

# Supporting Information

## Enantioselective Diarylcarbene Insertion into Si–H Bonds Induced by Electronic Properties of the Carbenes

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### This PDF file includes:

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Spectral Data  
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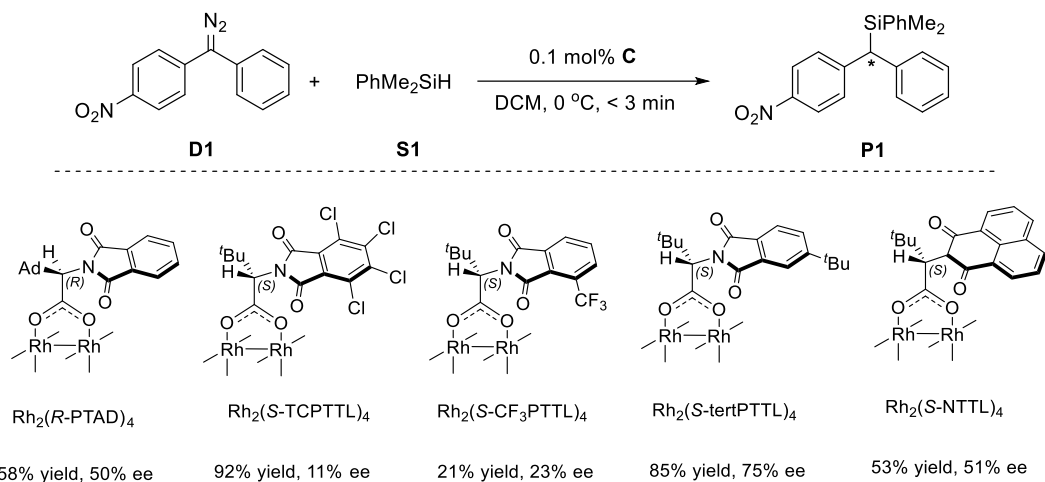
## 1. General information

NMR spectra were recorded with a Bruker AV 400 spectrometer at 400 MHz ( $^1\text{H}$  NMR), 101 MHz ( $^{13}\text{C}$  NMR), 79 MHz ( $^{29}\text{Si}$  NMR), 376 MHz ( $^{19}\text{F}$  NMR), 128 MHz ( $^{11}\text{B}$  NMR) and 162 MHz ( $^{31}\text{P}$  NMR). Chemical shifts ( $\delta$  values) were reported in ppm down field from internal  $\text{Me}_4\text{Si}$  ( $^1\text{H}$  and  $^{13}\text{C}$  NMR). High Resolution Mass Spectra (HRMS) were recorded on an IonSpec FT-ICR mass spectrometer with Electron Spray Ionization (ESI) resource and Waters GCT Premier mass spectrometer. Melting points were measured on a RY-I apparatus and uncorrected. Enantioselectivities were recorded on Agilent HPLC, using a chiral stationary phase column (Daicel Co. CHIRALPAK, CHIRALCEL, Phenomenex). The chiral HPLC methods were calibrated with the corresponding racemic mixtures.

All reactions and manipulations were performed using standard Schlenk techniques. All solvents were purified and dried using standard procedures. All chiral carboxylate dirhodium complexes were purchased from Strem and TCI.

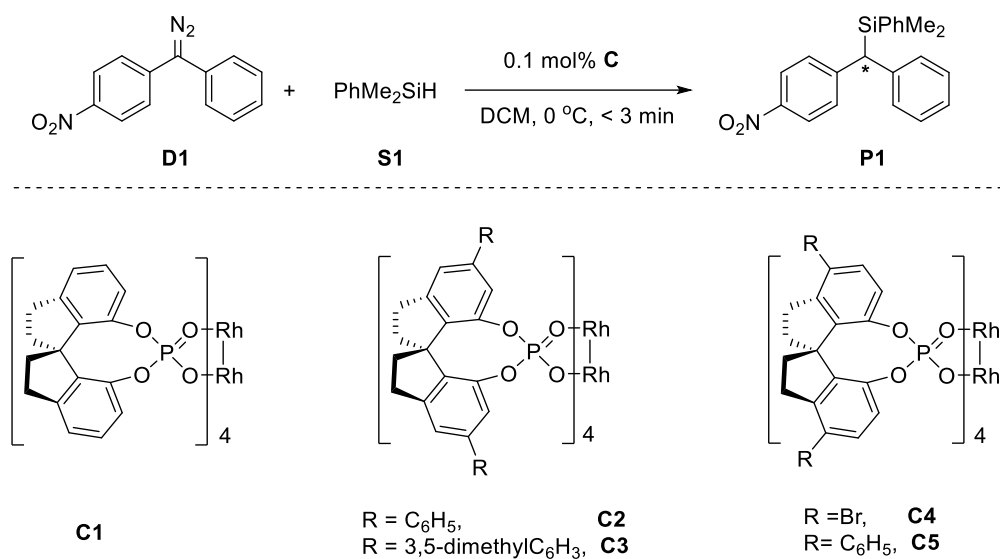
## 2. Condition optimization of enantioselective Si-H bond insertion

**Table S1. Initial screening of chiral carboxylic dirhodium catalysts<sup>a</sup>**



<sup>a</sup>Reaction conditions: **C/D1/S1**= 0.0002:0.2:0.24 (mmol), 1 mL solution of **D1** was dropped into 2 mL solution of **S1** and **C** at 0 °C, < 3 min, isolated yield.

**Table S2. Screening of chiral spiro phosphate dirhodium catalysts and optimization of conditions<sup>a</sup>**



Entry	C	Solvent	Yield/%	Ee/%
1	<b>C1</b>	DCM	56	95
2	<b>C2</b>	DCM	92	>99
3	<b>C3</b>	DCM	94	97
4	<b>C4</b>	DCM	56	66
5	<b>C5</b>	DCM	33	82
6	<b>C2</b>	toluene	95	99
7	<b>C2</b>	THF	65	99
8 <sup>b</sup>	<b>C2</b>	DCM	84	>99
9 <sup>c</sup>	<b>C2</b>	DCM	42	98

<sup>a</sup>Reaction conditions: **C/D1/S1** = 0.0002:0.2:0.24 (mmol), 1 mL solution of **D1** was dropped into 2 mL solution of **S1** and **C** at 0 °C, < 3 min, isolated yield. <sup>b</sup>**C/D1/S1** = 0.00002:0.2:0.24, the diazo compound disappeared completely for 10 min. <sup>c</sup>**C/D1/S1** = 0.000002:0.2:0.24, the diazo compound was not decomposed completely.

### 3. The correlation between enantioselectivity and electronic Hammett parameters.

R	NO <sub>2</sub>	CN	CF <sub>3</sub>	SCF <sub>3</sub>	OCF <sub>3</sub>	Cl	Br	I	F	Me	OMe	NMe <sub>2</sub>
$\Delta\sigma_p$	0.78	0.66	0.54	0.5	0.35	0.28	0.23	0.18	0.06	-0.17	-0.27	-0.6
ee/%	99.2	98	95(S)	97	76	66	76	82	25	18	64(R)	90
er (S/R)	99.6:0.4	99:1	97.5:2.5	98.5:1.5	88:12	83:17	88:12	91:9	62.5:37.5	41:59	18:82	5:95

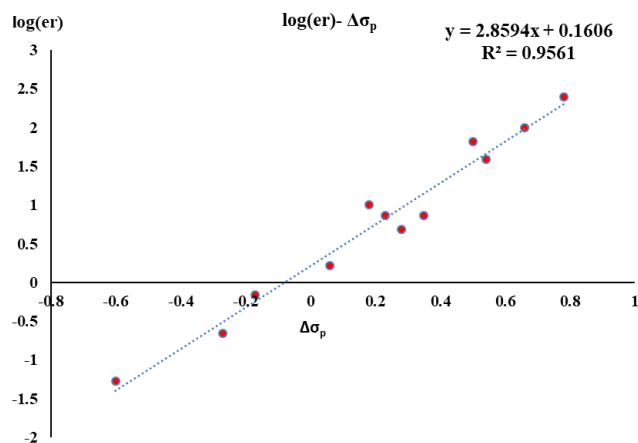


Figure S1. Plot of  $\log(er)$  vs Hammett constant  $\Delta\sigma_p$

R <sup>1</sup>	NO <sub>2</sub>	NO <sub>2</sub>	NO <sub>2</sub>	NO <sub>2</sub>	NO <sub>2</sub>	NO <sub>2</sub>	NO <sub>2</sub>	CN	CF <sub>3</sub>	CF <sub>3</sub>	CF <sub>3</sub>	CF <sub>3</sub>	CF <sub>3</sub>	OCF <sub>3</sub>	Br	Cl	F	Me
R <sup>2</sup>	NMe <sub>2</sub>	OMe	Me	F	Br	Cl	CF <sub>3</sub>	CF <sub>3</sub>	OMe	Me	F	Br	Cl	OMe	OMe	OMe	OMe	OMe
$\Delta\sigma_p$	1.38	1.05	0.95	0.72	0.55	0.5	0.24	0.12	0.81	0.71	0.48	0.31	0.26	0.62	0.5	0.55	0.33	0.1
ee/%	96	99	99	98	95	96	86	36	98	94	92	67	76	93	94	93	77	56
er	98:2	99.5:0.5	99.5:0.5	99:1	97.5:2.5	98:2	93:7	68:32	99:1	97:3	96:4	83.5:16.5	88:12	96.5:3.5	97:3	96.5:3.5	88.5:11.5	78:22

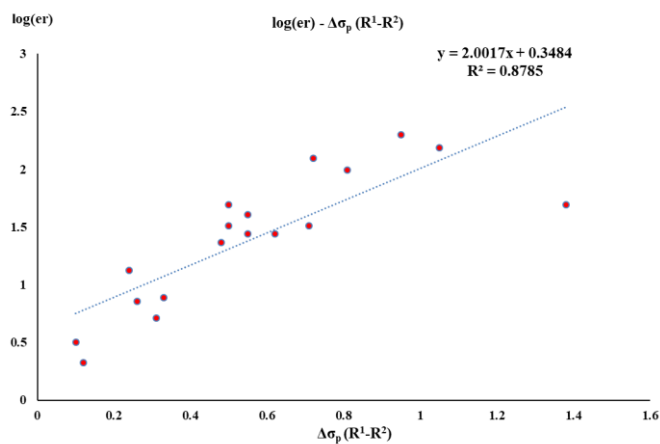


Figure S2. Plot of  $\log(er)$  vs Hammett constant  $\Delta\sigma_p(R^1-R^2)$

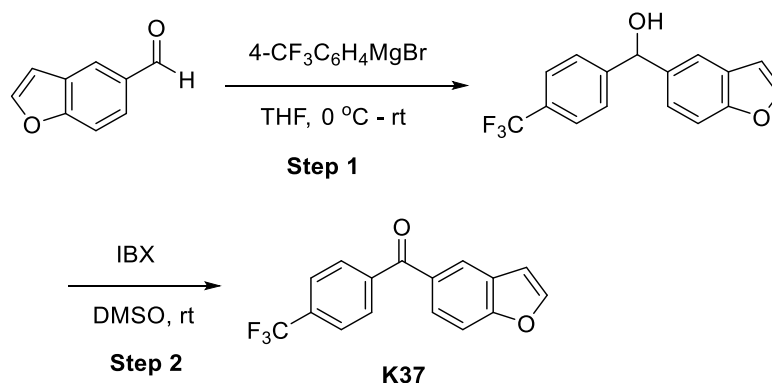
## 4. Preparation and analytical data of substrates

### 4.1 Preparation of diarylmethanones

(4-Nitrophenyl)(phenyl)methanone (**K1**), 4-benzoylbenzotrile (**K2**), phenyl(4-(trifluoromethyl)phenyl)methanone (**K3**), (4-chlorophenyl)(phenyl)methanone (**K6**), (4-bromophenyl)(phenyl)methanone (**K7**), (4-iodophenyl)(phenyl)methanone (**K8**), (4-fluorophenyl)(phenyl)methanone(**K9**), phenyl(*p*-tolyl)methanone (**K10**), (4-methoxyphenyl)(phenyl)methanone (**K11**), (4-(dimethylamino)phenyl)(phenyl)methanone (**K12**), (4-methoxyphenyl)(4-nitrophenyl)methanone (**K14**), (4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methanone (**K26**), (4-bromophenyl)(4-methoxyphenyl)methanone (**K27**), (4-chlorophenyl)(4-methoxyphenyl)methanone (**K28**), (4-fluorophenyl)(4-methoxyphenyl)methanone (**K29**), (4-methoxyphenyl)(*p*-tolyl)methanone (**K30**), naphthalen-2-yl(phenyl)methanone (**K31**), (2-methoxyphenyl)(phenyl)methanone (**K33**), (2-chlorophenyl)(phenyl)methanone (**K39**), (2-bromophenyl)(phenyl)methanone (**K40**), (2-fluorophenyl)(phenyl)methanone (**K41**) and (2-fluorophenyl)(4-methoxyphenyl)methanone (**K42**) were purchased from Aldrich, Alfa, or TCI chemical company.

The diarylmethanones **K4**<sup>1</sup>, **K5**<sup>2</sup>, **K13**<sup>3</sup>, **K15-K18**<sup>4</sup>, **K19**<sup>5</sup>, **K20**<sup>6</sup>, **K21-K25**<sup>5,6</sup>, **K32**<sup>7</sup>, **K34-K35**<sup>7</sup>, **K36**<sup>8</sup> were prepared according to literature methods.

The new diarylmethanones were prepared by using the following procedure (taking **K37** for example).

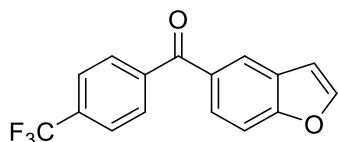


**Step 1:** A dry 250 mL Schlenk-tube equipped with a magnetic stir bar, was charged with benzofuran-5-carbaldehyde (1.5 g, 10.0 mmol) and THF (25 mL) under argon. Under vigorous stirring, a solution of bromo[4-(trifluoromethyl)phenyl]magnesium (15.0 mmol) in THF (40 mL) was slowly added under  $0\text{ }^\circ\text{C}$ . The reaction mixture was stirred under argon for 1.0 h and quenched with saturated aqueous  $\text{NH}_4\text{Cl}$  (20 mL). The aqueous layer was extracted with diethyl ether ( $3 \times 20\text{ mL}$ ). The combined organic extract was washed with brine, then dried over  $\text{MgSO}_4$ , filtered, and concentrated to give crude product. The crude product was purified by silica gel column

chromatography (eluting with petroleum ether/EtOAc, 8:1, v/v) to afford benzofuran-5-yl(4-(trifluoromethyl)phenyl)methanol (2.5 g, 85% yield) as an oil.

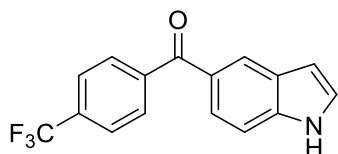
**Step 2:** A 100 mL Schlenk-tube equipped with a magnetic stir bar, was charged with benzofuran-5-yl(4-(trifluoromethyl)phenyl)methanol (2.3 g, 7.8 mmol) and THF (30 mL). Under vigorous stirring, 2-Iodoxybenzoic acid (3.3 g, 11.7 mmol) was added at one portion at ambient temperature. The reaction mixture was stirred for 2 h and diluted by water. The mixture was filtered and washed with EtOAc. The aqueous layer was extracted with EtOAc (3 × 40 mL). The combined organic extract was washed with brine, then dried over MgSO<sub>4</sub>, filtered, and concentrated to give a solid. The crude product was purified by silica gel column chromatography (eluting with petroleum ether/EtOAc, 15:1, v/v) to afford benzofuran-5-yl(4-(trifluoromethyl)phenyl)methanone (**K37**) (2.0 g, 86% yield) as a solid.

### benzofuran-5-yl(4-(trifluoromethyl)phenyl)methanone (**K37**)



Yield: 86%. White solid. m.p. = 100–102 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.08 (d, *J* = 1.8 Hz, 1H), 7.93 – 7.87 (d, *J* = 8.1 Hz, 2H), 7.84 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 2H), 7.73 (d, *J* = 2.2 Hz, 1H), 7.60 (d, *J* = 8.6 Hz, 1H), 6.86 (dd, *J* = 2.2, 0.9 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 195.3, 157.5, 146.7, 141.4, 133.4 (q, *J* = 32.0 Hz), 132.0, 130.0, 127.5, 126.7, 125.3 (q, *J* = 3.8 Hz), 124.6, 123.7 (q, *J* = 270.0 Hz), 111.6, 107.2. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –59.3 (s, 3F). HRMS (ESI) calcd for [C<sub>16</sub>H<sub>9</sub>F<sub>3</sub>O<sub>2</sub>, M + H]<sup>+</sup>: 291.0633, Found: 291.0634.

### (1*H*-indol-5-yl)(4-(trifluoromethyl)phenyl)methanone (**K38**)



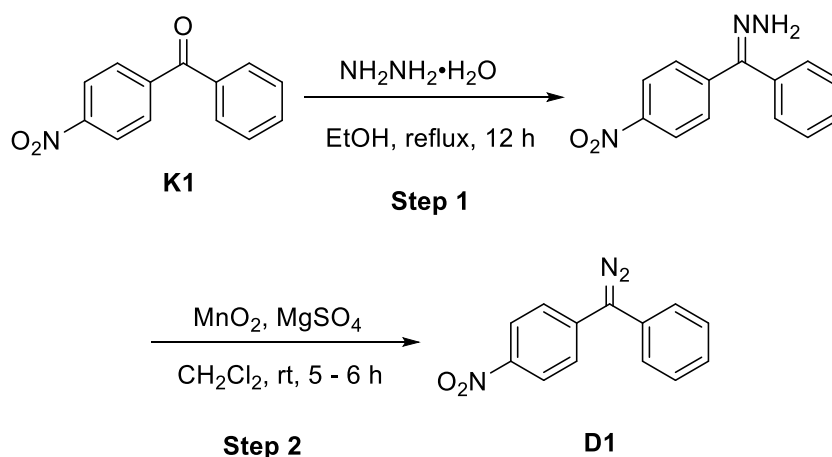
Yield: 80%. White solid. m.p. = 141–143 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.72 (s, 1H), 8.11 (s, 1H), 7.89 (d, *J* = 8.1 Hz, 2H), 7.79 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 1H), 7.31 (t, *J* = 2.8 Hz, 1H), 6.65 (t, *J* = 2.8 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 196.2, 142.2, 138.5, 133.0 (q, *J* = 33.0 Hz), 129.9, 128.9, 127.2, 126.1, 125.5, 125.1 (q, *J* = 4.1 Hz), 124.0, 123.8 (q, *J* = 271.0 Hz), 111.3, 104.3. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –59.3 (s, 3F). HRMS (ESI) calcd for [C<sub>16</sub>H<sub>10</sub>F<sub>3</sub>NO, M + H]<sup>+</sup>: 290.0793, Found: 290.0788.

## 4.2 Preparation of diaryl hydrazones and diazomethanes

Diaryl hydrazones and diazomethanes were prepared according to the literature methods.<sup>9</sup> The following are the typical procedure for the preparation of diaryl hydrazones and diazomethanes.



## Typical procedure for preparation of diaryl hydrazones and diazomethanes



**Step 1:** Hydrazine monohydrate (80% purity, 18 mL, 300.0 mmol) was added to (4-nitrophenyl)(phenyl)methanone (6.8 g, 30.0 mmol) in ethanol (100 mL). HOAc (0.5 mL) was added and the mixture was stirred at reflux for 12 h. After cooling to room temperature, (4-nitrophenyl)(phenyl)methanone hydrazone precipitated as yellow crystal. Filtration of the crude mixture gave pure (4-nitrophenyl)(phenyl)methanone hydrazone as a yellow solid in 70% yield (5.0 g, 21.0 mmol).

When the hydrazone could not precipitate. The EtOH was removed *in vacuo*, the residue was taken up in Et<sub>2</sub>O and water. The layers were separated and the aqueous layer was extracted with Et<sub>2</sub>O (3 x 20 mL). The combined organic layer was dried with MgSO<sub>4</sub>, filtered, then concentrated *in vacuo*. Column chromatography using 15–25% EtOAc/hexanes as the eluent afforded the desired product.

(Note: An inseparable mixture of two isomers of ketone hydrazone was obtained, which was used in the next step without further purification.)

**Step 2:** (4-Nitrophenyl)(phenyl)methanone hydrazone (2.9 g, 12.0 mmol) and anhydrous MgSO<sub>4</sub> (3.6 g) were placed into an oven-dried Schlenk tube under argon atmosphere and 50 mL DCM was introduced. After cooling to 0 °C, to this rapidly stirring mixture was added activated MnO<sub>2</sub> (3.7 g, 42.0 mmol) in one portion. The reaction mixture was warmed to room temperature and stirred for 5-6 h, and filtered off the solid. The solvent was removed under reduced pressure and the crude product was used for next reaction.

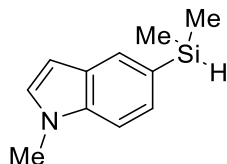
(Note: The purity of compounds were determined by <sup>1</sup>H NMR, which was generally 90%~100%. The impurity was identified as (Ar<sup>1</sup>Ar<sup>2</sup>)C=N-N=C(Ar<sup>1</sup>Ar<sup>2</sup>).)

### 4.3 Preparation of silanes.

Dimethyl(phenyl)silane (**S1**), ethoxydimethylsilane (**S2**), chlorodimethylsilane (**S3**), triethylsilane (**S4**), methyldiphenylsilane (**S5**) were purchased from Aldrich, Alfa, or TCI chemical company. Dimethyl(phenylethynyl)silane (**S7**)<sup>10</sup>, (3-

chloropropyl)dimethylsilane (**S8**)<sup>11</sup>, 5-(dimethylsilyl)-1-methyl-1*H*-indole (**S9**)<sup>10</sup> were prepared according to the methodology described by the literatures.

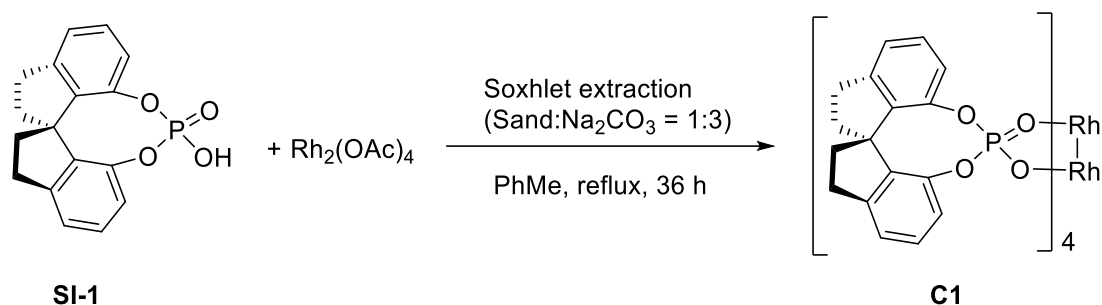
### 5-(dimethylsilyl)-1-methyl-1*H*-indole (**S9**)



Yield: 80%. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.84 (s, 1H), 7.45 – 7.23 (m, 2H), 7.01 (d, *J* = 3.1 Hz, 1H), 6.47 (d, *J* = 3.1 Hz, 1H), 4.53 (hept, *J* = 3.6 Hz, 1H), 3.74 (s, 3H), 0.37 (d, *J* = 3.7 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 137.3, 128.8, 128.5, 127.2, 126.7, 126.1, 109.0, 100.9, 32.7, –3.2. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>) δ –18.3. **HRMS (EI)** calcd for [C<sub>11</sub>H<sub>15</sub>NSi, M]<sup>+</sup>: 189.0974; Found 189.0966.

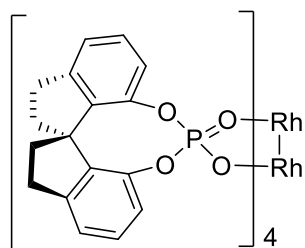
## 5. Preparation and analytical data of catalysts

### 5.1 Procedure for synthesis of C1<sup>12</sup>



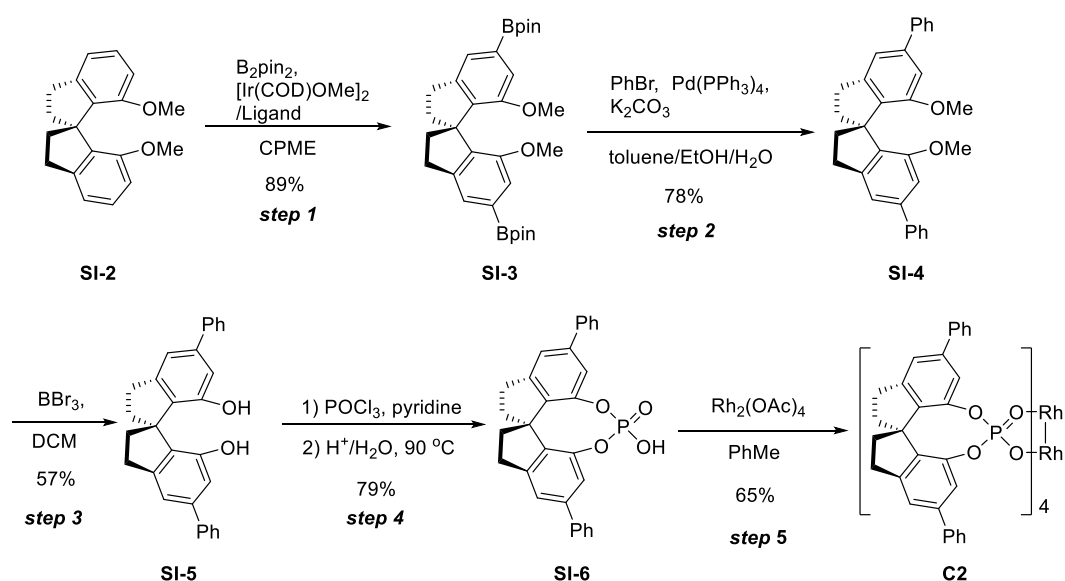
According to our previously reported procedure, **SI-1** (3.4 g, 10.8 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (0.6 g, 1.4 mmol) and 130 mL dry toluene were introduced into a 250 mL two-necked flask. The mixture was refluxed for 36 h at reflux using a Soxhlet apparatus filled with sand and Na<sub>2</sub>CO<sub>3</sub> for the removal of acetic acid. The mixture was then concentrated under vacuum and purified by column chromatography on silica gel using DCM as mobile phase to give the crude product. The crude product was recrystallized in a mixed solvent of DCM and MeOH to give **C1** as a green needle crystal (1.5 g, 93% yield).

#### tetrakis[(*S*)-1,1'-Spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II) (**C1**)



Green black needle crystal. m.p.: decomposed over 300 °C.  $[\alpha]_D^{26} +326$  (c 0.5, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.13 – 6.95 (m, 24H, ArH), 3.59 (s, 2H, OH), 3.12 – 2.95 (m, 8H, 4CH<sub>2</sub>), 2.86 – 2.68 (m, 16H, 4CH<sub>2</sub> + 2CH<sub>3</sub>O + H<sub>2</sub>O), 2.26 – 2.12 (m, 8H, 4CH<sub>2</sub>), 2.06 – 1.88 (m, 8H, 4CH<sub>2</sub>). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 146.4, 145.9, 139.4, 128.7, 122.2, 77.3, 59.0, 52.5 (MeOH), 38.3, 30.5. <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>) δ 5.3 (s) (methanol in coordination sphere).

### 5.2 Procedure for synthesis of C2 and C3

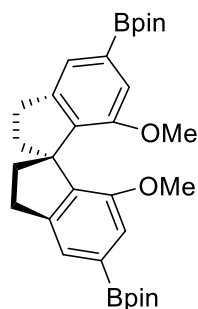


(*S*)-7,7'-dimethoxy-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] (**SI-2**) was prepared from the optically pure (*S*)-SPINOL according to our previously reported procedures.<sup>13</sup>

### Step 1. Synthesis of **SI-3**<sup>14</sup>

According to the reported procedure, in an oven-dried Schlenk tube (120 mL in volume) equipped with a stir bar were placed with **SI-2**, B<sub>2</sub>pin<sub>2</sub> (4.5 g, 17.6 mmol), [Ir(OMe)(cod)]<sub>2</sub> (212 mg, 0.32 mmol) and dipyridinyl tetraaminodiborane (248 mg, 0.64 mmol). After evacuation and refill with dry nitrogen for three times, dry methoxycyclopentane (30 mL) was added with syringe. The resulting mixture was stirred at 110 °C for 36 h. After cooling to room temperature, the reaction mixture was concentrated and the residue was purified by column chromatography on silica gel (eluting with petroleum ether/DCM = 1:1, v/v) to give **SI-3** as a white solid (3.8 g, 89% yield).

### (*S*)-2,2'-(7,7'-dimethoxy-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-5,5'-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (**SI-3**)



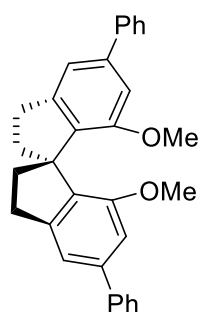
White solid. m.p.: 190–192 °C.  $[\alpha]_D^{25} -34.0$  (c 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.34 (s, 2H, ArH), 7.04 (s, 2H, ArH), 3.56 (s, 6H, 2OCH<sub>3</sub>), 3.10 – 2.90 (m, 4H, 2CH<sub>2</sub>), 2.33 – 2.25 (m, 2H, CH<sub>2</sub>), 2.16 – 2.10 (m, 2H, CH<sub>2</sub>), 1.34 (s, 24H, 8CH<sub>3</sub>). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 156.1, 145.0, 140.5, 123.6, 114.3, 83.6, 59.5, 55.3, 38.5, 31.3, 24.9, 24.9. <sup>11</sup>B NMR (128 MHz, CDCl<sub>3</sub>) δ 33.9. HRMS (ESI) calcd for [C<sub>31</sub>H<sub>42</sub>B<sub>2</sub>O<sub>6</sub>,

$M + Na]^+$ : 555.3065, Found: 555.3070.

### Step 2. Synthesis of SI-4

To a solution of **SI-3** (1.3 g, 2.5 mmol), phenylboronic acid (2.4 g, 15 mmol) and  $Pd(PPh_3)_4$  (433 mg, 0.375 mmol) in toluene (30 mL) and EtOH (14 mL), aqueous  $K_2CO_3$  (1 M, 20 mL) was added. The mixture was degassed by freezing and then heated at reflux for 24 h. The reaction mixture was cooled to ambient temperature and diluted by ethyl acetate. The aqueous layer was extracted with EtOAc ( $3 \times 20$  mL). The combined organic extract was washed with brine, then dried over  $MgSO_4$ , filtered, concentrated. The residue was purified by column chromatography (eluting with petroleum ether/DCM = 4:1, v/v) to give **SI-4** as a white solid (0.8 g, 78% yield).

### (S)-7,7'-dimethoxy-5,5'-diphenyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] (SI-4)

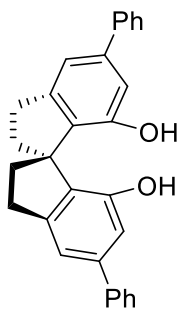


Yield: 78%. White solid. m.p.: 58–60 °C.  $[\alpha]_D^{25} -1.4$  (c 1.0,  $CHCl_3$ ).  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.61 (d,  $J = 7.3$  Hz, 4H, ArH), 7.44 – 7.38 (m, 4H, ArH), 7.33 – 7.28 (m, 2H, ArH), 7.10 (s, 2H, ArH), 6.85 (s, 2H, ArH), 3.61 (s, 6H, 2OCH<sub>3</sub>), 3.24 – 2.99 (m, 4H, 2CH<sub>2</sub>), 2.50 – 2.38 (m, 2H, CH<sub>2</sub>), 2.30 – 2.16 (m, 2H, CH<sub>2</sub>).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  156.7, 146.0, 142.0, 141.3, 136.1, 128.7, 127.2, 127.0, 115.9, 108.1, 58.9, 55.4, 39.2, 31.8. HRMS (ESI) calcd for  $[C_{31}H_{28}O_2, M + Na]^+$ : 455.1987, Found: 455.1985.

### Step 3. Synthesis of SI-5

To a dried Schlenk tube equipped with septum and stir bar, **SI-4** (850 mg, 2.0 mmol) was added. After three vacuum nitrogen cycles, dry DCM (20 mL) was added by syringe. The solution was cooled to  $-78$  °C, treated with  $BBr_3$  (1 M, 15 mmol) in DCM and allowed to warm to room temperature. After stirring overnight, the reaction mixture was diluted with DCM and washed sequentially with saturated  $NaHCO_3$  and brine. The organic layer was dried over anhydrous  $MgSO_4$  and then concentrated. The residue was purified by column chromatography (eluting with petroleum ether/DCM = 1:1, v/v) to give **SI-5** as a white solid (460 mg, 57% yield).

### (S)-5,5'-diphenyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diol (SI-5)

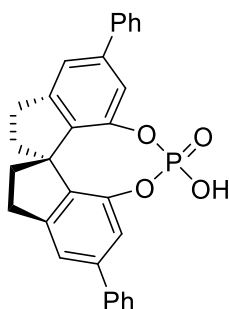


White solid. m.p.: 101–102 °C.  $[\alpha]_{\text{D}}^{25} +40.6$  (c 1.0,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.53 (d,  $J = 7.8$  Hz, 4H, ArH), 7.42 – 7.34 (m, 4H, ArH), 7.34 – 7.26 (m, 2H, ArH), 7.10 (s, 2H, ArH), 6.90 (s, 2H, ArH), 4.85 (s, 2H, 2OH), 3.15 – 2.92 (m, 4H, 2 $\text{CH}_2$ ), 2.39 – 2.14 (m, 4H, 2 $\text{CH}_2$ ).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  153.0, 146.6, 143.5, 140.9, 129.9, 128.8, 127.5, 127.2, 116.7, 113.4, 57.2, 37.8, 31.4. HRMS (ESI) calcd for  $[\text{C}_{29}\text{H}_{24}\text{O}_2, \text{M} + \text{Na}]^+$ : 427.1674, Found: 427.1673.

#### Step 4. Synthesis of SI-6

To a 50 mL oven-dried Schlenk flask containing **SI-5** (460 mg, 1.2 mmol) was added 4 mL anhydrous pyridine and freshly distilled  $\text{POCl}_3$  (370 mg, 2.4 mmol) under a nitrogen atmosphere. The mixture was stirred under 90 °C for 12 h. After cooling to room temperature, 4 mL of  $\text{H}_2\text{O}$  was added. The mixture was stirred under 90 °C for another 12 h, then cooled by an ice-bath, followed by a slow addition of  $\text{HCl}$  (aq. 3 N, 35 mL). After stirring for 1 h, the mixture was extracted by DCM ( $3 \times 20$  mL). The combined organic layer was concentrated and the residue was purified by column chromatography (eluting first with petroleum ether/EtOAc = 1:1, v/v, then MeOH/DCM = 1:5, v/v) to give 440 mg white solid. The white solid was dissolved with 100 mL DCM, washed with concentrated  $\text{HCl}$  (10 mL). The organic layer was dried by anhydrous  $\text{MgSO}_4$  and then concentrated. The residue was dried under vacuum to give **SI-6** as a white solid (430 mg, 79% yield).

#### (S)-5,5'-Diphenyl-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (SI-6)

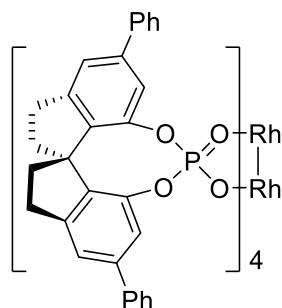


White solid. m.p.: 275–277 °C.  $[\alpha]_{\text{D}}^{25} -396$  (c 1.0,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  12.35 (s, 1H, OH), 7.48 (d,  $J = 7.2$  Hz, 4H, ArH), 7.38 – 7.17 (m, 10H, ArH), 3.20 – 3.05 (m, 2H,  $\text{CH}_2$ ), 2.88 – 2.77 (m, 2H,  $\text{CH}_2$ ), 2.35 – 2.25 (m, 2H,  $\text{CH}_2$ ), 2.15 – 1.92 (m, 2H,  $\text{CH}_2$ ).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  147.0 (d,  $J = 2.2$  Hz), 145.5 (d,  $J = 7.6$  Hz), 142.3 (d,  $J = 2.0$  Hz), 139.9, 137.9 (d,  $J = 3.6$  Hz), 128.6, 127.3, 127.1, 121.6, 120.1 (d,  $J = 3.3$  Hz), 58.8, 38.4, 30.6.  $^{31}\text{P}$  NMR (162 MHz,  $\text{CDCl}_3$ )  $\delta$  -9.2 (s). HRMS

(ESI) calcd for  $[C_{29}H_{23}O_4P, M + Na]^+$ : 489.1232, Found: 489.1230.

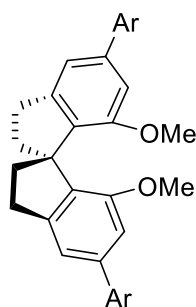
### Step 5. Synthesis of C2

#### tetrakis(*S*)-5,5'-diphenyl-1,1'-spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II) (C2)



By using the same procedure as for C1. The catalyst C2 was prepared in 65% yield. Green sheet crystal. m.p.: decomposed over 320 °C.  $[\alpha]_D^{25} +289$  (c 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (s, 8H, ArH), 7.42 – 7.37 (m, 16H, ArH), 7.33 (s, 8H, ArH), 7.22 – 7.13 (m, 24H, ArH), 3.17 – 3.06 (m, 8H, 4CH<sub>2</sub>), 2.94 (s, 3H, H<sub>2</sub>O), 2.92 – 2.80 (m, 8H, 4CH<sub>2</sub>), 2.33 – 2.24 (m, 8H, 4CH<sub>2</sub>), 2.07 – 1.95 (m, 13H, 4CH<sub>2</sub> + (CH<sub>3</sub>)<sub>2</sub>(CO)). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 146.6 (p, *J* = 3.3 Hz), 146.3, 141.7, 140.2, 138.4, 128.5, 127.1, 127.0, 120.8, 120.8, 58.6, 38.6, 30.9 ((CH<sub>3</sub>)<sub>2</sub>(CO)), 30.7. <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>) δ 6.6 (s). HRMS (MALDI) calcd for  $[C_{116}H_{88}O_{16}P_4Rh_2, M + Na]^+$ : 2090.3064, Found: 2090.3034.

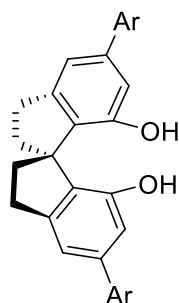
#### (*S*)-5,5'-bis(3,5-dimethylphenyl)-7,7'-dimethoxy-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] (SI-7)



Ar = 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>

By using the same procedure as for SI-4, the SI-7 was prepared in 91% yield. White solid. m.p.: 72–74 °C.  $[\alpha]_D^{25} -10.6$  (c 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.21 (s, 4H, ArH), 7.07 (s, 2H, ArH), 6.95 (s, 2H, ArH), 6.82 (s, 2H, ArH), 3.59 (s, 6H, 2OCH<sub>3</sub>), 3.18 – 2.96 (m, 4H, 2CH<sub>2</sub>), 2.46 – 2.39 (m, 2H, CH<sub>2</sub>), 2.35 (s, 12H, 4CH<sub>3</sub>), 2.25 – 2.17 (m, 2H, CH<sub>2</sub>). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 156.7, 145.9, 142.1, 141.6, 138.1, 136.0, 128.7, 125.3, 115.9, 108.2, 59.0, 55.4, 39.3, 31.9, 21.6. HRMS (ESI) calcd for  $[C_{35}H_{36}O_2, M + Na]^+$ : 511.2613, Found: 511.2610.

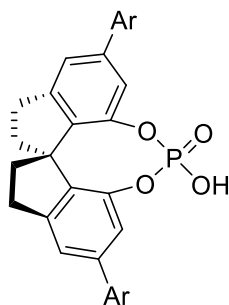
#### (*S*)-5,5'-bis(3,5-dimethylphenyl)-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diol

**(SI-8)**

Ar = 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>

By using the same procedure as for **SI-5**, the **SI-8** was prepared in 60% yield. White solid. m.p.: 72–73 °C.  $[\alpha]_D^{25} +35.6$  (c 0.5, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.20 (s, 4H, ArH), 7.12 (s, 2H, ArH), 6.98 (s, 2H, ArH), 6.92 (s, 2H, ArH), 4.74 (s, 2H, 2OH), 3.19 – 2.99 (m, 4H, 2CH<sub>2</sub>), 2.37 (s, 12H, 4CH<sub>3</sub>), 2.36 – 2.18 (m, 4H, 2CH<sub>2</sub>). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 152.9, 146.3, 143.7, 140.8, 138.1, 129.3, 129.0, 125.1, 116.6, 113.4, 57.0, 37.7, 31.3, 21.4. HRMS (ESI) calcd for [C<sub>33</sub>H<sub>32</sub>O<sub>2</sub>, M + Na]<sup>+</sup>: 483.2300, Found: 483.2298.

**(S)-5,5'-bis(3,5-dimethylphenyl)-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate**  
**(SI-9)**

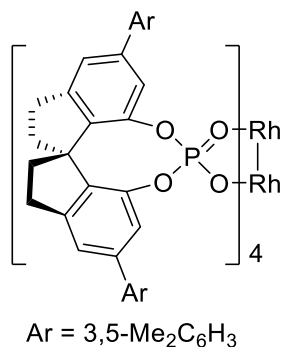


Ar = 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>

By using the same procedure as for **SI-6**, the **SI-9** was prepared in 90% yield. White solid. m.p.: decomposed over 320 °C.  $[\alpha]_D^{25} -382$  (c 0.5, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.40 – 7.23 (m, 4H, ArH), 7.15 (s, 4H, ArH), 6.94 (s, 2H, ArH), 3.21 – 3.08 (m, 2H, CH<sub>2</sub>), 2.93 – 2.81 (m, 2H, CH<sub>2</sub>), 2.41 – 2.21 (m, 14H, CH<sub>2</sub> + 4CH<sub>3</sub>), 2.11 – 2.01 (m, 2H, CH<sub>2</sub>). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 146.9, 145.5, 142.8, 140.0, 138.2, 137.8, 129.2, 125.1, 121.7, 120.2, 58.8, 38.6, 30.7, 21.4. <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>) δ –7.3 (s). **HRMS (ESI)** calcd for [C<sub>33</sub>H<sub>31</sub>O<sub>4</sub>P, M + Na]<sup>+</sup>: 545.1858, Found: 545.1856.

**tetrakis[(S)-5,5'-bis(3,5-dimethylphenyl)-1,1'-spirobiindanyl-7,7'-diyl-phosphate]dirhodium (II) (C3)**



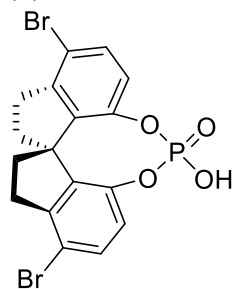


By using the same procedure as for **C1**, the **C3** was prepared in 30% yield. Green crystal. m.p.: decomposed over 320 °C.  $[\alpha]_{\text{D}}^{25} +172$  (c 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.42 (s, 8H, ArH), 7.25 (s, 8H, ArH), 7.12 – 7.01 (m, 16H, ArH), 6.84 (s, 8H, ArH), 3.12 – 2.98 (m, 8H, 4CH<sub>2</sub>), 2.83 (s, 2H, H<sub>2</sub>O), 2.81 -2.70 (m, 8H, 4CH<sub>2</sub>), 2.30 – 2.21 (m, 8H, 4CH<sub>2</sub>), 2.15 (s, 48H, 16CH<sub>3</sub>), 2.00 – 1.87 (m, 8H, 4CH<sub>2</sub>). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  146.7, 146.0, 141.6, 140.2, 138.2, 137.9, 128.6, 124.9, 121.1, 120.6, 58.6, 38.6, 30.8, 21.3. <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>)  $\delta$  5.33 (s). HRMS (MALDI) calcd for [C<sub>132</sub>H<sub>120</sub>O<sub>16</sub>P<sub>4</sub>Rh<sub>2</sub>, M + Na]<sup>+</sup>: 2314.5568, Found: 2314.5550.

### 5.3 Procedure for synthesis of **C4** and **C5**

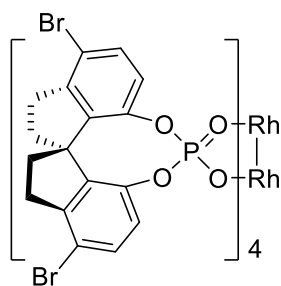
(*S*)-4,4'-dibromo-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diol (**SI-10**) and (*S*)-4,4'-diphenyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diol (**SI-11**) were prepared from the optically pure (*S*)-SPINOL according to our previously reported procedures.<sup>13</sup>

#### (*S*)-4,4'- dibromo-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (**SI-12**)



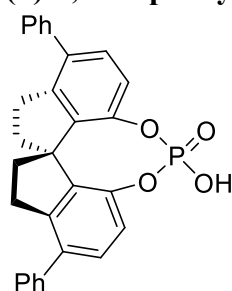
By using the same procedure as for **SI-6**, the **SI-12** was prepared in 80% yield. White solid. m.p.: 186–188 °C.  $[\alpha]_{\text{D}}^{25} -211$  (c 0.5, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.40 (d, *J* = 8.2 Hz, 2H, ArH), 6.95 (d, *J* = 8.2 Hz, 2H, ArH), 5.02 (s, 1H, OH), 3.31 (s, 1H, CH<sub>3</sub>O), 3.11 – 2.98 (m, 2H, CH<sub>2</sub>), 2.90 – 2.78 (m, 2H, CH<sub>2</sub>), 2.38 – 2.28 (m, 2H, CH<sub>2</sub>), 1.98 – 1.89 (m, 2H, CH<sub>2</sub>). <sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)  $\delta$  147.1 (d, *J* = 7.9 Hz), 145.2 (d, *J* = 2.0 Hz), 141.6 (d, *J* = 3.2 Hz), 130.9 (d, *J* = 2.1 Hz), 124.1 (d, *J* = 3.1 Hz), 115.0 (d, *J* = 3.1 Hz), 61.3, 37.2, 31.6. <sup>31</sup>P NMR (162 MHz, CD<sub>3</sub>OD)  $\delta$  -9.8 (s). HRMS (ESI) calcd for [C<sub>17</sub>H<sub>13</sub>Br<sub>2</sub>O<sub>4</sub>P, M – H]<sup>-</sup>: 470.8819, Found: 470.8830.

#### tetrakis(*S*)-4,4'-dibromo-1,1'-spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II) (**C4**)



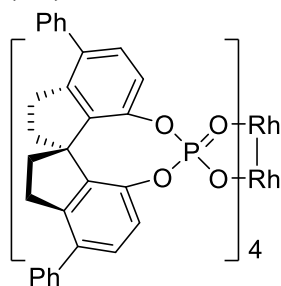
By using the same procedure as for **C1**, the **C4** was prepared in 85% yield. Greyish-green solid. m.p.: decomposed over 320 °C.  $[\alpha]_D^{25} +148$  (c 1.0,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.27 (d,  $J = 8.6$  Hz, 8H, ArH), 6.89 (d,  $J = 8.6$  Hz, 8H, ArH), 3.35 (s, 3H,  $\text{CH}_3\text{OH}$ ), 3.04 – 2.95 (m, 8H, 4 $\text{CH}_2$ ), 2.94 – 2.84 (m, 8H, 4 $\text{CH}_2$ ), 2.28 – 2.21 (m, 8H, 4 $\text{CH}_2$ ), 2.02 – 1.92 (m, 8H, 4 $\text{CH}_2$ ).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  145.8, 145.2 (d,  $J = 3.8$  Hz), 140.6, 132.1, 124.1, 117.1, 61.4, 37.6, 32.1.  $^{31}\text{P}$  NMR (162 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.5 (s). HRMS (MALDI) calcd for  $[\text{C}_{68}\text{H}_{48}\text{Br}_8\text{O}_{16}\text{P}_4\text{Rh}_2, \text{M} + \text{Na}]^+$ : 2112.3286, Found: 2112.3303.

**(S)-4,4'-diphenyl-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (SI-13)**



By using the same procedure as for **SI-6**, the **SI-13** was prepared in 84% yield. White solid. m.p.: 209–211 °C.  $[\alpha]_D^{25} -224$  (c 0.5,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  7.54 (d,  $J = 7.6$  Hz, 4H, ArH), 7.50 – 7.43 (m, 4H, ArH), 7.39 – 7.34 (m, 2H, ArH), 7.29 (d,  $J = 8.3$  Hz, 2H, ArH), 7.06 (d,  $J = 8.3$  Hz, 2H, ArH), 3.47 – 3.27 (m, 2H,  $\text{CH}_2$ ), 2.72 – 2.62 (m, 2H,  $\text{CH}_2$ ), 2.50 (s, 2H,  $\text{DMSO}$ ), 2.45 – 2.38 (m, 2H,  $\text{CH}_2$ ), 1.92 – 1.82 (m, 2H,  $\text{CH}_2$ ).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ )  $\delta$  146.1, 143.8, 140.5 (d,  $J = 3.5$  Hz), 140.2, 135.6, 129.0, 128.9, 128.9, 127.6, 122.9, 59.6, 38.6, 30.7.  $^{31}\text{P}$  NMR (162 MHz,  $\text{DMSO-d}_6$ )  $\delta$  -11.2 (s). HRMS (ESI) calcd for  $[\text{C}_{29}\text{H}_{23}\text{O}_4\text{P}, \text{M} + \text{Na}]^+$ : 489.1232, Found: 489.1230.

