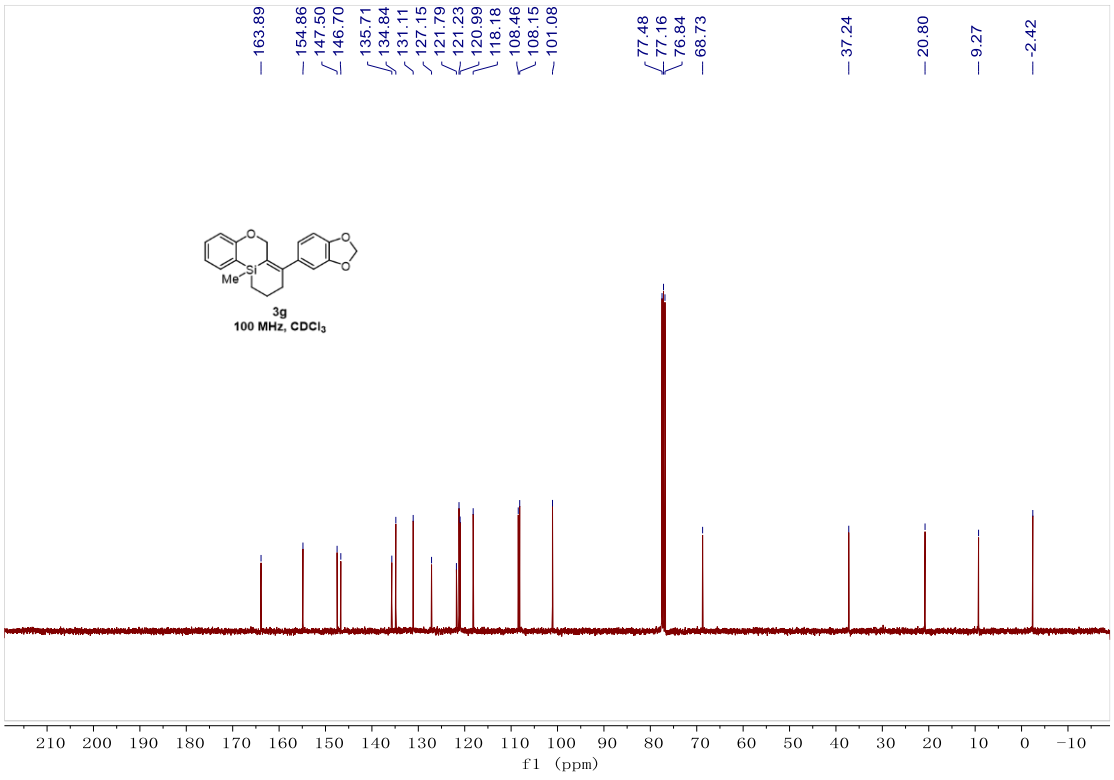
^{13}C NMR spectrum of 3f



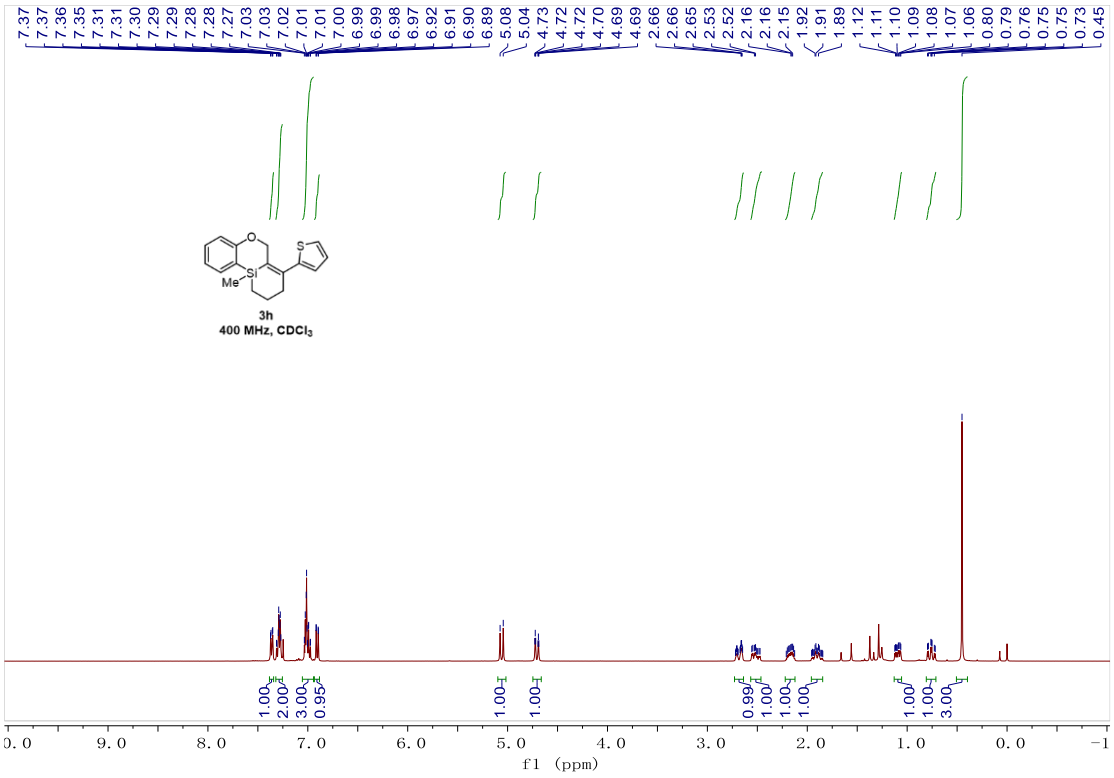
^{1}H NMR spectrum of 3g



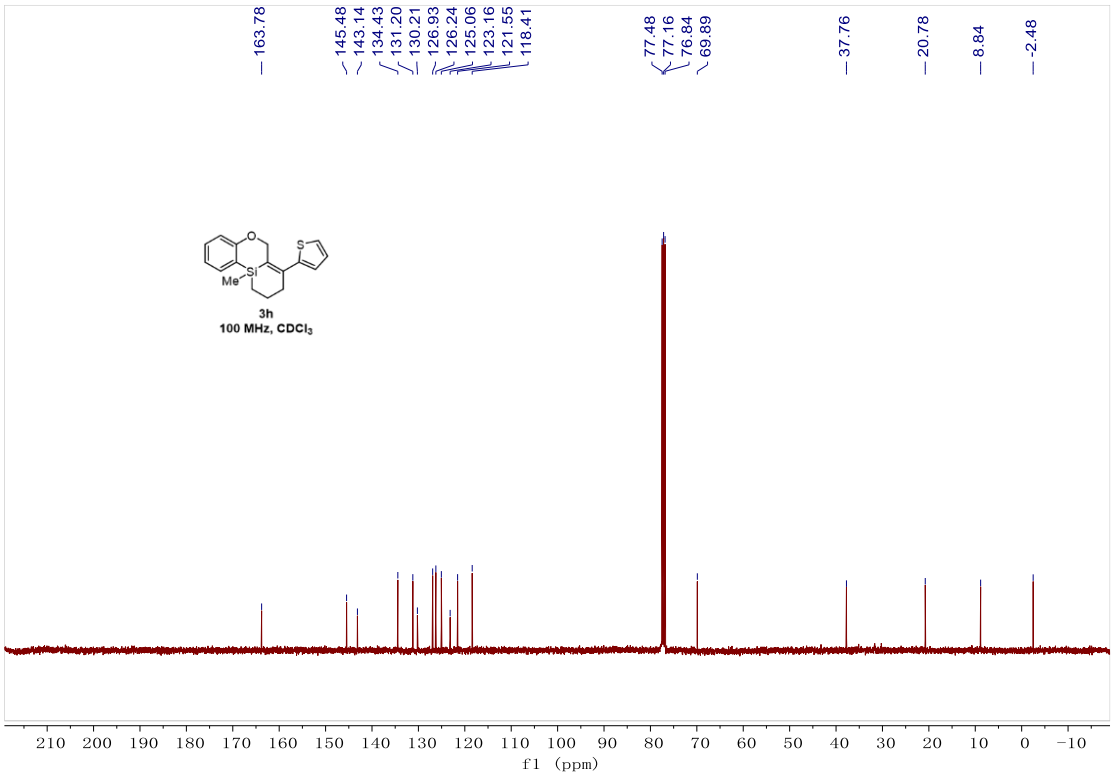