**tetrakis[(S)-4,4'-diphenyl-1,1'-spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II) (C5)**

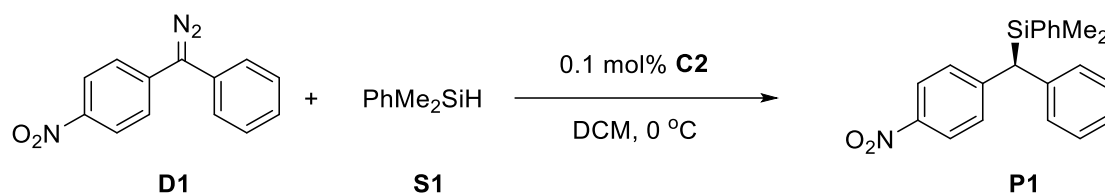


By using the same procedure as for **C1**, the **C5** was prepared in 95% yield. Greyish-

green solid. m.p.: decomposed over 320 °C.  $[\alpha]_{\text{D}}^{25} +143$  (c 1.0,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48 – 7.36 (m, 31H, ArH), 7.35 – 7.27 (m, 16H, ArH), 7.19 (d,  $J = 8.4$  Hz, 9H, ArH), 3.86 (s, 1H, OH), 3.43 (s, 3H,  $\text{CH}_3\text{O}$ ), 3.30 – 3.12 (m, 8H, 4 $\text{CH}_2$ ), 2.81 – 2.71 (m, 8H, 4 $\text{CH}_2$ ), 2.38 – 2.28 (m, 8H, 4 $\text{CH}_2$ ), 2.11 – 1.98 (m, 8H, 4 $\text{CH}_2$ ).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  145.7, 143.4, 140.4, 139.7, 136.3, 129.5, 128.7, 128.3, 127.0, 122.8, 59.7, 38.3, 30.8.  $^{31}\text{P}$  NMR (162 MHz,  $\text{CDCl}_3$ )  $\delta$  5.9 (s). HRMS (MALDI) calcd for  $[\text{C}_{116}\text{H}_{88}\text{O}_{16}\text{P}_4\text{Rh}_2, \text{M} + \text{Na}]^+$ : 2090.3064, Found: 2090.3030.

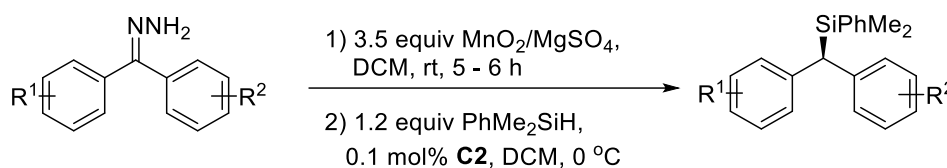
## 6. Typical procedure for Si–H bond insertion reaction

### 6.1 General procedure A



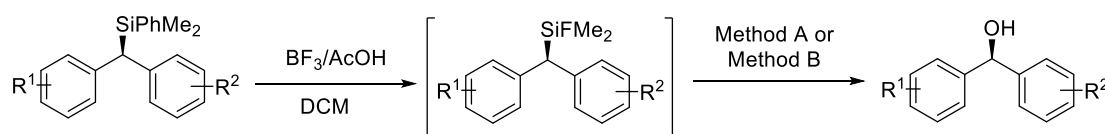
Dimethyl(phenyl)silane **S1** (32.7 mg, 0.24 mmol) and **C2** (0.42 mg, 0.0002 mmol, in 2 mL DCM) was injected into an oven-dried Schlenk tube under argon atmosphere. The mixture was cooled to 0 °C under ice-bath, a solution of **D1** (47.9 mg, 0.2 mmol, in 1 mL DCM) was introduced by syringe in 3 min. The color of diazo compound immediately disappeared after the addition. The TLC showed that the reaction completed as soon as the addition finished. Then the reaction mixture was concentrated and purified by a flash chromatography on silica gel (eluting with petroleum ether/EtOAc = 50:1, v/v) to give **P1** as a colorless oil (64.0 mg, 92% yield).

### 6.2 General procedure B



Hydrazone (0.2 mmol, 1 equiv) and anhydrous  $\text{MgSO}_4$  (70 mg, 350 mg/mmol) were placed into an oven-dried Schlenk tube under argon atmosphere and 2 mL DCM was introduced. After cooling to 0 °C, to this rapidly stirring mixture was added activated  $\text{MnO}_2$  (0.7 mmol, 3.5 equiv) in one portion. The reaction mixture was warmed to room temperature and kept stirring for 5-6 h, TLC indicated that the hydrazone was consumed completely. Then the solid was filtered off and washed with anhydrous DCM. The solution was concentrated to 1 mL, and was reacted with silane as in the procedure A.

*Notes: For the Si–H insertion products **P3–P5**, **P9**, **P22–P25** and **P29**, the enantiomeric excesses (*ee*) cannot be directly measured, but determined after converting to the corresponding alcohols.<sup>15</sup>*



Method A (taking **P3** for example):

The **P3** (68 mg, 0.18 mmol) was added into a 25 mL oven-dried Schlenk tube under argon atmosphere, and 2 mL of DCM was injected. The mixture was cooled to 0 °C under ice-bath, a solution of BF<sub>3</sub>/AcOH (28 μL, 143 μL/mmol) was introduced. The mixture was stirred at reflux for 4 h, and cooled to room temperature and quenched with saturated aqueous NaHCO<sub>3</sub> (2 mL). The mixture was extracted with Et<sub>2</sub>O for three times and the combined organic extract was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated to give a solid.

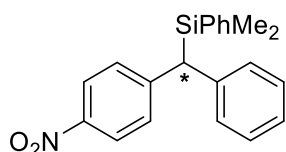
The solid was dissolved in Et<sub>2</sub>O (2 mL) and was successively added 3-chloroperoxybenzoic acid (155 mg, 0.9 mmol) and triethylamine (20 mg, 0.20 mmol) under ice-bath. The mixture was stirred at room temperature for 20 h and then diluted by Et<sub>2</sub>O (2 mL). The mixture was successively washed by saturated aqueous NaHSO<sub>3</sub> and saturated NaHCO<sub>3</sub>. The water layer was extracted with Et<sub>2</sub>O for three times. The combined extract was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated to give a solid. The crude product was purified by silica gel column chromatography (petroleum ether/EtOAc, 10:1, v/v) to afford alcohol **3ol** (34 mg, 75% yield) as a pale solid.

Method B (taking **P29** for example):

The **P29** (35 mg, 0.1 mmol) was fluorinated and then treated as in Method A. The **P29** was dissolved in THF/MeOH (2 mL, 1:1, v/v), and was successively added KHCO<sub>3</sub> (100 mg, 1.0 mmol, 10 equiv) and KF (58 mg, 1.0 mmol, 10 equiv) under ice-bath. After stirring for several minutes, the mixture was added aqueous H<sub>2</sub>O<sub>2</sub> (30%, 10 equiv). The resulting mixture was stirred at room temperature for 24 h, and extracted with Et<sub>2</sub>O for three times. The combined extract was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated to give a solid. The solid was purified by silica gel column chromatography (eluting with petroleum ether/EtOAc, 10:1, v/v) to afford alcohol **29ol** (10 mg, 45% yield).

## 7. Analytical data of Si-H bond insertion products

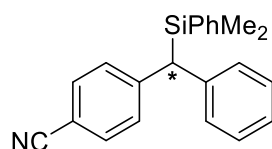
### (-)-dimethyl((4-nitrophenyl)(phenyl)methyl)(phenyl)silane (P1)



Yield: 92%. Colorless oil.  $[\alpha]_{\text{D}}^{25} -46.6$  (c 1.0,  $\text{CHCl}_3$ ), >99% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J = 8.8$  Hz, 2H), 7.40 – 7.35 (m, 1H), 7.33 – 7.22 (m, 6H), 7.21 – 7.13 (m, 5H), 3.87 (s, 1H), 0.32 (s, 3H), 0.3 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.7, 145.5, 140.4, 136.2, 134.2, 129.6, 129.1, 128.8, 128.6, 127.8, 126.0, 123.4, 46.6, –3.1, –3.8;  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –1.7. HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{21}\text{NO}_2\text{Si}$   $[\text{M}]^+$ : 347.1342; Found 347.1336.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 7.90$  min (minor) and  $t_2 = 8.51$  min (major).

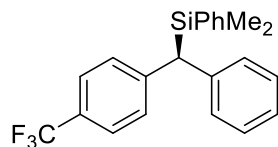
### (-)-4-((dimethyl(phenyl)silyl)(phenyl)methyl)benzonitrile (P2)



Yield: 96%. Colorless oil.  $[\alpha]_{\text{D}}^{25} -28.4$  (c 1.0,  $\text{CHCl}_3$ ), 98% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 (d,  $J = 8.2$  Hz, 2H), 7.40 – 7.33 (m, 1H), 7.33 – 7.21 (m, 6H), 7.20 – 7.07 (m, 5H), 3.80 (s, 1H), 0.30 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  147.3, 139.6, 135.3, 133.3, 130.9, 128.5, 128.1, 128.0, 127.5, 126.7, 124.9, 118.1, 107.7, 45.6, –4.1, –4.7.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –1.8. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{21}\text{NSi}$   $[\text{M}]^+$ : 327.1443; Found 327.1435.

HPLC condition: Chiralpak IG-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 5.27$  min (major) and  $t_2 = 5.84$  min (minor).

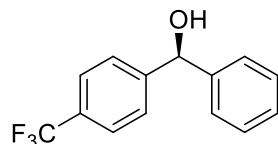
### (S)-dimethyl(phenyl)(phenyl(4-(trifluoromethyl)phenyl)methyl)silane (P3)



Yield: 91%. Colorless oil.  $[\alpha]_{\text{D}}^{25} -18.4$  (c 1.0,  $\text{CHCl}_3$ ), 95% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (d,  $J = 8.0$  Hz, 2H), 7.37 – 7.32 (m, 1H), 7.31 – 7.25 (m, 4H), 7.24 – 7.17 (m, 4H), 7.13 – 7.05 (m, 3H), 3.80 (s, 1H), 0.30 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.7, 141.3, 136.8, 134.4, 129.4, 129.1, 128.8, 128.5, 127.7, 127.4 (q,  $J = 32.0$  Hz), 125.7, 125.1 (q,  $J = 3.6$  Hz), 124.4 (q,  $J = 270.0$  Hz), 46.0, –3.2, –3.4.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  –62.2 (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –2.4. HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{18}\text{F}_3\text{Si}$   $[\text{M}-\text{CH}_3]^+$ : 355.1130; Found 355.1123.

**P3** was oxidized to alcohol **3ol** via Method A. The enantiomeric excess was determined to be 95% by chiral HPLC analysis. See alcohol **3ol** below.

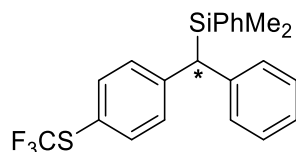
**(S)-phenyl(4-(trifluoromethyl)phenyl)methanol (3ol)**<sup>16</sup>



Yield: 75%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 8.1 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.32 (m, 4H), 7.31 – 7.24 (m, 1H), 5.85 (s, 1H), 2.39 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 147.5, 143.1, 129.7 (q, *J* = 31.6 Hz), 128.8, 128.1, 126.7, 126.6, 125.4 (q, *J* = 4.1 Hz), 124.1 (q, *J* = 270.0 Hz), 75.7. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –58.3 (s, 3F).

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 98:2, 1.0 mL/min, 220 nm UV detector, *t*<sub>1</sub> = 8.34 min (minor) and *t*<sub>2</sub> = 9.04 min (major), 95% ee. [α]<sub>D</sub><sup>25</sup> +31.6 (c 1.0, CHCl<sub>3</sub>) (*lit.* 16 [α]<sub>D</sub><sup>22</sup> +34.3 (c 1.0, CHCl<sub>3</sub>), 92% ee (*S*)).

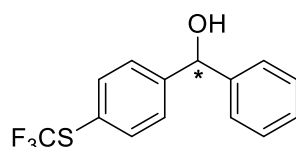
**(–)-dimethyl(phenyl)(phenyl(4-((trifluoromethyl)thio)phenyl)methyl)silane (P4)**



Yield: 68%. Colorless oil. [α]<sub>D</sub><sup>30</sup> –31.0 (c 1.0, CHCl<sub>3</sub>), 97% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.49 – 7.43 (m, 2H), 7.39 – 7.32 (m, 1H), 7.31 – 7.20 (m, 6H), 7.19 – 7.09 (m, 5H), 3.77 (s, 1H), 0.30 (s, 3H), 0.29 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 145.8, 141.2, 136.7, 136.2, 134.3, 129.8 (q, *J* = 271.0 Hz), 129.6, 129.4, 129.1, 128.4, 127.6, 125.7, 120.4, 45.9, –3.2, –3.6. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –43.1 (s, 3F). <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>) δ –2.6. HRMS (EI) calcd for C<sub>21</sub>H<sub>18</sub>F<sub>3</sub>SSi [M-CH<sub>3</sub>]<sup>+</sup>: 387.0851; Found 387.0845.

**P4** was oxidized to alcohol **4ol** via Method A. The enantiomeric excess was determined to be 97% by chiral HPLC analysis. See alcohol **4ol** below.

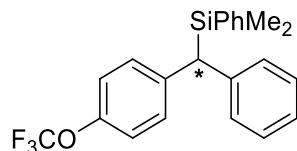
**(+)-phenyl(4-((trifluoromethyl)thio)phenyl)methanol (4ol)**<sup>17</sup>



Yield: 41%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.60 (d, *J* = 8.1 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.36 – 7.33 (m, 4H), 7.31 – 7.25 (m, 1H), 5.81 (s, 1H), 2.44 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 146.7, 143.1, 136.4, 129.8 (q, *J* = 262.0 Hz), 128.8, 128.1, 127.5, 126.7, 123.3, 75.7. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –53.5 (s, 3F).

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 99.2:0.8, 0.5 mL/min, 230 nm UV detector,  $t_1 = 10.66$  min (minor) and  $t_2 = 11.00$  min (major), 97% ee.  $[\alpha]_D^{25} +43.2$  (c 0.5,  $\text{CHCl}_3$ ).

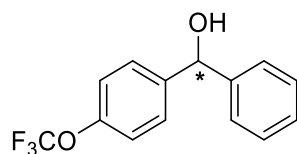
**(-)-dimethyl(phenyl)(phenyl(4-(trifluoromethoxy)phenyl)methyl)silane (P5)**



Yield: 66%. Colorless oil.  $[\alpha]_D^{30} -3.2$  (c 1.0,  $\text{CHCl}_3$ ), 76% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 – 7.34 (m, 1H), 7.31 – 7.19 (m, 6H), 7.18 – 7.07 (m, 5H), 7.03 (d,  $J = 8.4$  Hz, 2H), 3.74 (s, 1H), 0.30 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.9, 141.7, 141.1, 137.0, 134.3, 129.8, 129.3, 128.9, 128.4, 127.6, 125.5, 120.6, 120.6 (q,  $J = 255.0$  Hz), 45.2, -3.2, -3.4.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -57.9 (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -2.6. HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{18}\text{F}_3\text{OSi}$   $[\text{M}-\text{CH}_3]^+$ : 371.1079; Found 371.1074.

**P5** was oxidized to alcohol **5ol** via Method A. The enantiomeric excess was determined to be 76% by chiral HPLC analysis. See alcohol **5ol** below.

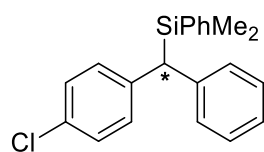
**(+)-phenyl(4-(trifluoromethoxy)phenyl)methanol (5ol)**<sup>17</sup>



Yield: 40%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 (d,  $J = 8.2$  Hz, 2H), 7.35 – 7.30 (m, 4H), 7.29 – 7.25 (m, 1H), 7.19 – 7.12 (m, 2H), 5.79 (d,  $J = 3.4$  Hz, 1H), 2.48 (d,  $J = 3.4$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.5, 143.4, 142.4, 128.7, 127.9 (2C signal), 126.6, 121.8, 120.1 (q,  $J = 255.0$  Hz), 75.6.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -38.3 (s, 3F).

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 99.2:0.8, 0.5 mL/min, 230 nm UV detector,  $t_1 = 10.42$  min (minor) and  $t_2 = 10.74$  min (major), 76% ee.  $[\alpha]_D^{25} +12.4$  (c 0.5,  $\text{CHCl}_3$ ).

**(+)-((4-chlorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P6)**



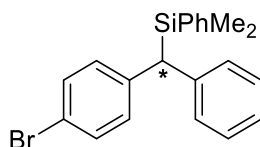
Yield: 95%. Colorless oil.  $[\alpha]_D^{30} +3.0$  (c 1.0,  $\text{CHCl}_3$ ), 66% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.32 (m, 1H), 7.31 – 7.25 (m, 4H), 7.21 (t,  $J = 8.1$  Hz, 2H), 7.18 – 7.07 (m, 5H), 7.02 (d,  $J = 7.7$  Hz, 2H), 3.70 (s, 1H), 0.29 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C}$  NMR



(101 MHz, CDCl<sub>3</sub>)  $\delta$  141.8, 140.9, 137.1, 134.4, 130.9, 130.1, 129.3, 128.9, 128.3, 128.2, 127.6, 125.4, 45.1, -3.2, -3.4. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -2.7. HRMS (EI) calcd for C<sub>21</sub>H<sub>21</sub>ClSi [M]<sup>+</sup>: 336.1101; Found 336.1100.

HPLC condition: phenomenex, Cellulose-3, methanol/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector, *t*<sub>1</sub> = 4.87 min (major) and *t*<sub>2</sub> = 5.91 min (minor).

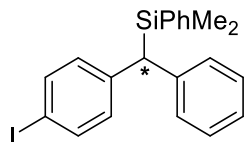
**(+)-((4-bromophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P7)**



Yield: 79%. Colorless oil. [ $\alpha$ ]<sub>D</sub><sup>28</sup> +3.4 (c 1.0, CHCl<sub>3</sub>), 77% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.36 – 7.32 (m, 1H), 7.31 – 7.26 (m, 6H), 7.21 (t, *J* = 7.3 Hz, 2H), 7.16 – 7.07 (m, 3H), 6.97 (d, *J* = 8.1 Hz, 2H), 3.69 (s, 1H), 0.29 (s, 3H), 0.28 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  141.6, 141.4, 137.0, 134.3, 131.2, 130.5, 129.3, 128.9, 128.3, 127.6, 125.4, 118.9, 45.2, -3.2, -3.4. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -2.8. HRMS (EI) calcd for C<sub>21</sub>H<sub>21</sub>BrSi [M]<sup>+</sup>: 380.0596; Found 380.0586.

HPLC condition: phenomenex, Cellulose-3, methanol/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector, *t*<sub>1</sub> = 5.08 min (major) and *t*<sub>2</sub> = 6.35 min (minor).

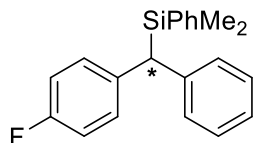
**(+)-((4-iodophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P8)**



Yield: 62%. Colorless oil. [ $\alpha$ ]<sub>D</sub><sup>28</sup> +21.2 (c 1.0, CHCl<sub>3</sub>), 82% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.48 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.32 (m, 1H), 7.32 – 7.24 (m, 4H), 7.24 – 7.17 (m, 2H), 7.16 – 7.05 (m, 3H), 6.84 (d, *J* = 8.4 Hz, 2H), 3.67 (s, 1H), 0.29 (s, 3H), 0.27 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  142.1, 141.7, 137.2, 137.1, 134.4, 130.9, 129.3, 129.0, 128.4, 127.7, 125.5, 90.2, 45.3, -3.1, -3.3. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -2.8. HRMS (EI) calcd for C<sub>20</sub>H<sub>18</sub>ISi [M-CH<sub>3</sub>]<sup>+</sup>: 413.0222; Found 413.0215.

HPLC condition: phenomenex, Cellulose-3, methanol/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector, *t*<sub>1</sub> = 5.48 min (major) and *t*<sub>2</sub> = 6.41 min (minor).

**(+)-((4-fluorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P9)**

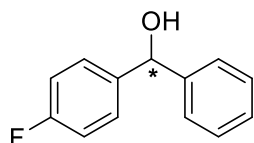


Yield: 88%. Colorless oil. [ $\alpha$ ]<sub>D</sub><sup>27</sup> +1.2 (c 1.0, CHCl<sub>3</sub>), 25% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.37 – 7.31 (m, 1H), 7.30 – 7.25 (m, 4H), 7.21 (t, *J* = 7.4 Hz, 2H), 7.16 – 7.01

(m, 5H), 6.88 (t,  $J = 8.7$  Hz, 2H), 3.71 (s, 1H), 0.29 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.9 (d,  $J = 242.0$  Hz), 142.2, 138.0 (d,  $J = 4.1$  Hz), 137.3, 134.4, 130.2 (d,  $J = 8.6$  Hz), 129.3, 128.9, 128.3, 127.6, 125.4, 115.0 (d,  $J = 21.0$  Hz), 44.9, -3.2, -3.3.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.6 (s, 1F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -2.8. HRMS (EI) calcd for  $\text{C}_{20}\text{H}_{18}\text{FSi}$   $[\text{M}-\text{CH}_3]^+$ :305.1162; Found 305.1159.

**P9** was oxidized to alcohol **9ol** via Method A. The enantiomeric excess was determined to be 25% by chiral HPLC analysis. See alcohol **9ol** below.

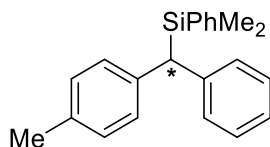
**(-)-(4-fluorophenyl)(phenyl)methanol (9ol)**<sup>18</sup>



Yield: 57%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.23 (m, 7H), 7.01 (t,  $J = 8.6$  Hz, 2H), 5.82 (s, 1H), 2.24 (s, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.2 (d,  $J = 245.9$  Hz), 143.7, 139.6 (d,  $J = 3.2$  Hz), 128.6, 128.2 (d,  $J = 8.1$  Hz), 127.8, 126.5, 115.3 (d,  $J = 21.3$  Hz), 75.6.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.1 (s, 1F).

HPLC condition: Chiralpak IB-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 10.31$  min (minor) and  $t_2 = 10.78$  min (major), 25% ee.  $[\alpha]_{\text{D}}^{25} -1.8$  (c 1.0,  $\text{CHCl}_3$ ).

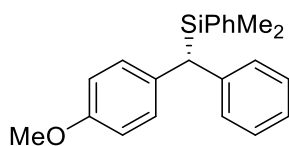
**(-)-dimethyl(phenyl)(phenyl(*p*-tolyl)methyl)silane (P10)**



Yield: 51%. Colorless oil.  $[\alpha]_{\text{D}}^{27} -0.02$  (c 1.0,  $\text{CHCl}_3$ ), 18% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 – 7.31 (m, 1H), 7.30 – 7.23 (m, 4H), 7.22 – 7.14 (m, 2H), 7.12 – 7.06 (m, 3H), 7.05 – 6.98 (m, 4H), 3.70 (s, 1H), 2.27 (s, 3H), 0.28 (s, 3H), 0.27 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  142.5, 139.1, 137.7, 134.6, 134.4, 129.0, 128.9, 128.9, 128.8, 128.1, 127.5, 125.0, 45.1, 20.9, -3.1, -3.2.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -3.1. HRMS (EI) Calcd for  $\text{C}_{22}\text{H}_{24}\text{Si}$   $[\text{M}]^+$ :316.1647; Found 316.1638.

HPLC condition: phenomenex, Cellulose-3, methanol/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 5.53$  min (minor) and  $t_2 = 7.53$  min (major).

**(R)-((4-methoxyphenyl)(phenyl)methyl)dimethyl(phenyl)silane (P11)**

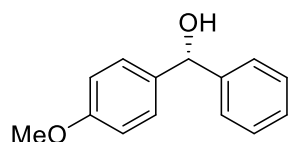


Yield: 47%. Colorless oil.  $[\alpha]_D^{27} -15.8$  (c 1.0,  $\text{CHCl}_3$ ), 64% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 – 7.31 (m, 1H), 7.31 – 7.24 (m, 4H), 7.22 – 7.16 (m, 2H), 7.13 – 7.02 (m, 5H), 6.76 (d,  $J = 8.8$  Hz, 2H), 3.75 (s, 3H), 3.68 (s, 1H), 0.29 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.3, 142.7, 137.6, 134.4, 134.3, 129.9, 129.0, 128.7, 128.1, 127.5, 125.0, 113.6, 55.2, 44.5, –3.1, –3.2.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –3.1. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{24}\text{OSi}$   $[\text{M}]^+$ : 332.1596; Found 332.1592.

HPLC condition: Chiralcel AS-3 column, n-hexane/2-propanol = 99.2:0.8, 0.5 mL/min, 230 nm UV detector,  $t_1 = 7.21$  min (minor) and  $t_2 = 7.45$  min (major).

**P11** was oxidized to alcohol **11ol** via Method B. The absolute configuration of **P11** was assigned by **11ol**. See alcohol **11ol** below.

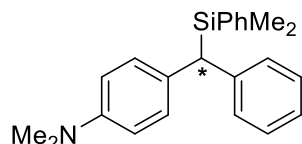
**(R)-(4-methoxyphenyl)(phenyl)methanol (11ol)**<sup>18</sup>



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 – 7.17 (m, 7H), 6.84 (d,  $J = 8.6$  Hz, 2H), 5.76 (s, 1H), 3.76 (s, 3H), 2.30 (s, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 144.0, 136.1, 128.4, 127.9, 127.4, 126.4, 113.8, 75.7, 55.2.

HPLC condition: Chiralpak AD-H column, n-hexane/2-propanol = 90:10, 0.8 mL/min, 230 nm UV detector,  $t_1 = 14.56$  min (major) and  $t_2 = 15.76$  min (minor), 64% ee.  $[\alpha]_D^{25} +4.0$  (c 0.5,  $\text{CHCl}_3$ ) (*lit.* 18  $[\alpha]_D^{23} -14.8$  (c 0.81,  $\text{CHCl}_3$ ), 92% ee (*S*)).

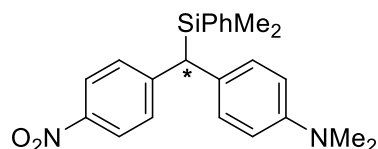
**(–)-4-((dimethyl(phenyl)silyl)(phenyl)methyl)-*N,N*-dimethylaniline (P12)**



Yield: 45%. Yellow oil.  $[\alpha]_D^{28} -19.6$  (c 0.5,  $\text{CHCl}_3$ ), 91% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 – 7.23 (m, 5H), 7.19 – 7.15 (m, 2H), 7.11 – 6.99 (m, 5H), 6.62 (d,  $J = 8.6$  Hz, 2H), 3.64 (s, 1H), 2.87 (s, 6H), 0.29 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.5, 143.2, 138.1, 134.4, 130.4, 129.8, 128.9, 128.7, 128.0, 127.4, 124.8, 112.8, 44.2, 40.8, –2.9, –3.2.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –3.0. HRMS (ESI) calcd for  $\text{C}_{23}\text{H}_{27}\text{NSi}$   $[\text{M}+\text{H}]^+$ : 346.1991; Found 346.1988.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99.5:0.5, 0.7 mL/min, 230 nm UV detector,  $t_1 = 6.41$  min (minor) and  $t_2 = 6.64$  min (major).

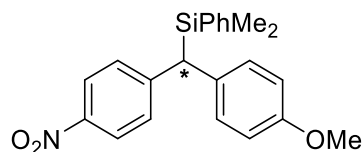
**(–)-4-((dimethyl(phenyl)silyl)(4-nitrophenyl)methyl)-*N,N*-dimethylaniline (P13)**



The solution of diazo compound was dropped for 30 min. Yield: 66%. Yellow oil.  $[\alpha]_D^{28} -84.8$  (c 0.5,  $\text{CHCl}_3$ ), 96% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 8.7$  Hz, 2H), 7.29 – 7.27 (m, 1H), 7.25 – 7.21 (m, 4H), 7.04 (d,  $J = 8.7$  Hz, 2H), 6.96 (d,  $J = 8.6$  Hz, 2H), 6.58 (d,  $J = 8.6$  Hz, 2H), 3.70 (s, 1H), 2.83 (s, 6H), 0.23 (s, 3H), 0.23 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.9, 148.8, 145.2, 136.7, 134.3, 130.1, 129.4, 128.6, 128.1, 127.7, 123.2, 112.8, 45.2, 40.6, -2.9, -3.8.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.9. HRMS (ESI) calcd for  $\text{C}_{23}\text{H}_{27}\text{N}_2\text{O}_2\text{Si}$   $[\text{M}+\text{H}]^+$ : 391.1842; Found 391.1840.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 4.73$  min (minor) and  $t_2 = 5.39$  min (major).

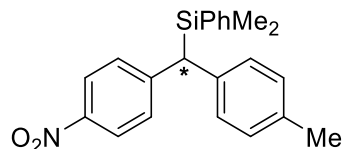
**(-)-((4-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P14)**



Yield: 78%. Colorless oil.  $[\alpha]_D^{28} -67.6$  (c 1.0,  $\text{CHCl}_3$ ), 99% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 8.7$  Hz, 2H), 7.41 – 7.37 (m, 1H), 7.34 – 7.22 (m, 4H), 7.14 (d,  $J = 8.7$  Hz, 2H), 7.08 (d,  $J = 8.6$  Hz, 2H), 6.81 (d,  $J = 8.6$  Hz, 2H), 3.82 (s, 1H), 3.76 (s, 3H), 0.31 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.8, 151.2, 145.4, 136.3, 134.2, 132.4, 130.2, 129.5, 128.7, 127.7, 123.3, 114.0, 55.2, 45.4, -3.1, -3.8.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.9. HRMS (ESI) calcd for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{Si}$   $[\text{M}+\text{Na}]^+$ : 400.1345; Found 400.1342.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 230 nm UV detector,  $t_1 = 9.20$  min (minor) and  $t_2 = 11.83$  min (major).

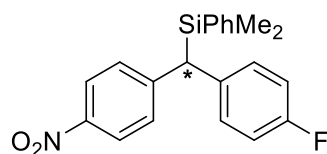
**(-)-dimethyl((4-nitrophenyl)(*p*-tolyl)methyl)(phenyl)silane (P15)**



Yield: 87%. Colorless oil.  $[\alpha]_D^{28} -60.6$  (c 1.0,  $\text{CHCl}_3$ ), 99% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 8.7$  Hz, 2H), 7.39 – 7.36 (m, 1H), 7.33 – 7.23 (m, 4H), 7.15 (d,  $J = 8.7$  Hz, 2H), 7.11 – 7.01 (m, 4H), 3.83 (s, 1H), 2.30 (s, 3H), 0.31 (s, 3H), 0.30 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.0, 145.4, 137.3, 136.3, 135.5, 134.2, 129.5, 129.3, 129.1, 128.7, 127.7, 123.3, 46.0, 20.9, -3.1, -3.8.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.9. HRMS (ESI) calcd for  $\text{C}_{22}\text{H}_{23}\text{NO}_2\text{Si}$   $[\text{M}+\text{Na}]^+$ : 384.1396; Found 384.1395.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1 = 8.47$  min (minor) and  $t_2 = 8.89$  min (major).

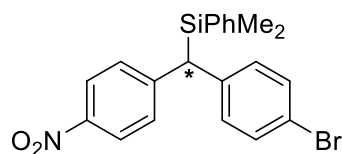
**(-)-((4-fluorophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P16)**



Yield: 86%. Colorless oil.  $[\alpha]_D^{28} -45.6$  (c 1.0,  $\text{CHCl}_3$ ), 98% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J = 8.8$  Hz, 2H), 7.43 – 7.36 (m, 1H), 7.35 – 7.29 (m, 2H), 7.28 – 7.24 (m, 2H), 7.16 (dd,  $J = 9.0, 2.3$  Hz, 2H), 7.13 – 7.06 (m, 2H), 6.96 (t,  $J = 8.6$  Hz, 2H), 3.85 (s, 1H), 0.32 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.2 (d,  $J = 244.0$  Hz), 150.5, 145.5, 136.2 (d,  $J = 3.6$  Hz), 135.9, 134.2, 130.5 (d,  $J = 8.1$  Hz), 129.7, 128.7, 127.8, 123.5, 115.4 (d,  $J = 21.0$  Hz), 45.6, -3.2, -3.8.  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -117.0 (s, 1F).  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.7. HRMS (EI) Calcd for  $\text{C}_{21}\text{H}_{20}\text{FNO}_2\text{Si}$   $[\text{M}]^+$ :365.1247; Found 365.1246.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 10.37$  min (minor) and  $t_2 = 12.38$  min (major).

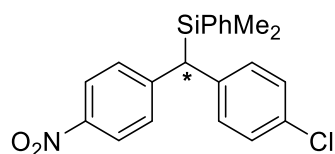
**(-)-((4-bromophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P17)**



Yield: 80%. Colorless oil.  $[\alpha]_D^{28} -45.6$  (c 1.0,  $\text{CHCl}_3$ ), 95% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (d,  $J = 8.7$  Hz, 2H), 7.37 (d,  $J = 8.4$  Hz, 3H), 7.31 (t,  $J = 7.4$  Hz, 2H), 7.25 (d,  $J = 6.5$  Hz, 2H), 7.16 (d,  $J = 8.7$  Hz, 2H), 7.01 (d,  $J = 8.4$  Hz, 2H), 3.83 (s, 1H), 0.31 (s, 3H), 0.30 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.9, 145.6, 139.5, 135.7, 134.2, 131.6, 130.7, 129.8, 128.8, 127.9, 123.5, 119.8, 45.9, -3.3, -3.8.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.7. HRMS (EI) Calcd for  $\text{C}_{21}\text{H}_{20}\text{BrNO}_2\text{Si}$   $[\text{M}]^+$ :425.0447; Found 425.0439.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 8.80$  min (minor) and  $t_2 = 9.53$  min (major).

**(-)-((4-chlorophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P18)**

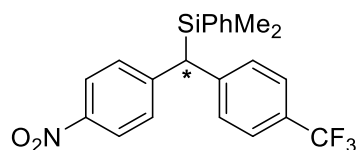


Yield: 88%. Colorless oil.  $[\alpha]_D^{28} -43.8$  (c 1.0,  $\text{CHCl}_3$ ), 96% ee.  $^1\text{H NMR}$  (400 MHz, Chloroform-*d*)  $\delta$  8.04 (d,  $J = 8.7$  Hz, 2H), 7.41 – 7.37 (m, 1H), 7.30 (t,  $J = 7.3$  Hz, 2H), 7.28 – 7.21 (m, 4H), 7.16 (d,  $J = 8.7$  Hz, 2H), 7.07 (d,  $J = 8.4$  Hz, 2H), 3.85 (s, 1H),

0.31 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 145.6, 139.0, 135.7, 134.2, 131.8, 130.3, 129.7, 128.8, 128.7, 127.8, 123.5, 45.8, -3.3, -3.8.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.7. HRMS (EI) Calcd for  $\text{C}_{21}\text{H}_{20}\text{ClNO}_2\text{Si}$   $[\text{M}]^+$ : 381.0952; Found 381.0946.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 10.55 min (minor) and  $t_2$  = 11.30 min (major).

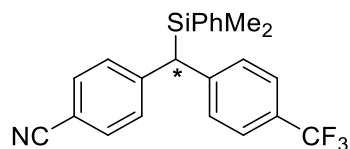
**(-)-dimethyl((4-nitrophenyl)(4-(trifluoromethyl)phenyl)methyl)(phenyl)silane (P19)**



Yield: 58%. Colorless oil.  $[\alpha]_{\text{D}}^{28}$  -17.8 (c 1.0,  $\text{CHCl}_3$ ), 86% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J$  = 8.8 Hz, 2H), 7.55 – 7.47 (m, 2H), 7.44 – 7.38 (m, 1H), 7.35 – 7.29 (m, 2H), 7.27 – 7.17 (m, 6H), 3.94 (s, 1H), 0.33 (s, 3H), 0.32 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.4, 145.8, 144.7, 135.4, 134.2, 129.9, 129.1, 129.0, 128.2 (q,  $J$  = 32.0 Hz), 127.9, 125.5 (q,  $J$  = 3.7 Hz), 124.0 (q,  $J$  = 238.0 Hz), 123.6, 46.6, -3.4, -3.7.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.4 (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.4. HRMS (EI) Calcd for  $\text{C}_{22}\text{H}_{20}\text{F}_3\text{NO}_2\text{Si}$   $[\text{M}]^+$ : 415.1215; Found 415.1205.

HPLC condition: Chiralpak AS-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 6.04 min (major) and  $t_2$  = 10.23 min (minor).

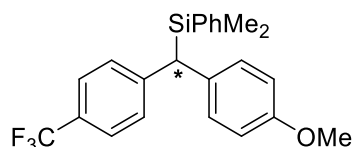
**(-)-4-((dimethyl(phenyl)silyl)(4-(trifluoromethyl)phenyl)methyl)benzonitrile (P20)**



Yield: 42%. Colorless oil.  $[\alpha]_{\text{D}}^{28}$  -2.6 (c 1.0,  $\text{CHCl}_3$ ), 36% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50 (d,  $J$  = 8.1 Hz, 4H), 7.44 – 7.36 (m, 1H), 7.31 (t,  $J$  = 7.3 Hz, 2H), 7.25 – 7.18 (m, 4H), 7.16 (d,  $J$  = 8.1 Hz, 2H), 3.86 (s, 1H), 0.31 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  147.1, 144.9, 135.6, 134.2, 132.1, 129.8, 129.2, 129.1, 128.1 (q,  $J$  = 32.0 Hz), 127.9, 125.4 (q,  $J$  = 3.4 Hz), 124.3 (q,  $J$  = 271.0 Hz), 118.9, 109.3, 46.7, -3.4, -3.7.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.9 (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.6. HRMS (EI) calcd for  $\text{C}_{23}\text{H}_{20}\text{F}_3\text{NSi}$   $[\text{M}]^+$ : 395.1317; Found 395.1307.

HPLC condition: Chiralpak AS-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 7.29 min (major) and  $t_2$  = 7.88 min (minor).

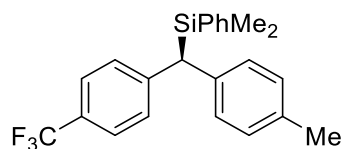
**(-)-((4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P21)**



Yield: 78%. Colorless oil.  $[\alpha]_D^{30}$   $-36.8$  (c 1.0,  $\text{CHCl}_3$ ), 98% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42 (d,  $J = 8.0$  Hz, 2H), 7.38 – 7.35 (m, 1H), 7.33 – 7.25 (m, 4H), 7.15 (d,  $J = 8.0$  Hz, 2H), 7.06 (d,  $J = 8.6$  Hz, 2H), 6.78 (d,  $J = 8.6$  Hz, 2H), 3.76 (s, 3H), 3.75 (s, 1H), 0.29 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 147.2, 137.0, 134.4, 133.3, 130.1, 129.4, 128.6, 127.7, 127.2 (q,  $J = 32.0$  Hz), 125.0 (q,  $J = 4.2$  Hz), 124.5 (q,  $J = 270.0$  Hz), 113.9, 55.2, 44.8,  $-3.1$ ,  $-3.5$ .  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-62.1$  (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.6$ . HRMS (EI) calcd for  $\text{C}_{23}\text{H}_{23}\text{F}_3\text{OSi}$   $[\text{M}]^+$ : 400.1470; Found 400.1460.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1 = 4.06$  min (minor) and  $t_2 = 4.30$  min (major).

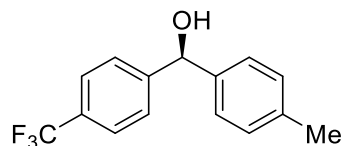
**(S)-dimethyl(phenyl)(p-tolyl(4-(trifluoromethyl)phenyl)methyl)silane (P22)**



Yield: 85%. Colorless oil.  $[\alpha]_D^{30}$   $-31.0$  (c 1.0,  $\text{CHCl}_3$ ), 94% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 (d,  $J = 8.1$  Hz, 2H), 7.37 – 7.33 (m, 1H), 7.32 – 7.26 (m, 4H), 7.16 (d,  $J = 8.1$  Hz, 2H), 7.04 (s, 4H), 3.76 (s, 1H), 2.28 (s, 3H), 0.30 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.9 (q,  $J = 1.2$  Hz), 138.1, 136.9, 135.1, 134.3, 129.3, 129.1, 129.0, 128.7, 127.7, 127.2 (q,  $J = 32.0$  Hz), 125.0 (q,  $J = 3.9$  Hz), 124.9 (q,  $J = 271.0$  Hz), 45.4, 20.9,  $-3.1$ ,  $-3.5$ .  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-62.1$  (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.6$ . HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{20}\text{F}_3\text{Si}$   $[\text{M}-\text{CH}_3]^+$ : 369.1286; Found 369.1275.

**P22** was oxidized to alcohol **22ol** via Method A. The enantiomeric excess was determined to be 94% by chiral HPLC analysis. See alcohol **22ol** below.

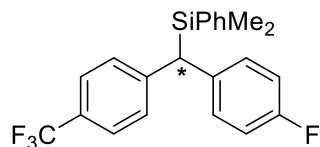
**(S)-p-tolyl(4-(trifluoromethyl)phenyl)methanol (22ol)<sup>19</sup>**



Yield: 46%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 8.2$  Hz, 2H), 7.52 (d,  $J = 8.2$  Hz, 2H), 7.25 (d,  $J = 8.0$  Hz, 2H), 7.18 (d,  $J = 8.0$  Hz, 2H), 5.85 (d,  $J = 3.2$  Hz, 1H), 2.40 (d,  $J = 3.2$  Hz, 1H), 2.36 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  147.7, 140.3, 137.9, 129.5 (q,  $J = 33.0$  Hz), 129.5, 126.6, 126.6, 125.4 (q,  $J = 4.0$  Hz), 124.2 (q,  $J = 271.0$  Hz), 75.6, 21.1.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-58.0$  (s, 3F).

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 5.20$  min (minor) and  $t_2 = 5.57$  min (major), 94% ee.  $[\alpha]_D^{25} +33.2$  (c 0.5, CHCl<sub>3</sub>). (*lit.* 19  $[\alpha]_D + 40.6$  (c 0.4, C<sub>6</sub>H<sub>6</sub>), 95% ee (S)).

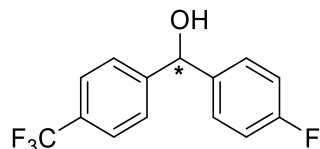
**(-)-((4-fluorophenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P23)**



Yield: 63%. Colorless oil.  $[\alpha]_D^{28} -25.0$  (c 1.0, CHCl<sub>3</sub>), 92% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.45 (d,  $J = 8.1$  Hz, 2H), 7.37 (t,  $J = 7.1$  Hz, 1H), 7.34 – 7.22 (m, 4H), 7.16 (d,  $J = 8.1$  Hz, 2H), 7.07 (dd,  $J = 8.5, 5.4$  Hz, 2H), 6.92 (t,  $J = 8.7$  Hz, 2H), 3.78 (s, 1H), 0.30 (s, 3H), 0.30 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  161.1 (d,  $J = 243.0$  Hz), 146.5, 136.9 (d,  $J = 3.3$  Hz), 136.5, 134.3, 130.3 (d,  $J = 7.6$  Hz), 129.5, 128.7, 128.2 (q,  $J = 40.0$  Hz), 127.8, 125.1 (q,  $J = 3.5$  Hz), 124.3 (q,  $J = 270.0$  Hz), 115.2 (d,  $J = 21.0$  Hz), 45.0, -3.3, -3.5. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -62.1 (s, 3F), -117.8 (s, 1F). <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -2.2. HRMS (EI) calcd for C<sub>21</sub>H<sub>17</sub>F<sub>4</sub>Si [M-CH<sub>3</sub>]<sup>+</sup>: 373.1036; Found 373.1034.

**P23** was oxidized to alcohol **23ol** via Method A. The enantiomeric excess was determined to be 92% by chiral HPLC analysis. See alcohol **23ol** below.

**(+)-(4-fluorophenyl)(4-(trifluoromethyl)phenyl)methanol (23ol)<sup>20</sup>**

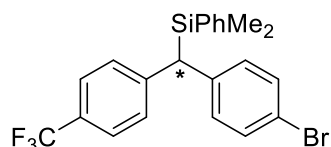


Yield: 44%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.60 (d,  $J = 8.1$  Hz, 2H), 7.48 (d,  $J = 8.1$  Hz, 2H), 7.35 – 7.28 (m, 2H), 7.08 – 6.97 (m, 2H), 5.84 (s, 1H), 2.48 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.4 (d,  $J = 246.7$  Hz), 147.3, 138.9 (d,  $J = 2.9$  Hz), 129.8 (q,  $J = 32.0$  Hz), 128.4 (d,  $J = 7.7$  Hz), 126.6, 125.5 (q,  $J = 4.2$  Hz), 124.1 (q,  $J = 271.0$  Hz), 115.6 (d,  $J = 21.5$  Hz), 75.1. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -58.1 (s, 3F), -109.7 (s, 1F).

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 99.2:0.8, 0.5 mL/min, 230 nm UV detector,  $t_1 = 9.60$  min (minor) and  $t_2 = 9.96$  min (major), 92% ee.  $[\alpha]_D^{25} +26.0$  (c 0.5, CHCl<sub>3</sub>).

**(-)-((4-bromophenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P24)**

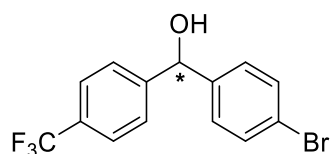




Yield: 71%. Colorless oil.  $[\alpha]_D^{28}$   $-16.2$  (c 1.0,  $\text{CHCl}_3$ ), 67% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 (d,  $J = 8.2$  Hz, 2H), 7.41 – 7.23 (m, 7H), 7.16 (d,  $J = 8.2$  Hz, 2H), 6.98 (d,  $J = 8.4$  Hz, 2H), 3.75 (s, 1H), 0.30 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.0, 140.3, 136.2, 134.3, 131.4, 130.6, 129.6, 128.8, 127.8, 127.6 (q,  $J = 32.0$  Hz), 125.2 (q,  $J = 4.2$  Hz), 124.3 (q,  $J = 270.0$  Hz), 119.4, 45.4,  $-3.4$ ,  $-3.5$ .  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-62.4$  (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.3$ . HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{17}\text{BrF}_3\text{Si}$   $[\text{M}-\text{CH}_3]^+$ : 433.0235; Found 433.0232.

**P24** was oxidized to alcohol **24ol** via Method A. The enantiomeric excess was determined to be 67% by chiral HPLC analysis. See alcohol **24ol** below.

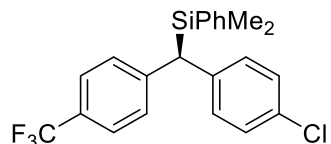
**(+)-(4-bromophenyl)(4-(trifluoromethyl)phenyl)methanol (24ol)<sup>21</sup>**



Yield: 32%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J = 8.2$  Hz, 2H), 7.51 – 7.42 (m, 4H), 7.22 (d,  $J = 8.2$  Hz, 2H), 5.81 (d,  $J = 3.0$  Hz, 1H), 2.41 (d,  $J = 3.0$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  147.0, 142.0, 131.9, 130.0 (q,  $J = 33.0$  Hz), 128.3, 126.7, 125.6 (q,  $J = 3.6$  Hz), 124.0 (q,  $J = 270.0$  Hz), 122.0, 75.1.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-58.2$  (s, 3F).

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 10.60$  min (minor) and  $t_2 = 11.15$  min (major), 67% ee.  $[\alpha]_D^{25}$   $+7.6$  (c 0.5,  $\text{CHCl}_3$ ).

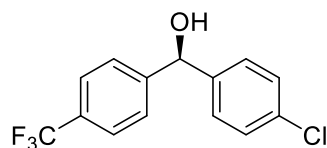
**(R)-((4-chlorophenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P25)**



Yield: 73%. Colorless oil.  $[\alpha]_D^{28}$   $-18.2$  (c 1.0,  $\text{CHCl}_3$ ), 76% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 (d,  $J = 8.1$  Hz, 2H), 7.40 – 7.35 (m, 1H), 7.33 – 7.24 (m, 4H), 7.22 – 7.13 (m, 4H), 7.03 (d,  $J = 8.8$  Hz, 2H), 3.77 (s, 1H), 0.30 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.1, 139.8, 136.3, 134.3, 131.4, 130.2, 129.6, 128.8, 128.5, 127.8, 126.5 (q,  $J = 32.0$  Hz), 125.2 (q,  $J = 3.7$  Hz), 124.3 (q,  $J = 270.0$  Hz), 45.3,  $-3.4$ ,  $-3.5$ .  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-62.3$  (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.2$ . HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{17}\text{ClF}_3\text{Si}$   $[\text{M}-\text{CH}_3]^+$ : 389.0740; Found 389.0740.

**P25** was oxidized to alcohol **25ol** via Method A. The enantiomeric excess was determined to be 76% by chiral HPLC analysis. See alcohol **25ol** below.

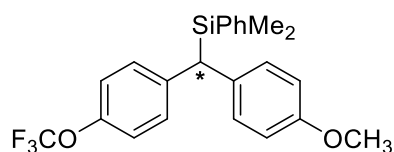
**(R)-(4-chlorophenyl)(4-(trifluoromethyl)phenyl)methanol (25ol)<sup>6</sup>**



Yield: 40%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.46 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.22 (m, 4H), 5.83 (s, 1H), 2.39 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 147.1, 141.5, 133.9, 130.0 (q, *J* = 32.4 Hz), 128.9, 128.0, 126.7, 125.6 (q, *J* = 3.5 Hz), 124.0 (q, *J* = 271.0 Hz), 75.1. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –58.1 (s, 3F).

HPLC condition: Chiralcel IB-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector, *t*<sub>1</sub> = 9.67 min (minor) and *t*<sub>2</sub> = 10.31 min (major), 76% ee. [α]<sub>D</sub><sup>25</sup> +10.8 (c 0.5, CHCl<sub>3</sub>). (*lit.* *6* [α]<sub>D</sub> –27.1 (c 2.3, C<sub>6</sub>H<sub>6</sub>), 96% ee (*S*)).

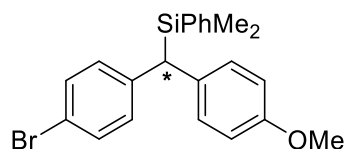
**(–)-((4-methoxyphenyl)(4-(trifluoromethoxy)phenyl)methyl)dimethyl(phenyl)silane (P26)**



Yield: 58%. Colorless oil. [α]<sub>D</sub><sup>28</sup> –46.8 (c 1.0, CHCl<sub>3</sub>), 93% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.34 (m, 1H), 7.32 – 7.24 (m, 4H), 7.10 – 6.99 (m, 6H), 6.78 (d, *J* = 8.7 Hz, 2H), 3.75 (s, 3H), 3.68 (s, 1H), 0.29 (s, 3H), 0.29 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 157.5, 146.8, 141.6, 137.1, 134.3, 133.7, 130.0, 129.6, 129.2, 127.6, 120.6, 120.5 (q, *J* = 255.0 Hz), 113.8, 55.2, 44.0, –3.2, –3.5. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ –58.2 (s, 3F). <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>) δ –3.0. **HRMS (EI)** calcd for C<sub>23</sub>H<sub>23</sub>F<sub>3</sub>O<sub>2</sub>Si [M]<sup>+</sup>: 416.1419; Found 416.1411.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99.5:0.5, 0.5 mL/min, 230 nm UV detector, *t*<sub>1</sub> = 8.47 min (minor) and *t*<sub>2</sub> = 8.83 min (major).

**(–)-((4-bromophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P27)**

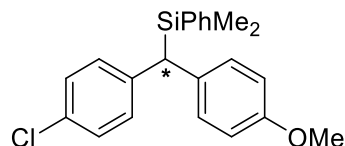


Yield: 58%. Colorless oil. [α]<sub>D</sub><sup>28</sup> –13.4 (c 1.0, CHCl<sub>3</sub>), 94% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.35 (m, 1H), 7.32 – 7.24 (m, 6H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.2 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.75 (s, 3H), 3.63 (s, 1H), 0.28 (s, 3H), 0.28 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 157.4, 141.9, 137.2, 134.4, 133.7, 131.1, 130.3, 129.9,

129.2, 127.6, 118.7, 113.7, 55.2, 44.0, -3.1, -3.4.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -3.0. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{23}\text{BrOSi}$   $[\text{M}]^+$ : 410.0702; Found 410.0694.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 4.56 min (minor) and  $t_2$  = 4.82 min (major).

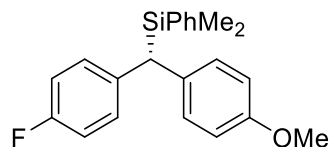
**(-)-((4-chlorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P28)**



Yield: 59%. Colorless oil.  $[\alpha]_{\text{D}}^{28}$  -17.0 (c 1.0,  $\text{CHCl}_3$ ), 93% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 – 7.34 (m, 1H), 7.31 – 7.28 (m, 4H), 7.14 (d,  $J$  = 8.4 Hz, 2H), 7.00 (dd,  $J$  = 15.7, 6.8 Hz, 4H), 6.76 (d,  $J$  = 7.0 Hz, 2H), 3.75 (s, 3H), 3.65 (s, 1H), 0.28 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.4, 141.3, 137.2, 134.3, 133.8, 130.7, 129.9, 129.9, 129.2, 128.2, 127.6, 113.7, 55.2, 43.9, -3.2, -3.4.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -3.0. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{23}\text{ClOSi}$   $[\text{M}]^+$ : 366.1207; Found 366.1196.

HPLC condition: Chiralpak AS-3 column, n-hexane/2-propanol = 99.2:0.8, 0.8 mL/min, 230 nm UV detector,  $t_1$  = 5.02 min (minor) and  $t_2$  = 5.31 min (major).

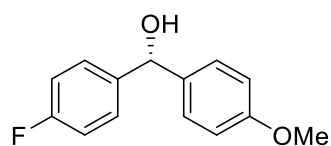
**(R)-((4-fluorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P29)**



Yield: 43%. Colorless oil.  $[\alpha]_{\text{D}}^{30}$  -34.0 (c 1.0,  $\text{CHCl}_3$ ), 77% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 – 7.32 (m, 1H), 7.29 – 7.26 (m, 4H), 7.05 – 6.98 (m, 4H), 6.87 (t,  $J$  = 8.7 Hz, 2H), 6.80 – 6.72 (m, 2H), 3.75 (s, 3H), 3.65 (s, 1H), 0.28 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.8 (d,  $J$  = 242.0 Hz), 157.4, 138.4 (d,  $J$  = 4.1 Hz), 137.4, 134.4, 134.2, 129.9 (d,  $J$  = 7.6 Hz), 129.8, 129.1, 127.6, 114.8 (d,  $J$  = 21.0 Hz), 113.7, 55.2, 43.6, -3.2, -3.4.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -119.0 (s, 1F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -3.0. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{23}\text{FOSi}$   $[\text{M}]^+$ : 350.1502; Found 350.1494.

**P29** was oxidized to alcohol **29ol** via Method B. The enantiomeric excess was determined to be 77% by chiral HPLC analysis. See alcohol **29ol** below.

**(R)-((4-fluorophenyl)(4-methoxyphenyl)methanol (29ol)<sup>22</sup>**

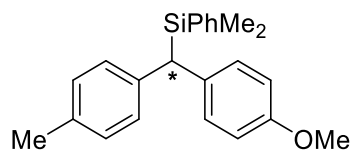


Yield: 45%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.29 (m, 2H), 7.25 (d,  $J$  = 7.5 Hz,

2H), 7.05 – 6.95 (m, 2H), 6.87 (d,  $J = 7.5$  Hz, 2H), 5.76 (s, 1H), 3.79 (s, 3H), 2.38 (s, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.1 (d,  $J = 245.4$  Hz), 159.1, 139.8 (d,  $J = 2.9$  Hz), 136.0, 128.1 (d,  $J = 7.8$  Hz), 127.9, 115.2 (d,  $J = 21.7$  Hz), 114.0, 75.2, 55.3.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.4 (s, 1F).

HPLC condition: Chiralpak AS-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 15.98$  min (major) and  $t_2 = 17.07$  min (minor), 77% ee.  $[\alpha]_{\text{D}}^{25} +10.4$  (c 0.5,  $\text{CHCl}_3$ ). (*lit.*  $[\alpha]_{\text{D}}^{20} +13.8$  (c 0.195, THF), 93% ee (*R*)).

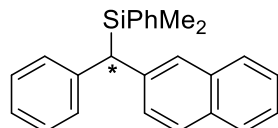
**(-)-((4-methoxyphenyl)(*p*-tolyl)methyl)dimethyl(phenyl)silane (P30)**



Yield: 40%. Colorless oil.  $[\alpha]_{\text{D}}^{30} -3.8$  (c 1.0,  $\text{CHCl}_3$ ), 56% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 – 7.21 (m, 5H), 7.05 – 6.96 (m, 6H), 6.76 – 6.71 (m, 2H), 3.74 (s, 3H), 3.64 (s, 1H), 2.27 (s, 3H), 0.28 (s, 3H), 0.27 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  157.2, 139.6, 137.9, 134.7, 134.4, 129.8 (2C signal), 129.0, 128.9, 128.7, 127.5, 113.6, 55.2, 43.9, 20.9, -3.1, -3.2.  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -3.4. **HRMS (ESI)** calcd for  $[\text{C}_{23}\text{H}_{26}\text{OSi} + \text{NH}_4]^+$ : 364.2097; Found 364.2100.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1 = 4.11$  min (minor) and  $t_2 = 4.34$  min (major).

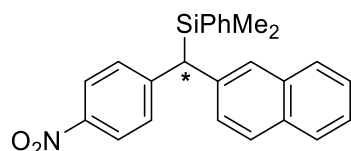
**(+)-dimethyl(naphthalen-2-yl(phenyl)methyl)(phenyl)silane (P31)**



Yield: 85%. Colorless oil.  $[\alpha]_{\text{D}}^{30} +11.8$  (c 1.0,  $\text{CHCl}_3$ ), 53% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 – 7.71 (m, 1H), 7.66 (d,  $J = 8.2$  Hz, 2H), 7.56 (s, 1H), 7.42 – 7.16 (m, 12H), 7.12 (td,  $J = 6.8, 2.2$  Hz, 1H), 3.91 (s, 1H), 0.32 (s, 3H), 0.32 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  142.3, 140.0, 137.6, 134.5, 133.6, 131.6, 129.2, 129.1, 128.3, 127.7 (2C signal), 127.6 (2C signal), 127.5, 126.9, 125.8, 125.3, 125.0, 45.9, -3.0 (2C signal).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -2.7. **HRMS (EI)** calcd for  $\text{C}_{25}\text{H}_{24}\text{Si}$   $[\text{M}]^+$ : 352.1647; Found 352.1647.

HPLC condition: phenomenex, Cellulose-3, methanol/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 8.14$  min (major) and  $t_2 = 9.19$  min (minor).

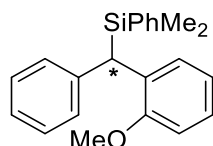
**(-)-dimethyl(naphthalen-2-yl(4-nitrophenyl)methyl)(phenyl)silane (P32)**



Yield: 89%. Colorless oil.  $[\alpha]_D^{30} -75.0$  (c 1.0,  $\text{CHCl}_3$ ), 96% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J = 8.8$  Hz, 2H), 7.80 – 7.70 (m, 3H), 7.60 (s, 1H), 7.47 – 7.34 (m, 3H), 7.34 – 7.18 (m, 7H), 4.03 (s, 1H), 0.35 (s, 3H), 0.33 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.6, 145.5, 138.0, 136.2, 134.3, 133.5, 131.7, 129.6, 128.9, 128.2, 128.0, 127.8, 127.5 (2C signal), 127.3, 126.1, 125.5, 123.4, 46.5, –3.0, –3.7.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –1.7. HRMS (EI) calcd for  $\text{C}_{25}\text{H}_{23}\text{NO}_2\text{Si}$   $[\text{M}]^+$ : 397.1498; Found 397.1493.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 8.77$  min (minor) and  $t_2 = 9.85$  min (major).

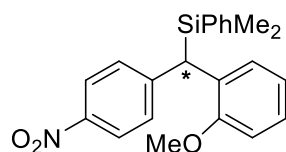
**(–)-((2-methoxyphenyl)(phenyl)methyl)dimethyl(phenyl)silane (P33)**



Yield: 60%. Colorless oil.  $[\alpha]_D^{27} -5.0$  (c 1.0,  $\text{CHCl}_3$ ), 32% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.27 (m, 5H), 7.26 – 7.08 (m, 7H), 6.92 – 6.79 (m, 2H), 4.34 (s, 1H), 3.70 (s, 3H), 0.33 (s, 3H), 0.30 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.8, 142.6, 138.6, 134.3, 131.1, 130.3, 129.0, 128.8, 128.0, 127.4, 126.4, 124.8, 120.2, 110.5, 55.1, 36.8, –2.8, –3.2.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –1.8. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{24}\text{OSi}$   $[\text{M}]^+$ : 332.1596; Found 332.1587.

HPLC condition: Chiralcel OJ-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 5.40$  min (major) and  $t_2 = 7.02$  min (minor).

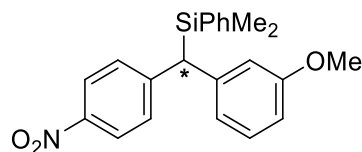
**(–)-((2-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P34)**



Yield: 45%. Colorless oil.  $[\alpha]_D^{30} -58.0$  (c 1.0,  $\text{CHCl}_3$ ), >99% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 (d,  $J = 8.8$  Hz, 2H), 7.40 – 7.33 (m, 1H), 7.34 – 7.30 (m, 4H), 7.25 – 7.16 (m, 2H), 7.16 – 7.09 (m, 2H), 6.89 (td,  $J = 7.5, 1.2$  Hz, 1H), 6.84 (dd,  $J = 8.2, 1.1$  Hz, 1H), 4.35 (s, 1H), 3.70 (s, 3H), 0.32 (s, 3H), 0.28 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.9, 151.4, 145.3, 137.4, 134.1, 130.5, 129.3, 129.2, 128.9, 127.7, 127.4, 123.2, 120.4, 110.8, 55.1, 38.5, –2.8, –3.6.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –1.9. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{Si}$   $[\text{M}]^+$ : 377.1447; Found 377.1440.

HPLC condition: Chiralpak AS-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 5.58$  min (minor) and  $t_2 = 7.35$  min (major).

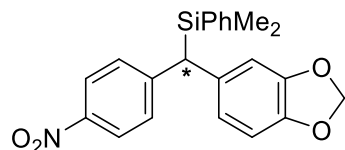
**(-)-((3-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P35)**



Yield: 73%. Colorless oil.  $[\alpha]_D^{30} -37.2$  (c 1.0,  $\text{CHCl}_3$ ), 99% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J = 8.8$  Hz, 2H), 7.38-7.36 (m, 1H), 7.35 – 7.25 (m, 4H), 7.18-7.16 (m, 3H), 6.79 – 6.71 (m, 2H), 6.68 (t,  $J = 2.1$  Hz, 1H), 3.84 (s, 1H), 3.71 (s, 3H), 0.33 (s, 3H), 0.32 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.6, 150.5, 145.5, 141.9, 136.2, 134.3, 129.6, 129.5, 128.9, 127.8, 123.4, 121.6, 115.1, 111.2, 55.0, 46.6, -3.1, -3.8.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -1.8. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{Si}$   $[\text{M}]^+$ : 377.1447; Found 377.1440.

HPLC condition: Chiralpak AS-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 7.31$  min (major) and  $t_2 = 7.68$  min (minor).

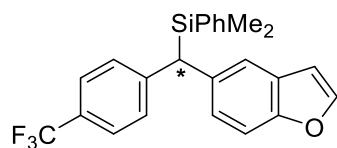
**(-)-((benzo[d][1,3]dioxol-5-yl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P36)**



Yield: 49%. Colorless oil.  $[\alpha]_D^{30} -62.0$  (c 1.0,  $\text{CHCl}_3$ ), 97% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (d,  $J = 8.8$  Hz, 2H), 7.43 – 7.35 (m, 1H), 7.34 – 7.22 (m, 4H), 7.18 – 7.08 (m, 2H), 6.72 (d,  $J = 7.8$  Hz, 1H), 6.68 – 6.58 (m, 2H), 5.92 (s, 2H), 3.79 (s, 1H), 0.33 (s, 3H), 0.32 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.9, 147.8, 145.8, 145.5, 136.2, 134.2, 134.2, 129.6, 128.7, 127.8, 123.4, 122.3, 109.8, 108.3, 101.0, 46.0, -3.0, -3.8.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  -2.1. HRMS (EI) calcd for  $\text{C}_{22}\text{H}_{21}\text{NO}_4\text{Si}$   $[\text{M}]^+$ : 391.1240; Found 391.1234.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1 = 12.92$  min (minor) and  $t_2 = 15.61$  min (major).

**(-)-((benzofuran-5-yl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P37)**

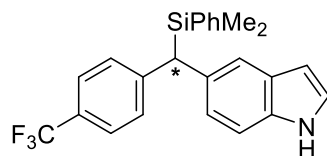


Yield: 82%. Colorless oil.  $[\alpha]_D^{30} -42.4$  (c 1.0,  $\text{CHCl}_3$ ), 98% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 (d,  $J = 2.2$  Hz, 1H), 7.43 (d,  $J = 8.3$  Hz, 2H), 7.38 – 7.34 (m, 3H), 7.30 – 7.28 (m, 4H), 7.20 (d,  $J = 8.2$  Hz, 2H), 7.07 (dd,  $J = 8.6, 1.9$  Hz, 1H), 6.66 (d,  $J = 1.3$

Hz, 1H), 3.90 (s, 1H), 0.32 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  153.4, 147.2, 145.2, 136.9, 135.8, 134.4, 129.4, 128.7, 127.7, 127.6, 127.3 (q,  $J = 32.0$  Hz), 125.8, 125.0 (q,  $J = 4.2$  Hz), 124.4 (q,  $J = 270.0$  Hz), 121.2, 111.1, 106.5, 45.6,  $-3.0$ ,  $-3.5$ .  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-62.8$  (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.5$ . HRMS (EI) calcd for  $\text{C}_{23}\text{H}_{18}\text{F}_3\text{OSi}$   $[\text{M}-\text{CH}_3]^+$ : 395.1079; Found 395.1067.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1 = 3.91$  min (minor) and  $t_2 = 4.31$  min (major).

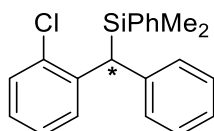
**(-)-5-((dimethyl(phenyl)silyl)(4-(trifluoromethyl)phenyl)methyl)-1H-indole (P38)**



Yield: 44%. Colorless oil.  $[\alpha]_{\text{D}}^{30} -59.0$  (c 1.0,  $\text{CHCl}_3$ ), 99% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (s, 1H), 7.43 (s, 1H), 7.39 (d,  $J = 8.2$  Hz, 2H), 7.37 – 7.25 (m, 5H), 7.25 – 7.15 (m, 3H), 7.15 – 7.11 (m, 1H), 6.97 (dd,  $J = 8.2, 1.6$  Hz, 1H), 6.45 (s, 1H), 3.90 (s, 1H), 0.32 (s, 3H), 0.30 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  147.8, 137.4, 134.4, 134.2, 132.6, 129.2, 128.7, 128.1, 127.6, 126.9 (q,  $J = 32.0$  Hz), 124.9 (q,  $J = 4.3$  Hz), 124.5 (q,  $J = 270.0$  Hz), 124.4, 124.2, 120.9, 110.9, 102.4, 45.6,  $-2.8$ ,  $-3.4$ .  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$   $-62.8$  (s, 3F).  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.7$ . HRMS (EI) calcd for  $\text{C}_{24}\text{H}_{22}\text{F}_3\text{NSi}$   $[\text{M}]^+$ : 409.1474; Found 409.1467.

HPLC condition: Chiralpak AD-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 7.63$  min (minor) and  $t_2 = 8.63$  min (major).

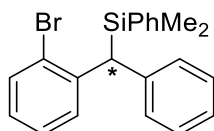
**(+)-((2-chlorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P39)**



The diazo compound disappeared completely for 15 min. Yield: 92%. Colorless oil.  $[\alpha]_{\text{D}}^{25} +7.0$  (c 1.0,  $\text{CHCl}_3$ ), 99% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 – 7.23 (m, 7H), 7.21 – 7.14 (m, 2H), 7.14 – 7.08 (m, 4H), 7.04 (td,  $J = 7.7, 1.8$  Hz, 1H), 4.44 (s, 1H), 0.34 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  141.3, 140.1, 137.3, 134.6, 134.5, 130.9, 129.8, 129.3, 129.1, 128.2, 127.7, 126.7, 126.4, 125.3, 40.6,  $-2.7$ ,  $-3.3$ .  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-2.3$ . HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{21}\text{ClSi}$   $[\text{M}-\text{CH}_3]^+$ : 321.0866; Found 321.0854.

HPLC condition: Chiralcel OJ-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 4.91$  min (minor) and  $t_2 = 7.32$  min (major).

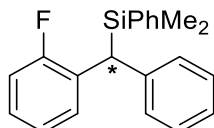
**(+)-((2-bromophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P40)**



The diazo compound disappeared completely for 10 min. Yield: 82%. Colorless oil.  $[\alpha]_D^{25} +4.0$  (c 1.0,  $\text{CHCl}_3$ ), 98% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.52 (dd,  $J = 8.0$ , 1.4 Hz, 1H), 7.38 – 7.25 (m, 6H), 7.21 – 7.14 (m, 3H), 7.13 – 7.05 (m, 3H), 6.97 (ddd,  $J = 7.9$ , 7.3, 1.7 Hz, 1H), 4.44 (s, 1H), 0.34 (s, 3H), 0.31 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  141.8, 141.2, 137.2, 134.5, 133.2, 130.9, 129.3, 129.0, 128.2, 127.7, 127.1, 127.0, 126.3, 125.3, 43.6, –2.6, –3.4.  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –2.2. HRMS (EI) calcd for  $\text{C}_{20}\text{H}_{18}\text{BrSi}$   $[\text{M}-\text{CH}_3]^+$ : 365.0361; Found 365.0353.

HPLC condition: Chiralcel OJ-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 5.04$  min (minor) and  $t_2 = 7.79$  min (major).

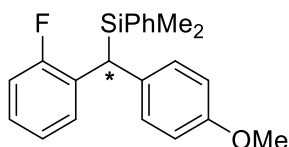
**(+)-((2-fluorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P41)**



The diazo compound disappeared completely for 5.0 h. Yield: 69%. Colorless oil.  $[\alpha]_D^{25} +1.8$  (c 0.5,  $\text{CHCl}_3$ ), 83% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 – 7.16 (m, 8H), 7.14 – 7.06 (m, 4H), 7.03 – 6.94 (m, 2H), 4.13 (s, 1H), 0.33 (s, 3H), 0.30 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.4 (d,  $J = 242.0$  Hz), 141.6, 137.4, 134.4, 130.8 (d,  $J = 3.7$  Hz), 129.6 (d,  $J = 15.5$  Hz), 129.2, 129.0, 128.2, 127.6, 126.9 (d,  $J = 8.0$  Hz), 125.3, 123.8 (d,  $J = 3.7$  Hz), 115.4 (d,  $J = 23.5$  Hz), 36.5, –3.0, –3.4.  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$  –115.9 (s, 1F).  $^{29}\text{Si NMR}$  (79 MHz,  $\text{CDCl}_3$ )  $\delta$  –2.2. HRMS (EI) calcd for  $\text{C}_{21}\text{H}_{21}\text{FSi}$   $[\text{M}]^+$ : 320.1397; Found 320.1387.

HPLC condition: Chiralcel OJ-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 4.94$  min (minor) and  $t_2 = 5.82$  min (major).

**(–)-((2-fluorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P42)**



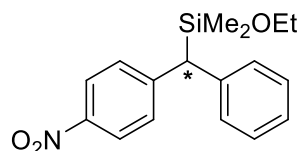
Yield: 36%. Colorless oil.  $[\alpha]_D^{25} -12.0$  (c 1.0,  $\text{CHCl}_3$ ), 91% ee.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 – 7.25 (m, 5H), 7.18 (td,  $J = 8.0$ , 2.0 Hz, 1H), 7.11 – 7.01 (m, 3H), 7.00 – 6.93 (m, 2H), 6.77 – 6.70 (m, 2H), 4.07 (s, 1H), 3.74 (s, 3H), 0.32 (s, 3H), 0.29 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.2 (d,  $J = 242.0$  Hz), 157.3, 137.4, 134.3, 133.5, 130.6 (d,  $J = 3.8$  Hz), 130.0, 129.9 (d,  $J = 15.7$  Hz), 129.1, 127.5, 126.6 (q,  $J = 8.0$  Hz), 123.7 (d,  $J = 3.6$  Hz), 115.3 (d,  $J = 23.5$  Hz), 113.6, 55.1, 35.2, –3.1, –3.5.  $^{19}\text{F NMR}$



(376 MHz, CDCl<sub>3</sub>)  $\delta$  -116.9 (s, 1F). <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -2.5. HRMS (EI) calcd for C<sub>22</sub>H<sub>23</sub>FOSi [M]<sup>+</sup>: 350.1502; Found 350.1498.

HPLC condition: Chiralcel OJ-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 6.01 min (minor) and  $t_2$  = 7.40 min (major).

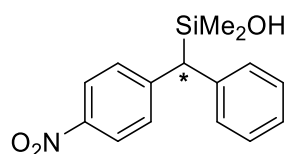
**(-)-ethoxydimethyl((4-nitrophenyl)(phenyl)methyl)silane (P43)**



Yield: 76%. Colorless oil.  $[\alpha]_D^{25}$  -0.2 (c 1.0, CHCl<sub>3</sub>), >99% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.14 (d,  $J$  = 8.8 Hz, 2H), 7.47 (d,  $J$  = 8.8 Hz, 2H), 7.36 – 7.32 (m, 4H), 7.25 – 7.23 (m, 1H), 3.73 (s, 1H), 3.62 (q,  $J$  = 7.0 Hz, 2H), 1.17 (t,  $J$  = 6.9 Hz, 3H), 0.15 (s, 3H), 0.14 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  150.7, 145.6, 140.2, 129.3, 129.1, 128.7, 126.0, 123.5, 59.0, 46.8, 18.4, -2.4, -2.5. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  +12.1. HRMS (EI) calcd for C<sub>17</sub>H<sub>21</sub>NO<sub>3</sub>Si [M]<sup>+</sup>: 315.1291; Found 315.1283.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 7.16 min (minor) and  $t_2$  = 7.93 min (major).

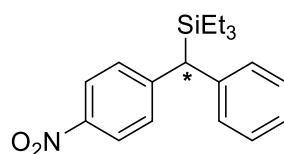
**(-)-dimethyl((4-nitrophenyl)(phenyl)methyl)silanol (P44)**



Yield: 56%. Colorless oil.  $[\alpha]_D^{25}$  -0.1 (c 0.5, CHCl<sub>3</sub>), 98% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.96 (d,  $J$  = 8.8 Hz, 2H), 7.30 (d,  $J$  = 8.8 Hz, 2H), 7.18 – 7.15 (m, 4H), 7.14 – 7.02 (m, 1H), 3.55 (s, 1H), 1.97 (s, 1H), 0.01 (s, 3H), 0.00 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  150.4, 145.6, 140.0, 129.1, 129.0, 128.8, 126.1, 123.6, 47.6, -0.8, -0.9. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  +13.0. HRMS (ESI) calcd for C<sub>15</sub>H<sub>17</sub>NO<sub>3</sub>Si [M+Na]<sup>+</sup>: 310.0875; Found 310.0873.

HPLC condition: Chiralcel OD-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 8.37 min (minor) and  $t_2$  = 9.75 min (major).

**(-)-triethyl((4-nitrophenyl)(phenyl)methyl)silane (P45)**

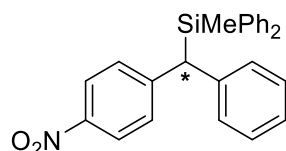


Yield: 64%. Colorless oil.  $[\alpha]_D^{25}$  -74.0 (c 0.3, CHCl<sub>3</sub>), 96% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.14 (d,  $J$  = 8.8 Hz, 2H), 7.42 (d,  $J$  = 8.8 Hz, 2H), 7.38 – 7.27 (m, 4H), 7.26 – 7.19 (m, 1H), 3.84 (s, 1H), 0.89 (t,  $J$  = 7.9 Hz, 9H), 0.69 – 0.61 (m, 6H). <sup>13</sup>C NMR

(101 MHz, CDCl<sub>3</sub>)  $\delta$  151.6, 145.5, 141.0, 129.1, 128.7, 128.7, 125.9, 123.6, 43.8, 7.4, 3.4. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  +8.4. HRMS (EI) calcd for C<sub>19</sub>H<sub>25</sub>NO<sub>2</sub>Si [M]<sup>+</sup>: 327.1655; Found 327.1647.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 7.26 min (minor) and  $t_2$  = 8.15 min (major).

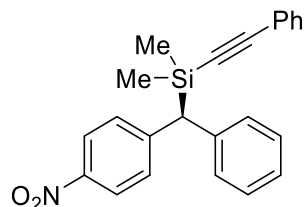
**(-)-methyl((4-nitrophenyl)(phenyl)methyl)diphenylsilane (P46)**



Yield: 62%. Colorless oil.  $[\alpha]_D^{25}$  -41.4 (c 1.0, CHCl<sub>3</sub>), 94% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.04 – 7.92 (m, 2H), 7.43 – 7.34 (m, 4H), 7.33 – 7.26 (m, 6H), 7.24 – 7.15 (m, 3H), 7.14 – 7.08 (m, 4H), 4.27 (s, 1H), 0.55 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  150.5, 145.7, 140.2, 135.3, 135.2, 134.8, 134.4, 129.9, 129.8, 129.7, 129.4, 128.7, 128.0 (2C signal), 126.2, 123.4, 45.2, -3.9. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -8.2. HRMS (EI) calcd for C<sub>26</sub>H<sub>23</sub>NO<sub>2</sub>Si [M]<sup>+</sup>: 409.1498; Found 409.1491.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 99:1, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 9.32 min (minor) and  $t_2$  = 9.69 min (major).

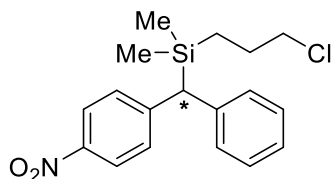
**(S)-dimethyl((4-nitrophenyl)(phenyl)methyl)(phenylethynyl)silane (P47)**



Yield: 93%. white solid. m.p.: 50–52 °C.  $[\alpha]_D^{28}$  -20.4 (c 1.0, CHCl<sub>3</sub>), >99% ee. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.13 (d,  $J$  = 8.8 Hz, 2H), 7.55 (d,  $J$  = 8.8 Hz, 2H), 7.48 – 7.38 (m, 4H), 7.38 – 7.27 (m, 5H), 7.27 – 7.17 (m, 1H), 3.79 (s, 1H), 0.25 (s, 3H), 0.23 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  150.4, 145.7, 140.1, 131.8, 129.3, 129.0, 129.0, 128.7, 128.3, 126.2, 123.5, 122.4, 108.2, 91.1, 45.5, -1.9, -2.2. <sup>29</sup>Si NMR (79 MHz, CDCl<sub>3</sub>)  $\delta$  -14.9. HRMS (EI) calcd for C<sub>23</sub>H<sub>21</sub>NO<sub>2</sub>Si [M]<sup>+</sup>: 371.1342; Found 371.1336. The absolute configuration of **P47** is *S* determined by X-ray single crystal analysis, see below.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1$  = 7.75 min (minor) and  $t_2$  = 8.20 min (major).

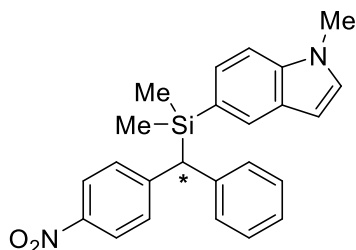
**(-)-(3-chloropropyl)dimethyl((4-nitrophenyl)(phenyl)methyl)silane (P48)**



Yield: 89%. Colorless oil.  $[\alpha]_{\text{D}}^{28}$   $-47.6$  (c 1.0,  $\text{CHCl}_3$ ), 99% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 (d,  $J = 8.8$  Hz, 2H), 7.50 – 7.36 (m, 4H), 7.36 – 7.26 (m, 3H), 3.80 (s, 1H), 3.48 (t,  $J = 6.8$  Hz, 2H), 1.81 – 1.66 (m, 2H), 0.78 – 0.65 (m, 2H), 0.16 (s, 3H), 0.15 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.0, 145.6, 140.6, 129.0, 128.9, 128.7, 126.1, 123.7, 47.7, 45.7, 27.3, 12.2,  $-3.5$ ,  $-3.7$ .  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-10.0$ . HRMS (EI) calcd for  $\text{C}_{18}\text{H}_{22}\text{ClNO}_2\text{Si}$   $[\text{M}]^+$ : 347.1108; Found 347.1100.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 230 nm UV detector,  $t_1 = 10.37$  min (minor) and  $t_2 = 12.38$  min (major).

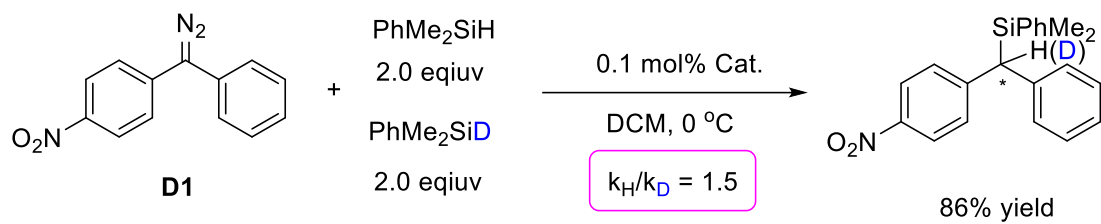
**(-)-5-(dimethyl((4-nitrophenyl)(phenyl)methyl)silyl)-1-methyl-1H-indole (P49)**



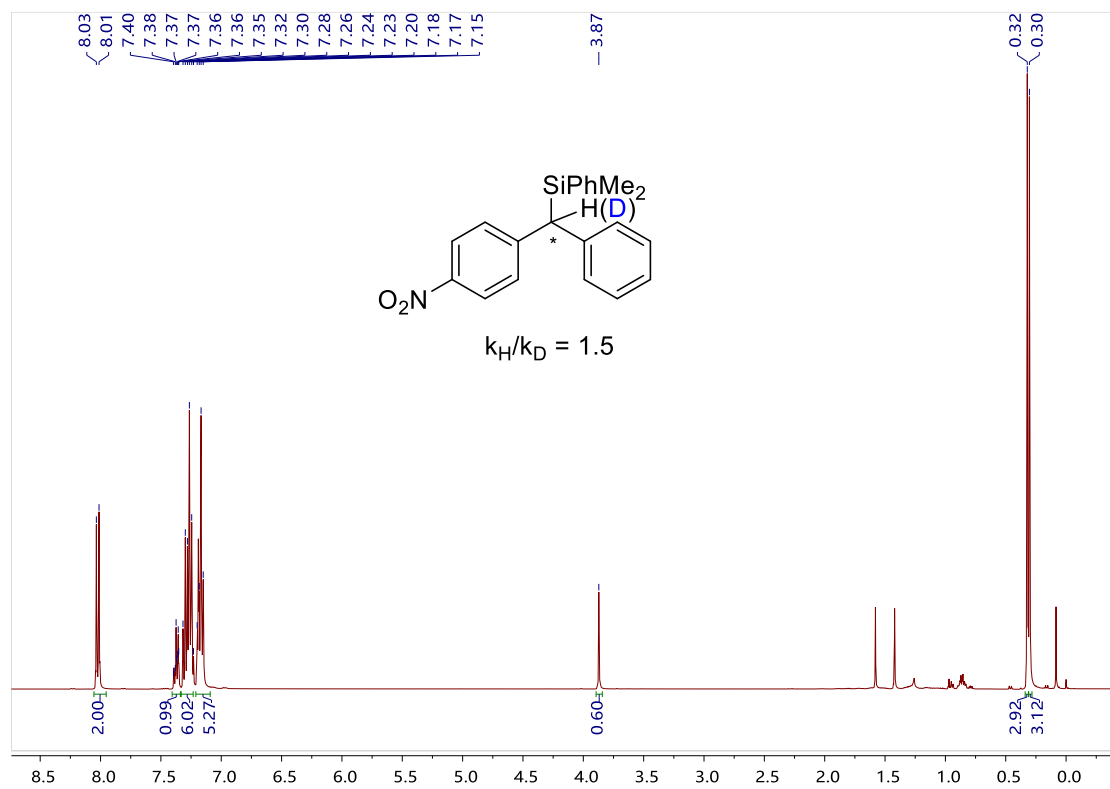
Yield: 53%. Colorless oil.  $[\alpha]_{\text{D}}^{28}$   $-83.2$  (c 1.0,  $\text{CHCl}_3$ ), >99% ee.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 (d,  $J = 8.8$  Hz, 2H), 7.63 (s, 1H), 7.35 – 7.26 (m, 3H), 7.25 – 7.21 (m, 5H), 7.12 – 7.05 (m, 2H), 6.51 (dd,  $J = 3.1, 0.9$  Hz, 1H), 3.96 (s, 1H), 3.84 (s, 3H), 0.40 (s, 3H), 0.38 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.3, 145.4, 141.0, 137.5, 129.3, 129.1, 128.9, 128.6, 128.4, 127.9, 127.1, 125.9, 124.8, 123.3, 108.9, 101.2, 47.3, 32.8,  $-2.5$ ,  $-3.3$ .  $^{29}\text{Si}$  NMR (79 MHz,  $\text{CDCl}_3$ )  $\delta$   $-1.5$ . HRMS (EI) calcd for  $\text{C}_{24}\text{H}_{24}\text{N}_2\text{O}_2\text{Si}$   $[\text{M}]^+$ : 400.1607; Found 400.1601.

HPLC condition: Chiralpak IC-3 column, n-hexane/2-propanol = 98:2, 1.0 mL/min, 230 nm UV detector,  $t_1 = 17.28$  min (minor) and  $t_2 = 18.11$  min (major).

## 8. Competition experiments for kinetic isotope effect



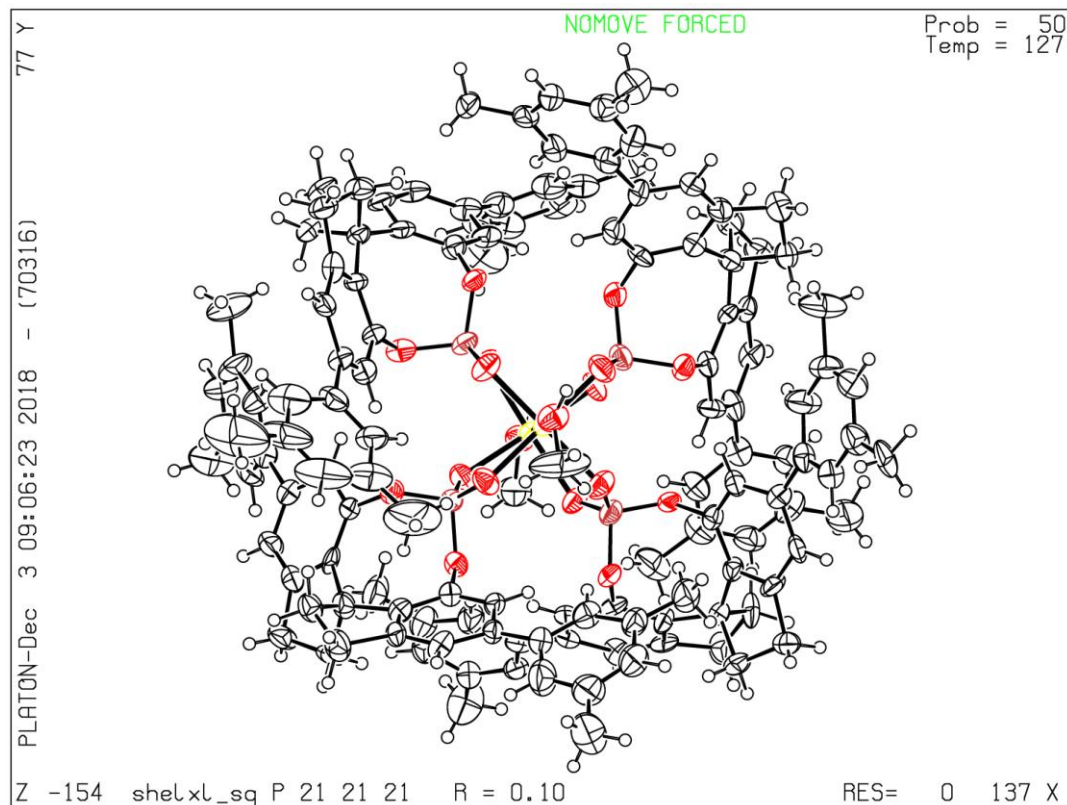
$^1\text{H NMR}$



## 9. Crystal data and structures refinement

### Crystal data and structures refinement of $C_3(MeOH)_2$

**$C_3(MeOH)_2$** : (The crystal structure of compound  $C_3(MeOH)_2$  has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1888695). The data is available free of charge at [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html).)

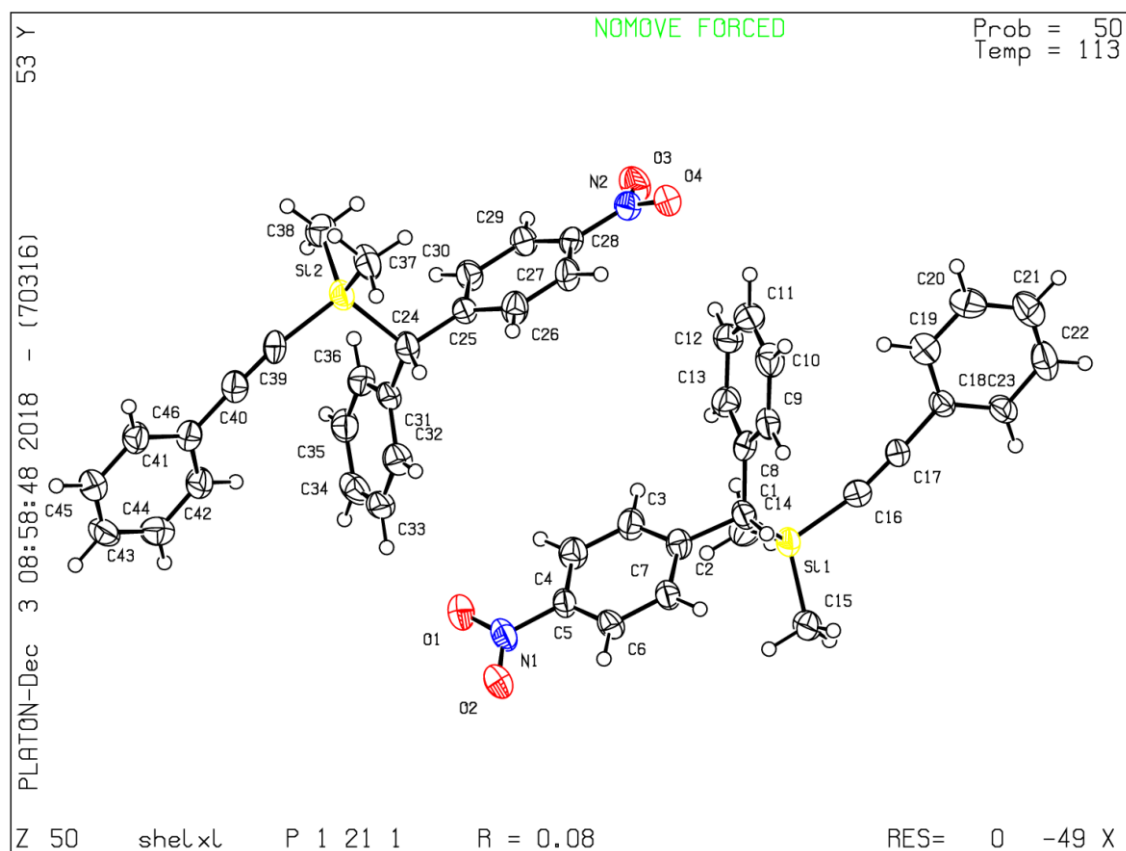


**Table S3. Crystal data and structure refinement for C<sub>3</sub>(MeOH)<sub>2</sub>**

Identification code	shelxl_sq
Empirical formula	C <sub>134</sub> H <sub>128</sub> O <sub>18</sub> P <sub>4</sub> Rh <sub>2</sub>
Formula weight	2356.06
Temperature/K	127.15
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	14.423(3)
b/Å	28.903(6)
c/Å	31.726(6)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	13226(5)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.183
μ/mm <sup>-1</sup>	0.358
F(000)	4904.0
Crystal size/mm <sup>3</sup>	0.32 × 0.18 × 0.16
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.096 to 50.698
Index ranges	-14 ≤ h ≤ 17, -34 ≤ k ≤ 34, -38 ≤ l ≤ 38
Reflections collected	74686
Independent reflections	23598 [R <sub>int</sub> = 0.1188, R <sub>sigma</sub> = 0.1387]
Data/restraints/parameters	23598/12/1447
Goodness-of-fit on F <sup>2</sup>	1.125
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.1017, wR <sub>2</sub> = 0.2024
Final R indexes [all data]	R <sub>1</sub> = 0.1192, wR <sub>2</sub> = 0.2163
Largest diff. peak/hole / e Å <sup>-3</sup>	0.95/-0.69
Flack parameter	0.00(3)

### Crystal data and structures refinement of P47

**Compound P47:** (The crystal structure of compound **P47** has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1888689). The data is available free of charge at [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html).)