^{13}C NMR spectrum of 3g



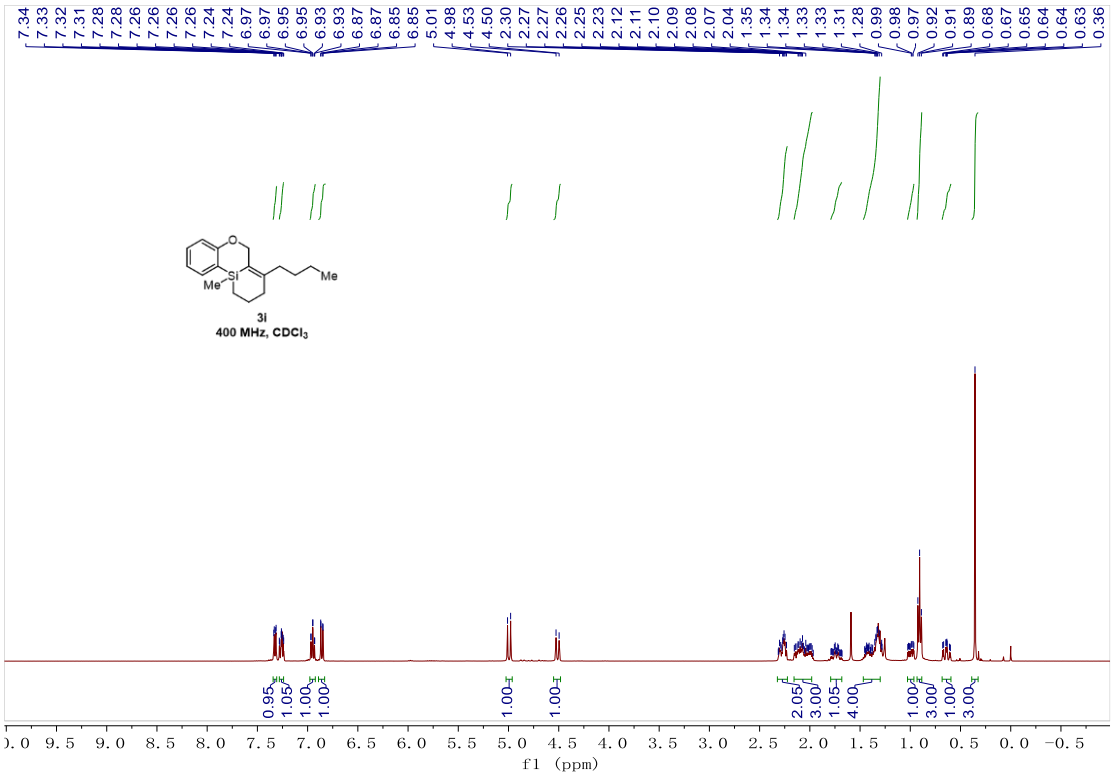
^{1}H NMR spectrum of 3h



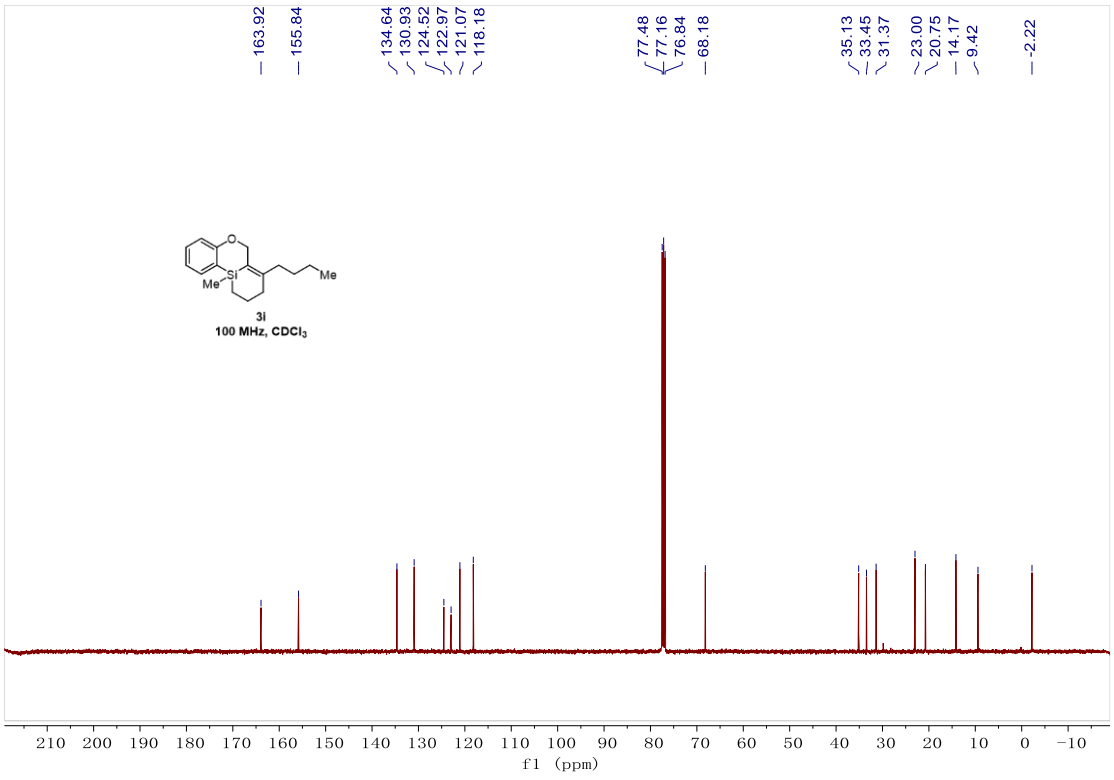
^{13}C NMR spectrum of 3h