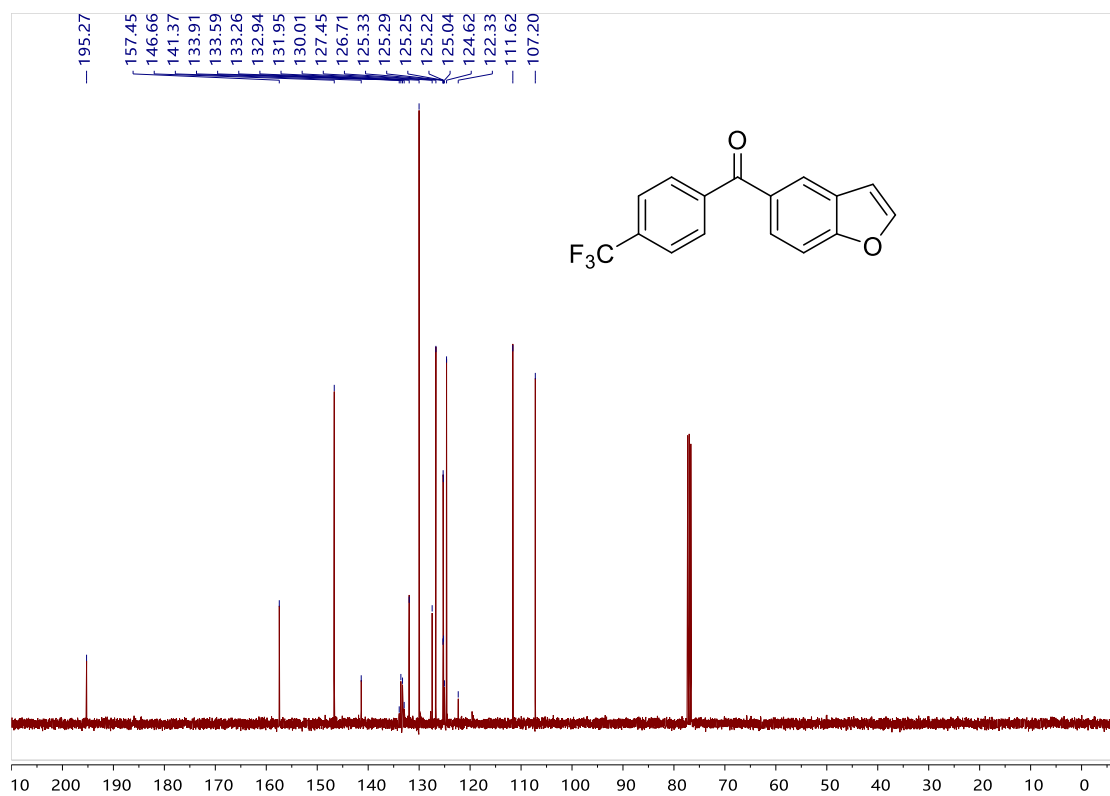
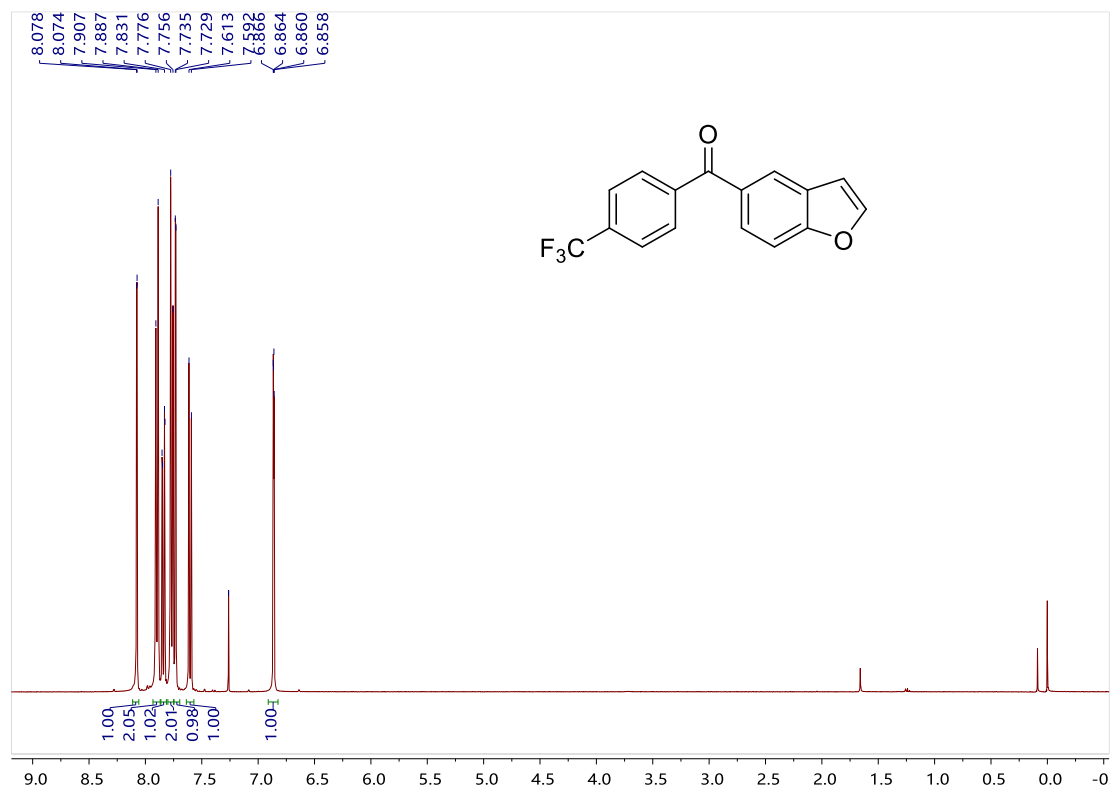
**Table S4. Crystal data and structure refinement for P47**

Identification code	shelxl
Empirical formula	C <sub>23</sub> H <sub>21</sub> NO <sub>2</sub> Si
Formula weight	371.50
Temperature/K	113.15
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	9.952(2)
b/Å	19.926(4)
c/Å	10.453(2)
α/°	90
β/°	90.60(3)
γ/°	90
Volume/Å <sup>3</sup>	2072.7(7)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.190
μ/mm <sup>-1</sup>	0.130
F(000)	784.0
Crystal size/mm <sup>3</sup>	0.2 × 0.18 × 0.12
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.092 to 50.038
Index ranges	-11 ≤ h ≤ 11, -23 ≤ k ≤ 23, -12 ≤ l ≤ 12
Reflections collected	16192
Independent reflections	7292 [R <sub>int</sub> = 0.0564, R <sub>sigma</sub> = 0.0802]
Data/restraints/parameters	7292/1/492
Goodness-of-fit on F <sup>2</sup>	1.078
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0763, wR <sub>2</sub> = 0.1955
Final R indexes [all data]	R <sub>1</sub> = 0.0912, wR <sub>2</sub> = 0.2095
Largest diff. peak/hole / e Å <sup>-3</sup>	0.70/-0.33
Flack parameter	0.01(11)

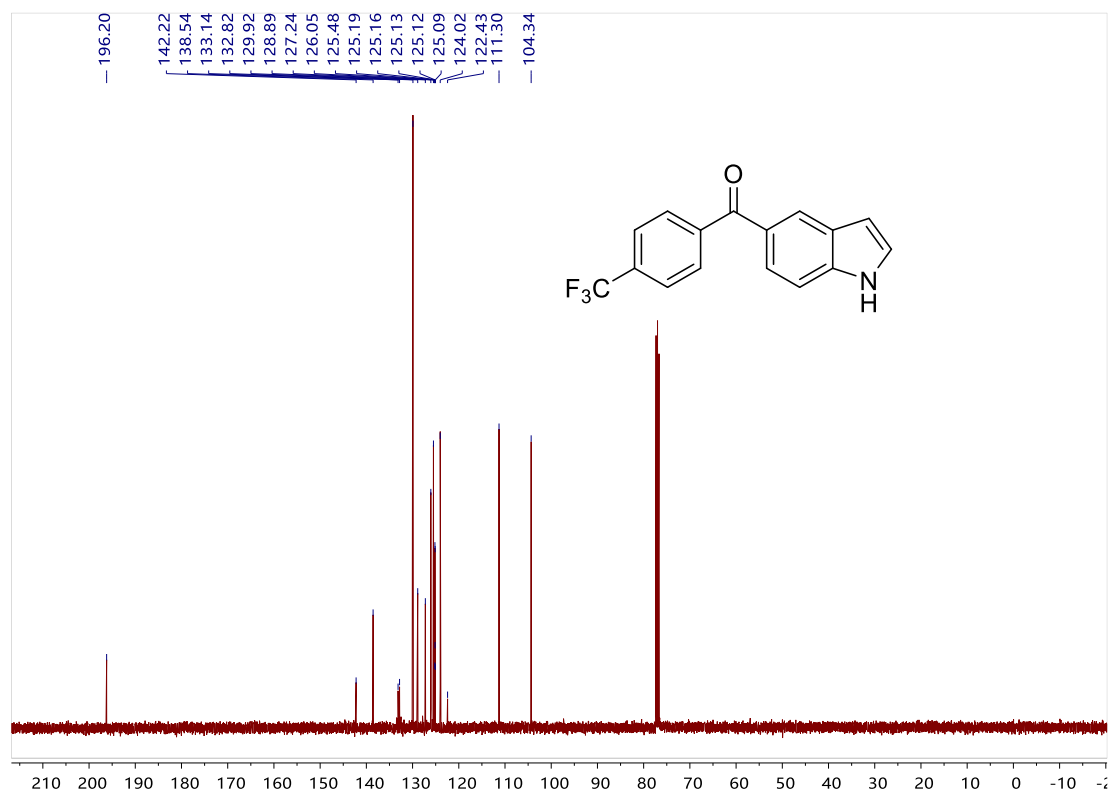
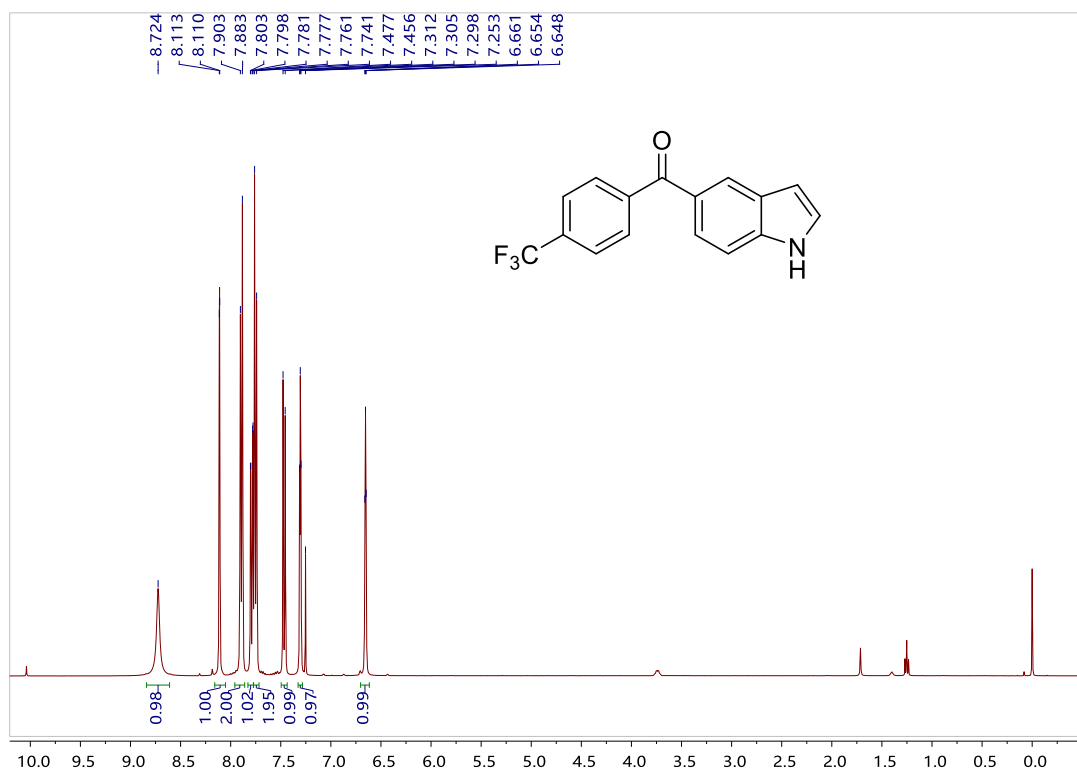


## 10. NMR spectra for new compounds

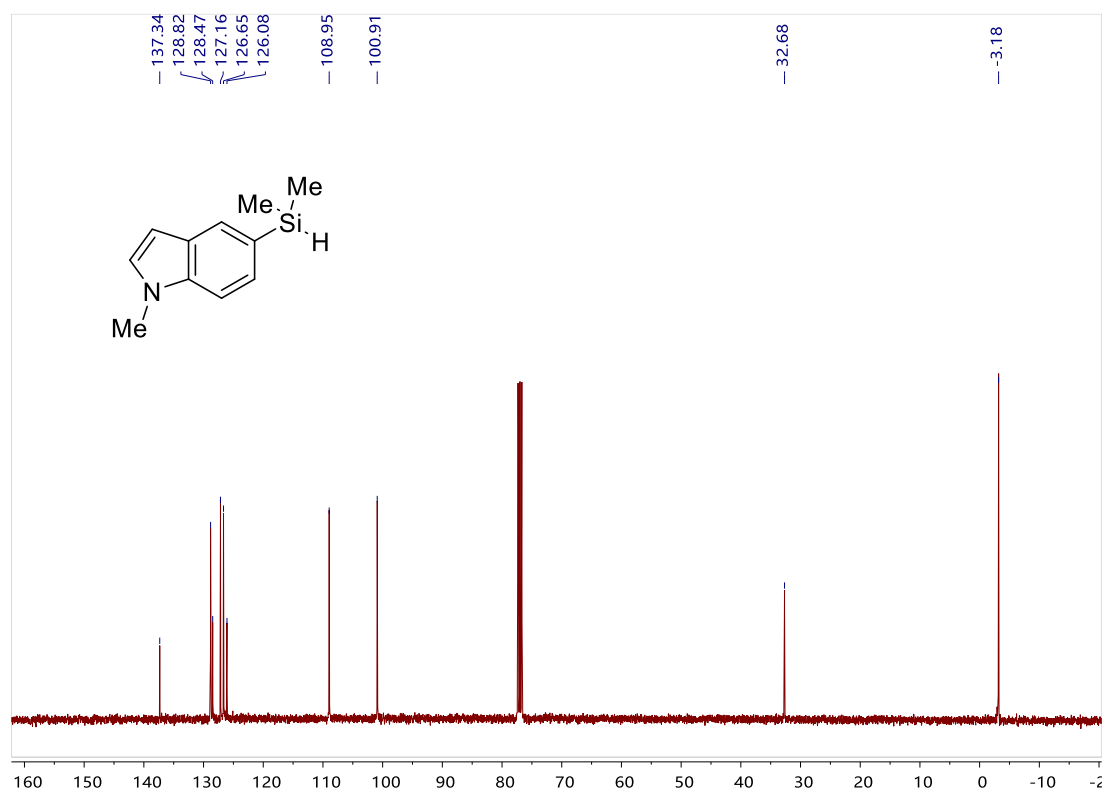
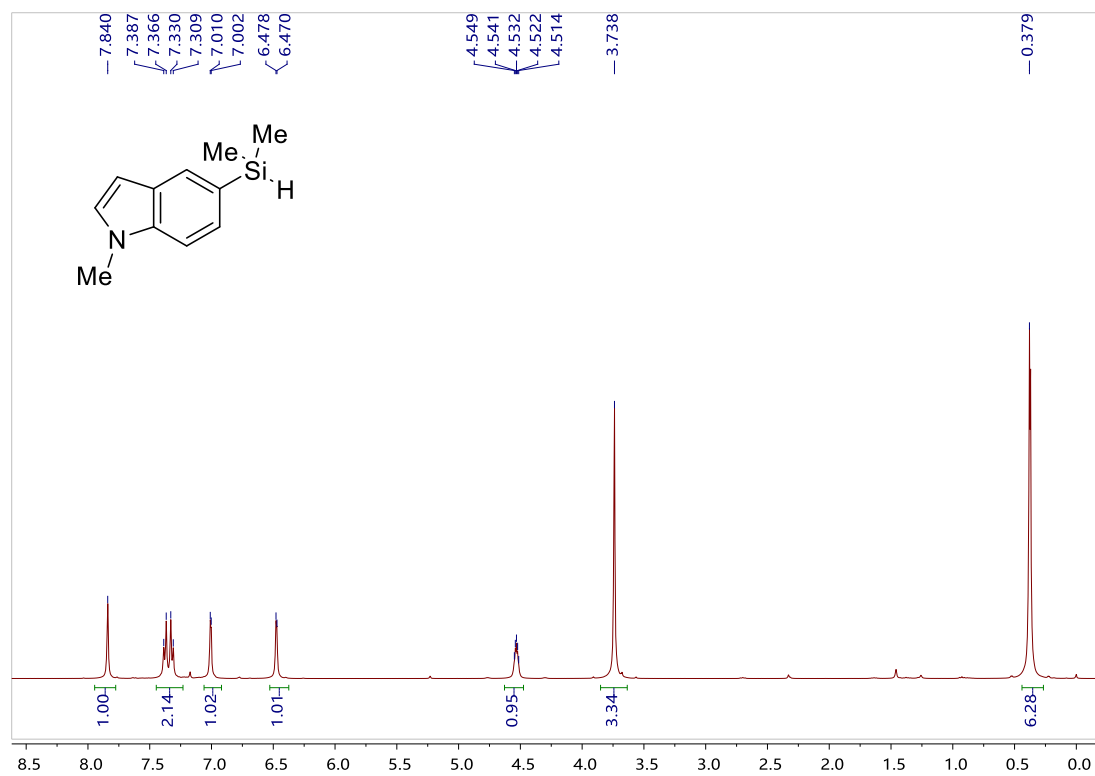
### benzofuran-5-yl(4-(trifluoromethyl)phenyl)methanone (K37)



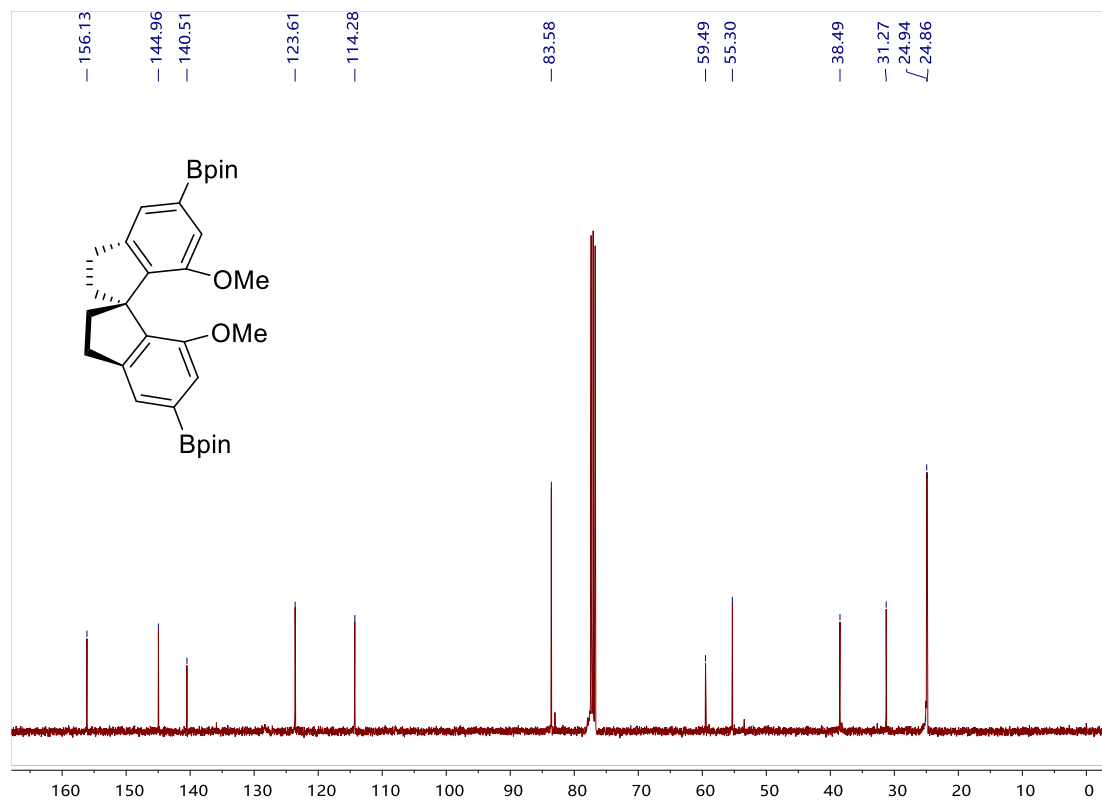
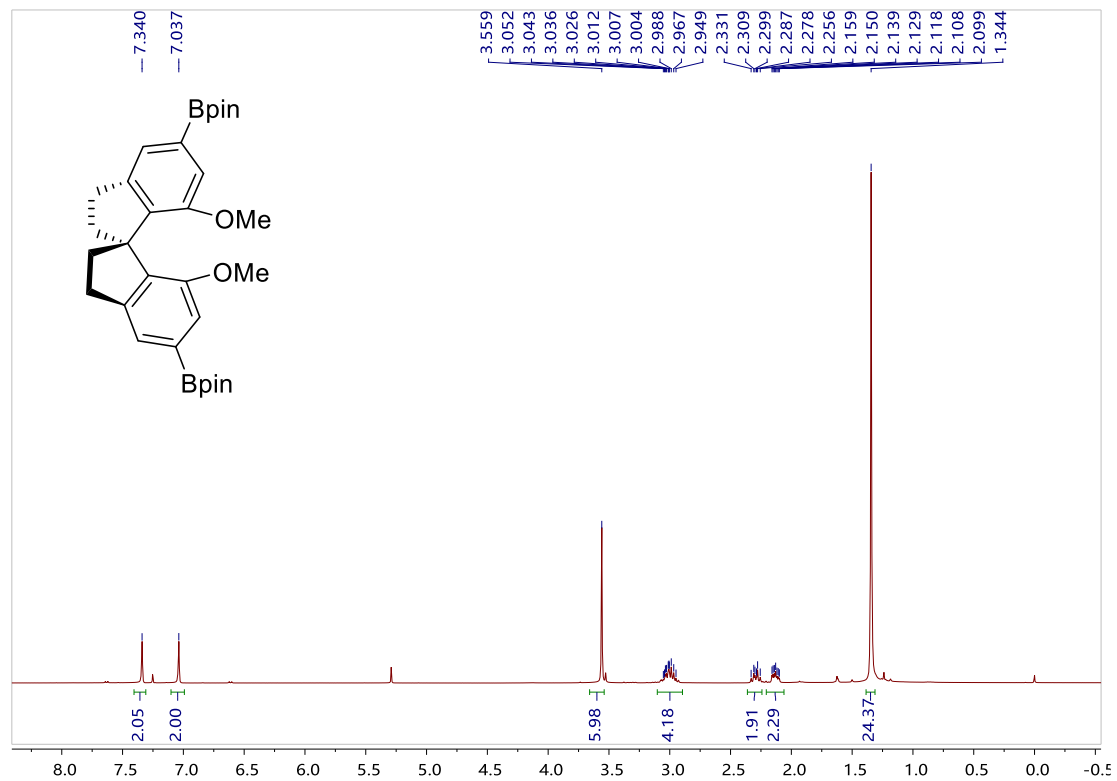
**(1H-indol-5-yl)(4-(trifluoromethyl)phenyl)methanone (K38)**



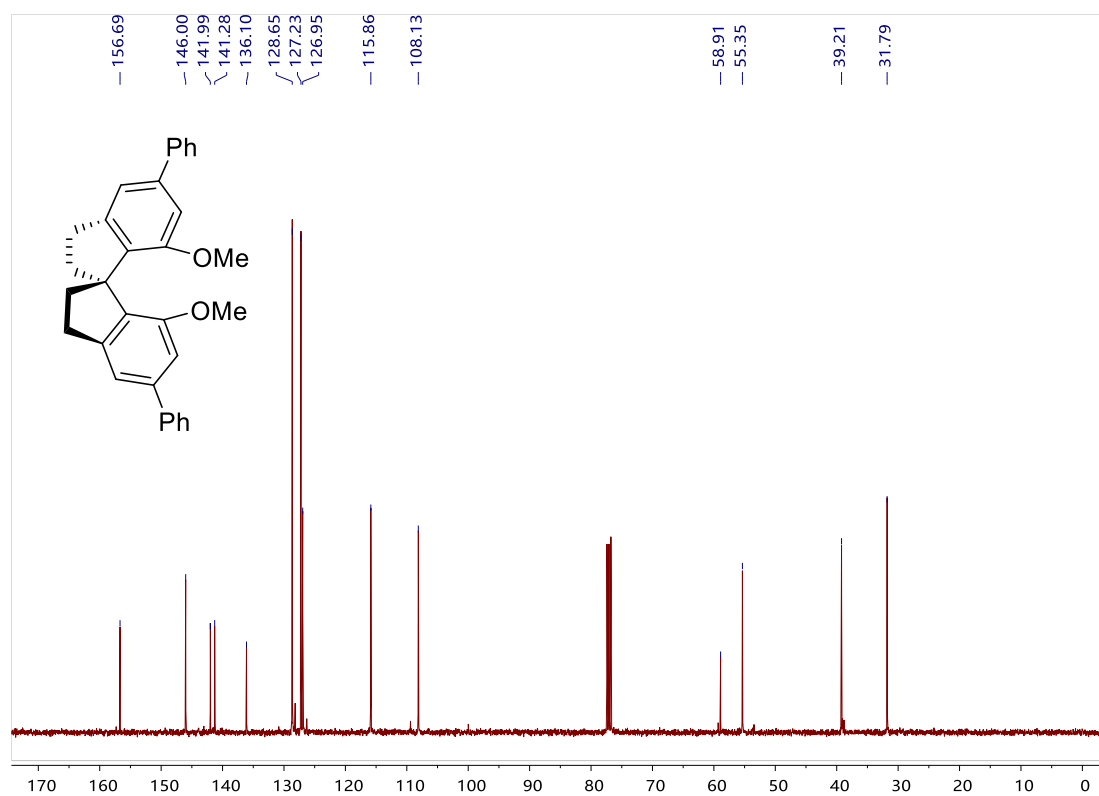
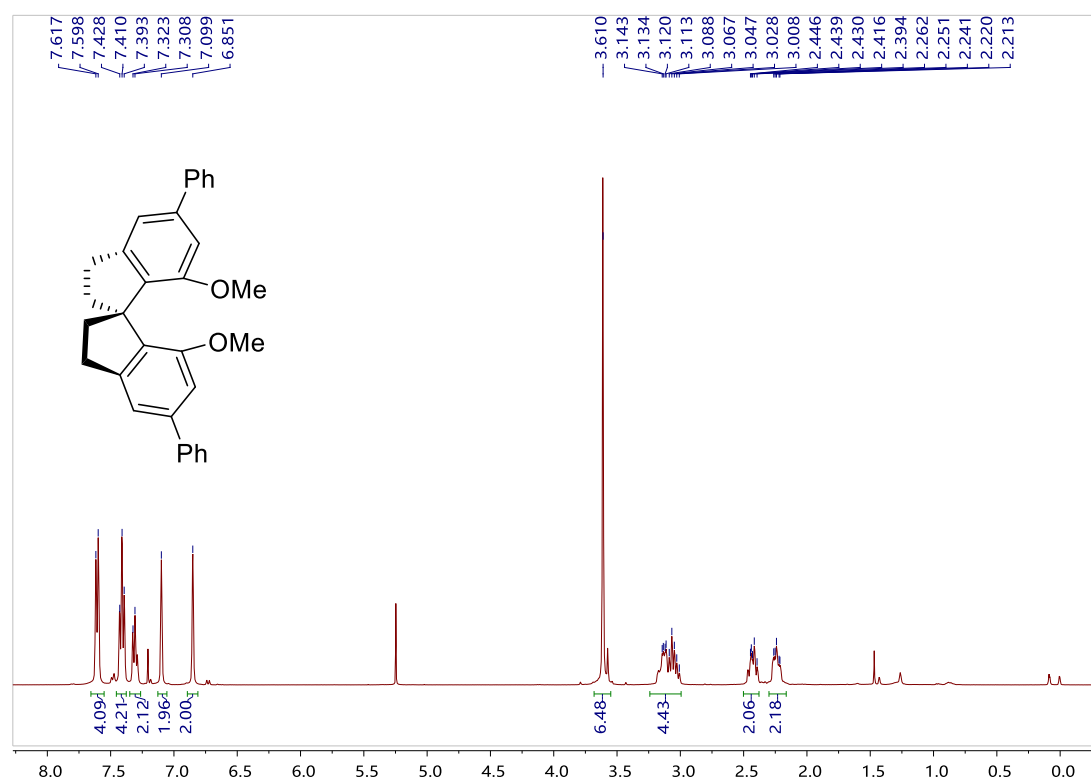
### 5-(dimethylsilyl)-1-methyl-1H-indole (S9)



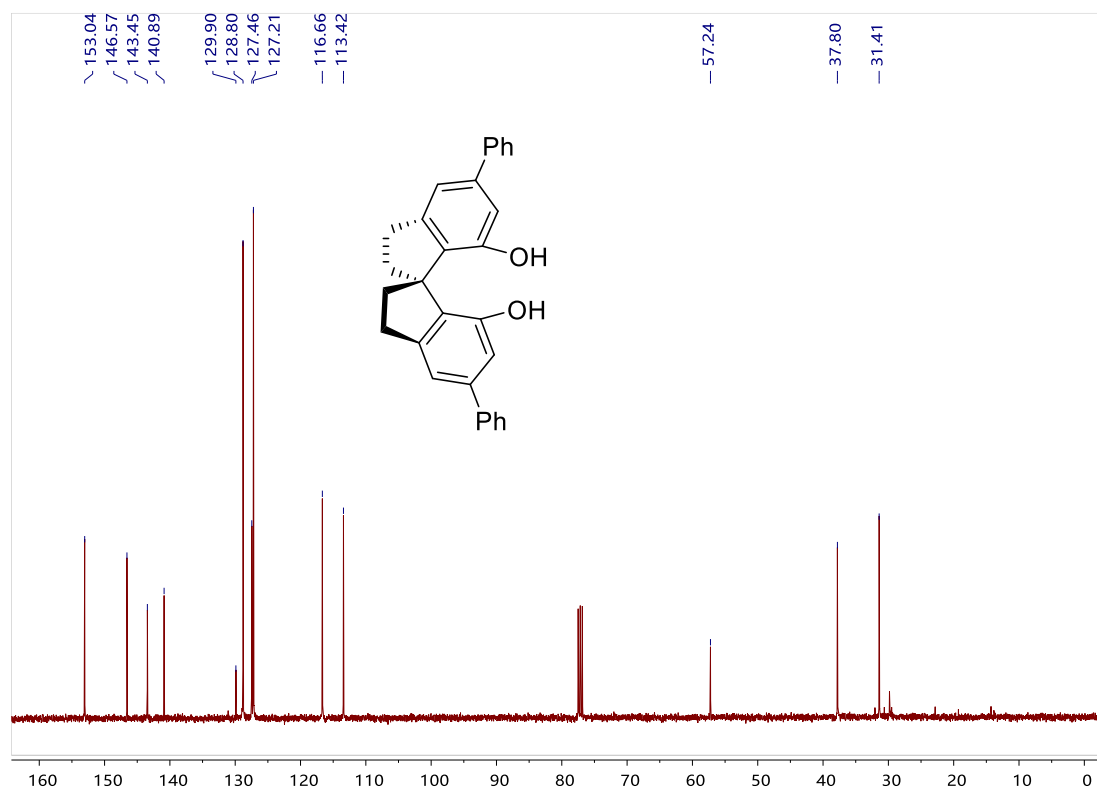
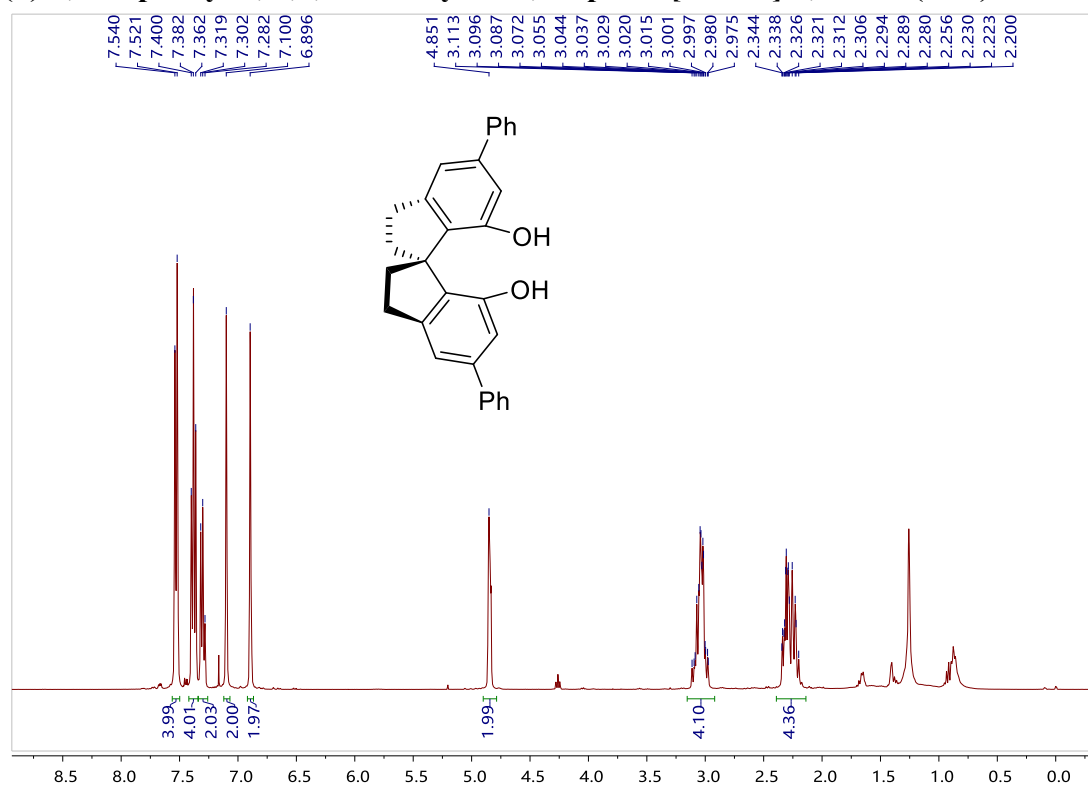
**(S)-2,2'-(7,7'-dimethoxy-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-5,5'-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (SI-3)**



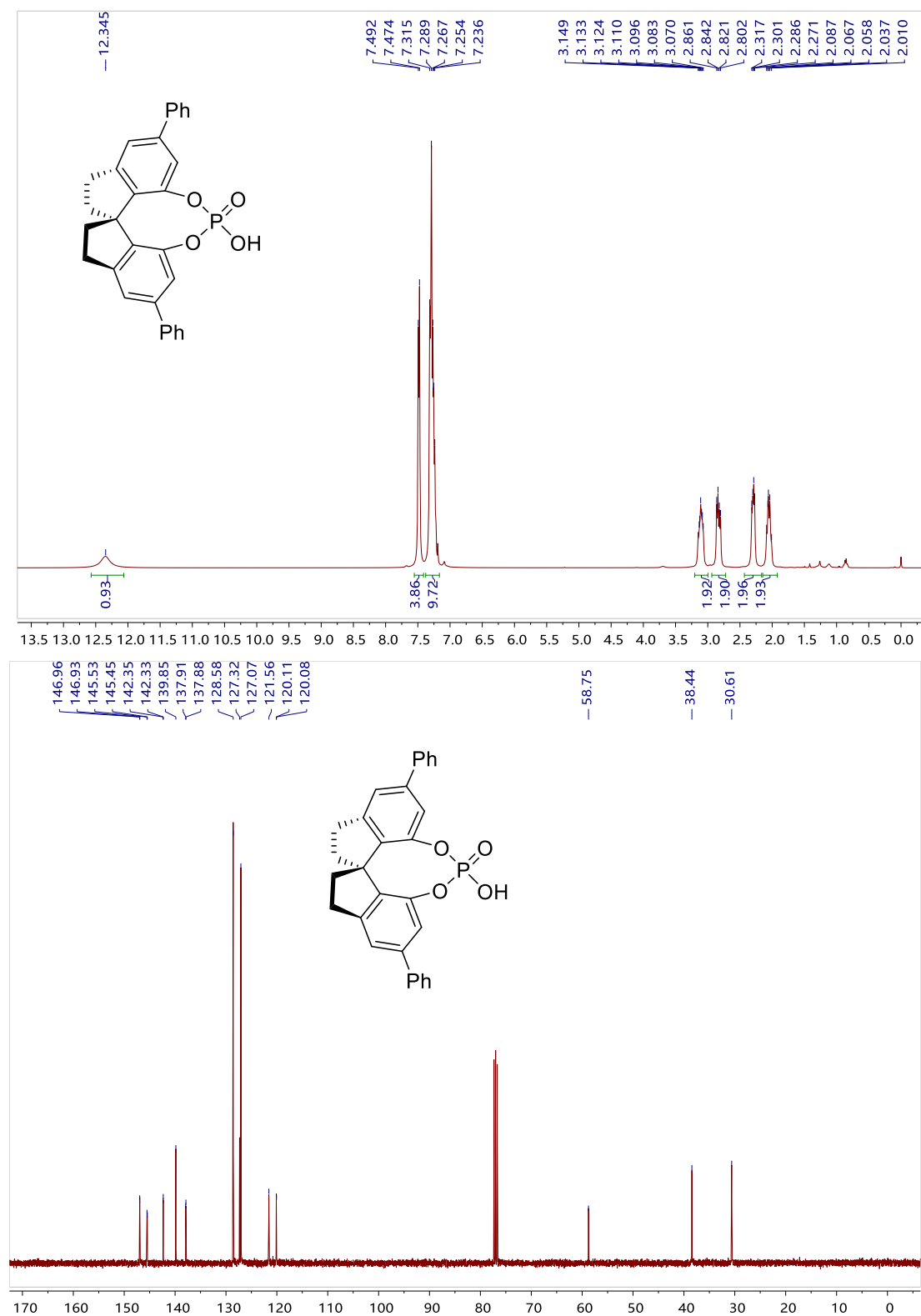
**(S)-7,7'-dimethoxy-5,5'-diphenyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] (SI-4)**

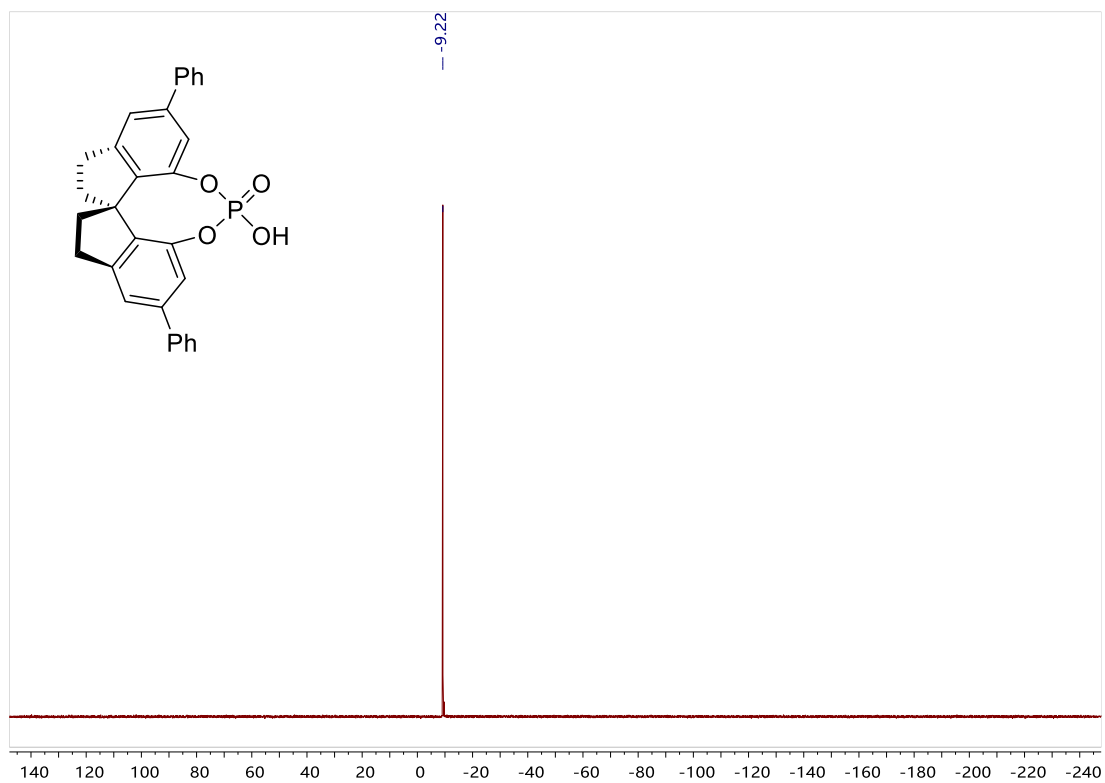


**(S)-5,5'-diphenyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diol (SI-5)**



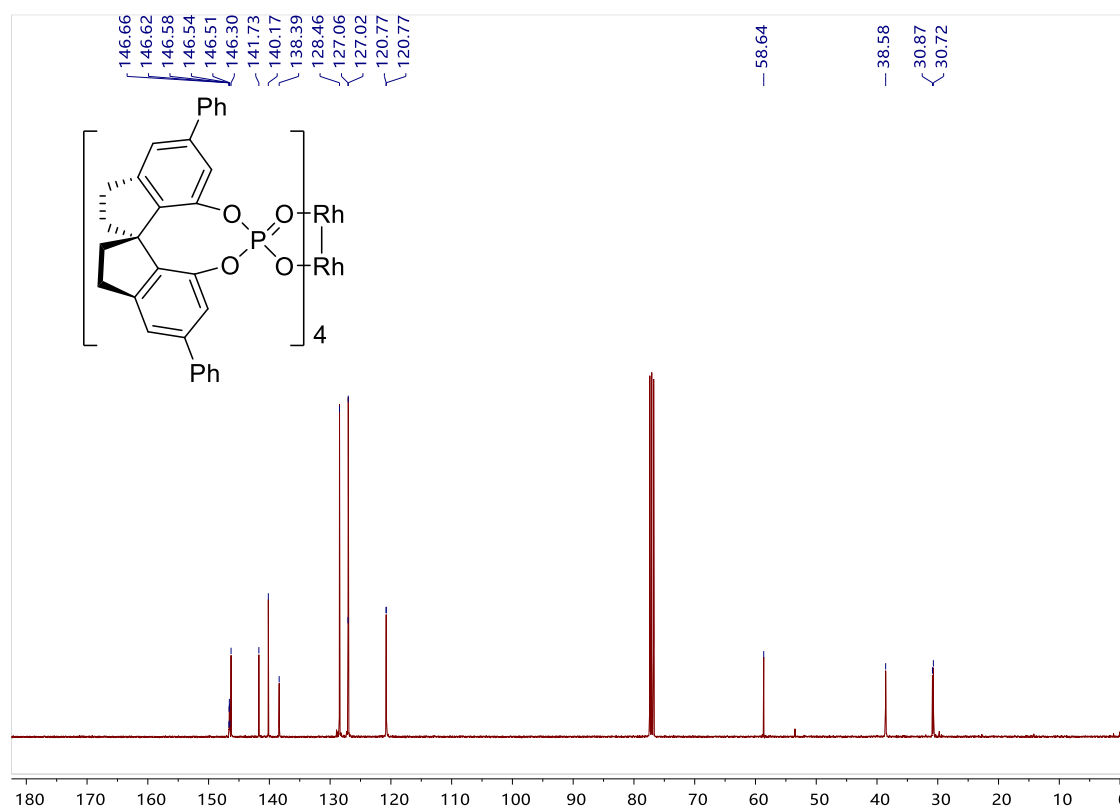
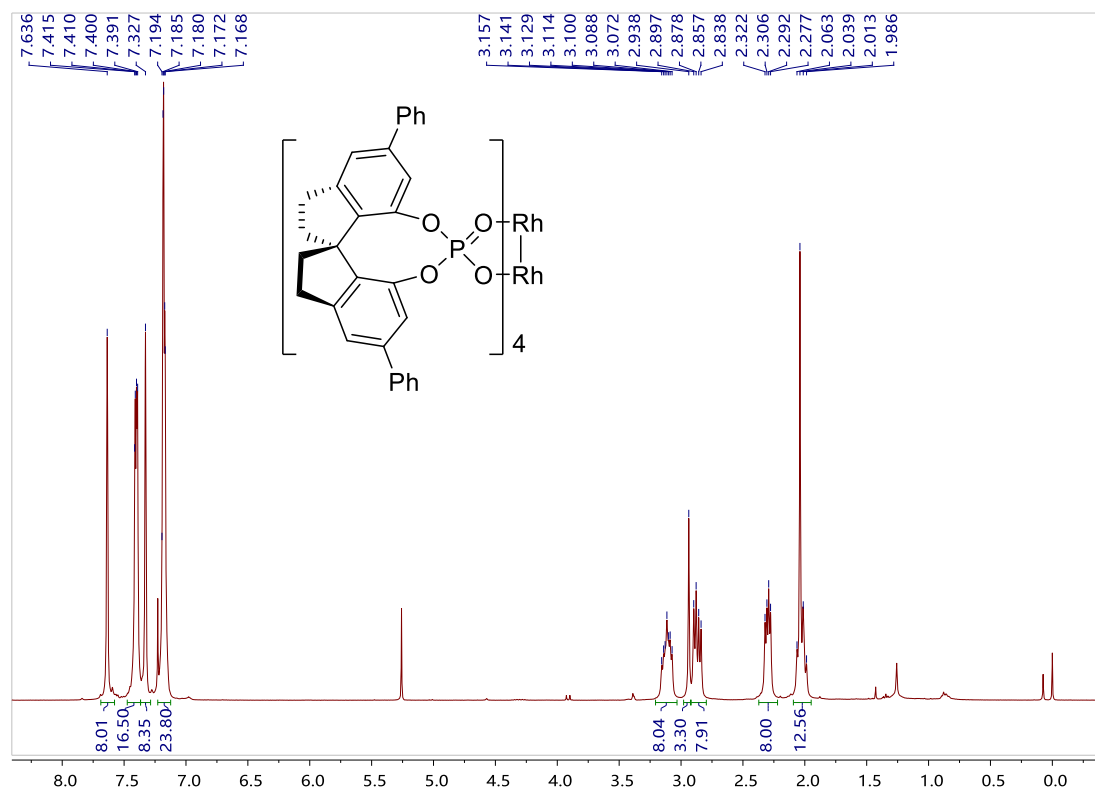
**(S)-5,5'-Diphenyl-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (SI-6)**

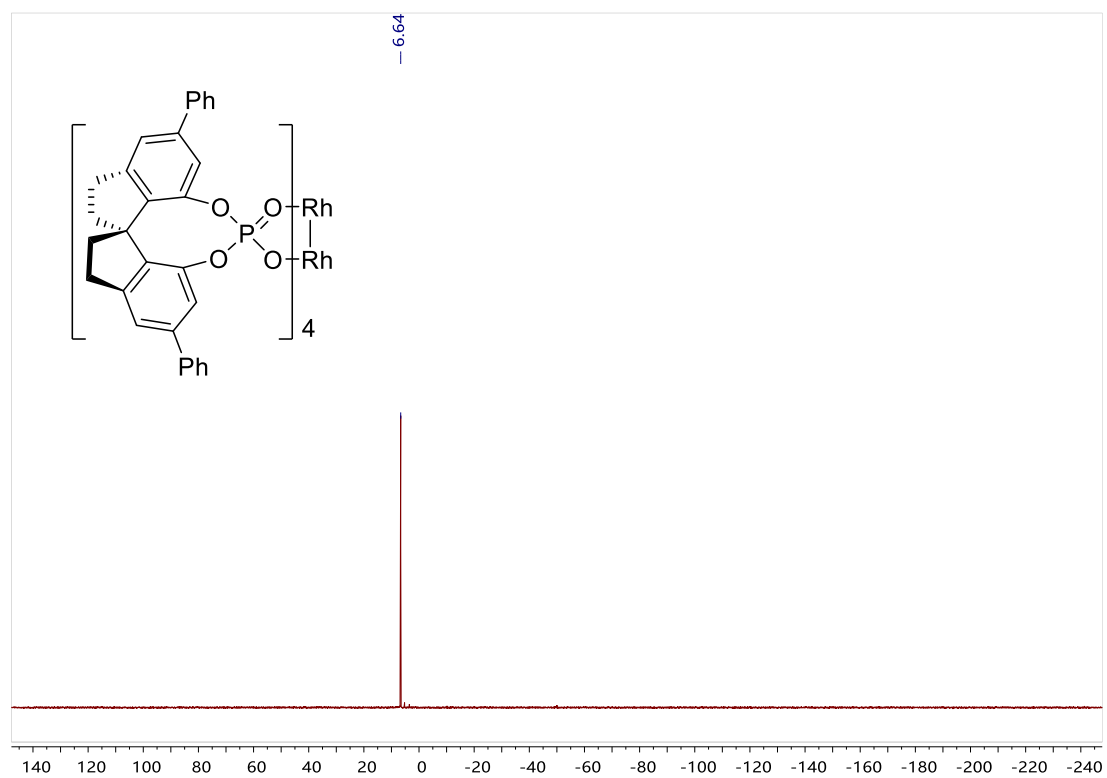




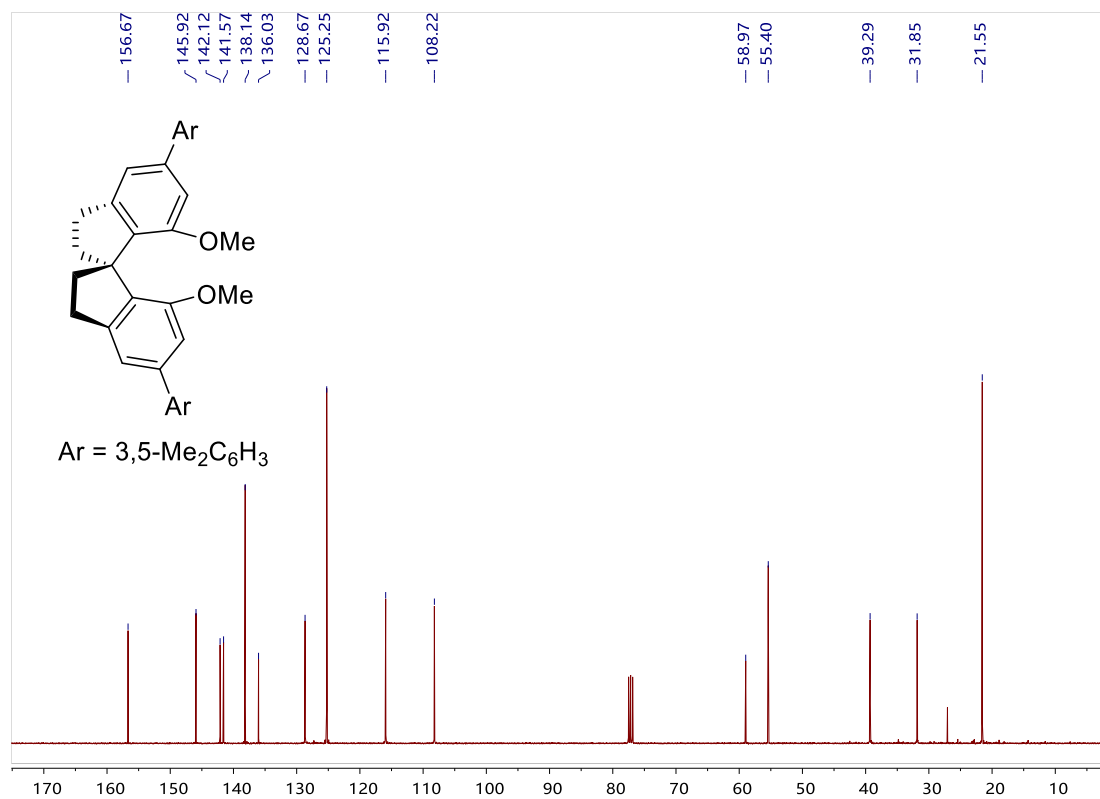
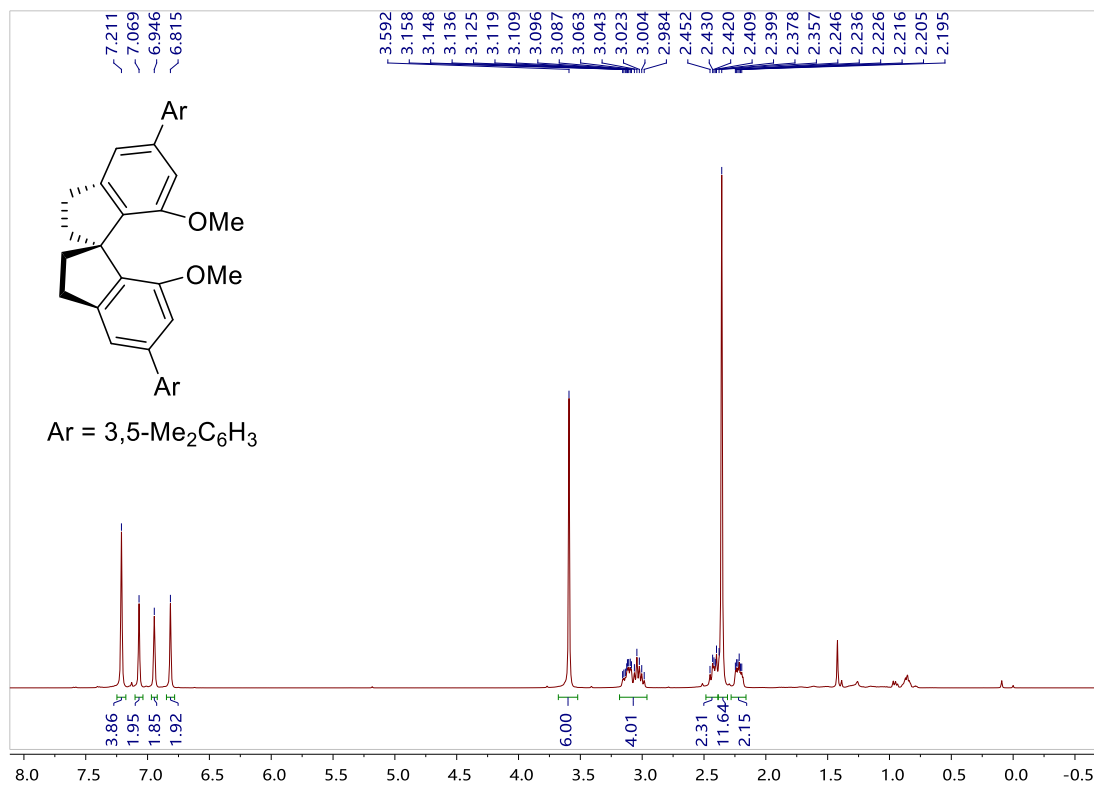


**Tetrakis[(*S*)-5,5'-diphenyl-1,1'-spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II)  
(C2)**

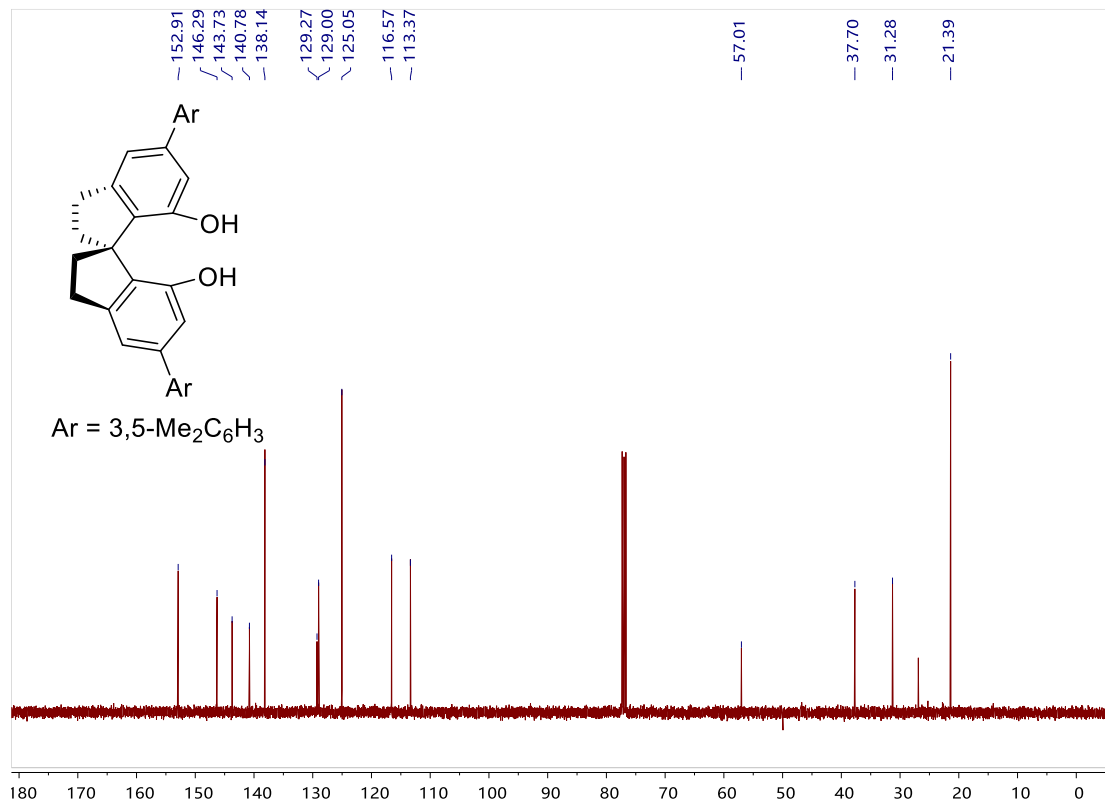
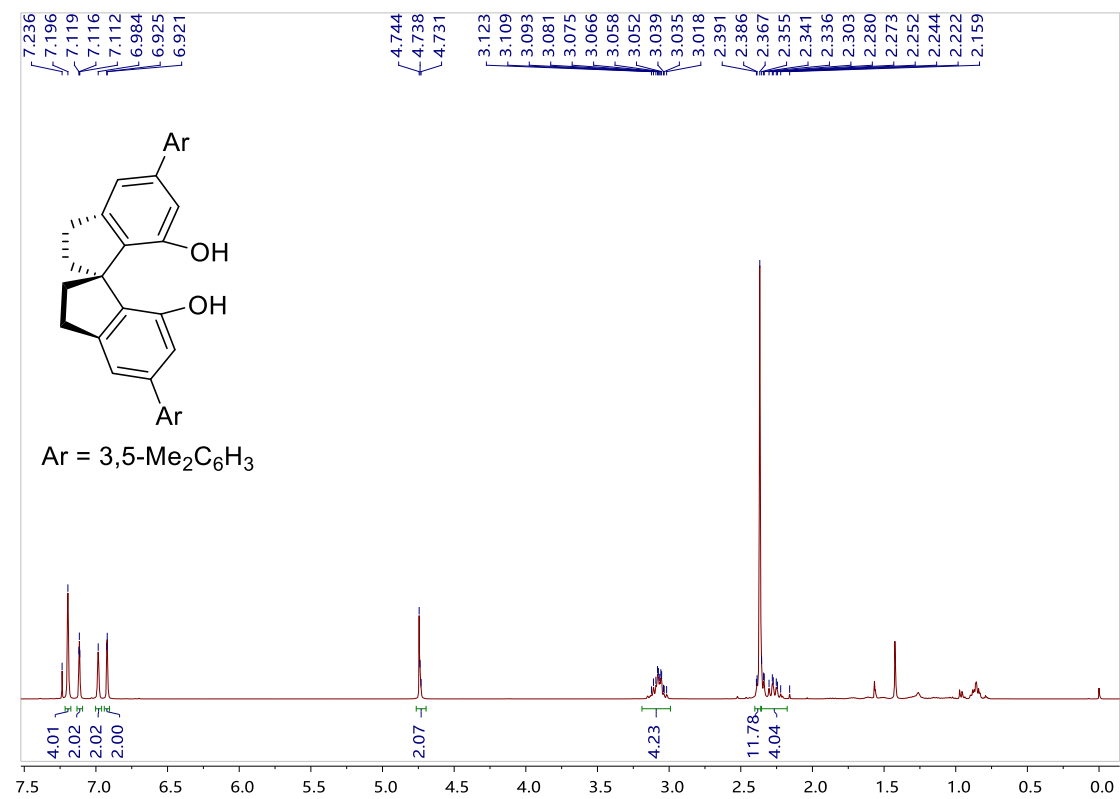




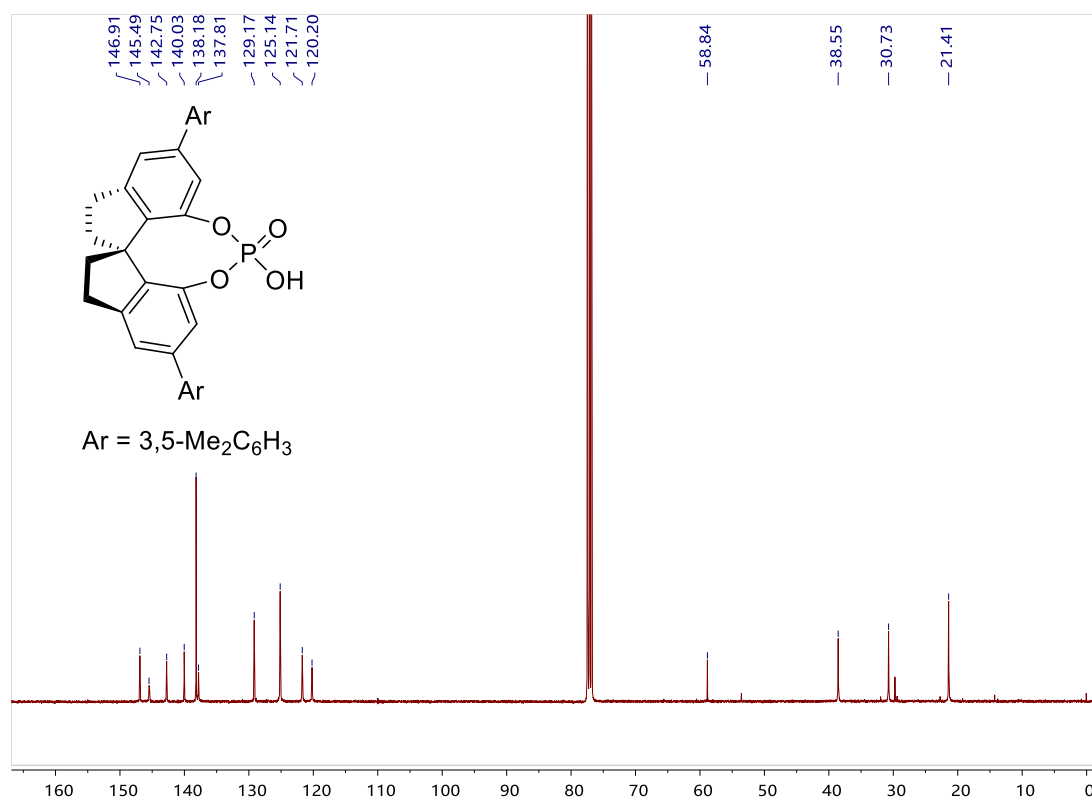
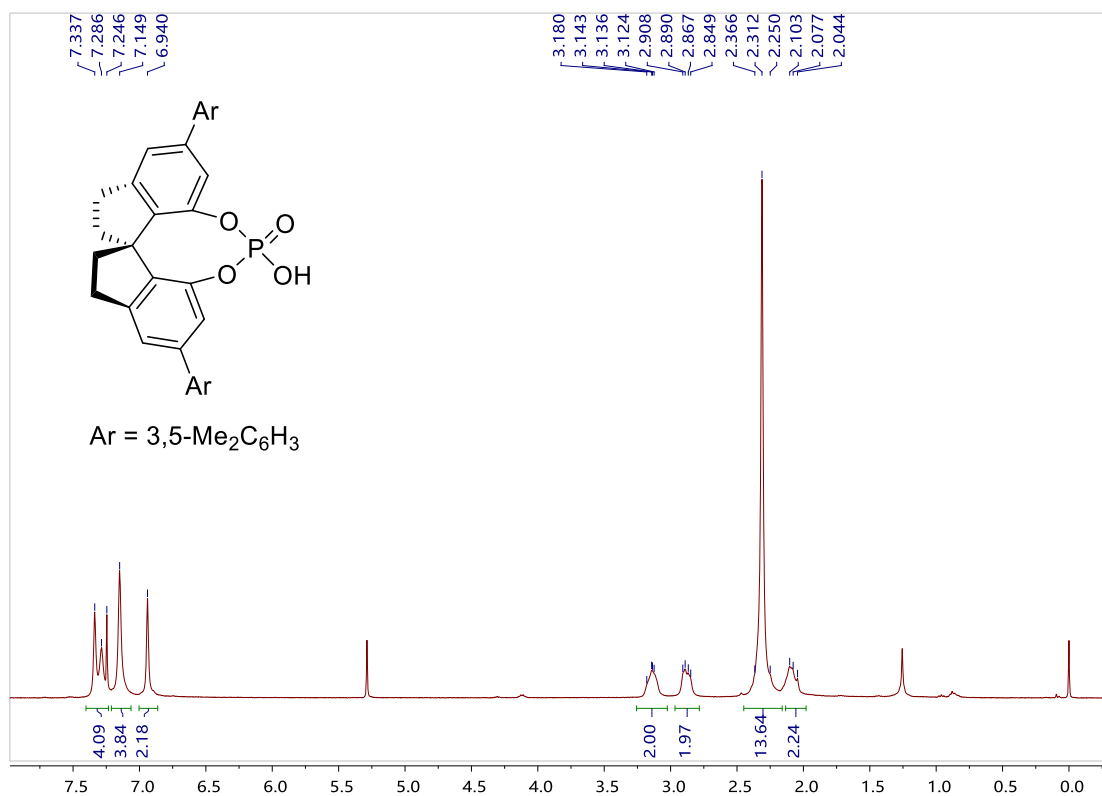
**(S)-5,5'-bis(3,5-dimethylphenyl)-7,7'-dimethoxy-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] (SI-7)**

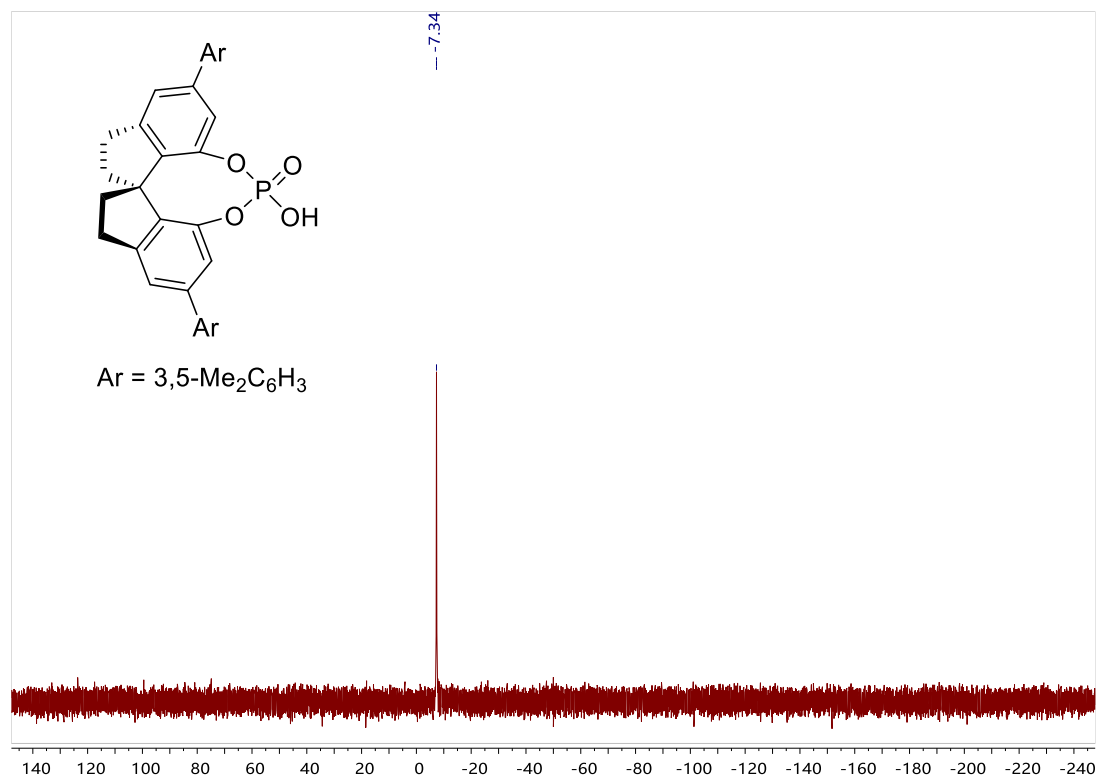


**(S)-5,5'-bis(3,5-dimethylphenyl)-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diol (SI-8)**

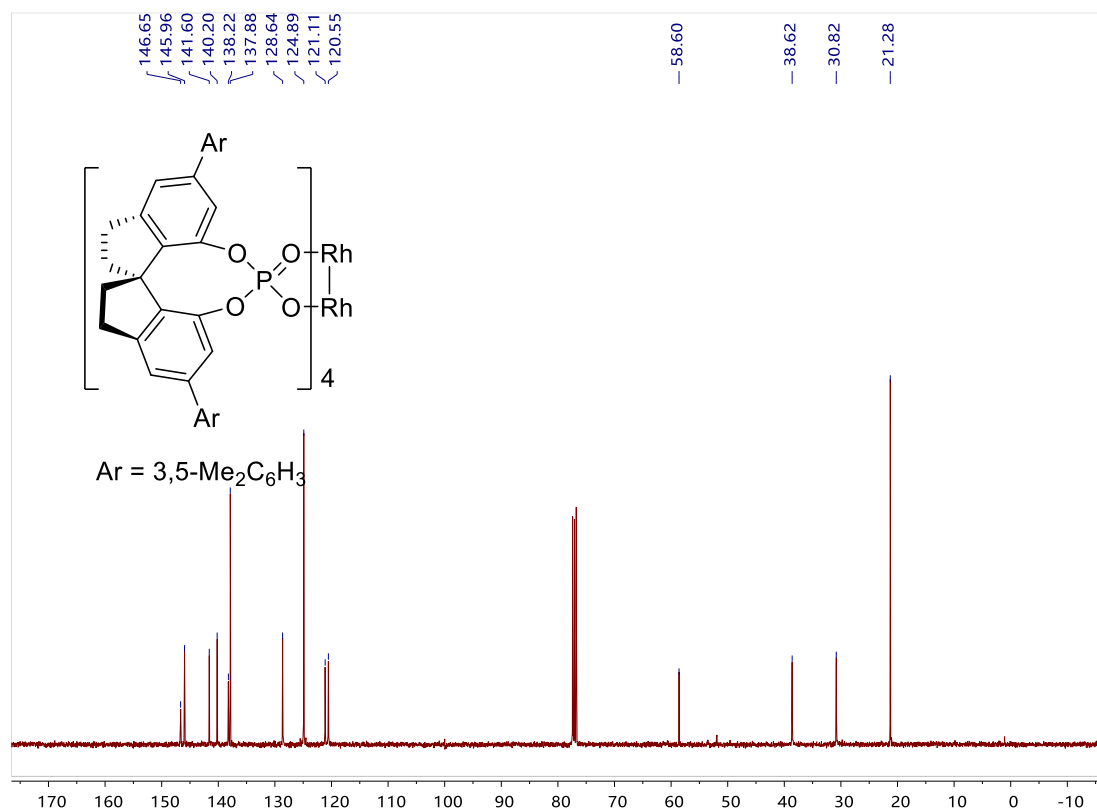
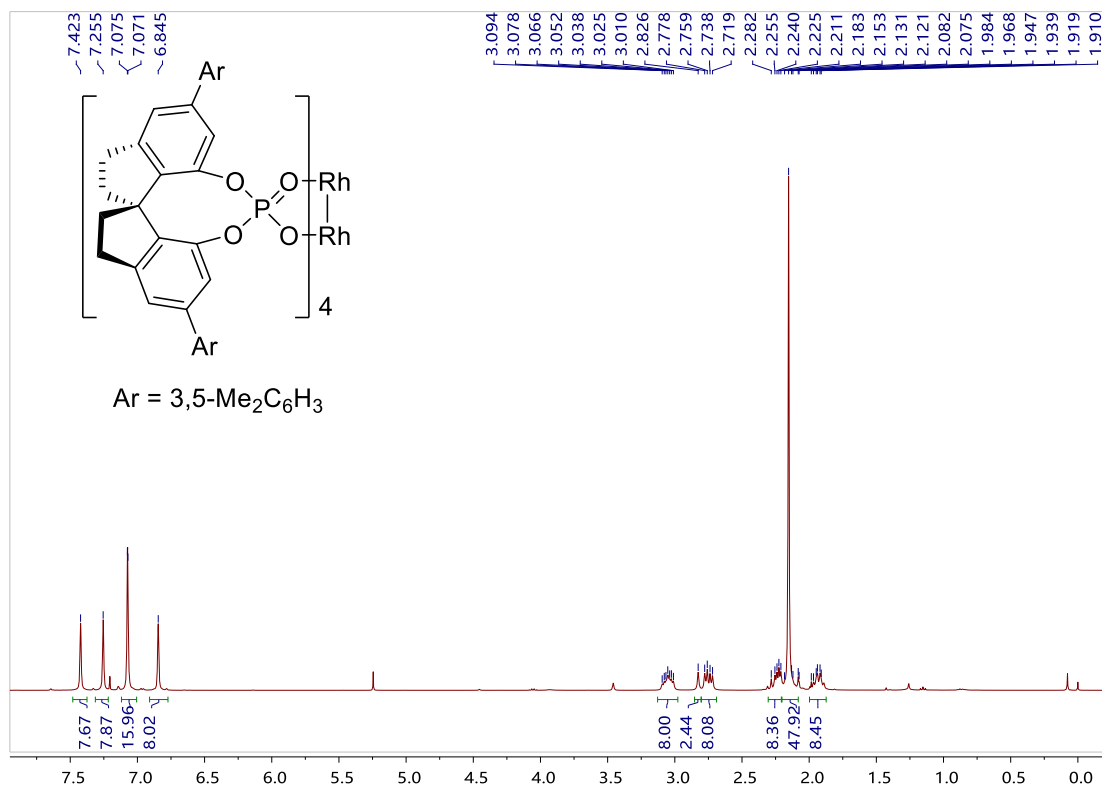


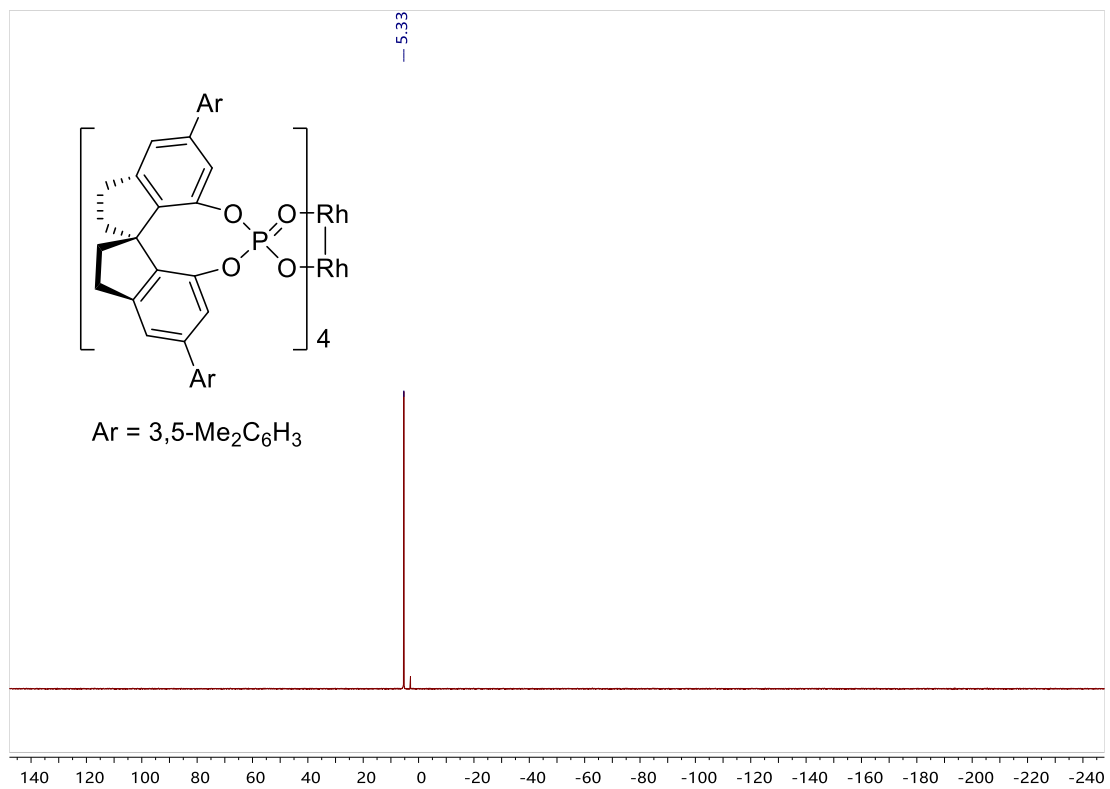
**(S)-5,5'-bis(3,5-dimethylphenyl)-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (SI-9)**





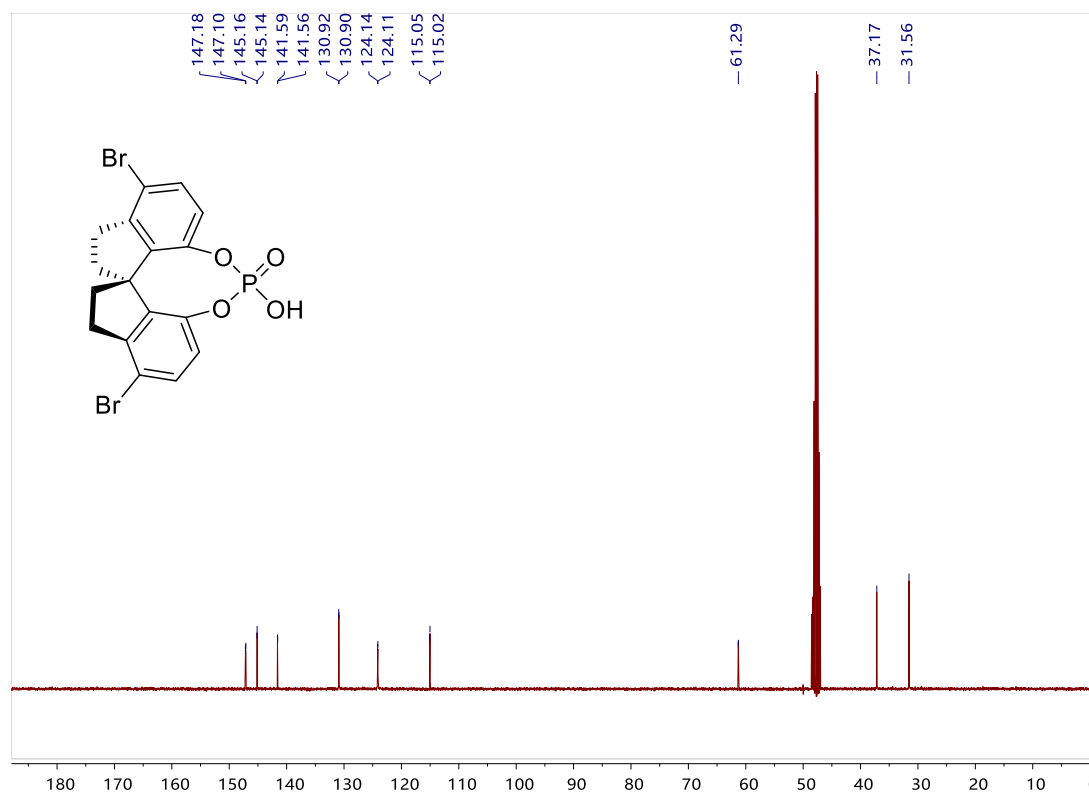
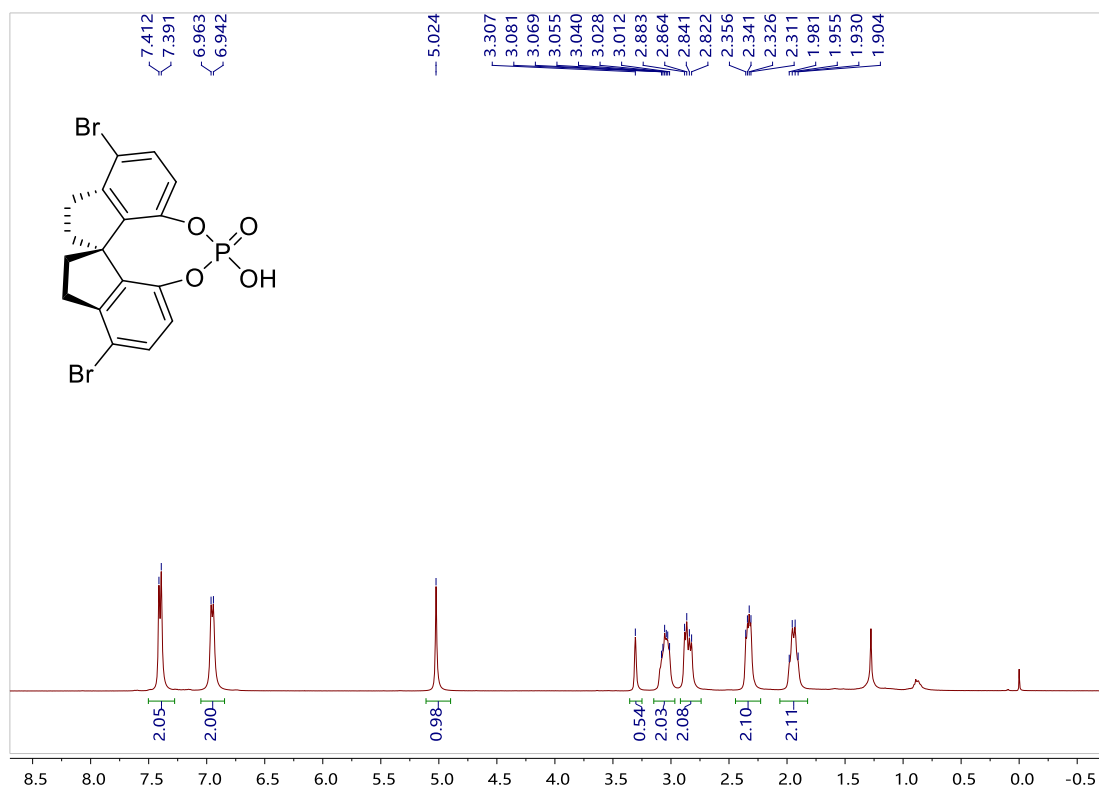
**Tetrakis[(*S*)-5,5'-bis(3,5-dimethylphenyl)-1,1'-spirobiindanyl-7,7'-diyl-phosphate]dirhodium (II) (C3)**

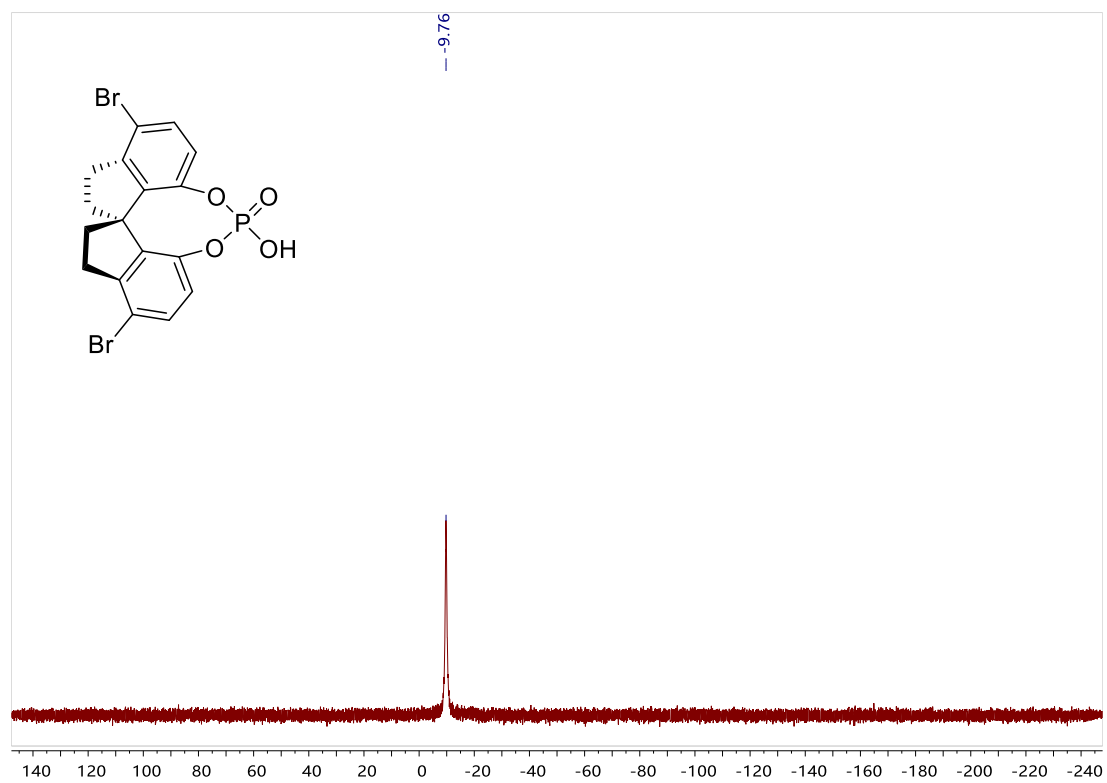




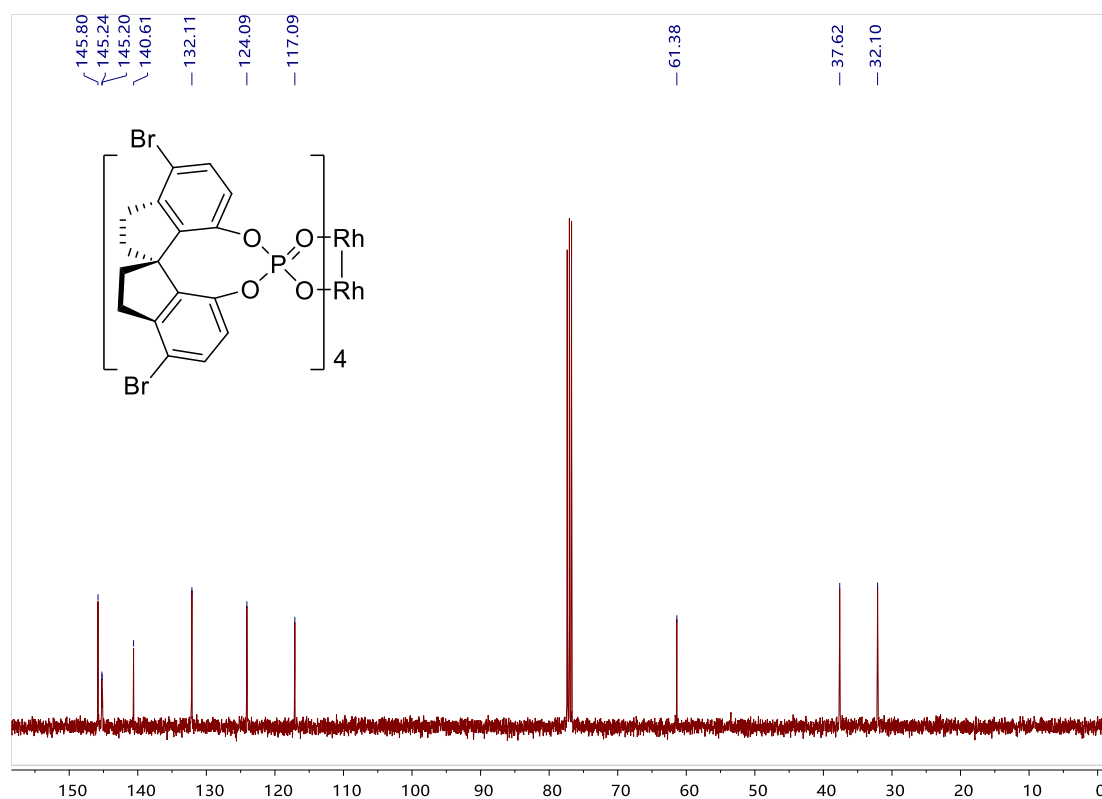
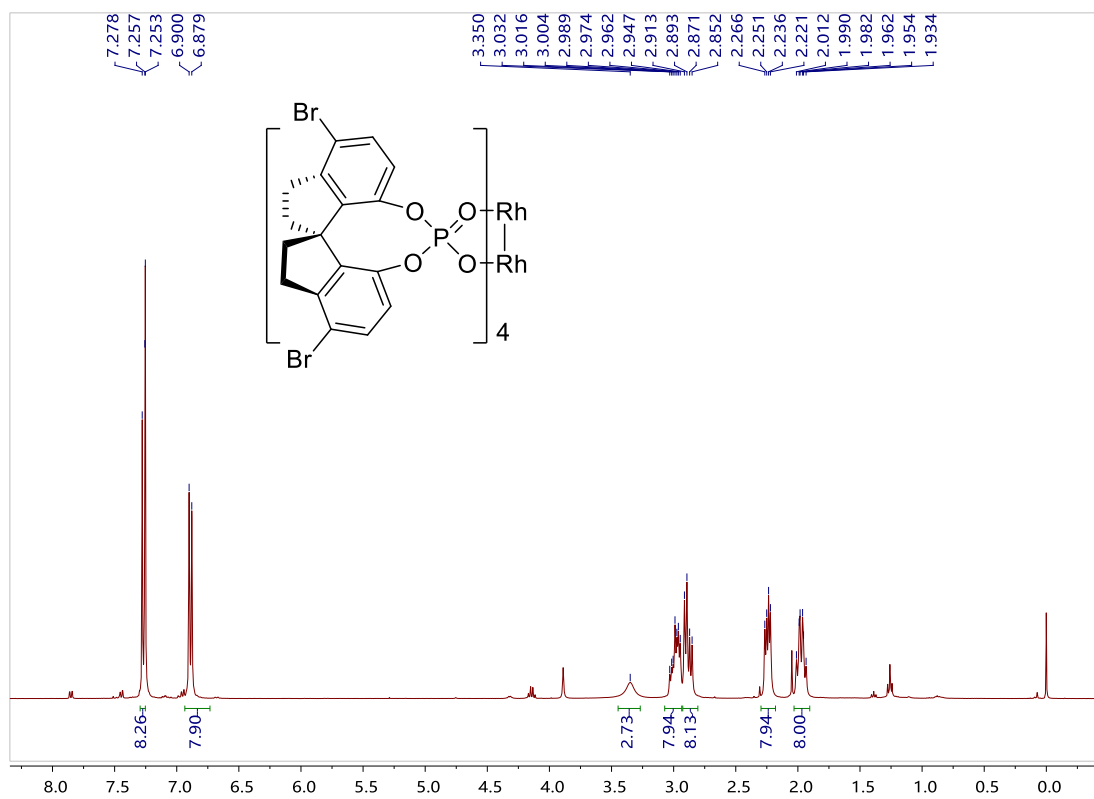


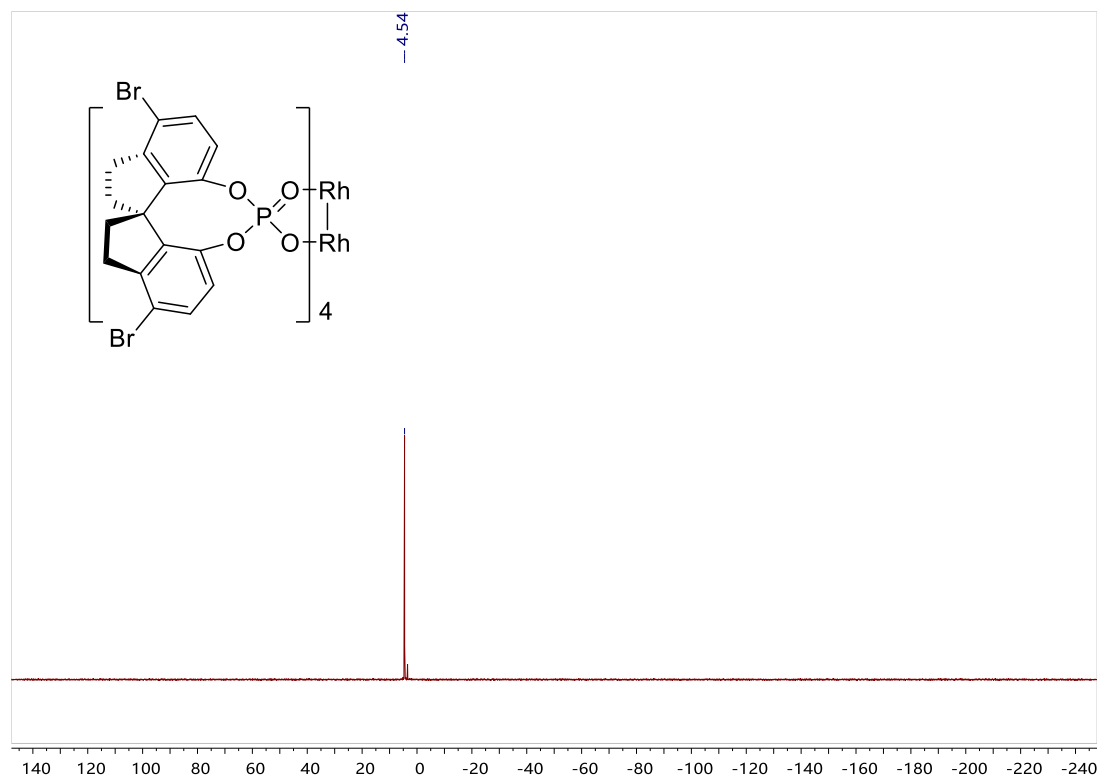
**(S)-4,4'- dibromo-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (SI-12)**



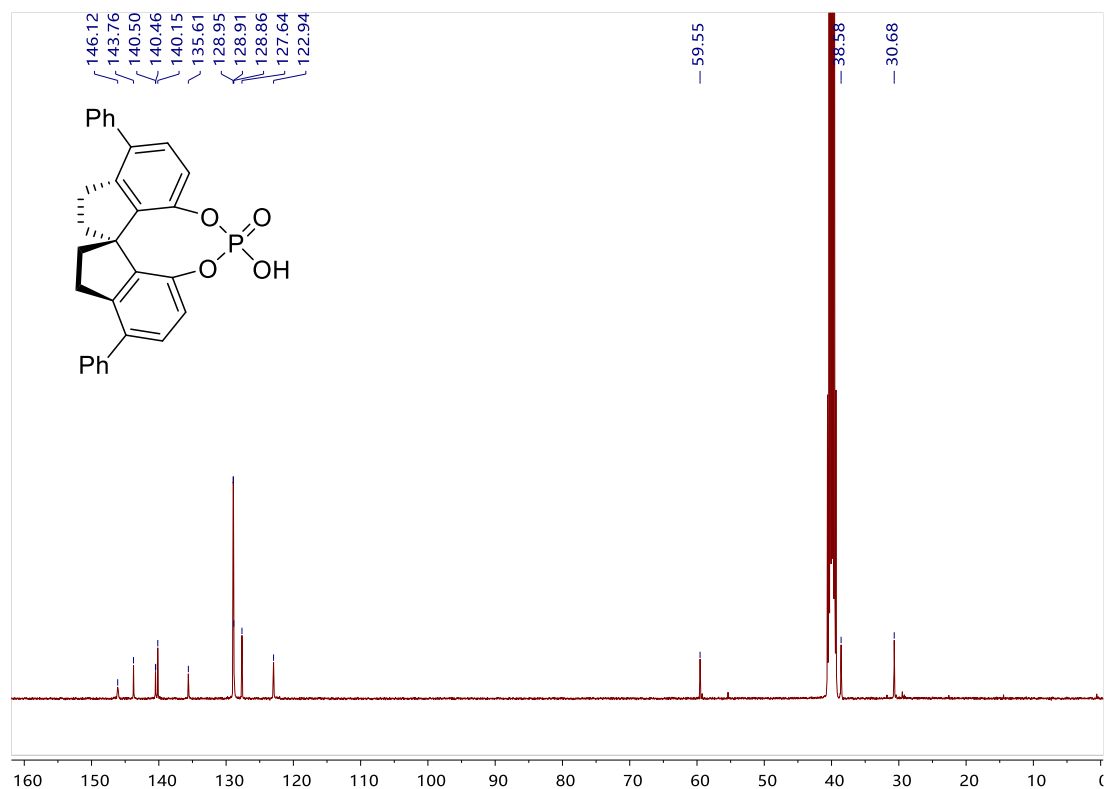
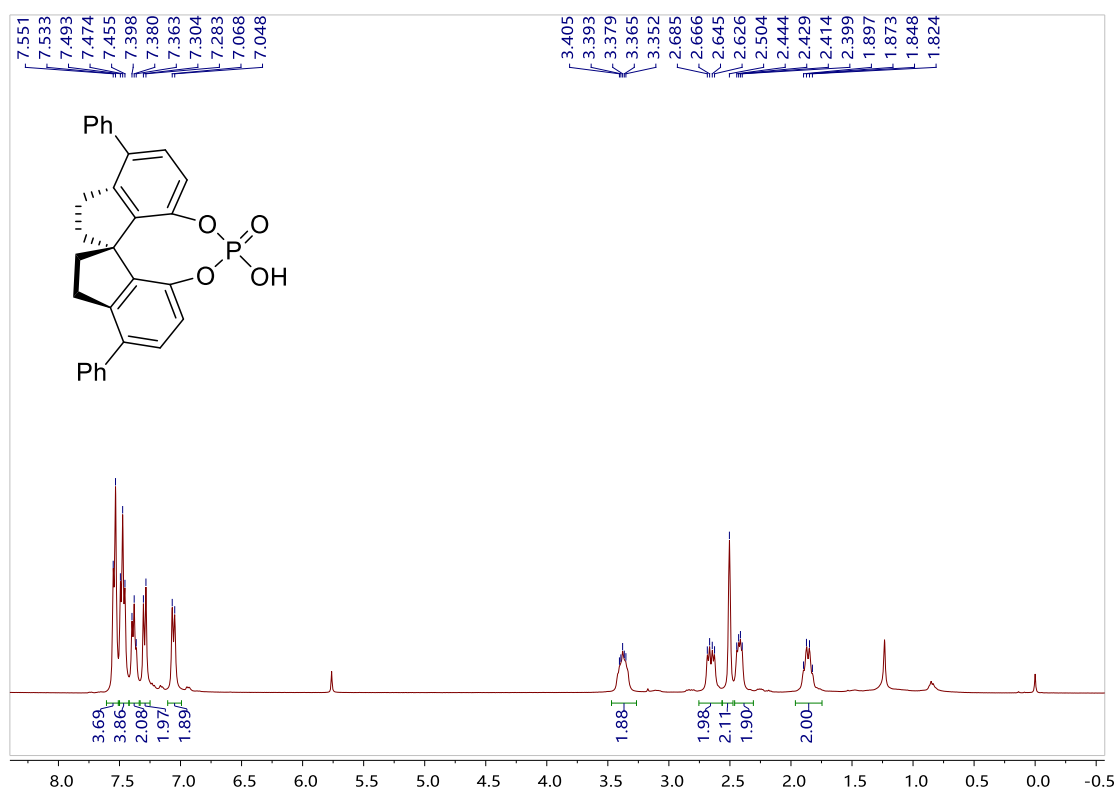


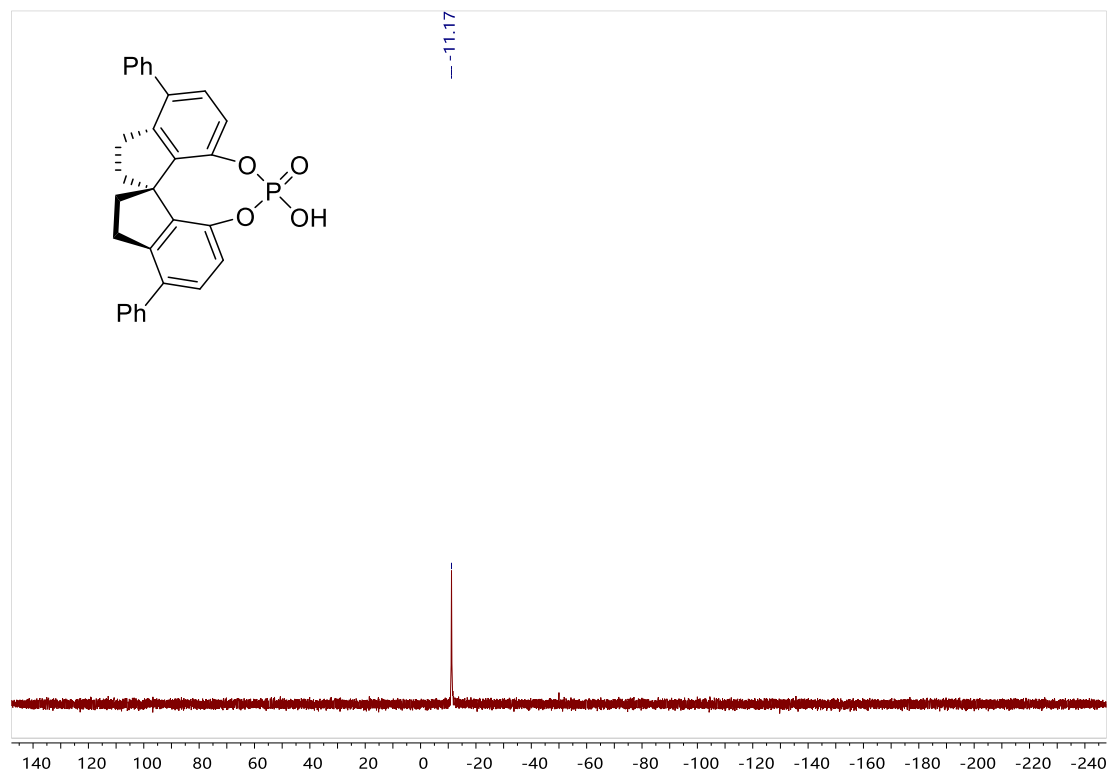
**Tetrakis[(S)-4,4'-dibromo-1,1'-spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II)  
(C4)**



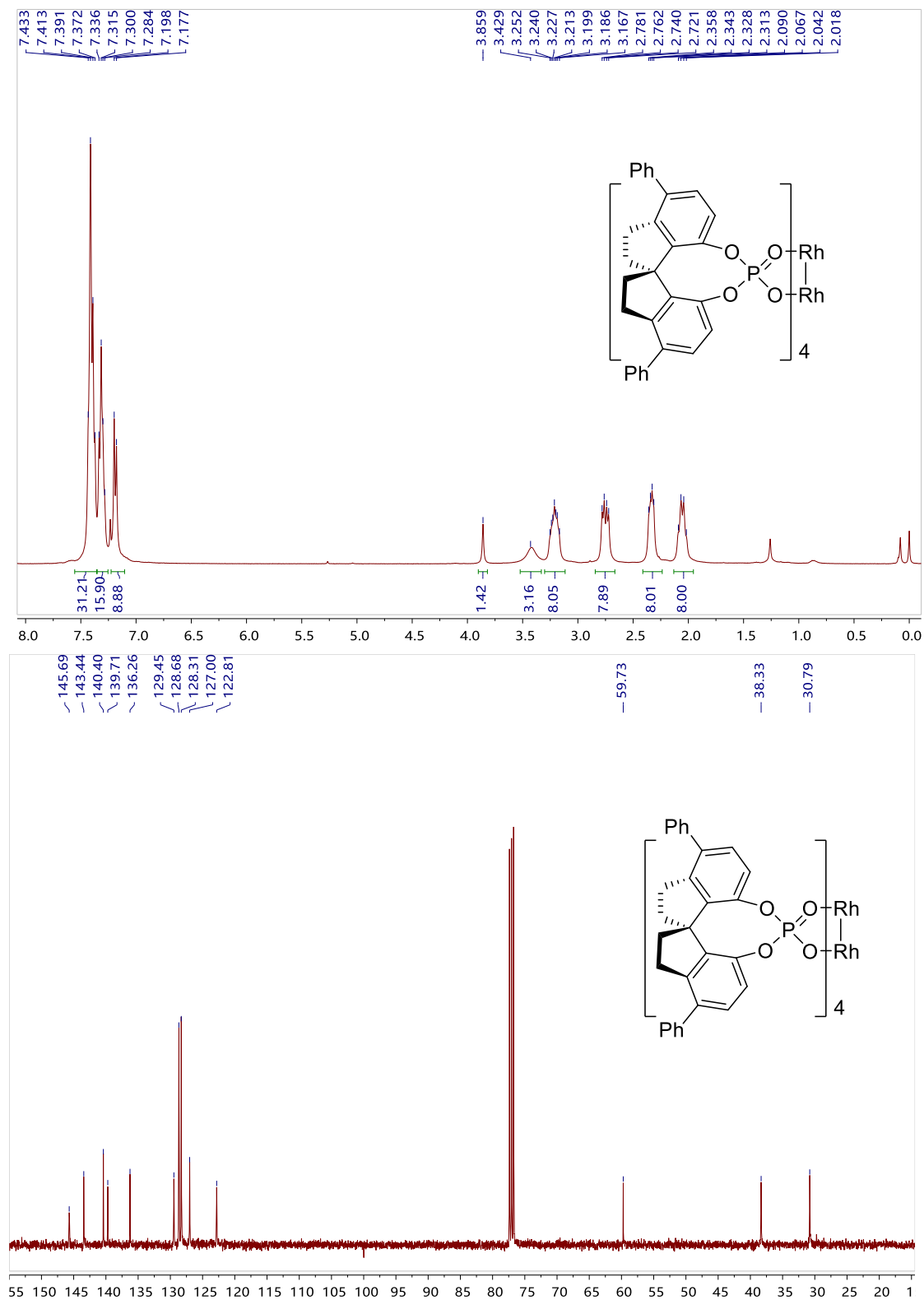


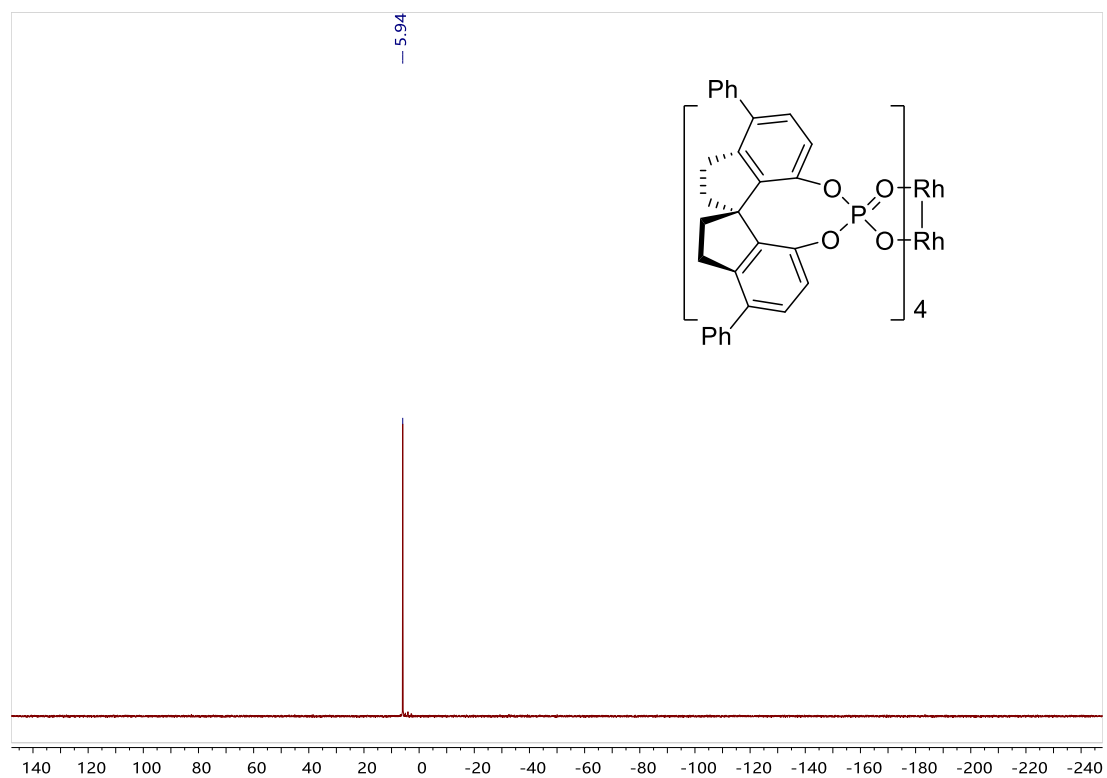
**(S)-4,4'- diphenyl-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate (SI-13)**