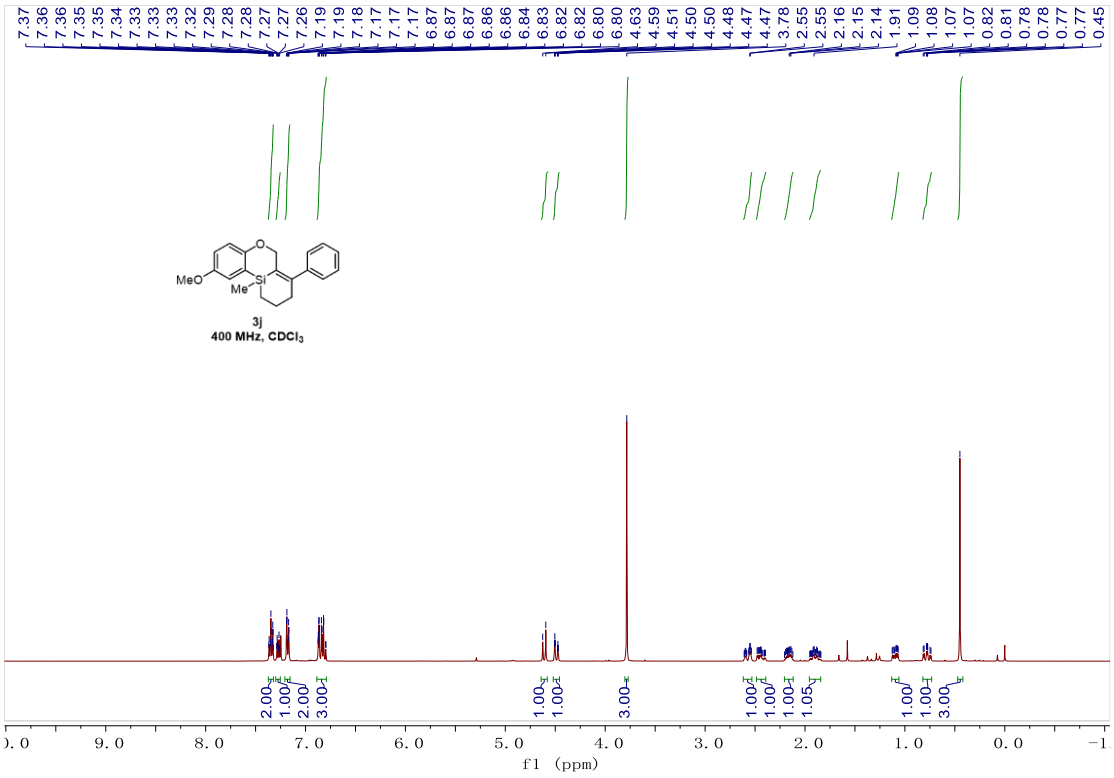
^{1}H NMR spectrum of 3i



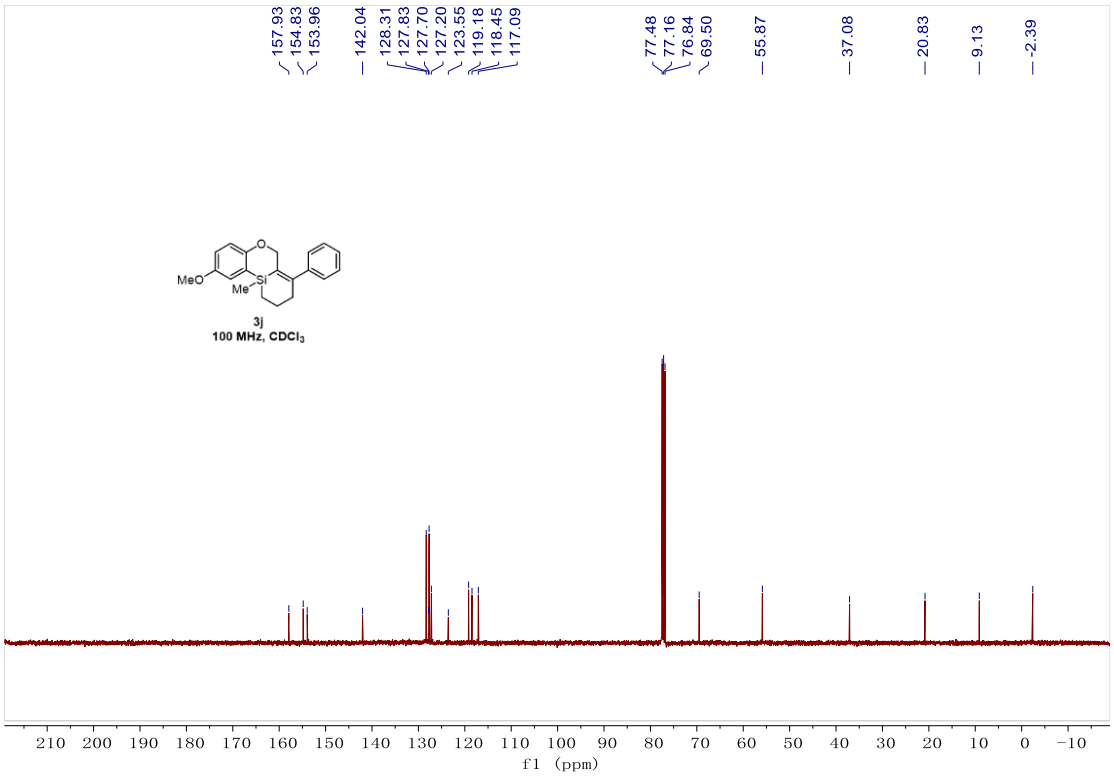
^{13}C NMR spectrum of 3i



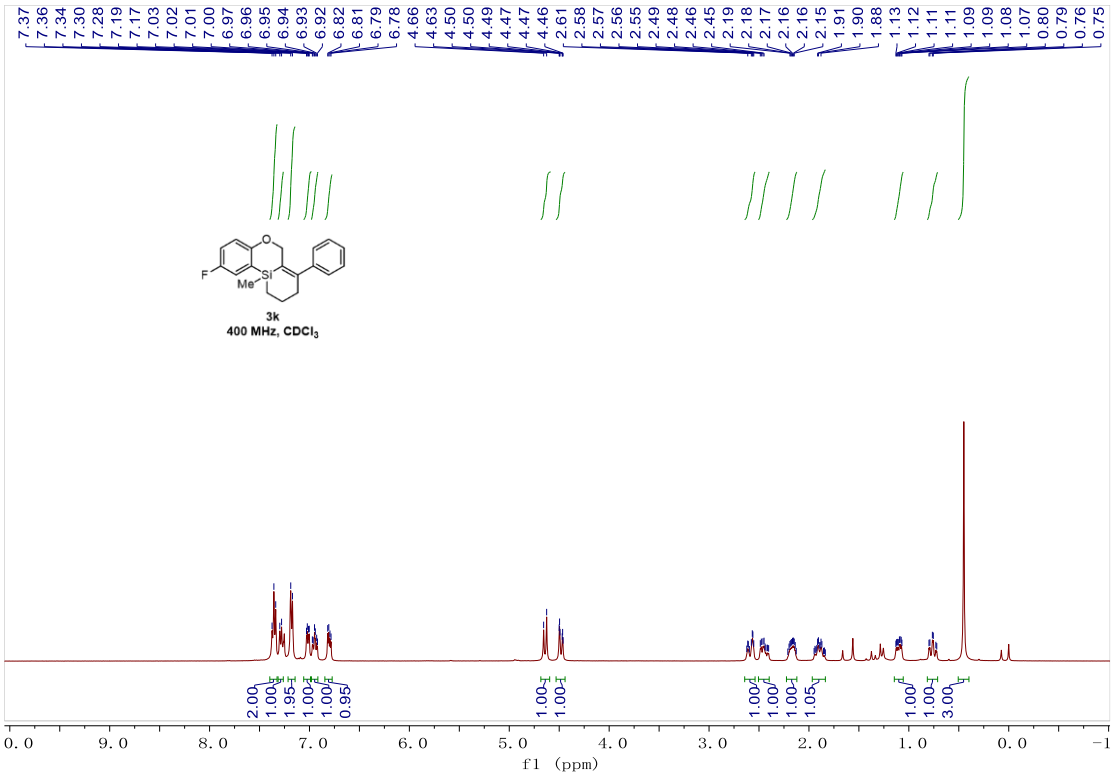