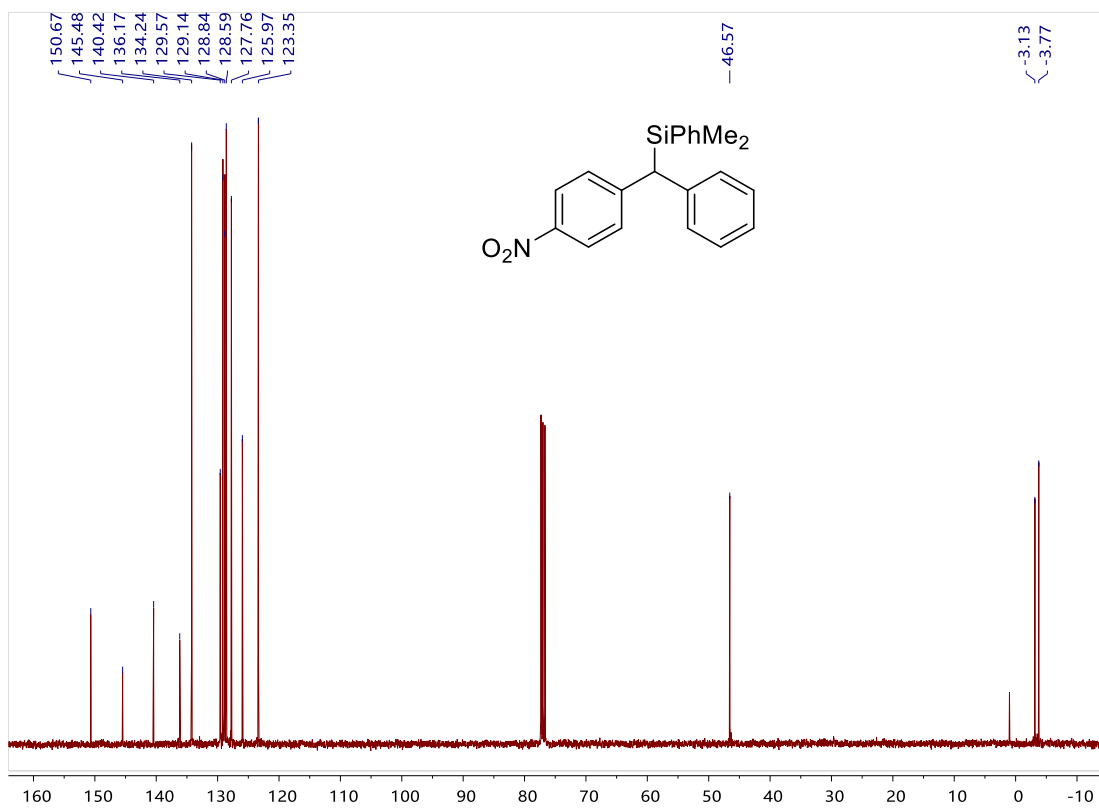
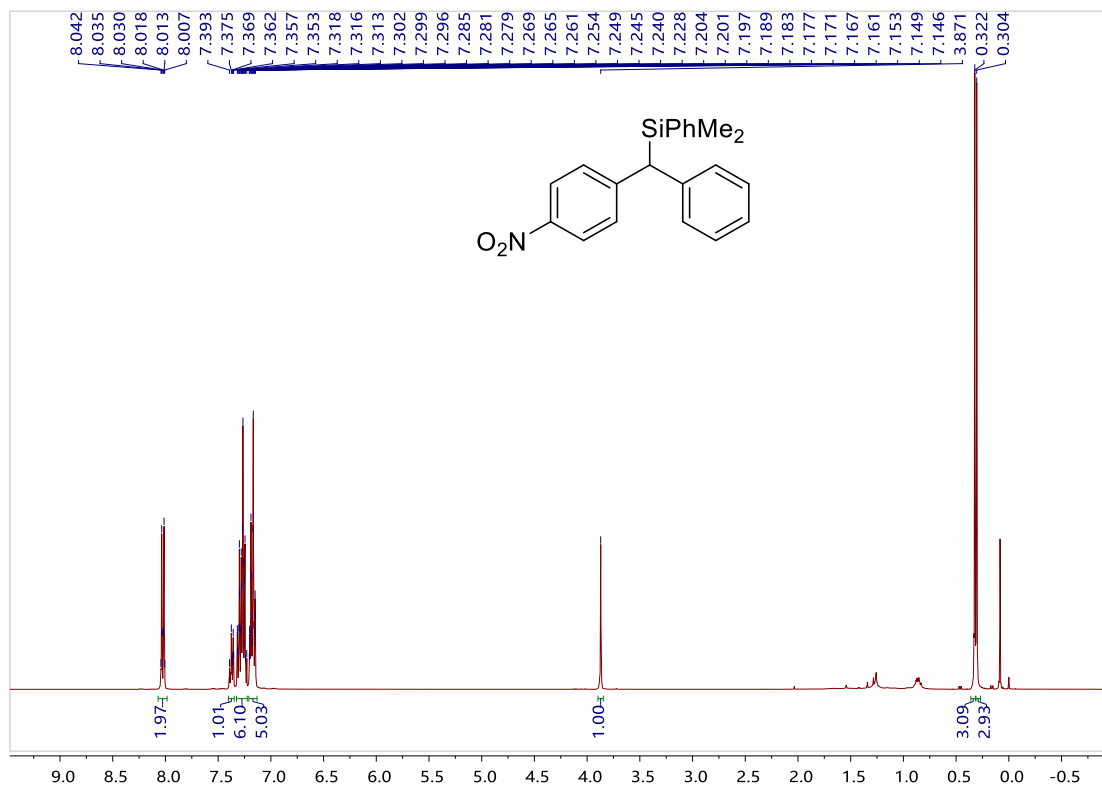
**Tetrakis[(S)-4,4'-diphenyl-1,1'-spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II)**  
**(C5)**



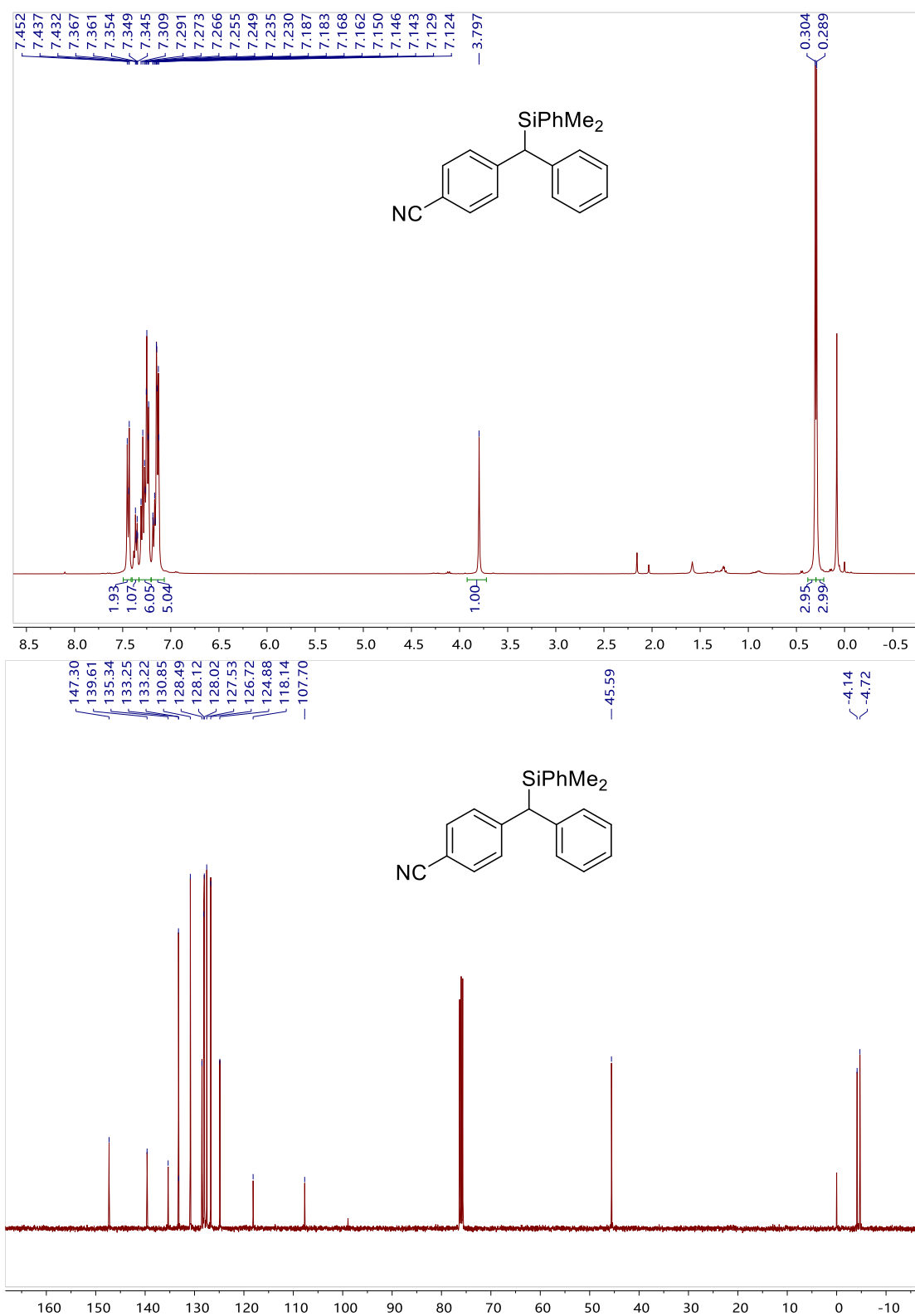




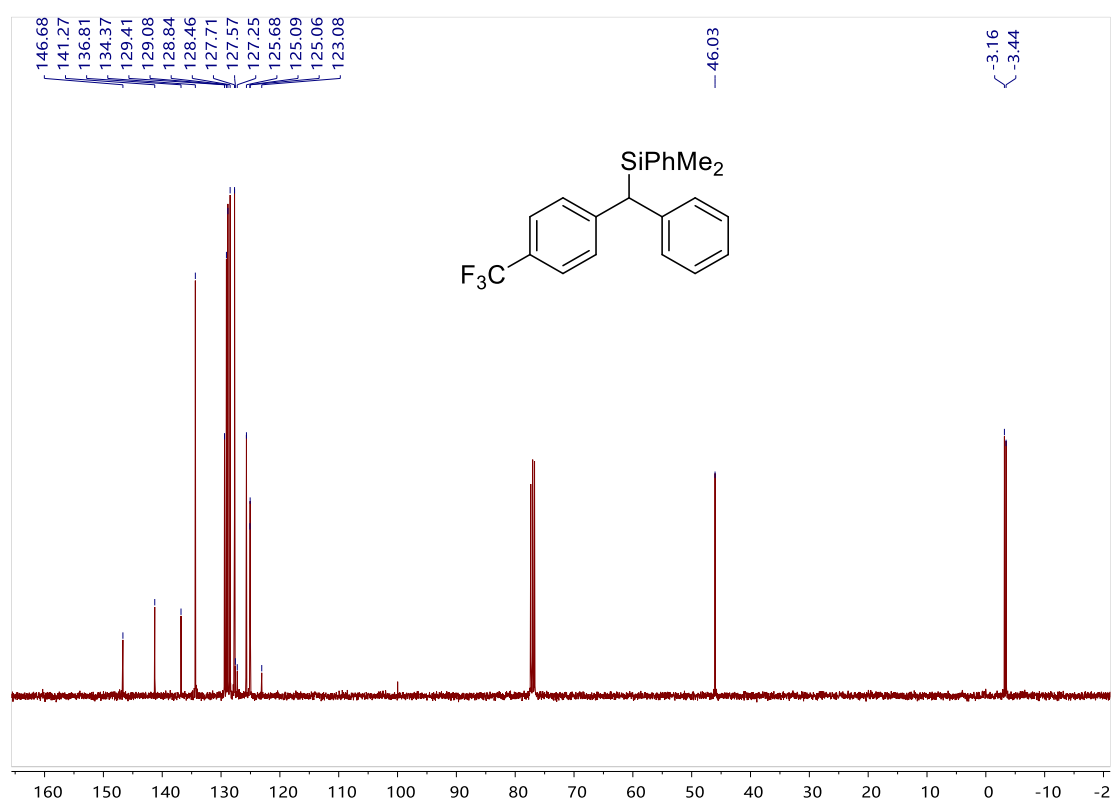
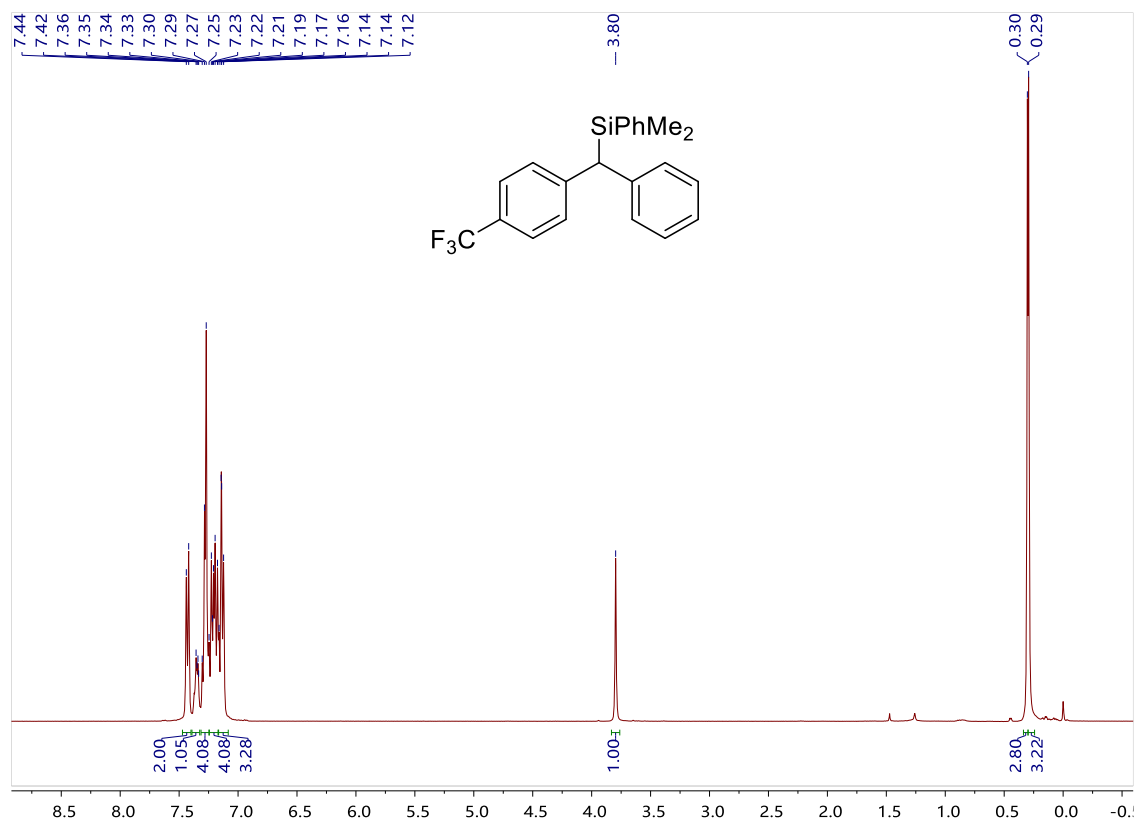
**(-)-dimethyl((4-nitrophenyl)(phenyl)methyl)(phenyl)silane (P1)**



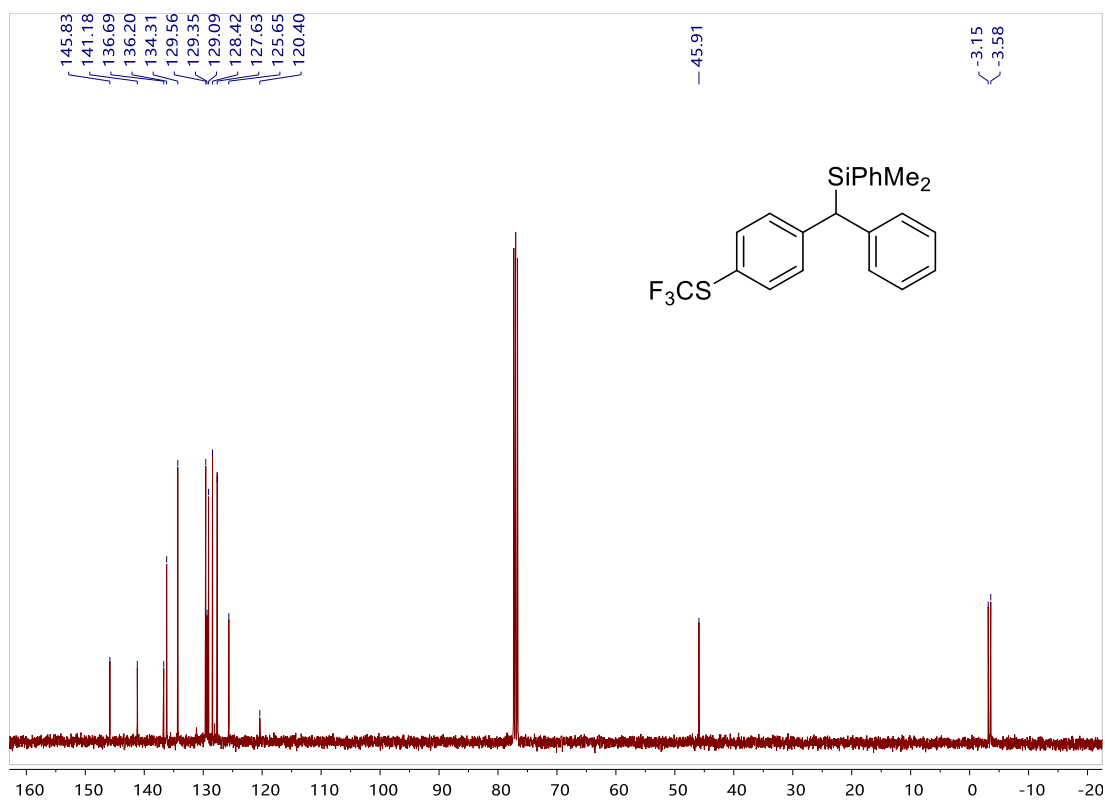
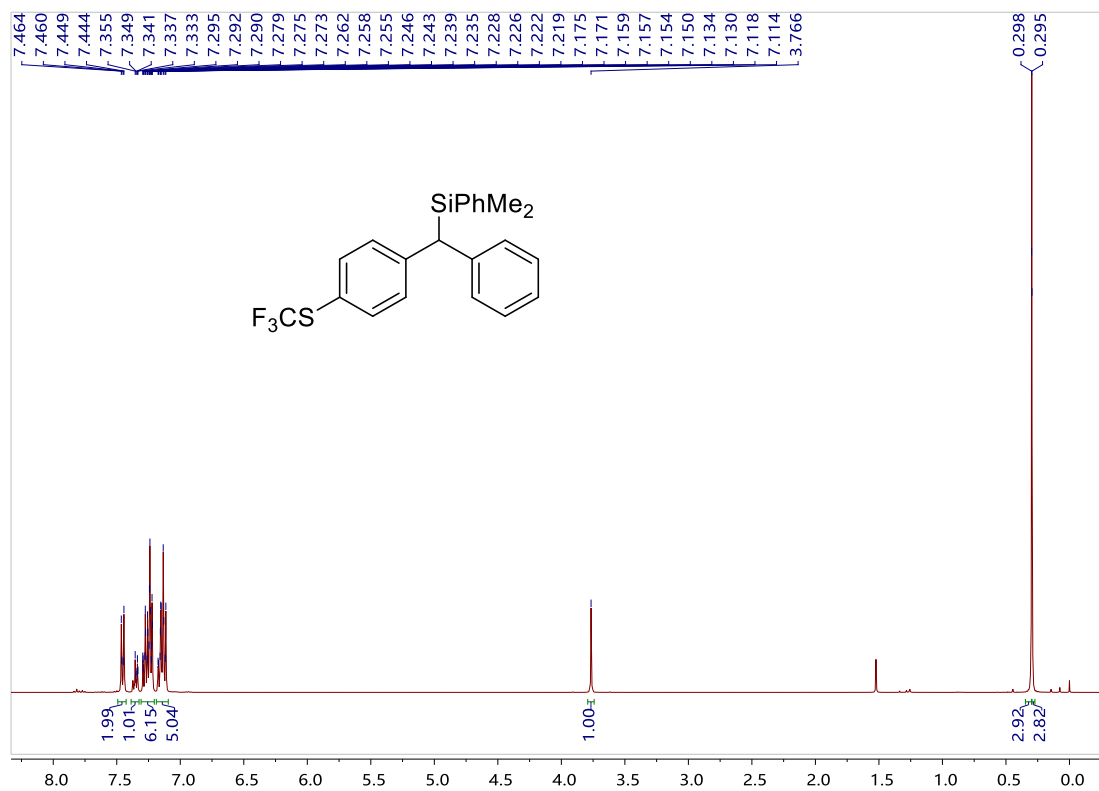
**(-)-4-((dimethyl(phenyl)silyl)(phenyl)methyl)benzonitrile (P2)**



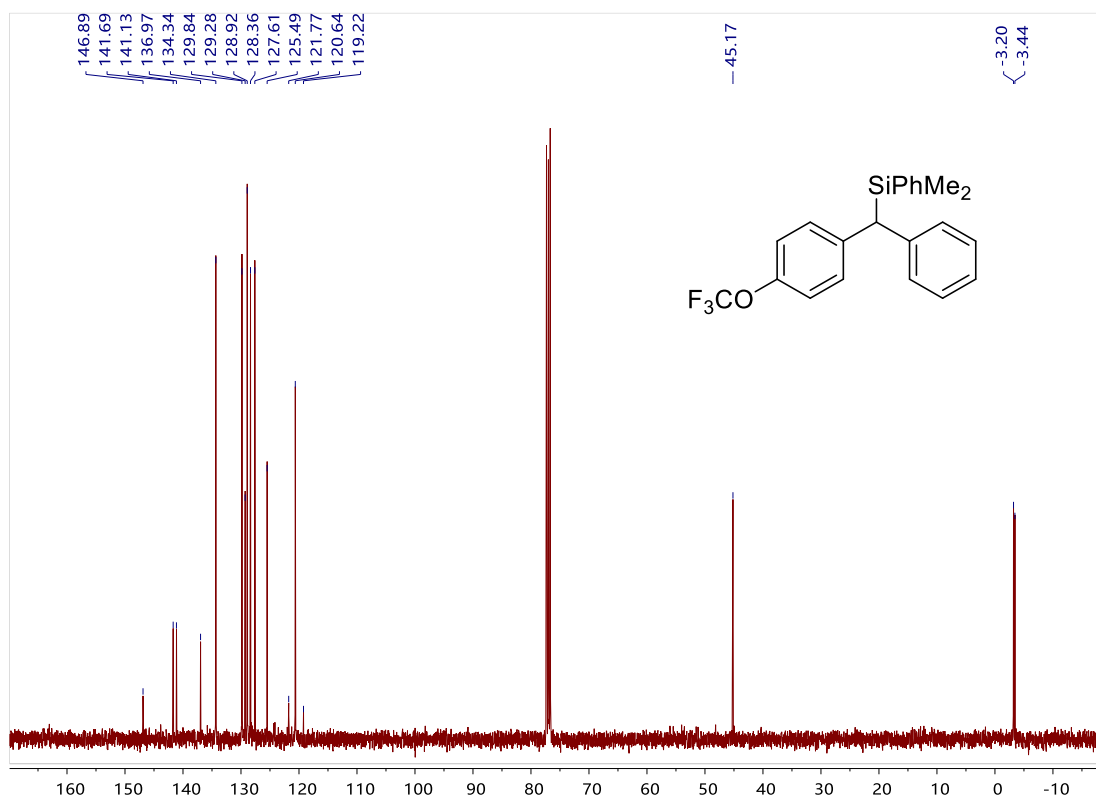
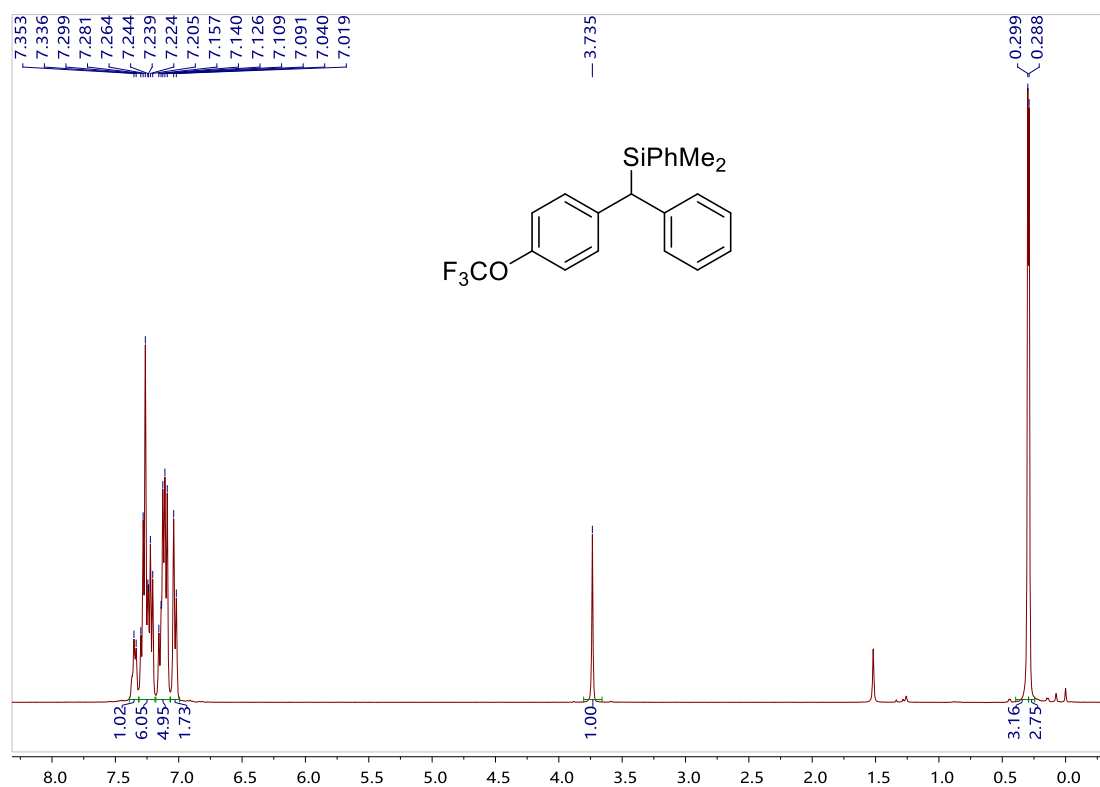
**(S)-dimethyl(phenyl)(phenyl(4-(trifluoromethyl)phenyl)methyl)silane (P3)**



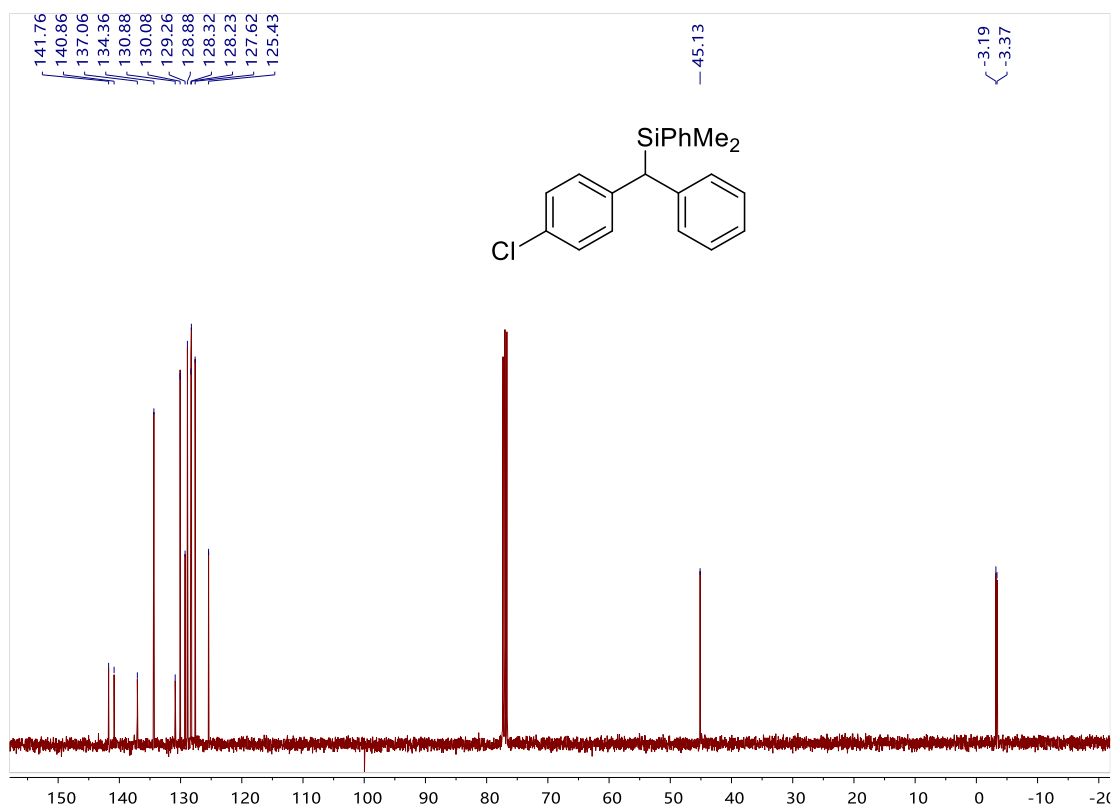
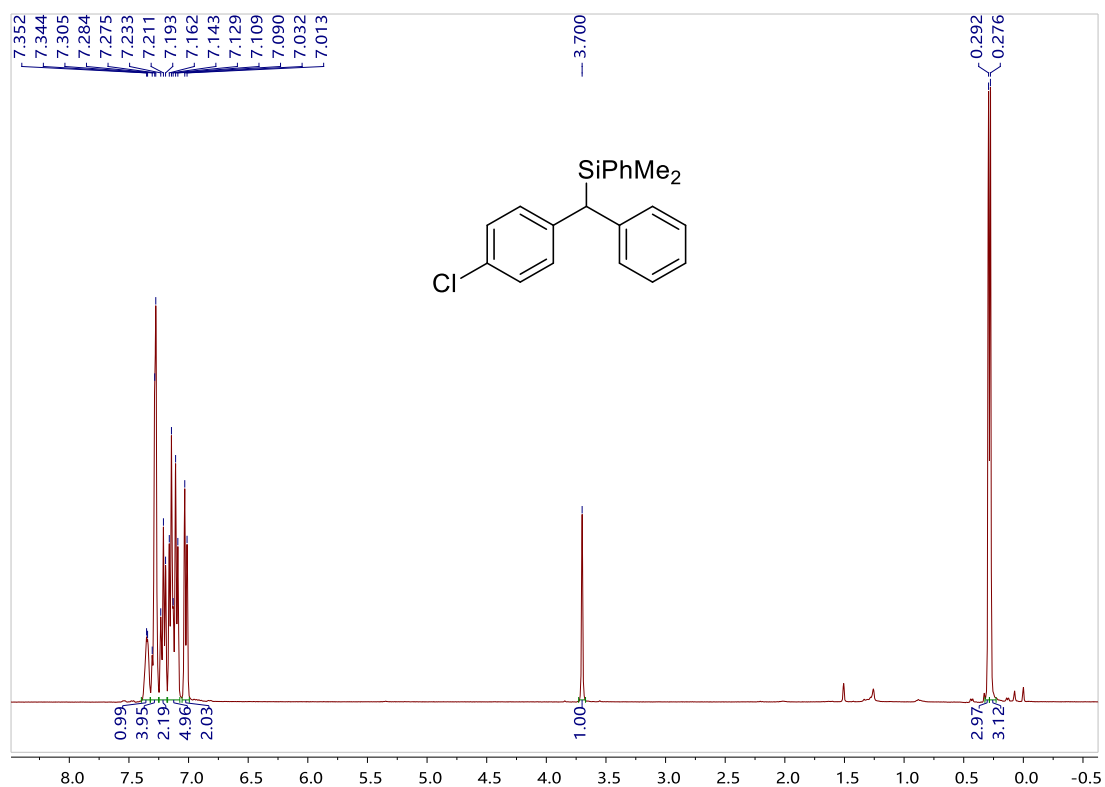
**(-)-dimethyl(phenyl)(phenyl(4-((trifluoromethyl)thio)phenyl)methyl)silane (P4)**



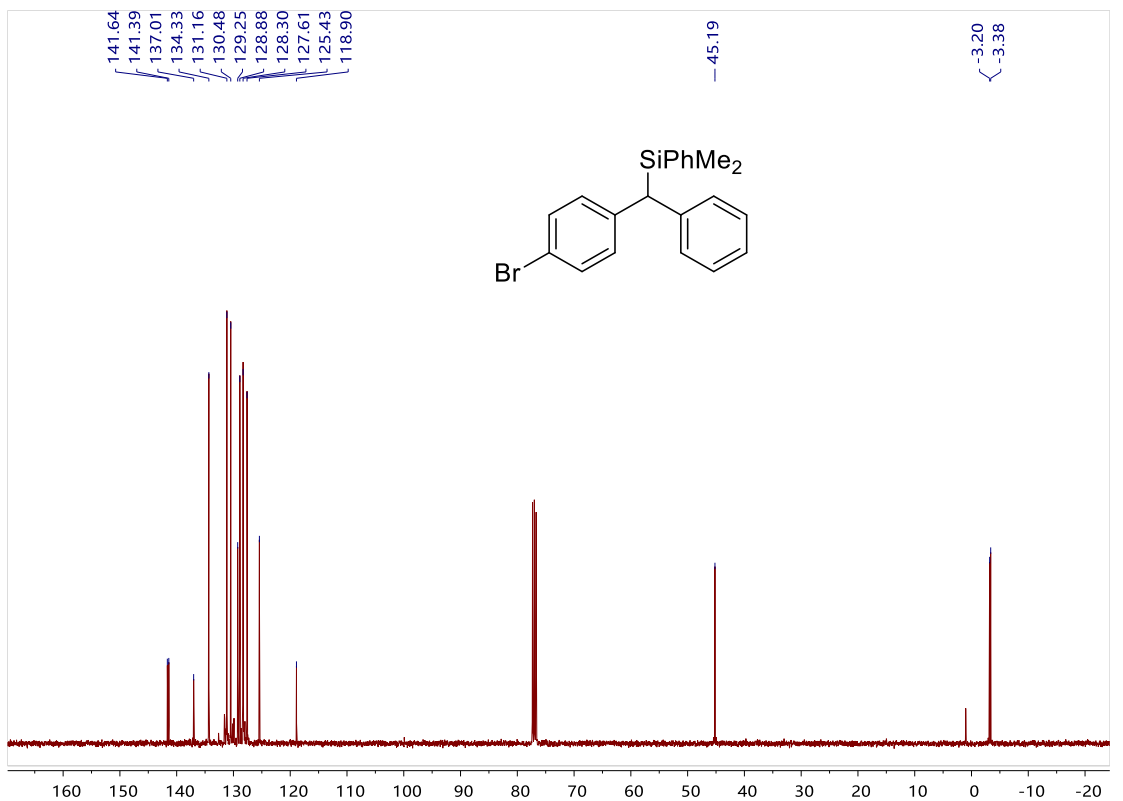
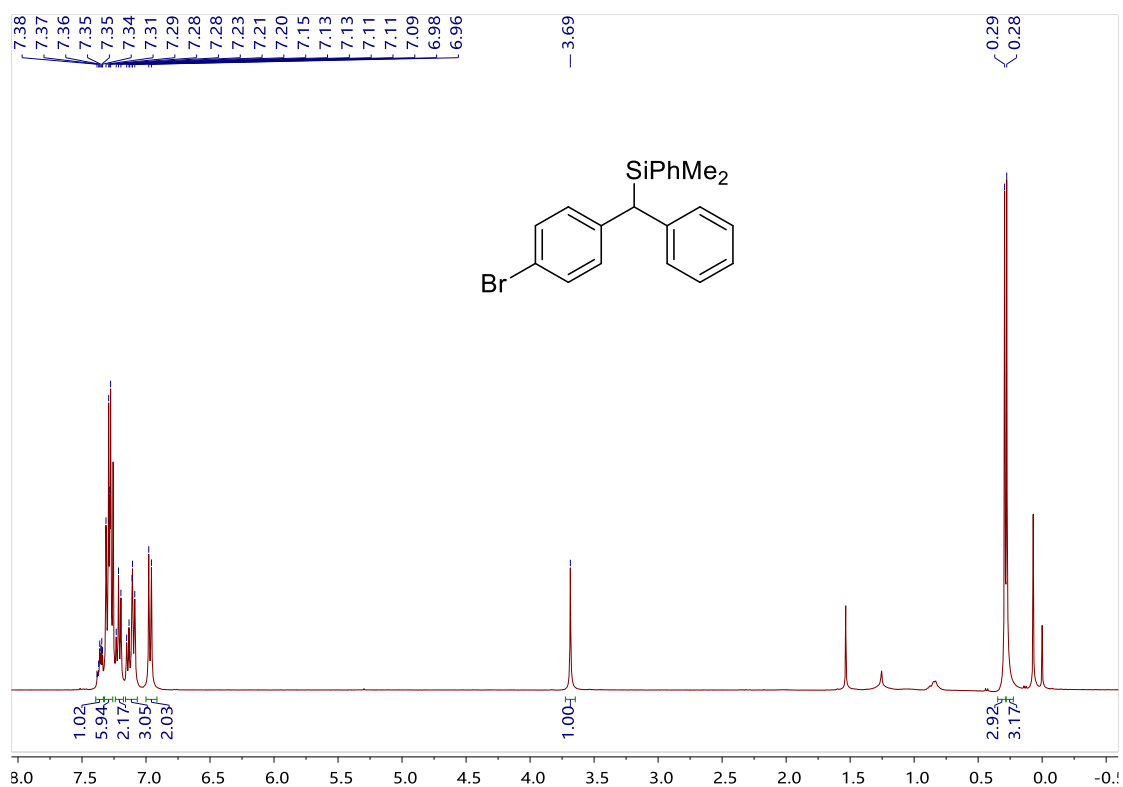
**(-)-dimethyl(phenyl)(phenyl(4-(trifluoromethoxy)phenyl)methyl)silane (P5)**



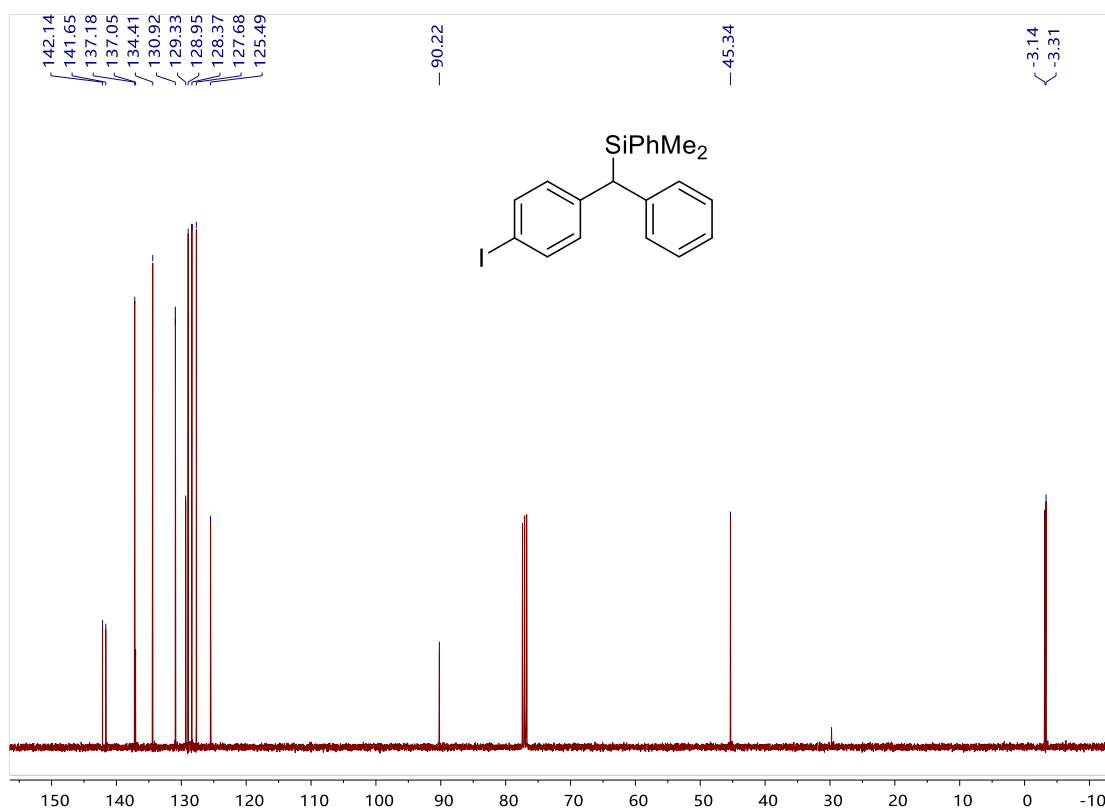
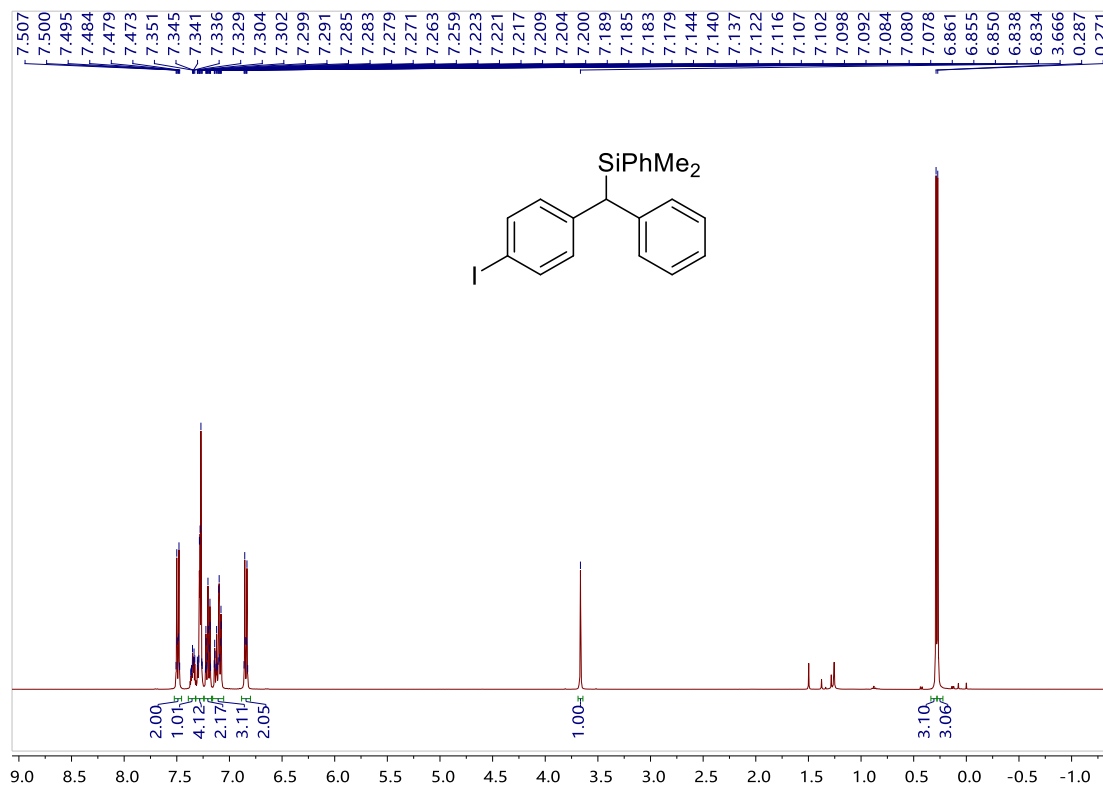
**(+)-((4-chlorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P6)**



**(+)-((4-bromophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P7)**

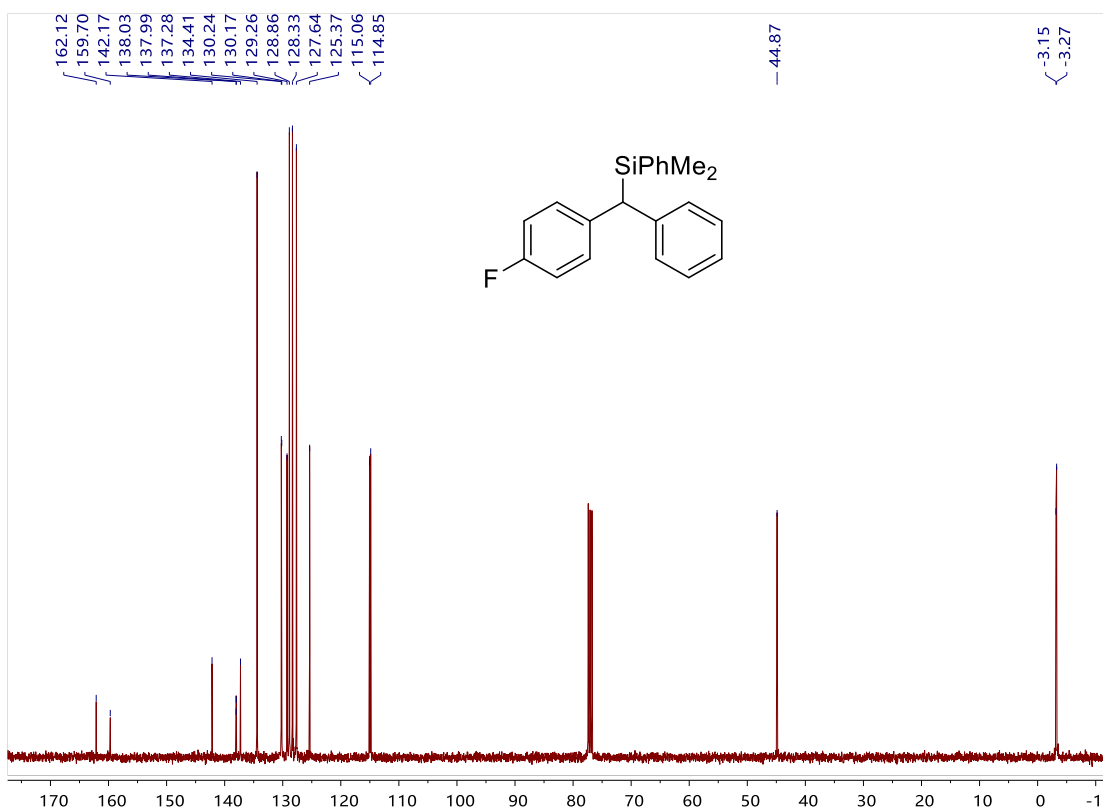
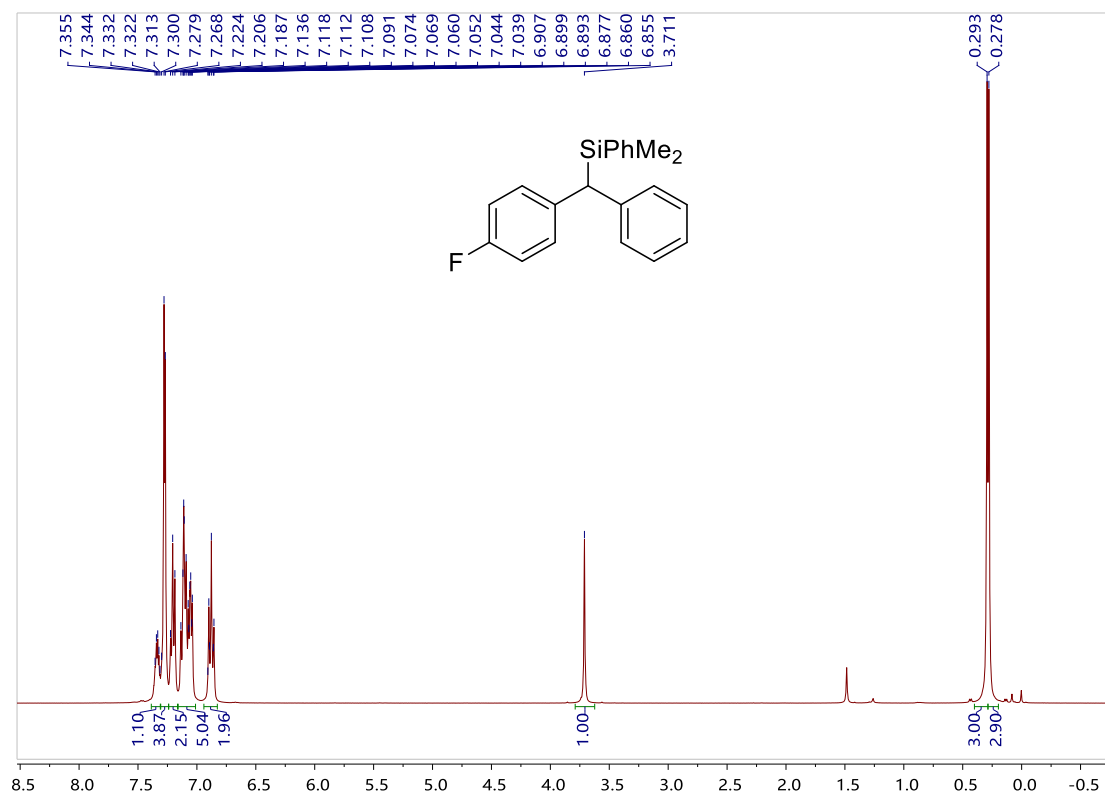