^{1}H NMR spectrum of 3j



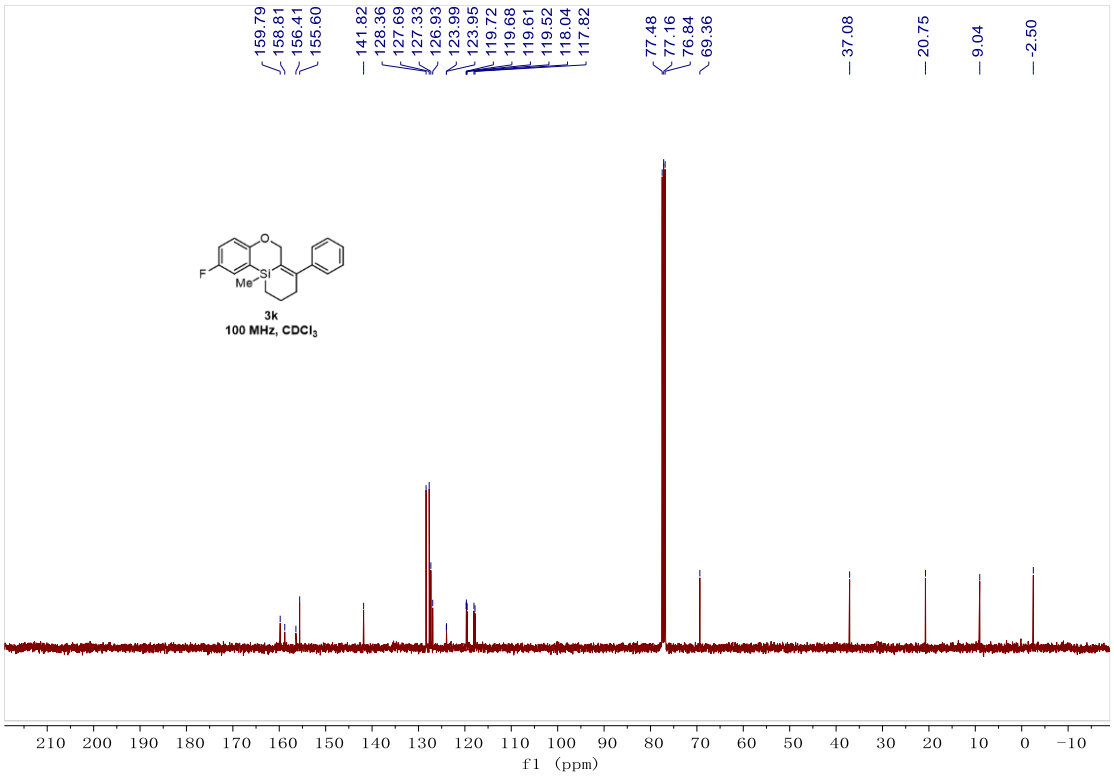
^{13}C NMR spectrum of 3j



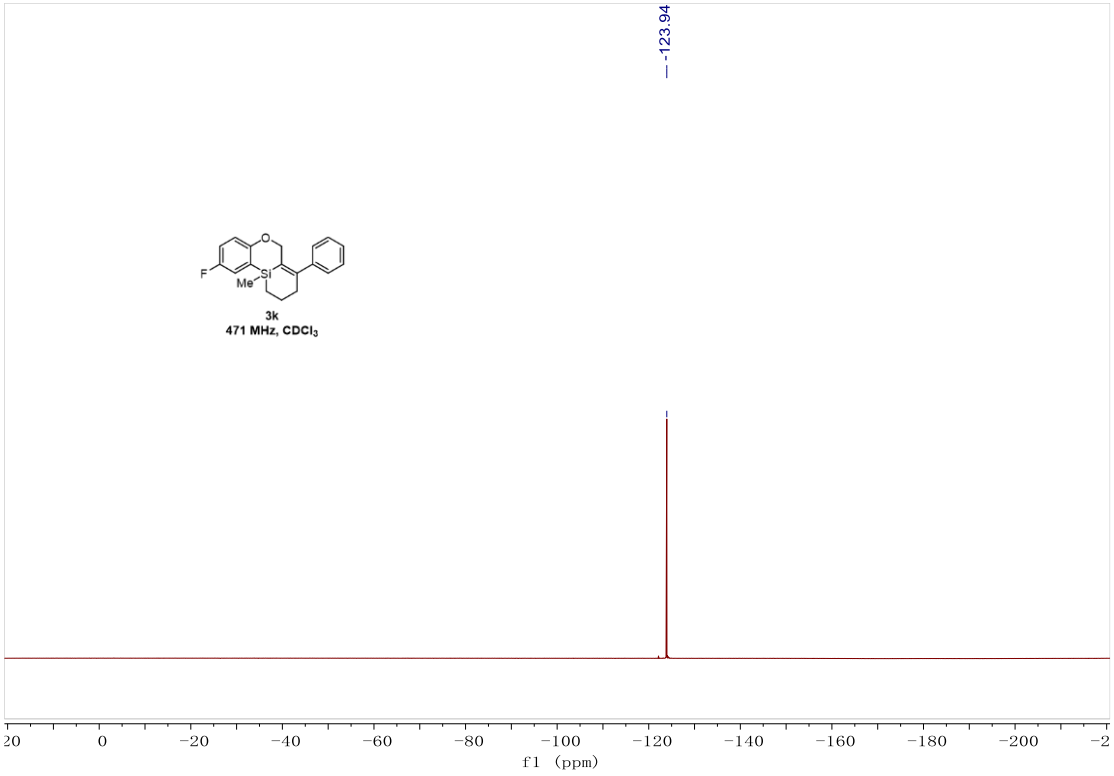
^{1}H NMR spectrum of 3k