**(+)-((4-iodophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P8)**

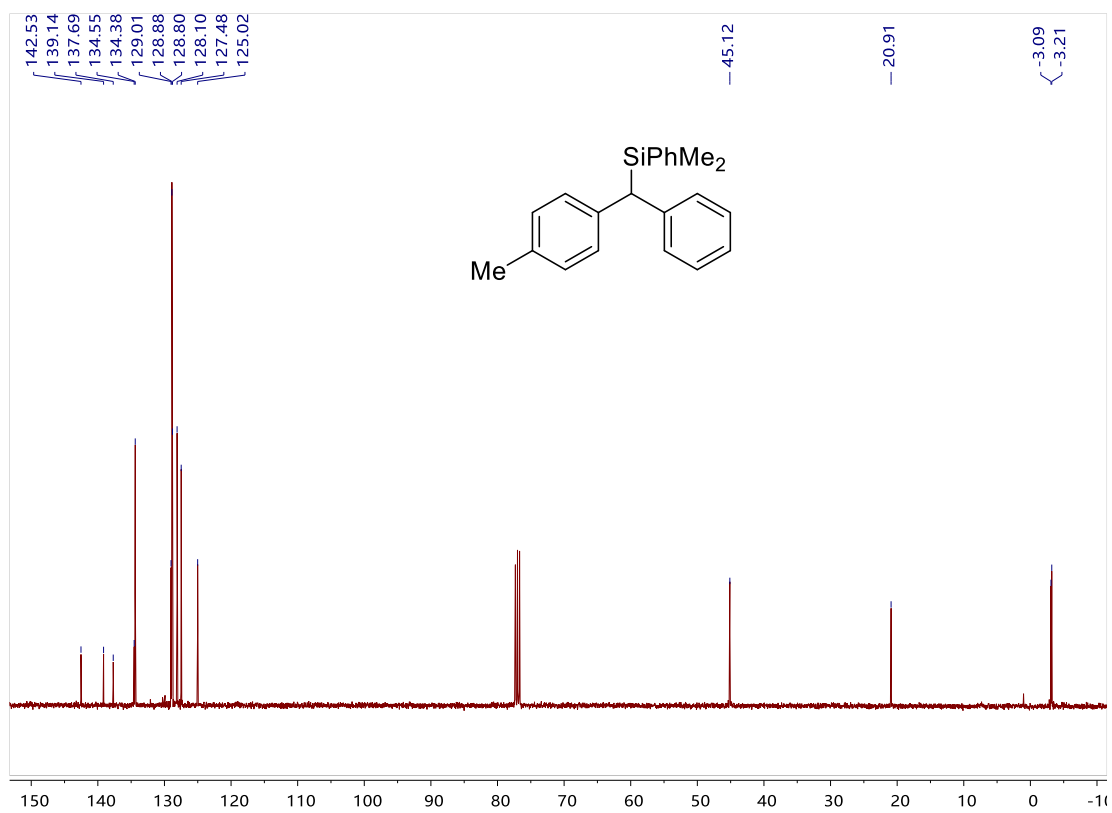
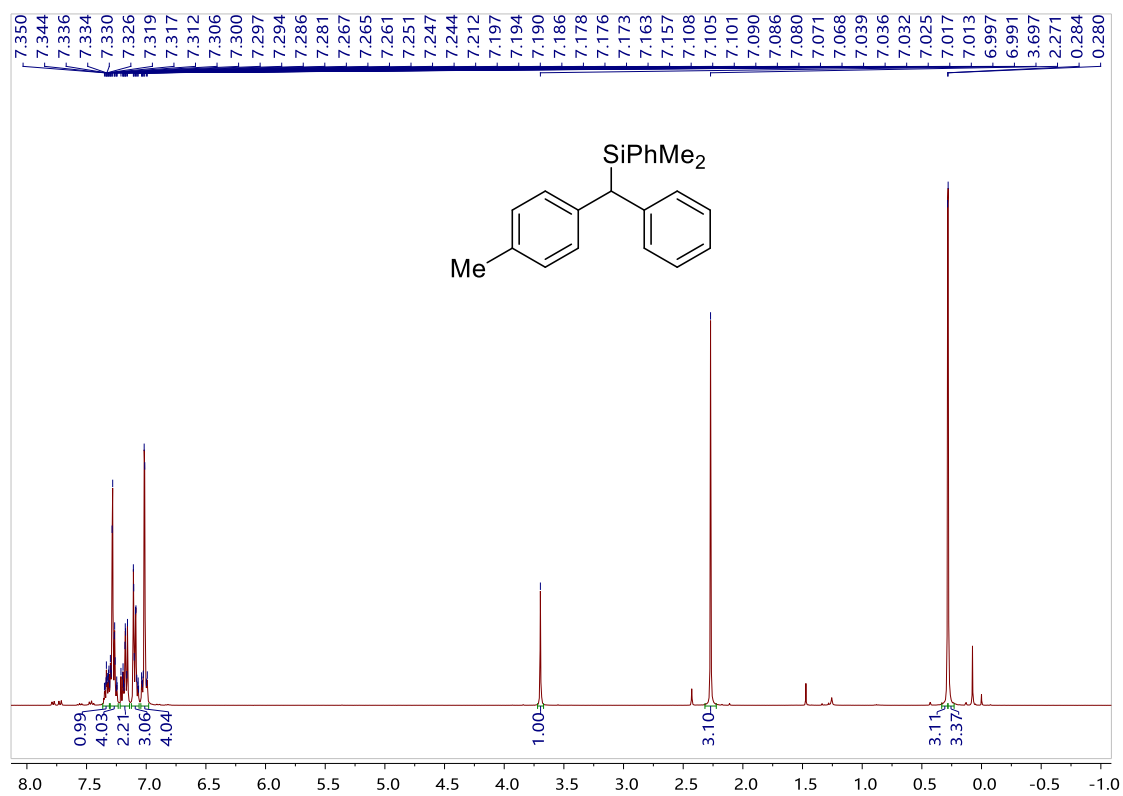




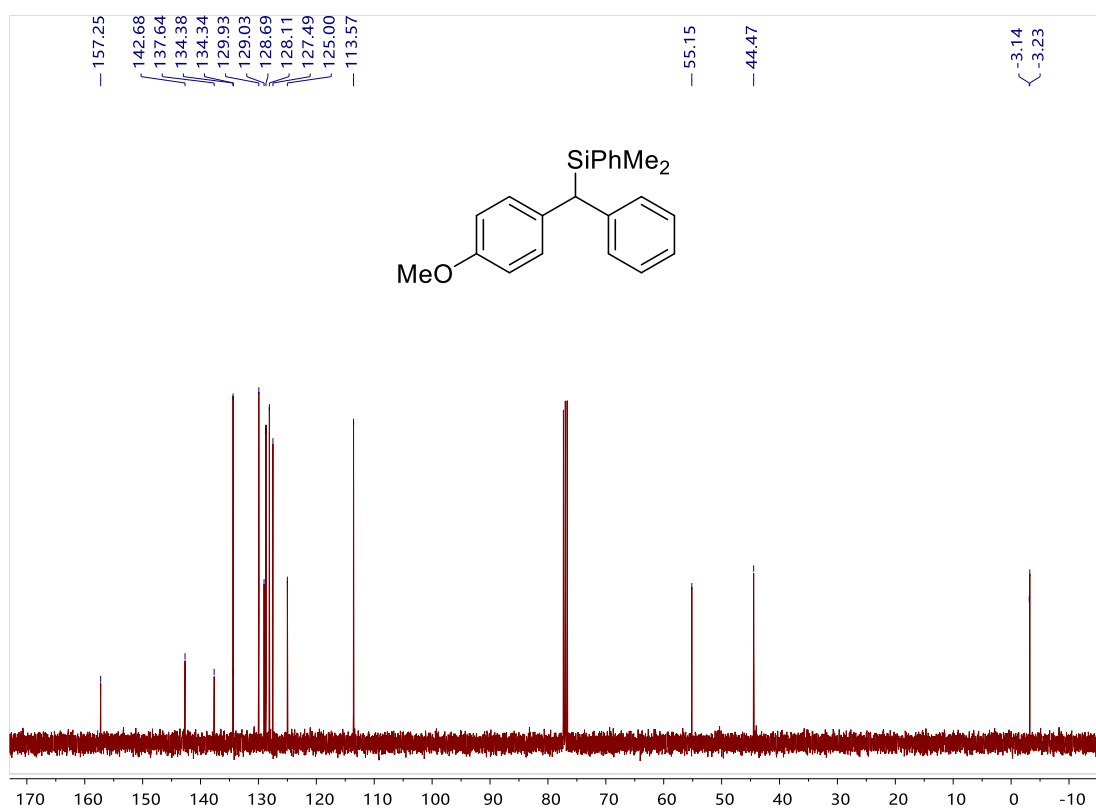
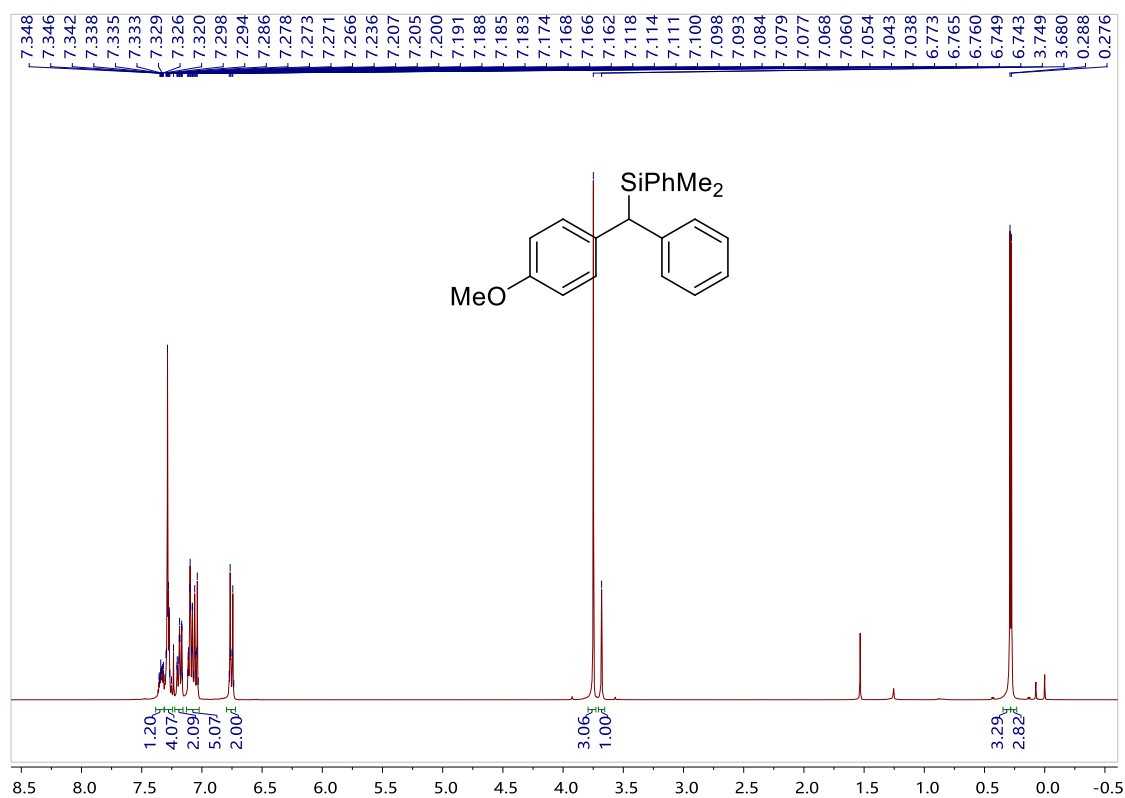
**(+)-((4-fluorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P9)**



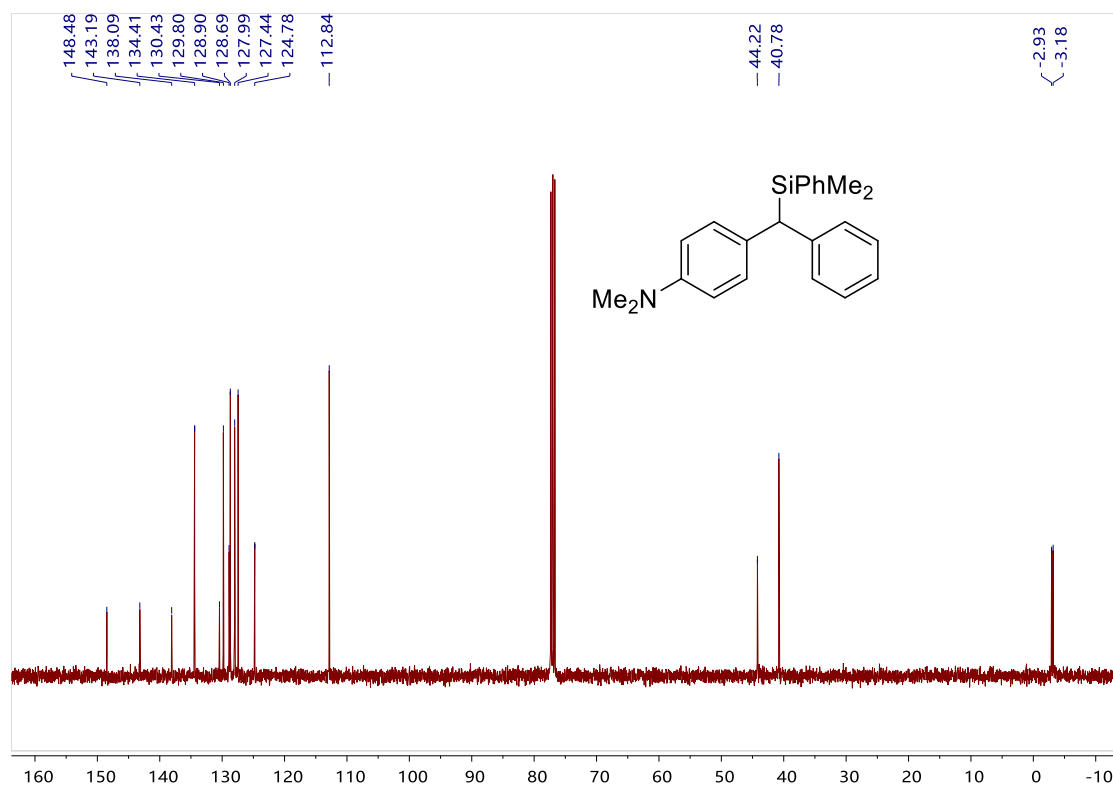
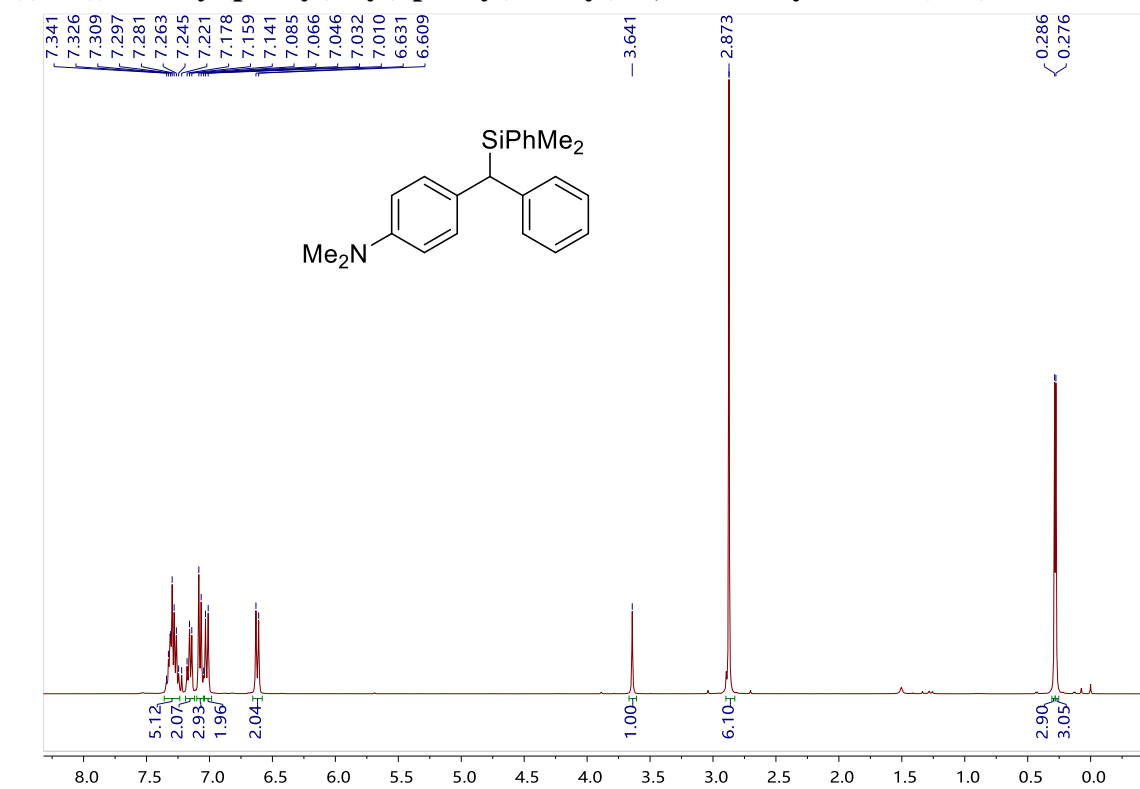
**(-)-dimethyl(phenyl)(phenyl(p-tolyl)methyl)silane (P10)**



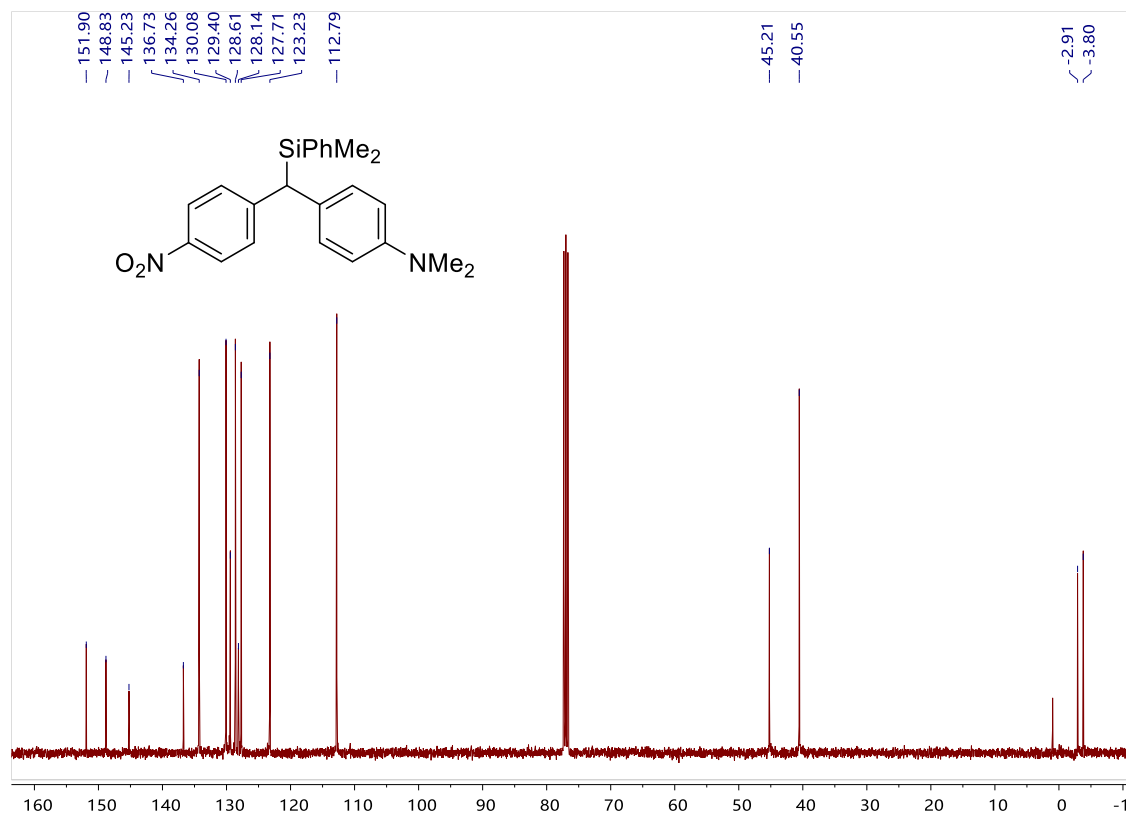
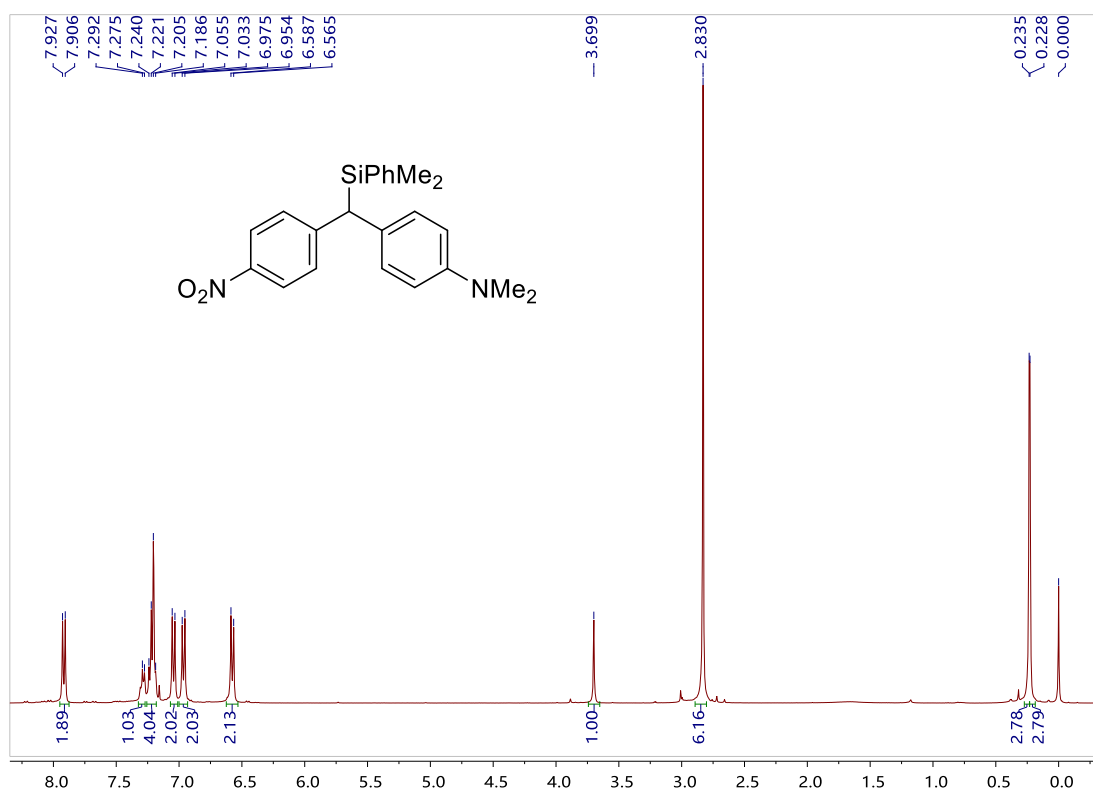
**(R)-((4-methoxyphenyl)(phenyl)methyl)dimethyl(phenyl)silane (P11)**



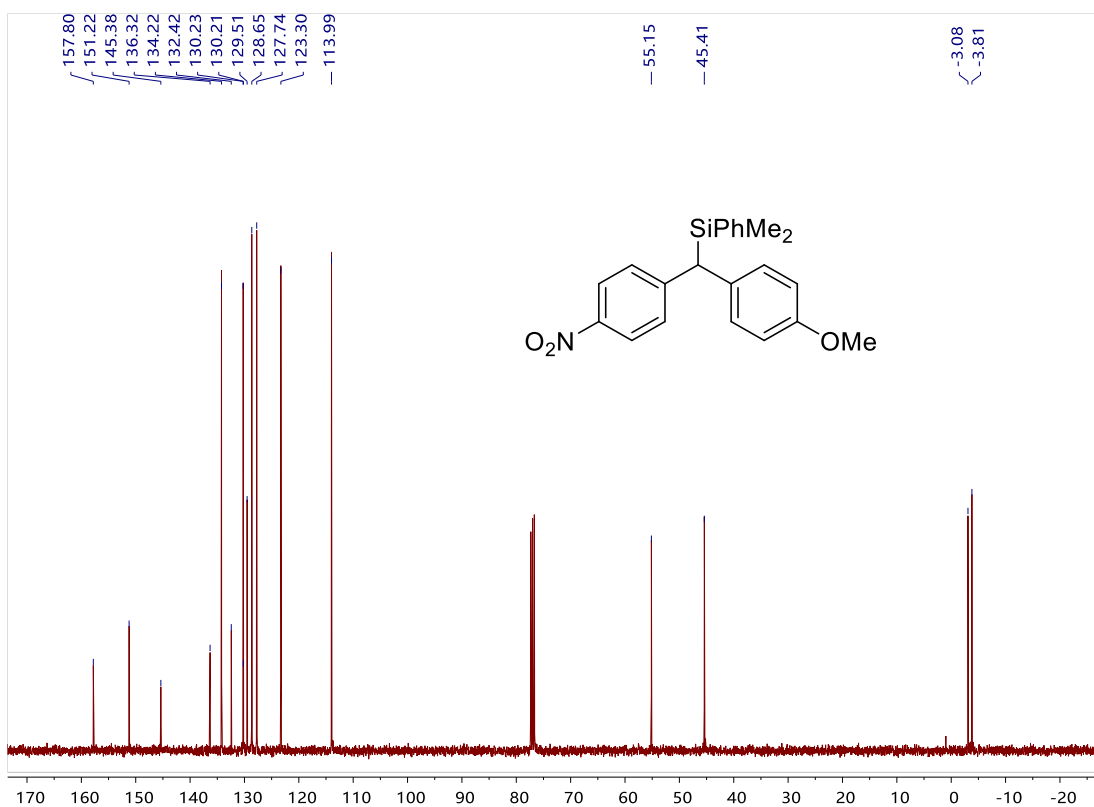
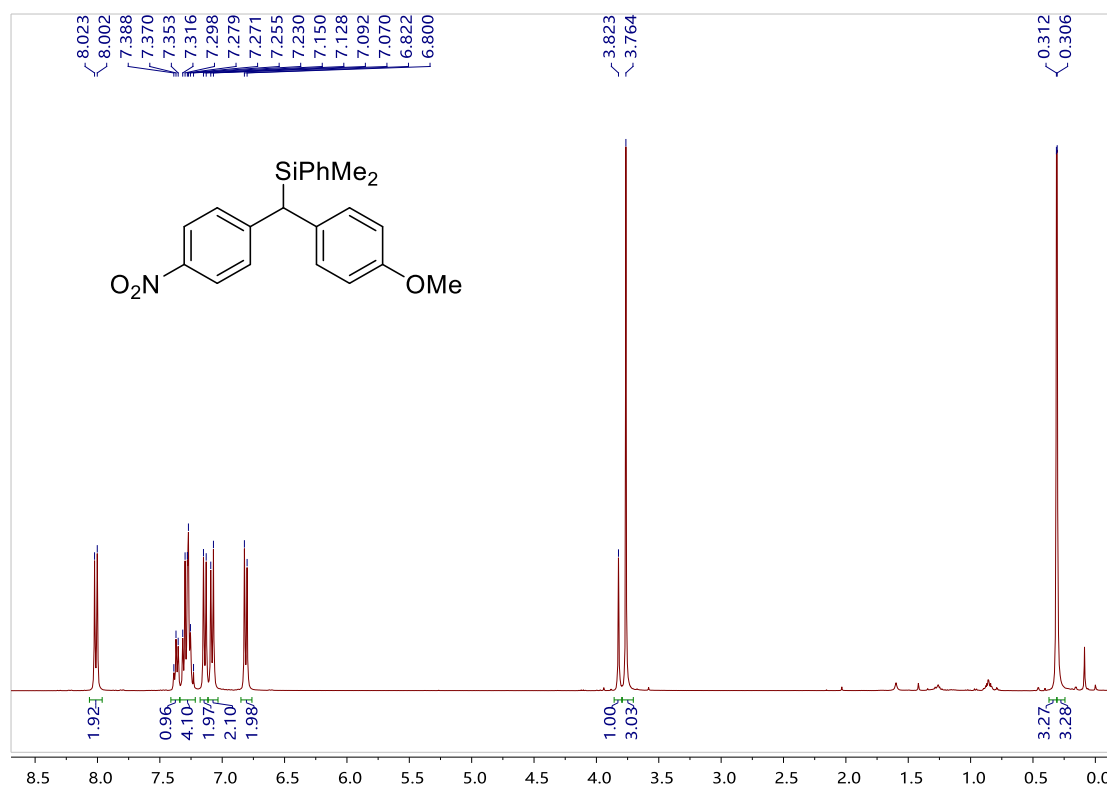
**(-)-4-((dimethyl(phenyl)silyl)(phenyl)methyl)-*N,N*-dimethylaniline (P12)**



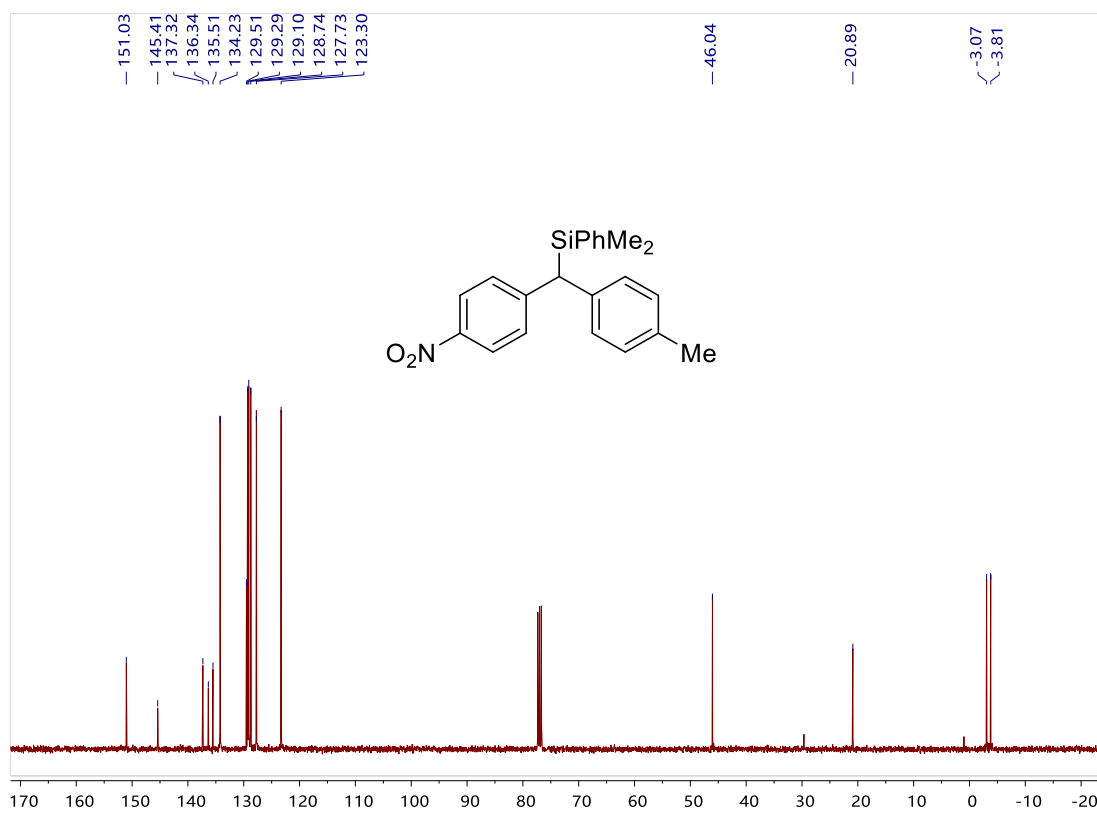
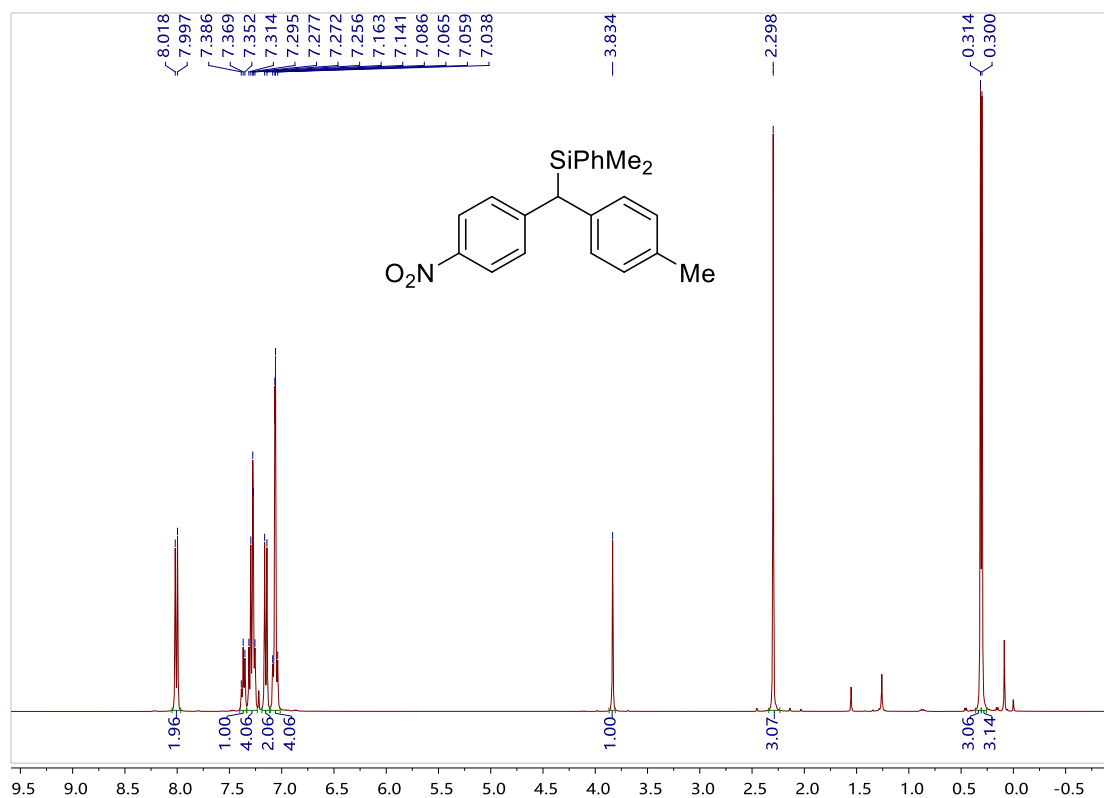
**(-)-4-((dimethyl(phenyl)silyl)(4-nitrophenyl)methyl)-*N,N*-dimethylaniline (P13)**



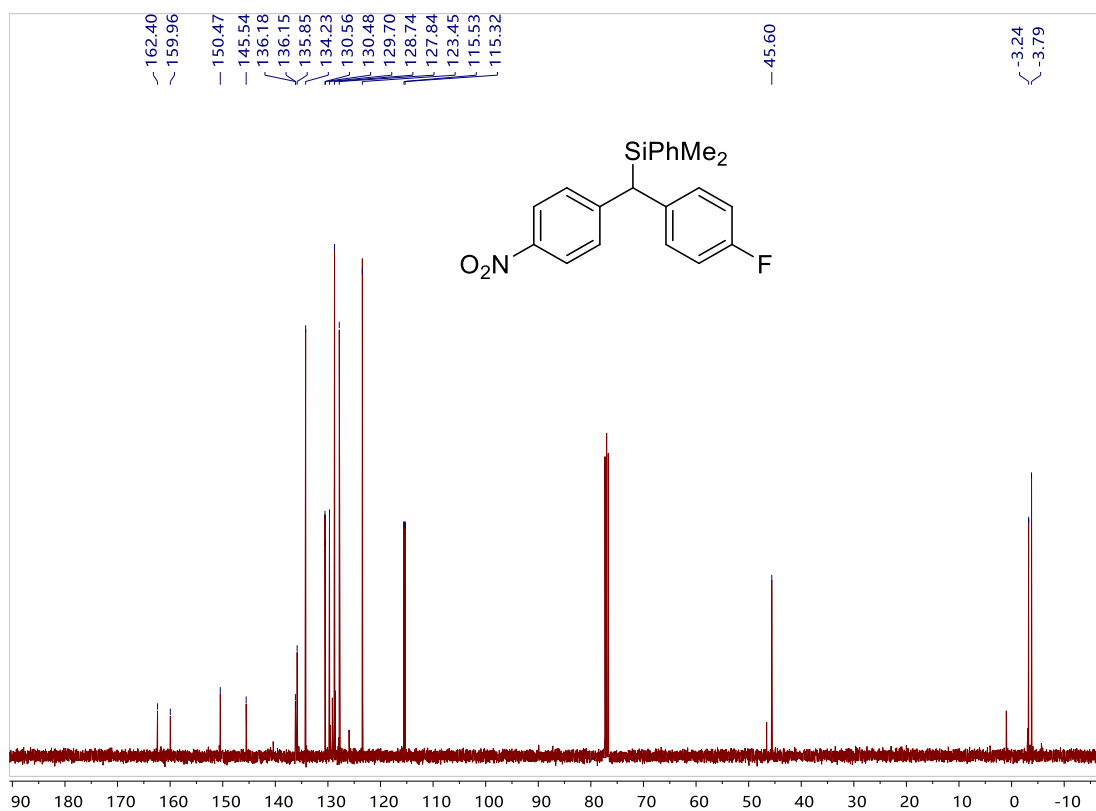
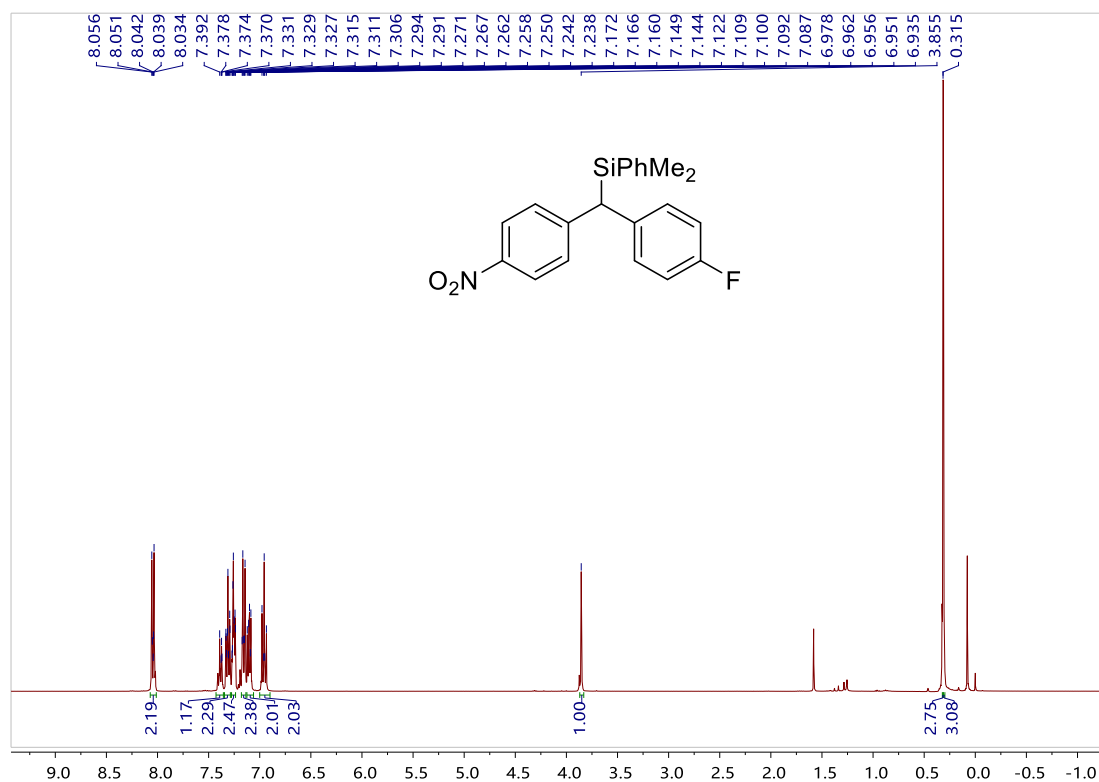
**(-)-((4-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P14)**



**(-)-dimethyl((4-nitrophenyl)(p-tolyl)methyl)(phenyl)silane (P15)**

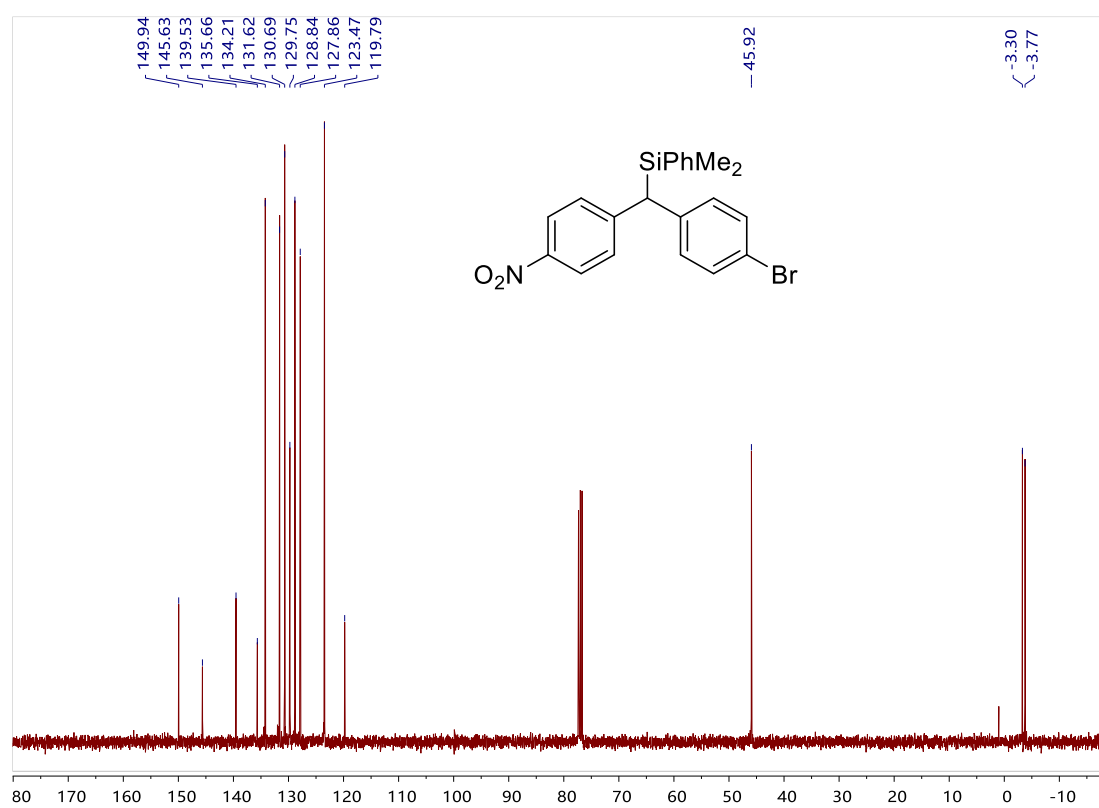
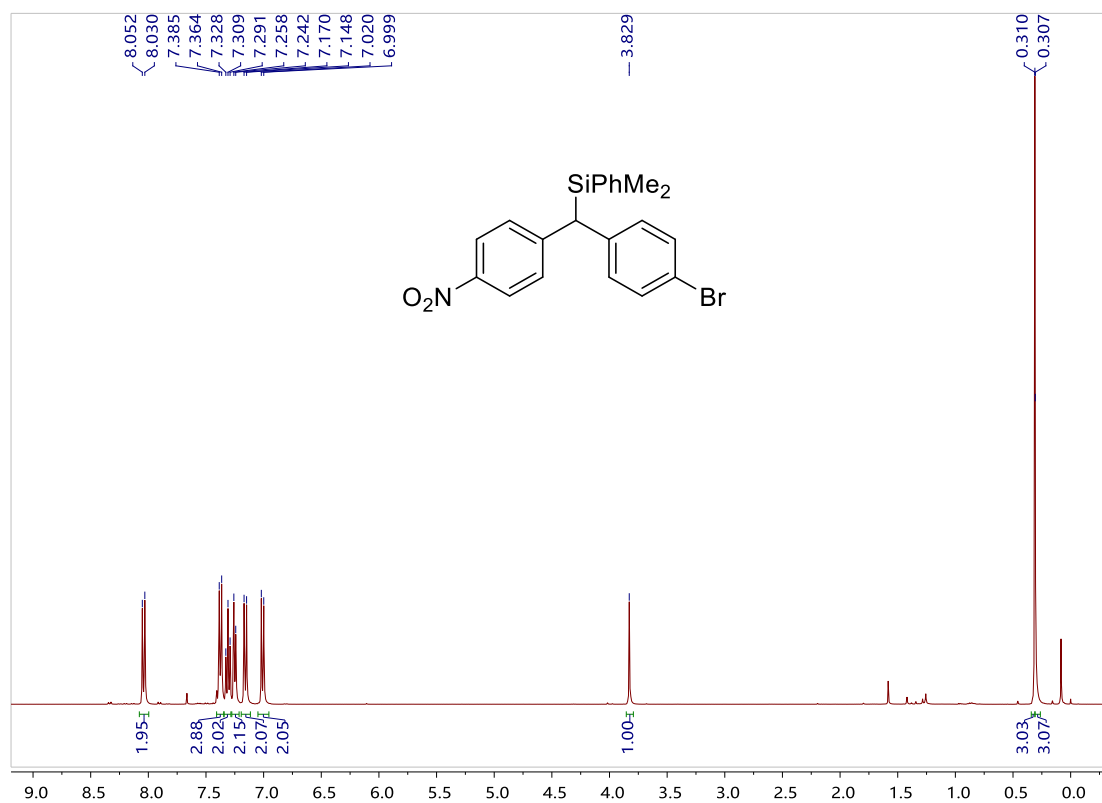