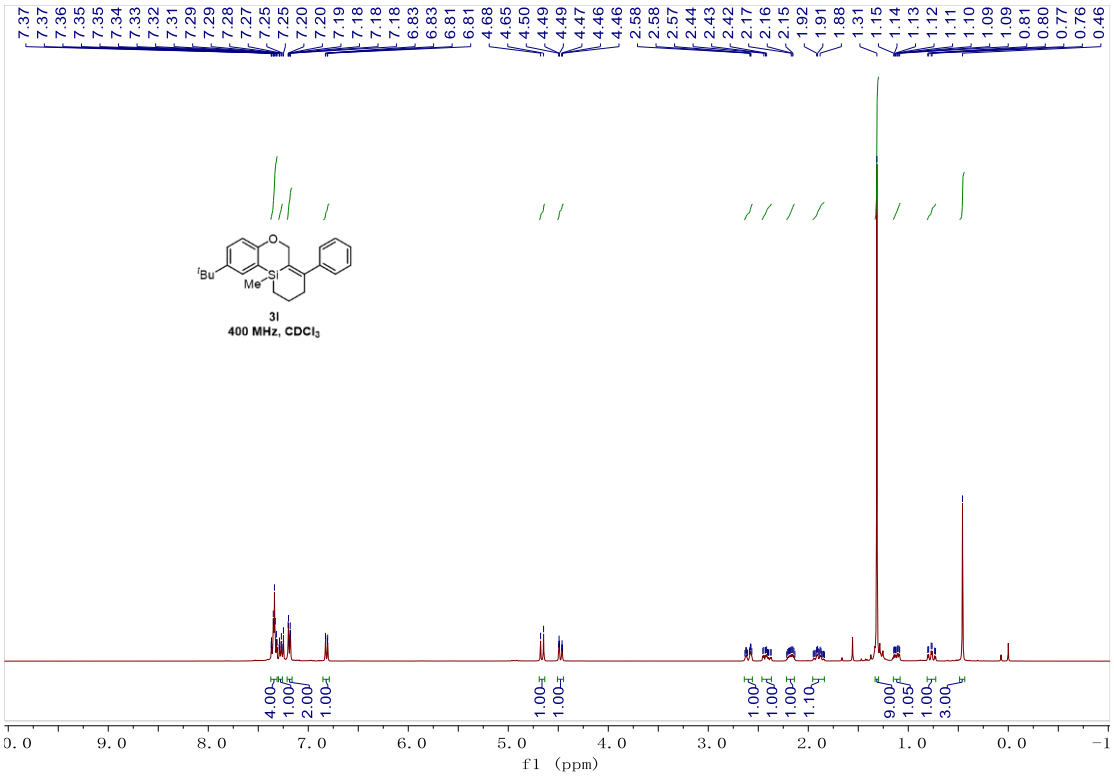
^{13}C NMR spectrum of 3k



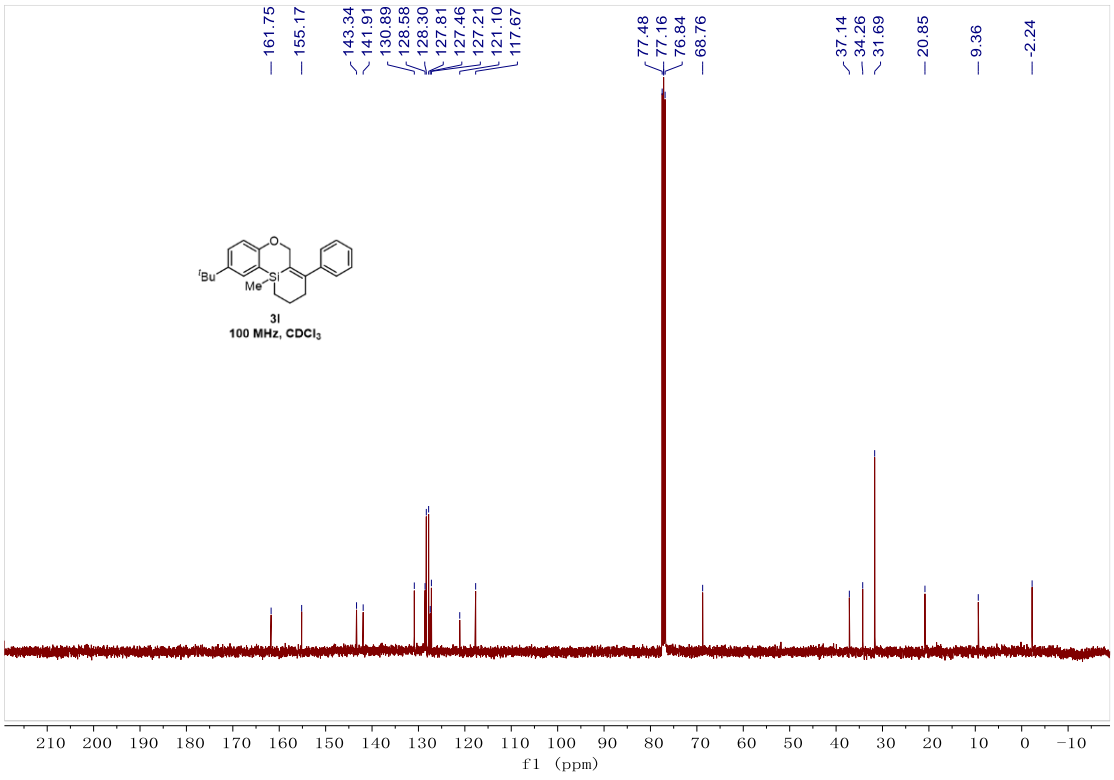
^{19}F NMR spectrum of 3k



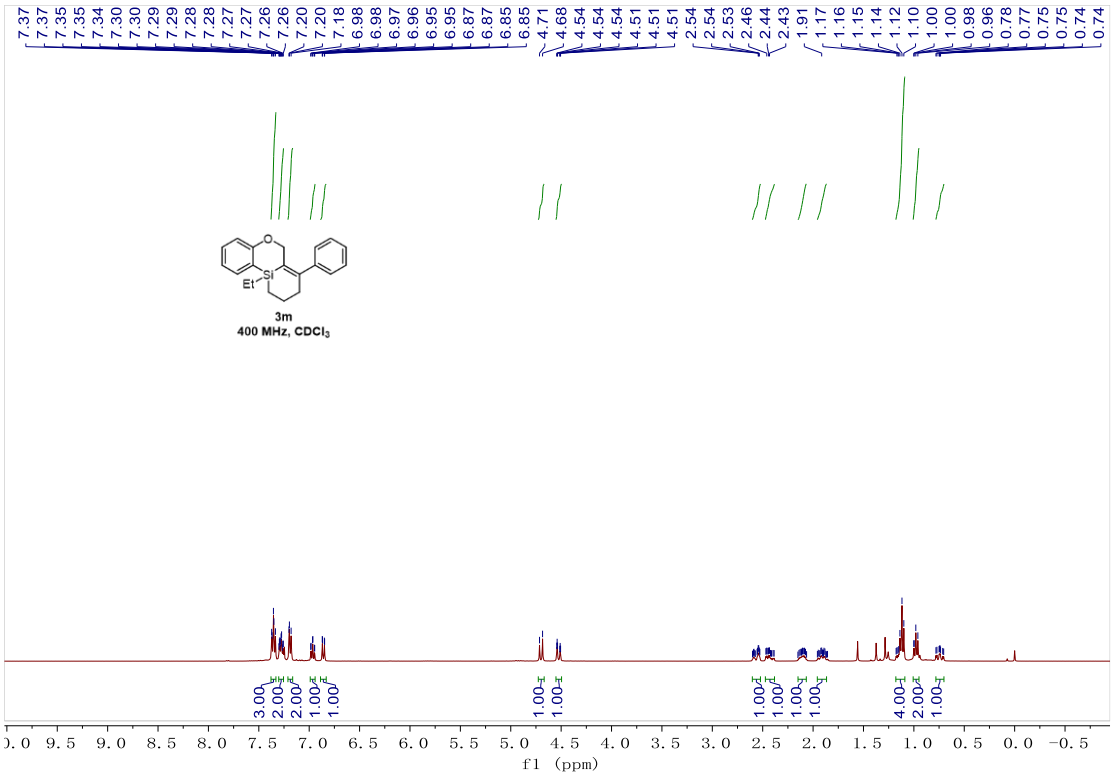
^{1}H NMR spectrum of 3l



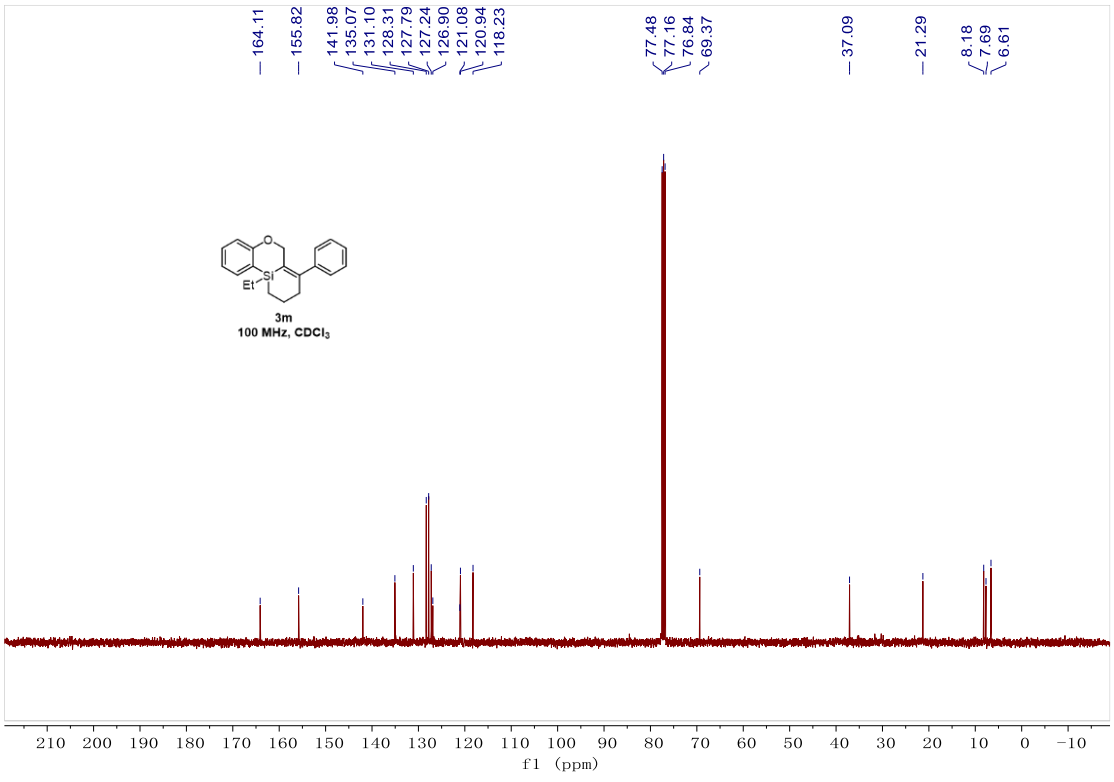
^{13}C NMR spectrum of 3l



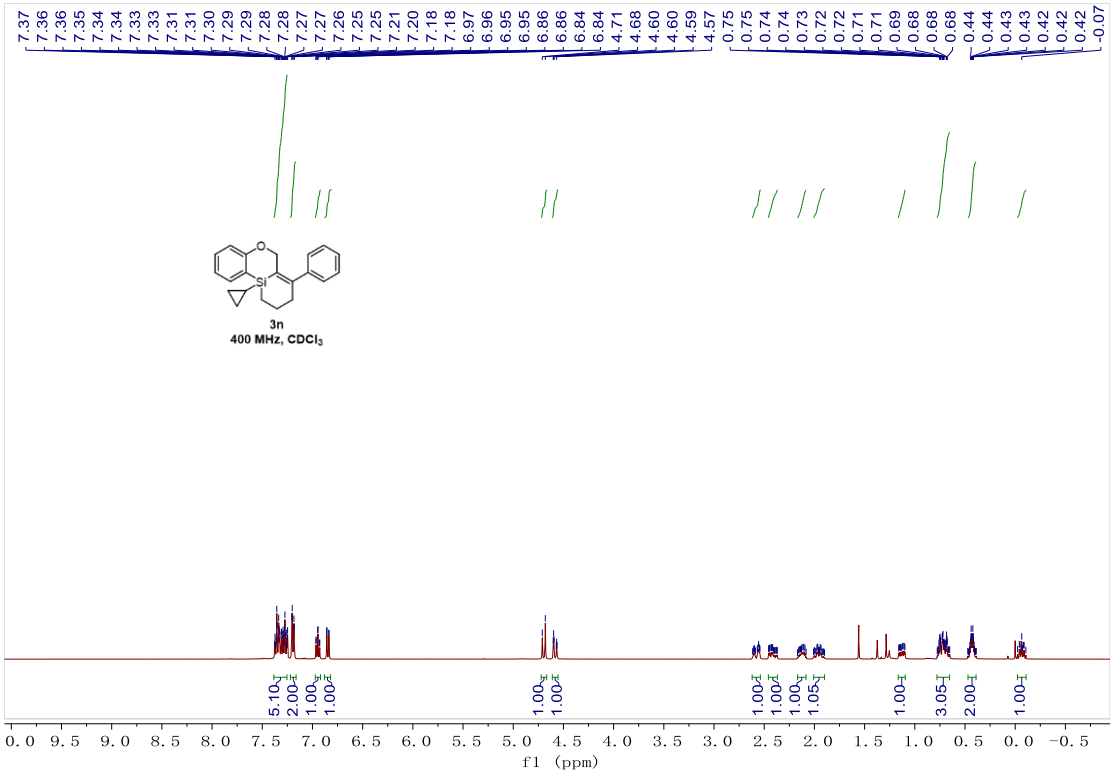
^{1}H NMR spectrum of 3m



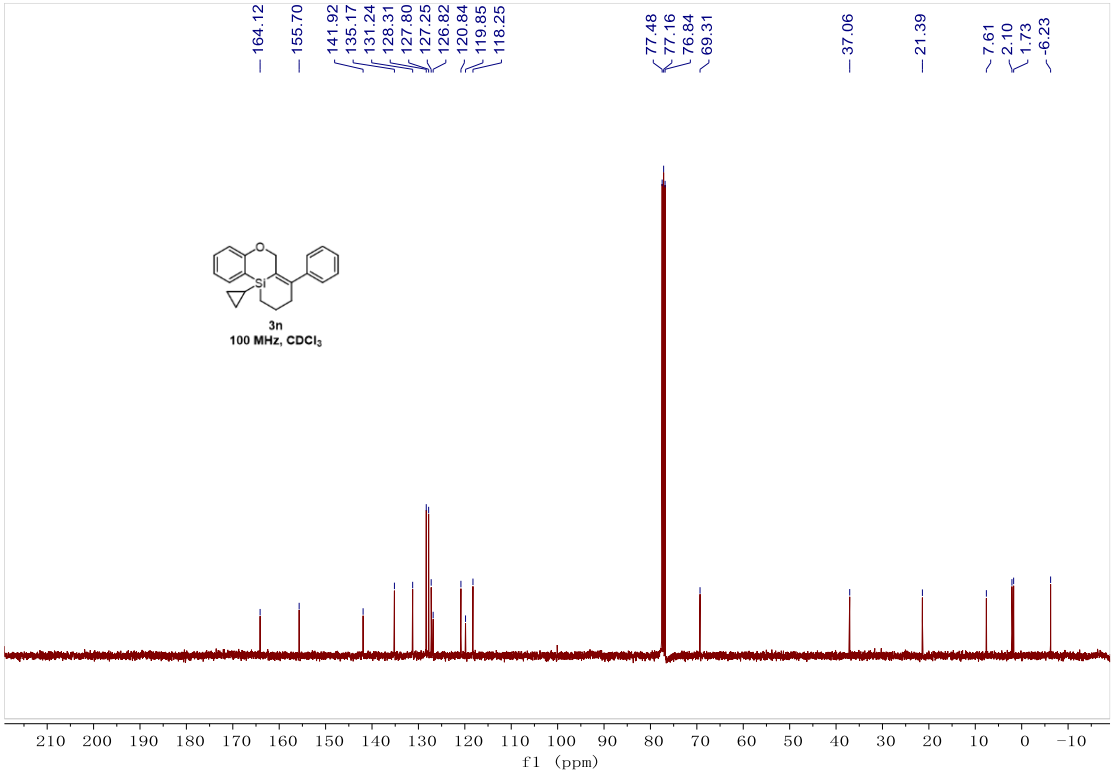
^{13}C NMR spectrum of 3m



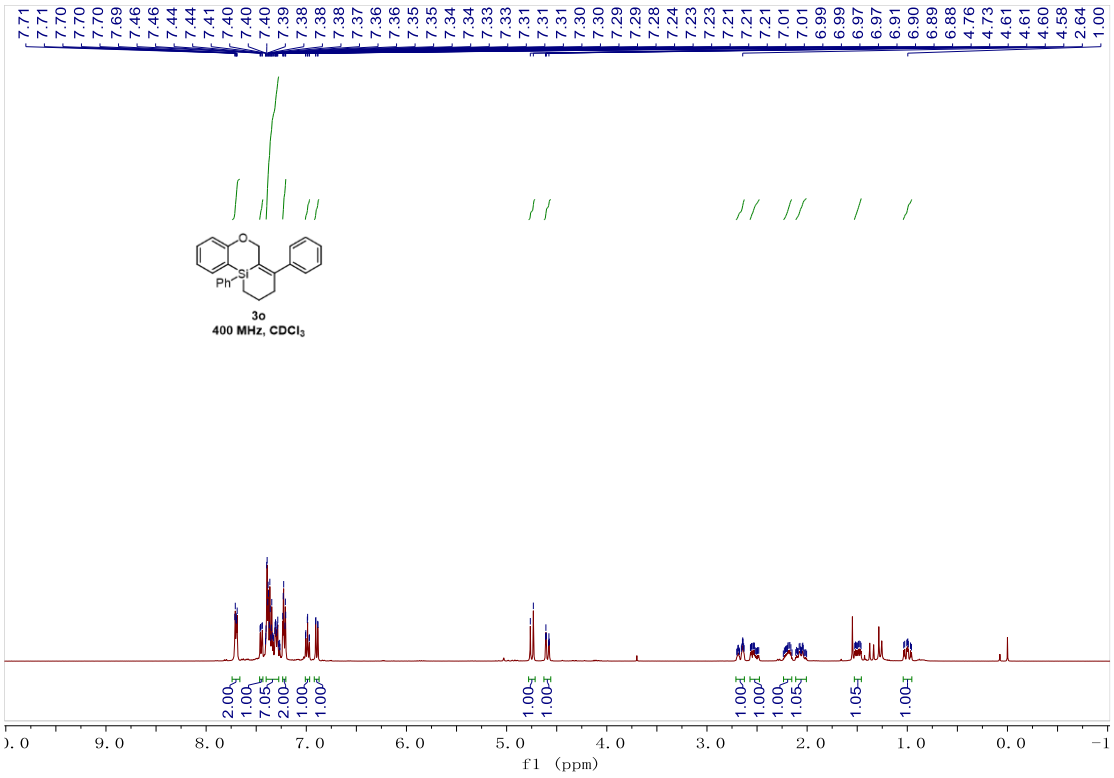
^{1}H NMR spectrum of 3n



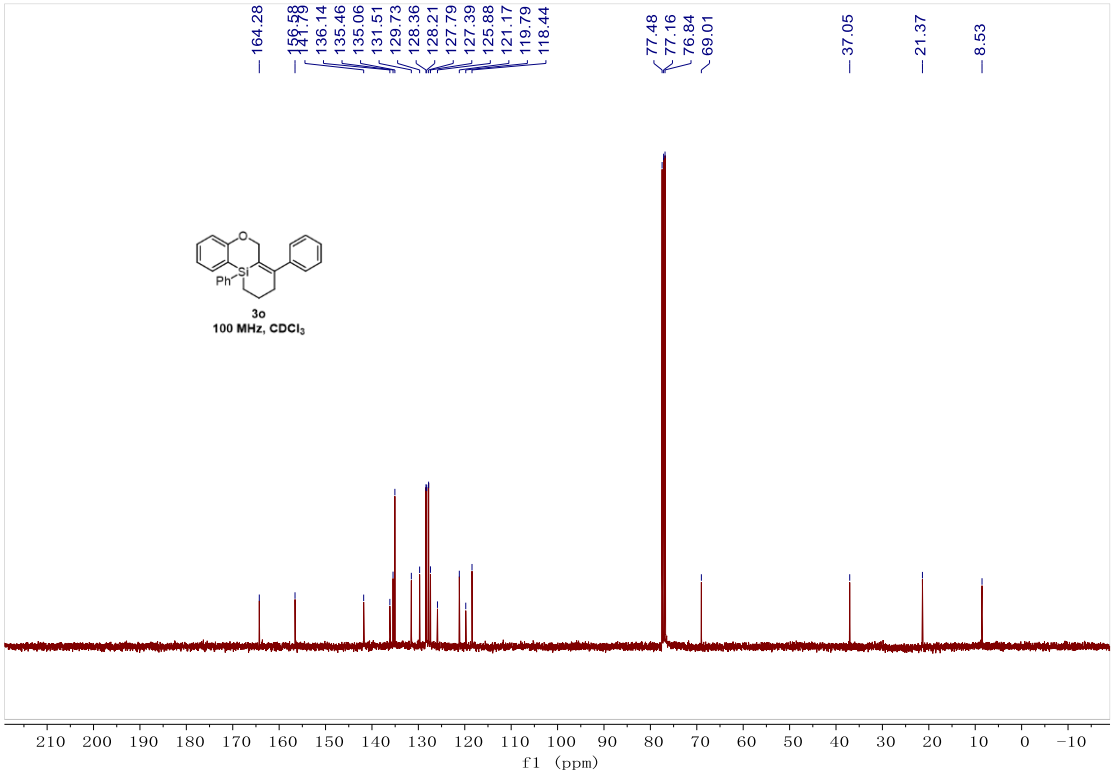
^{13}C NMR spectrum of 3n



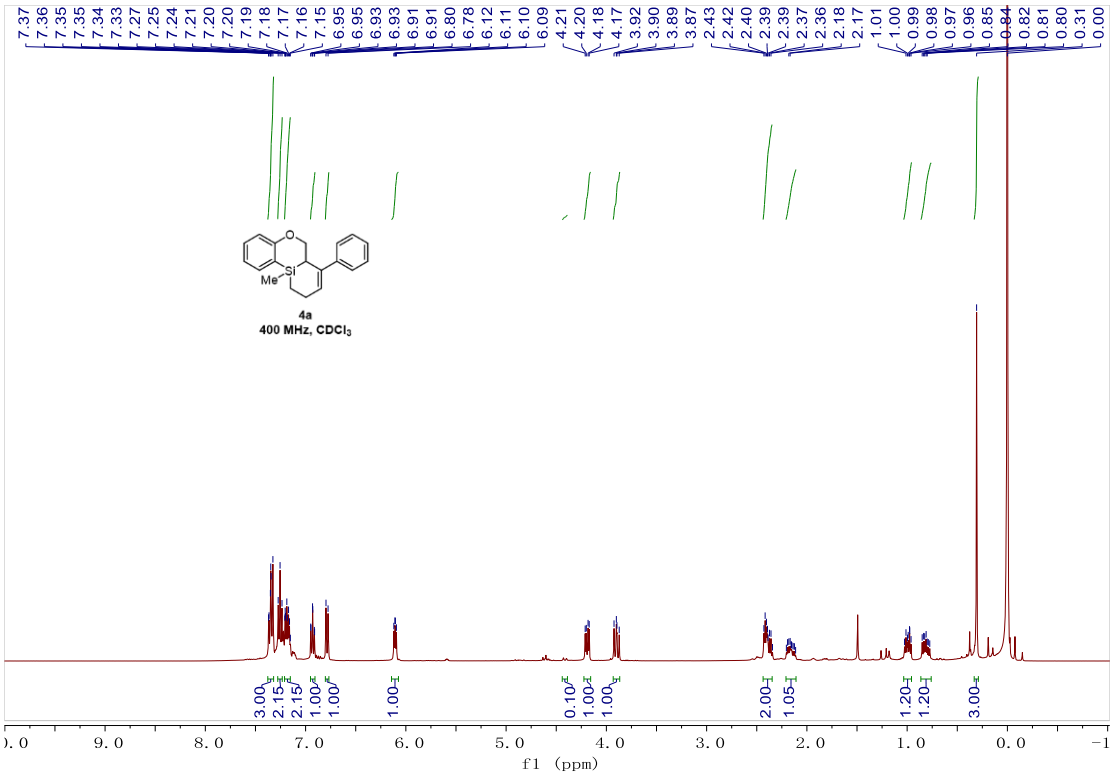
^{1}H NMR spectrum of 3o



^{13}C NMR spectrum of 3o



^{1}H NMR spectrum of 4a



^{13}C NMR spectrum of 4a