**(-)-((4-fluorophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P16)**

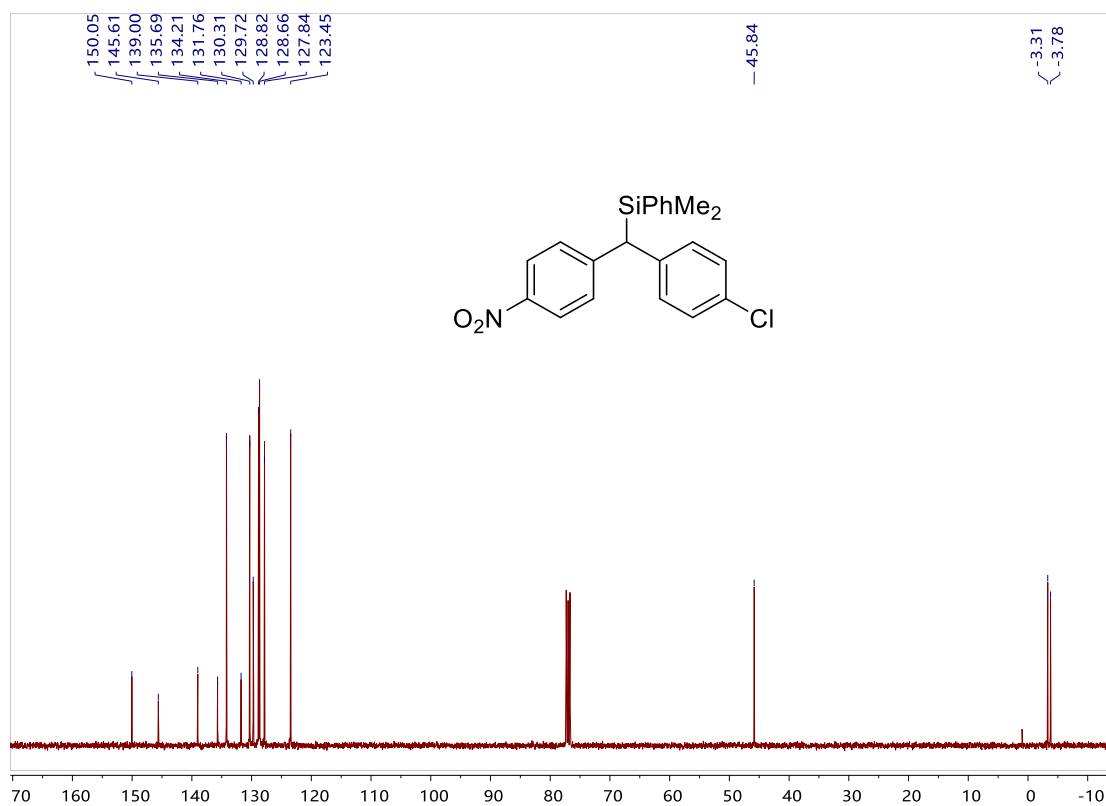
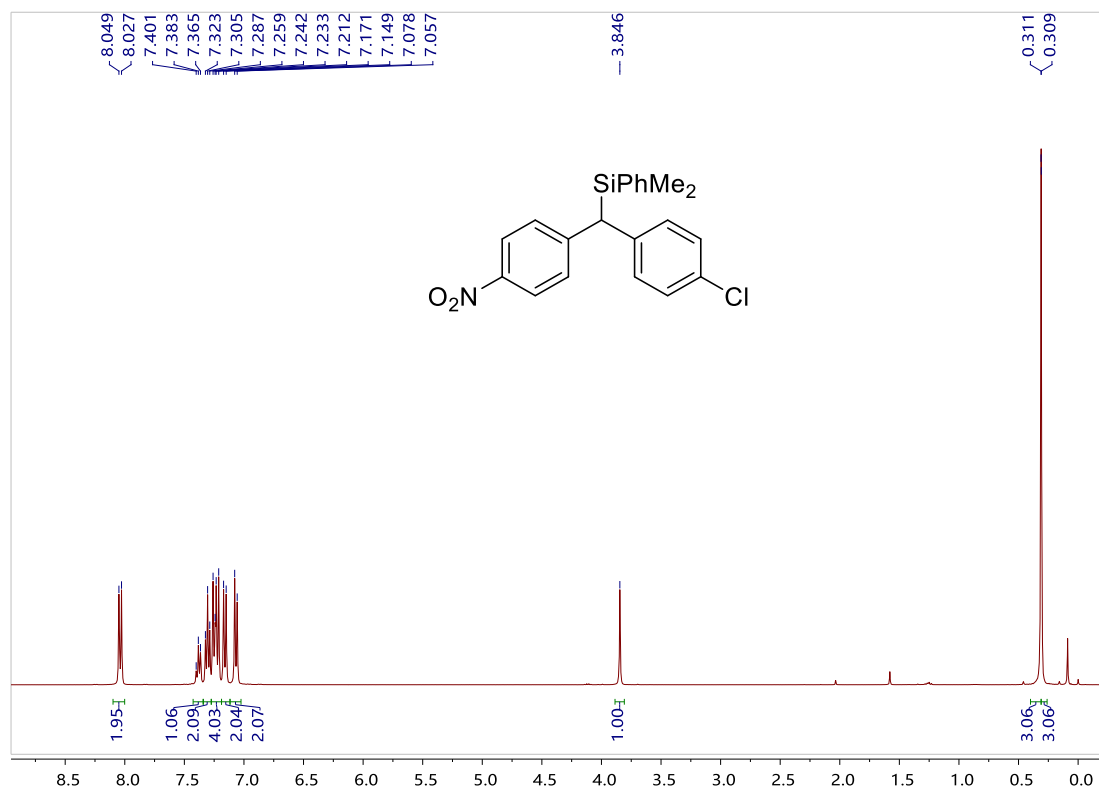




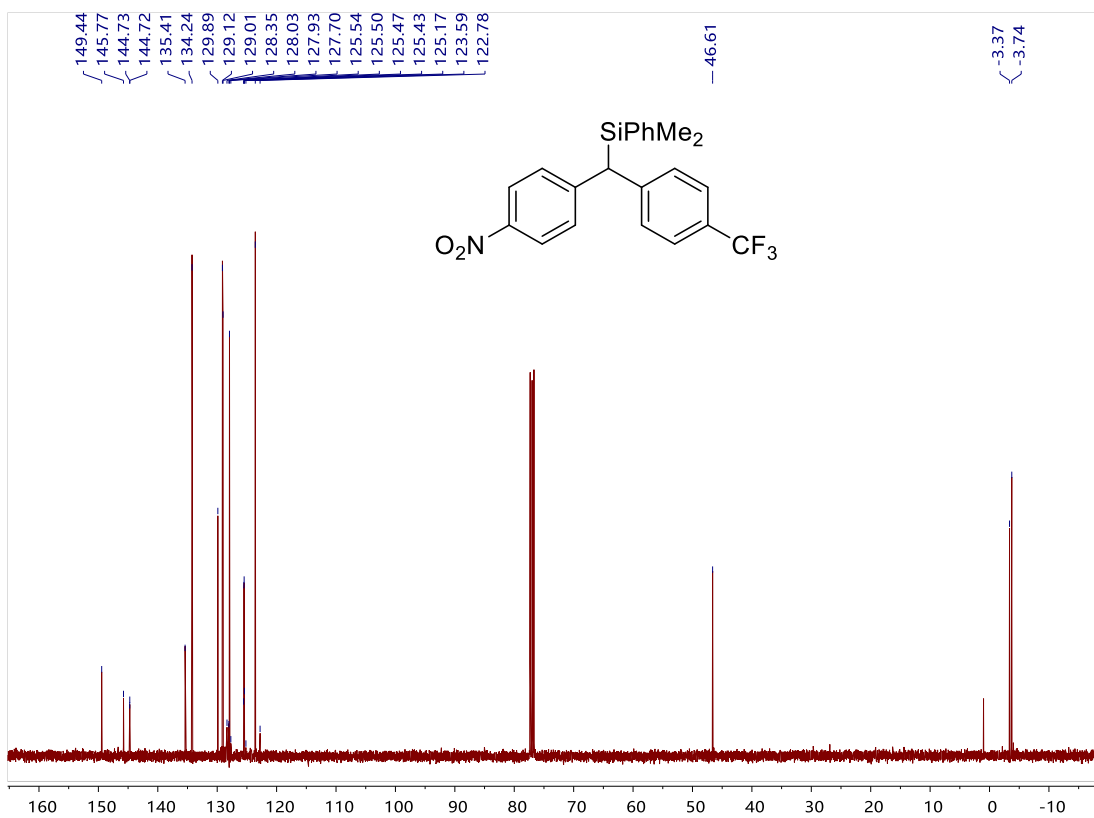
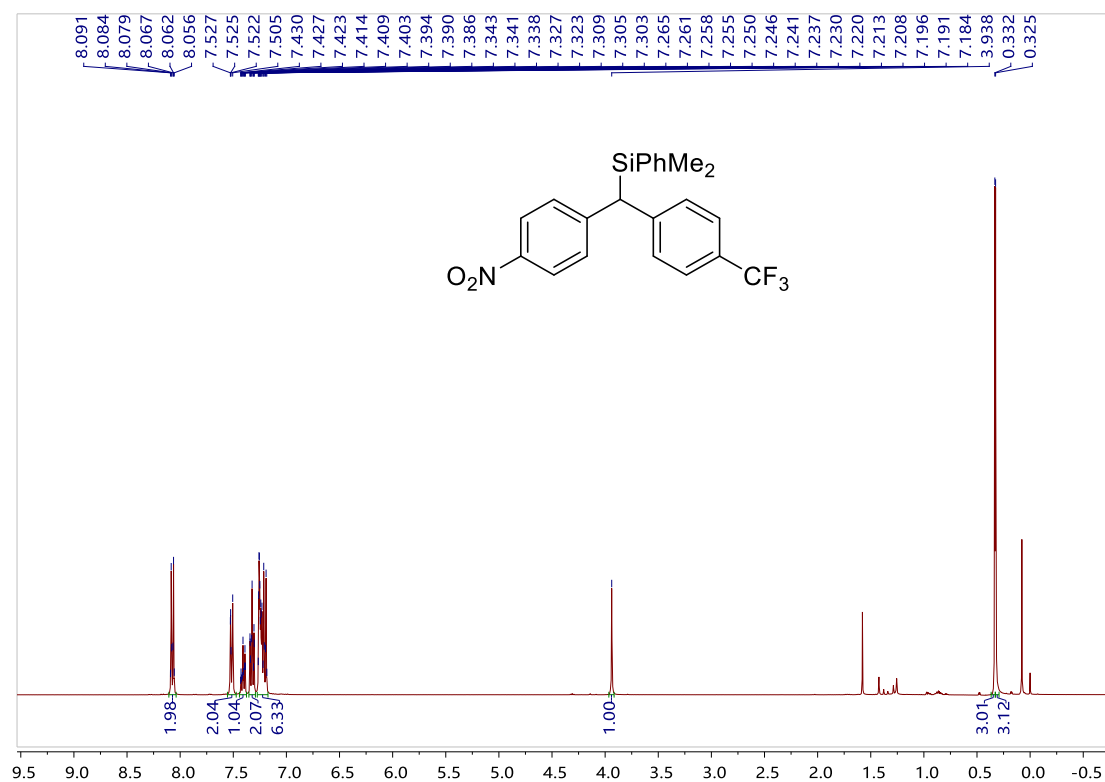
**(-)-((4-bromophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P17)**



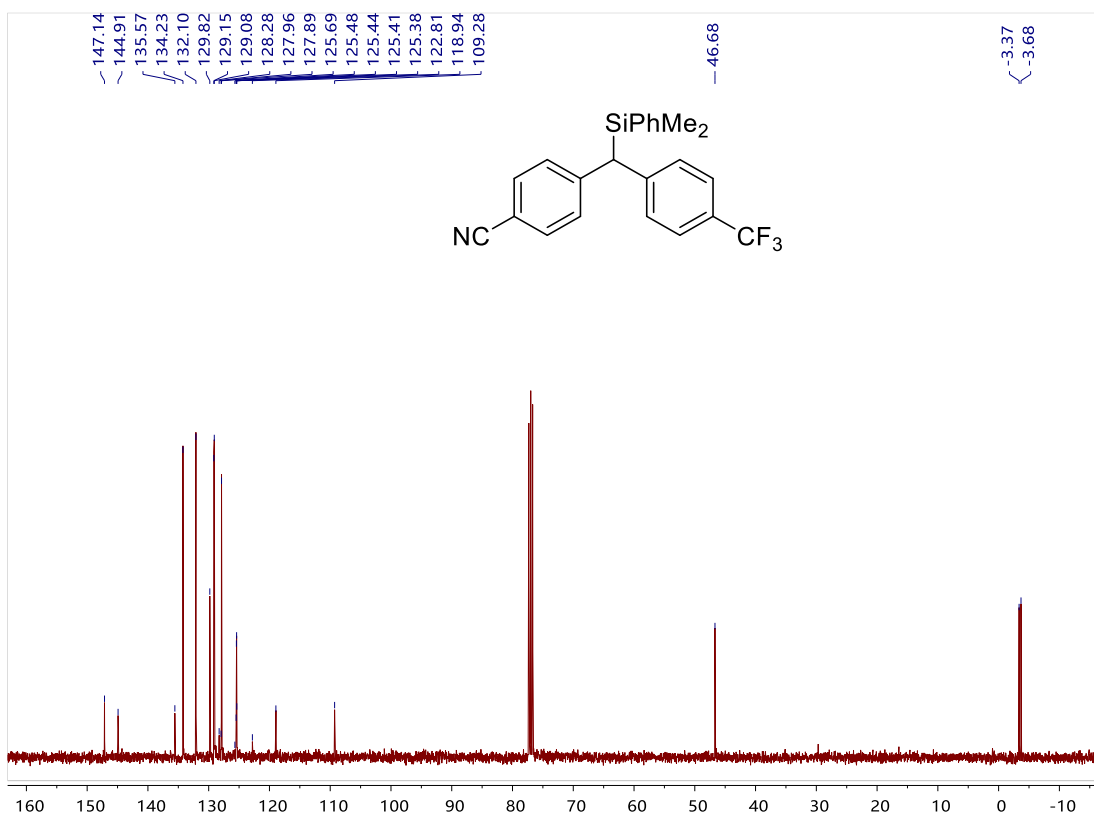
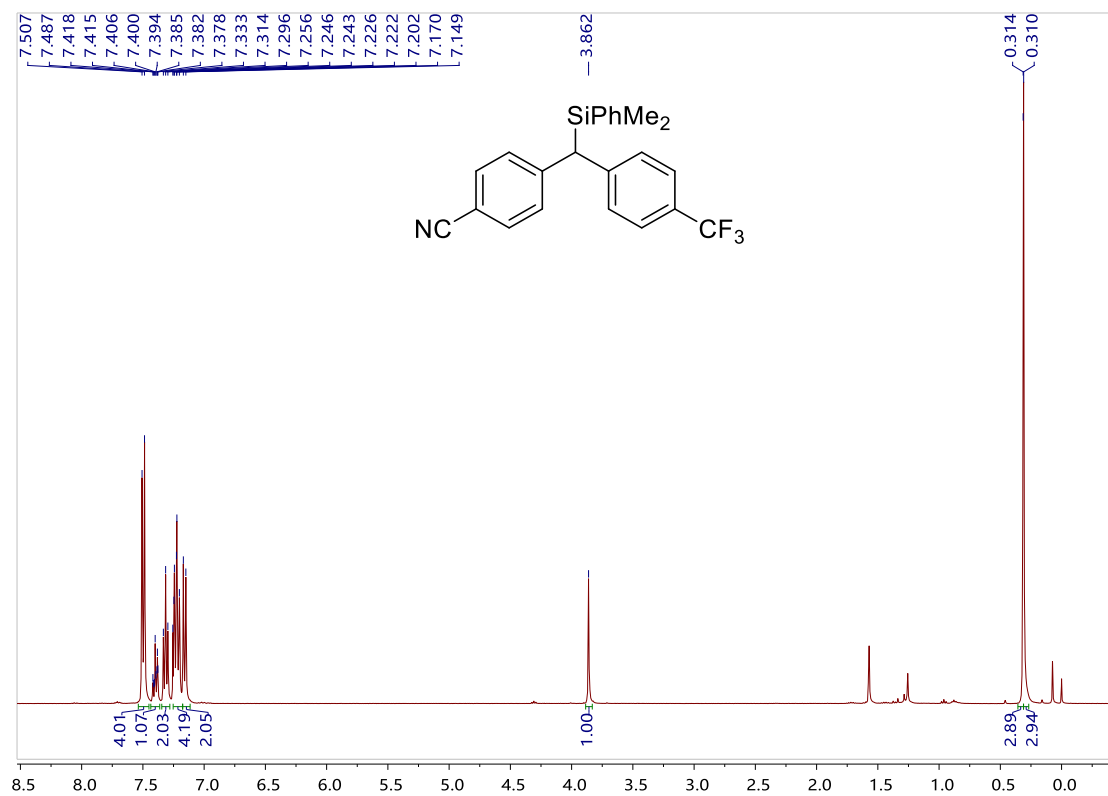
**(-)-((4-chlorophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P18)**



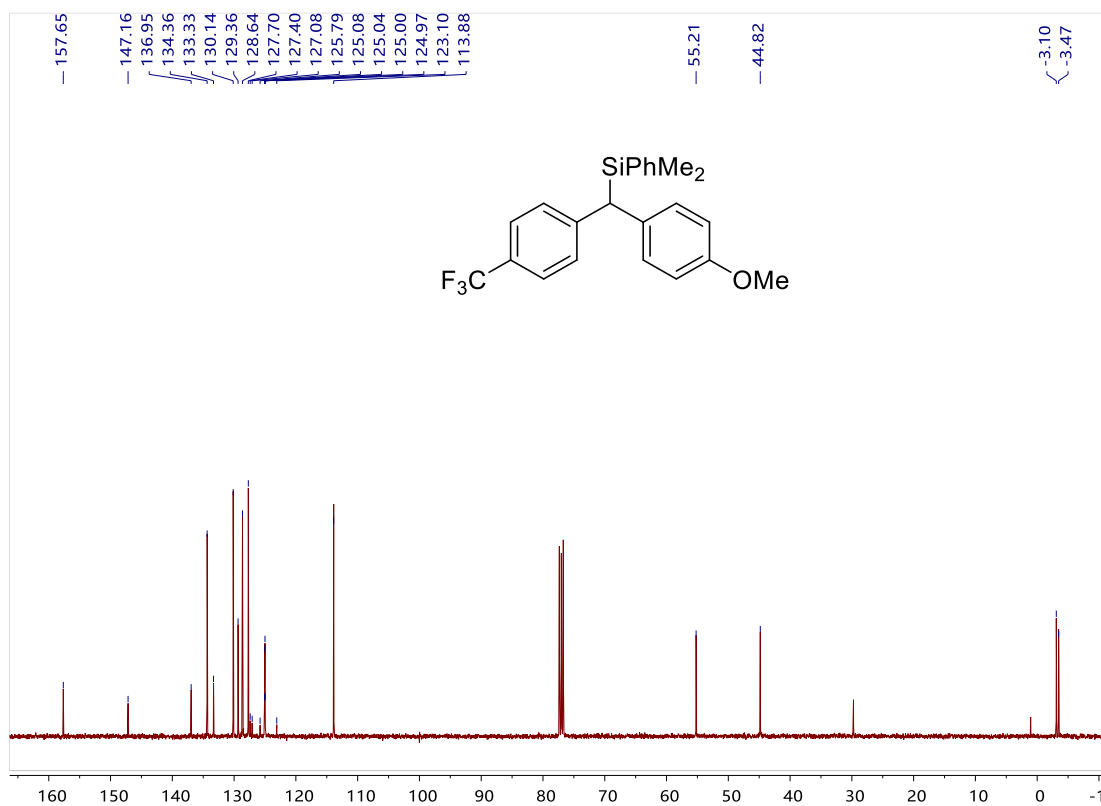
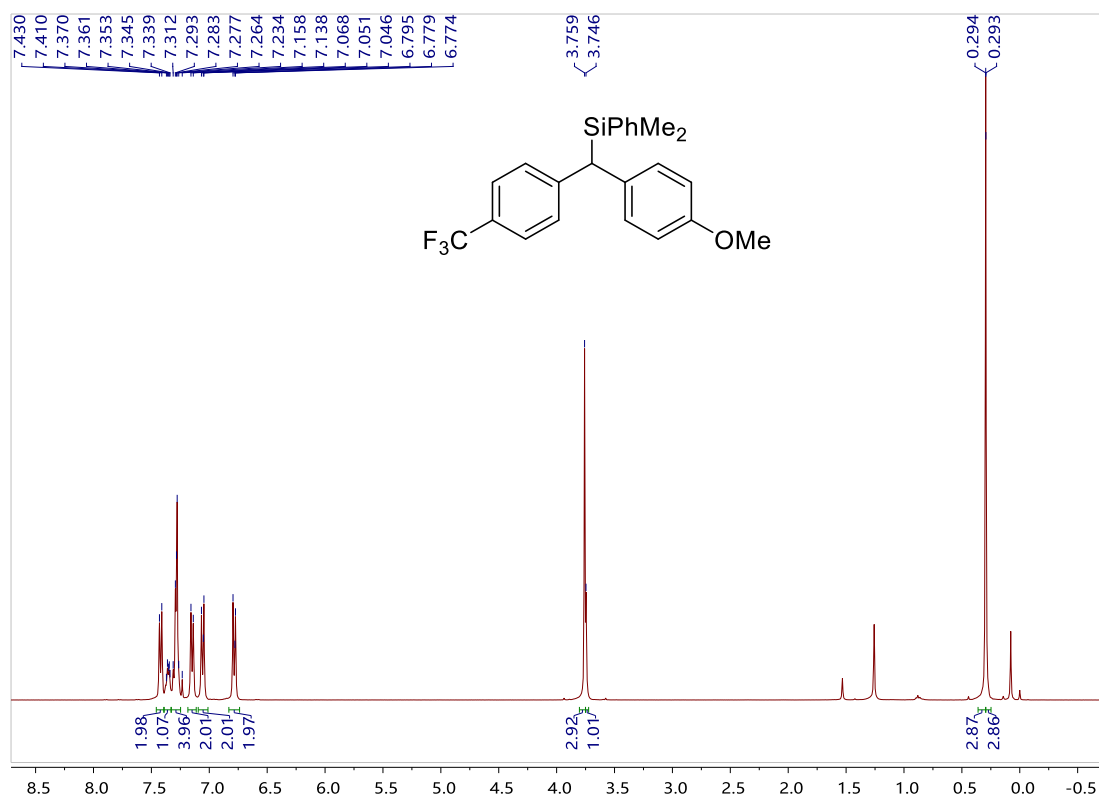
**(-)-dimethyl((4-nitrophenyl)(4-(trifluoromethyl)phenyl)methyl)(phenyl)silane (P19)**



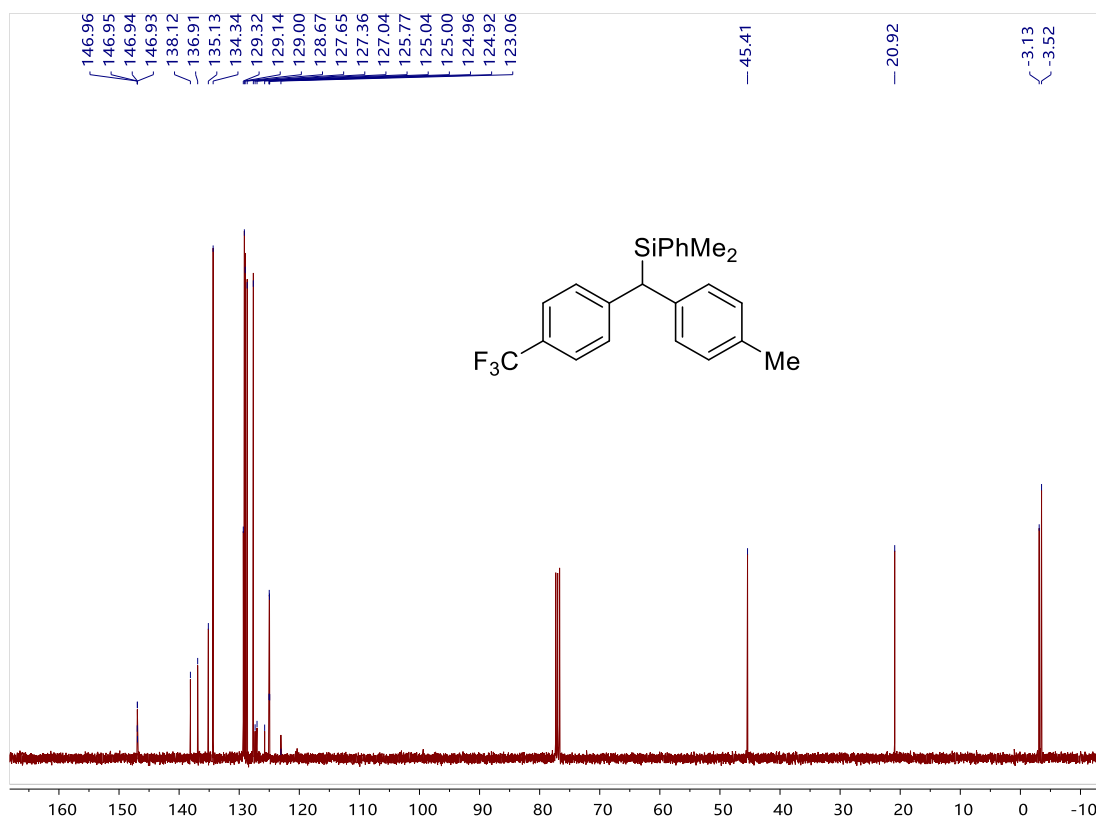
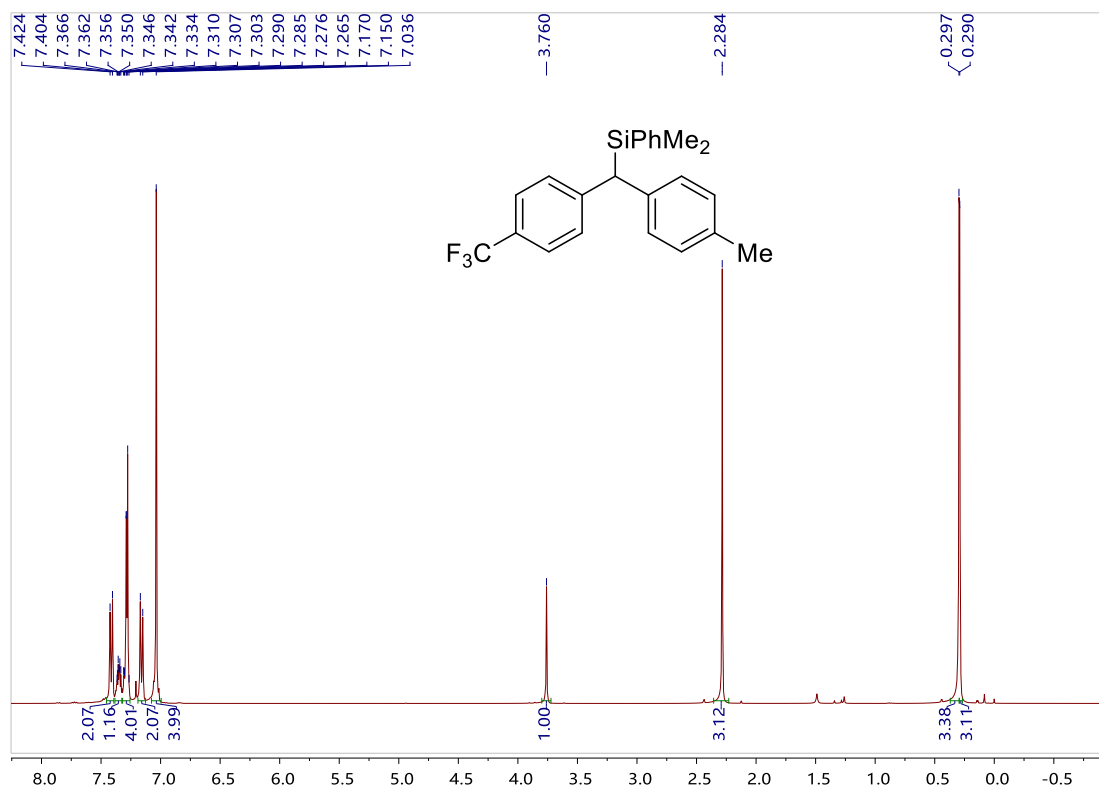
**(-)-4-((dimethyl(phenyl)silyl)(4-(trifluoromethyl)phenyl)methyl)benzonitrile (P20)**



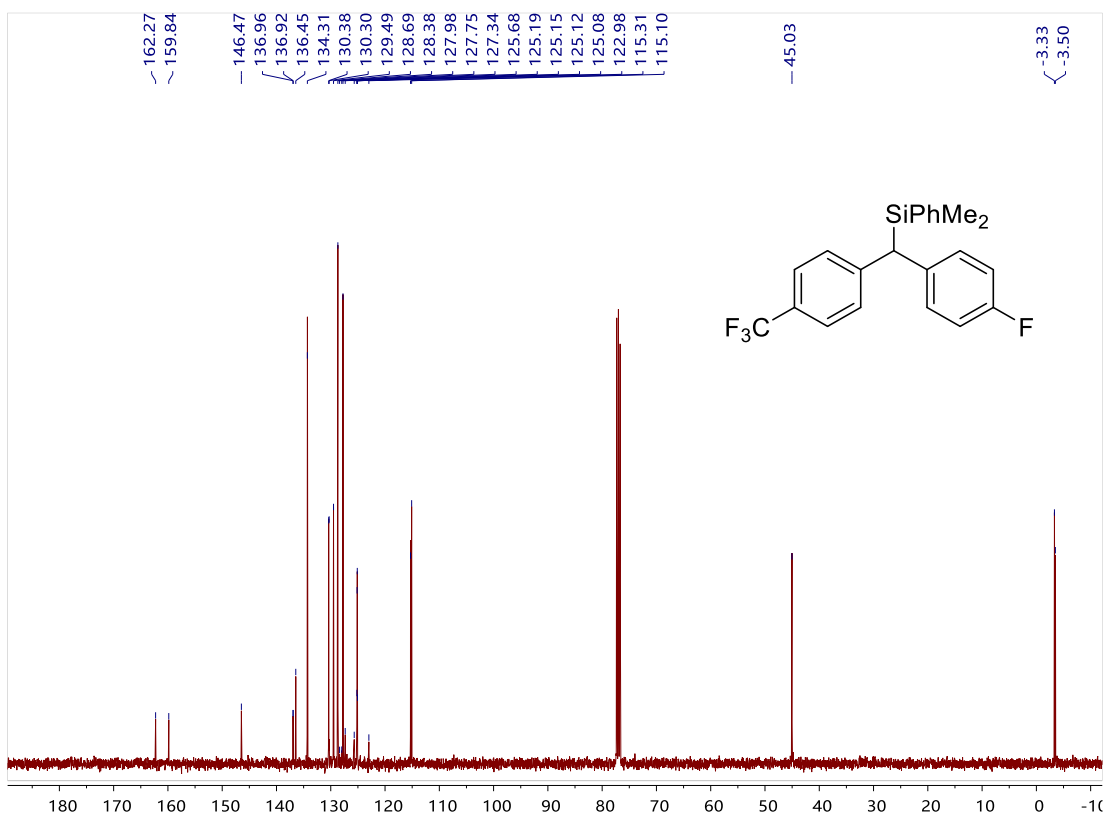
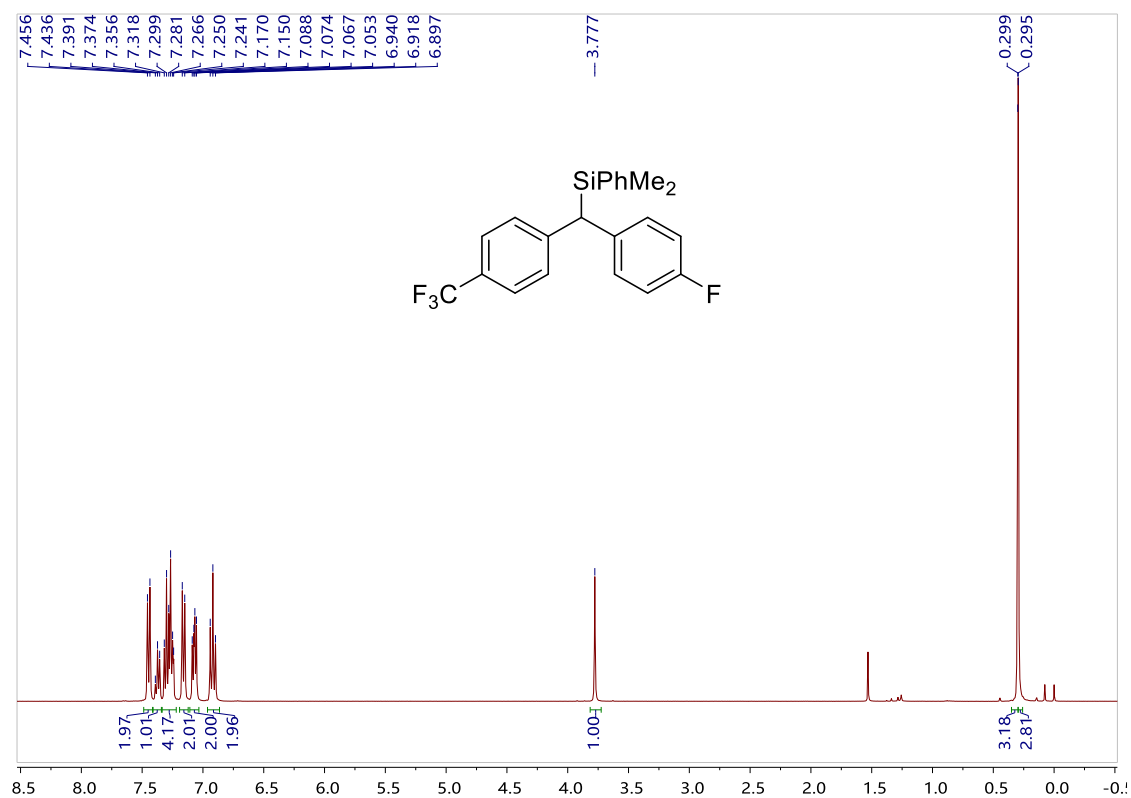
**(-)-((4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P21)**



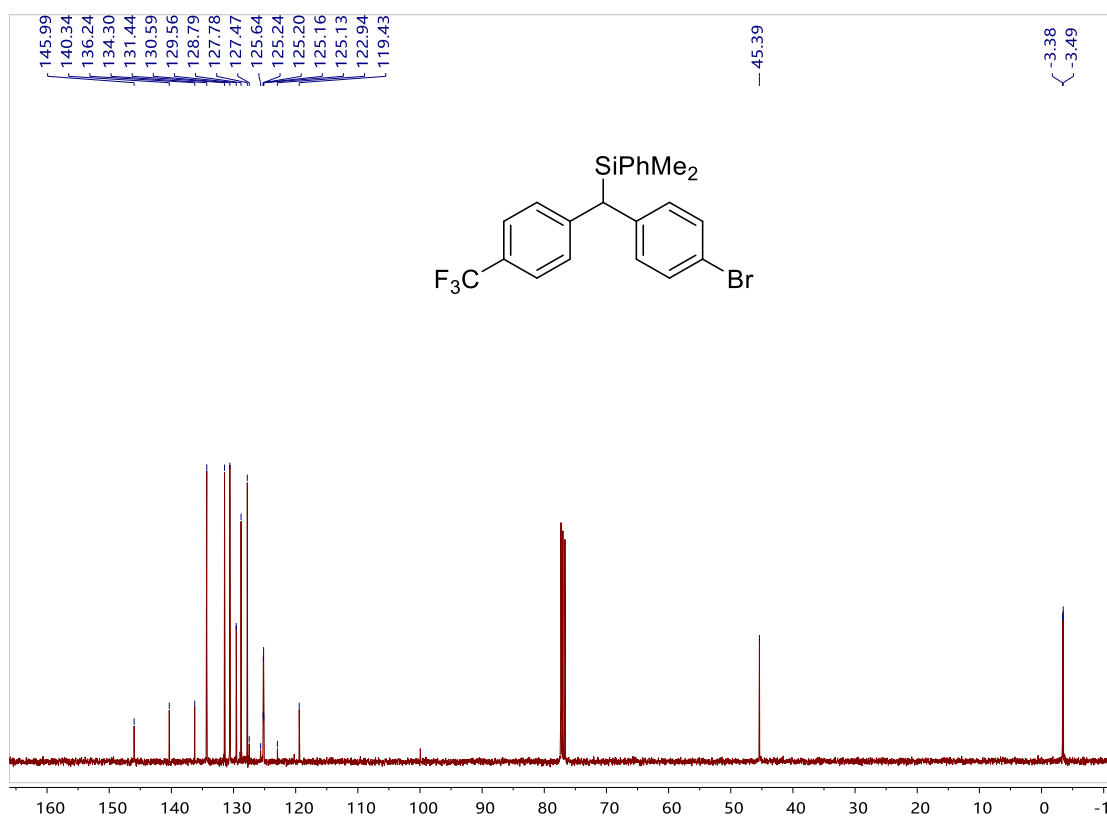
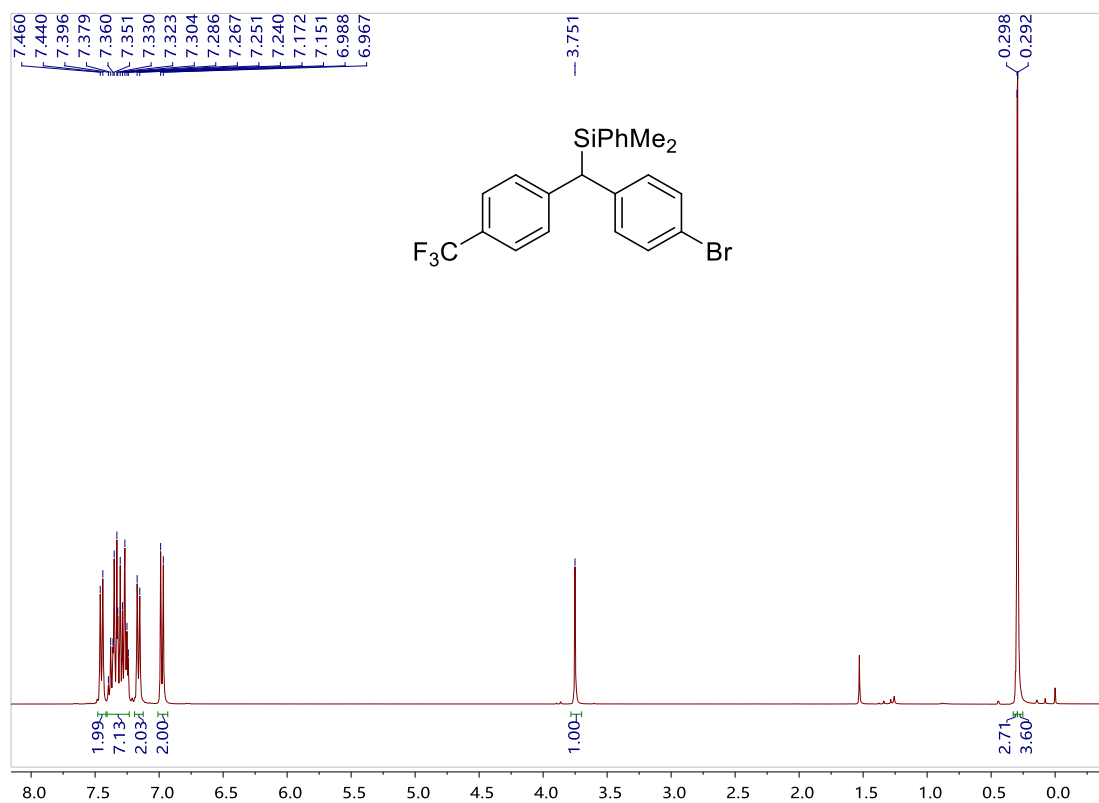
**(S)-dimethyl(phenyl)(p-tolyl(4-(trifluoromethyl)phenyl)methyl)silane (P22)**



**(-)-((4-fluorophenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P23)**

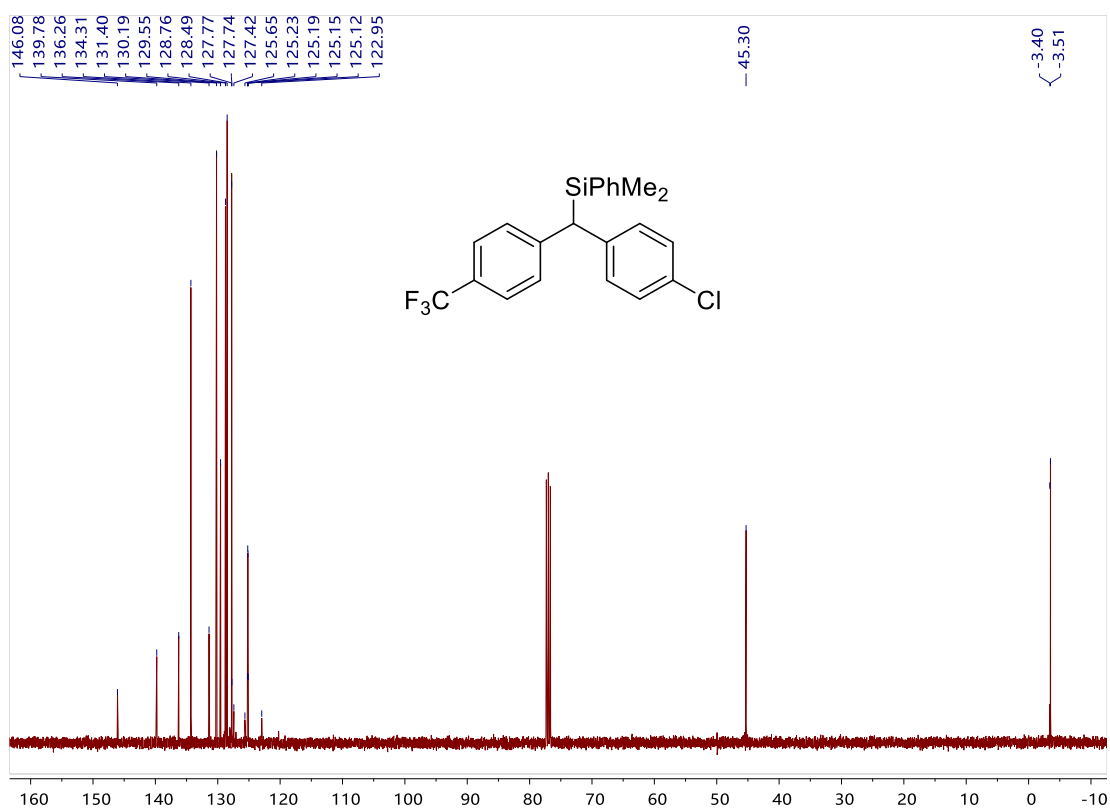
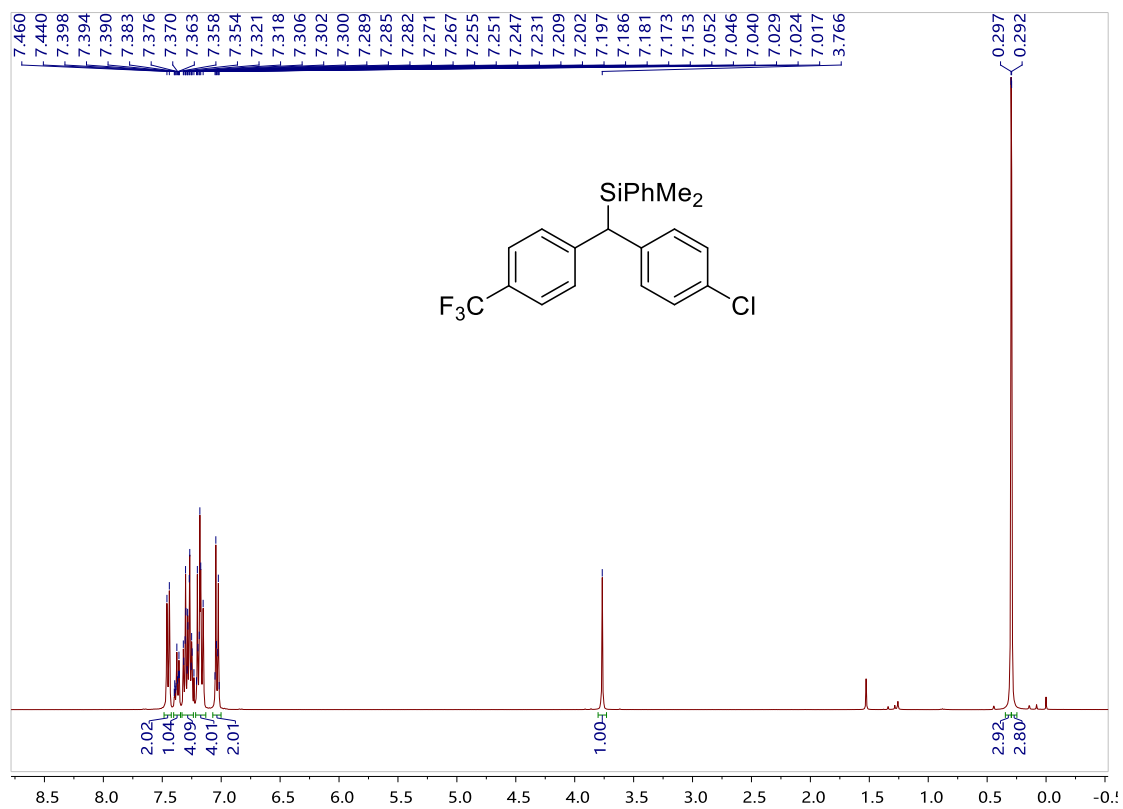


**(-)-((4-bromophenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P24)**

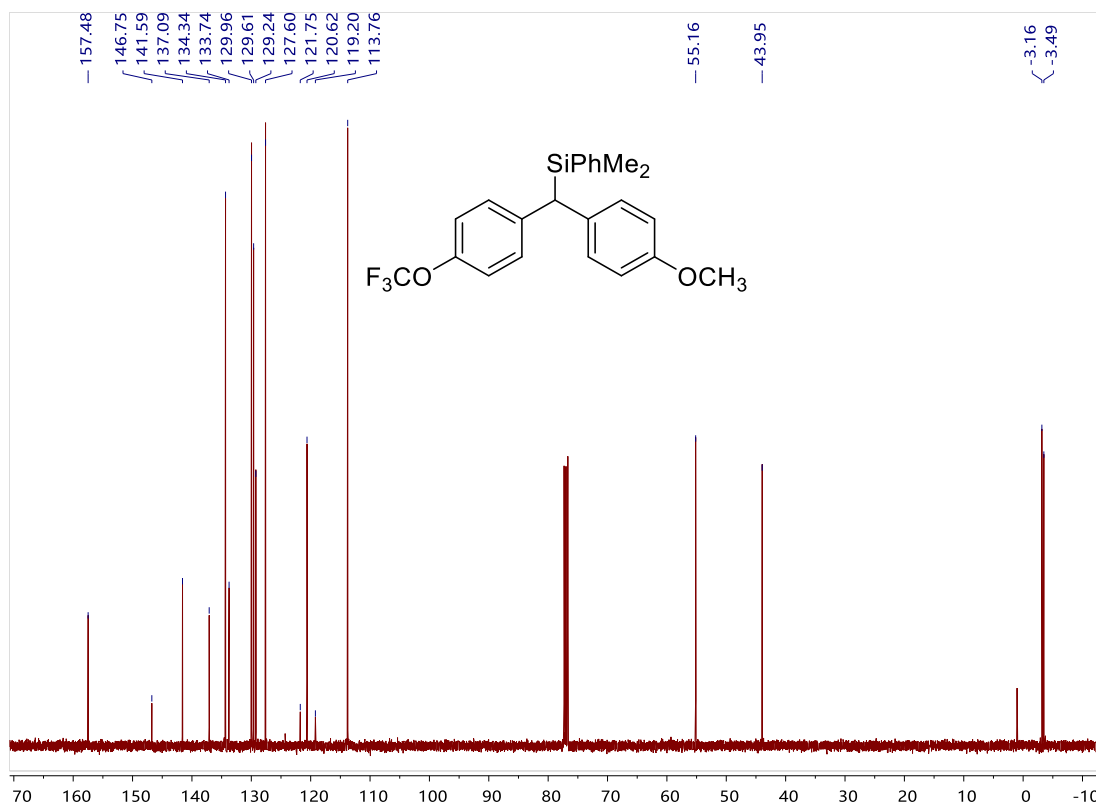
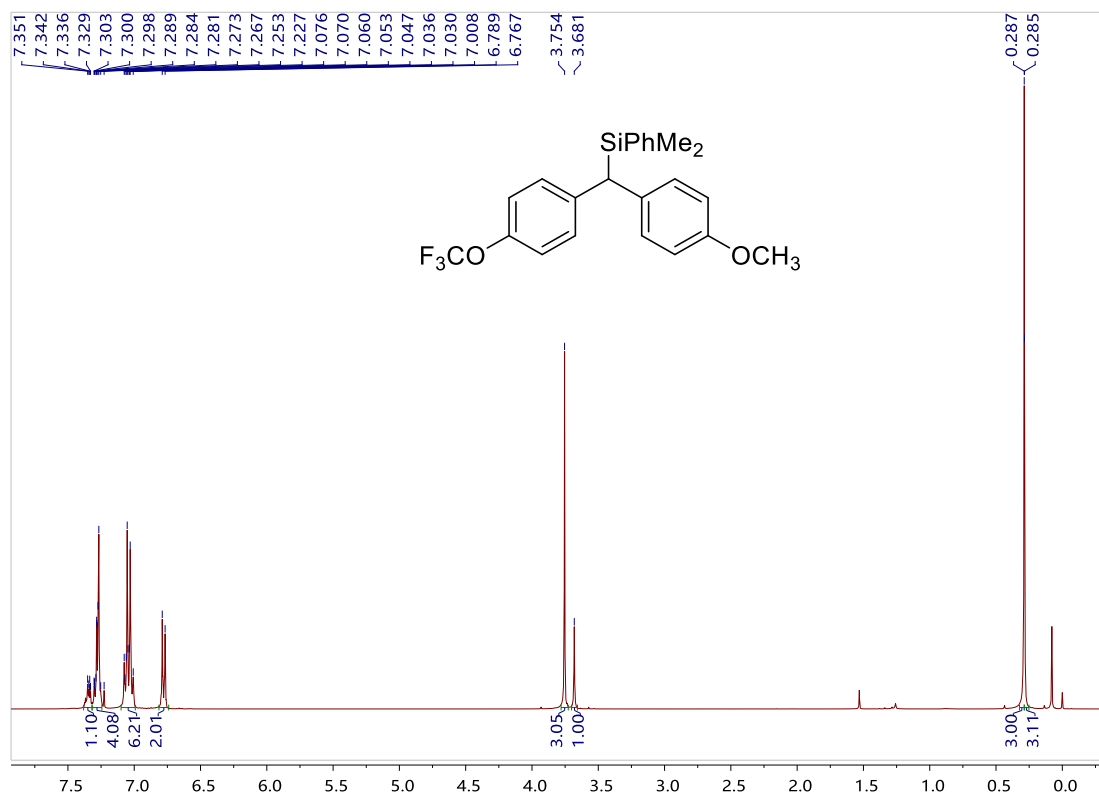




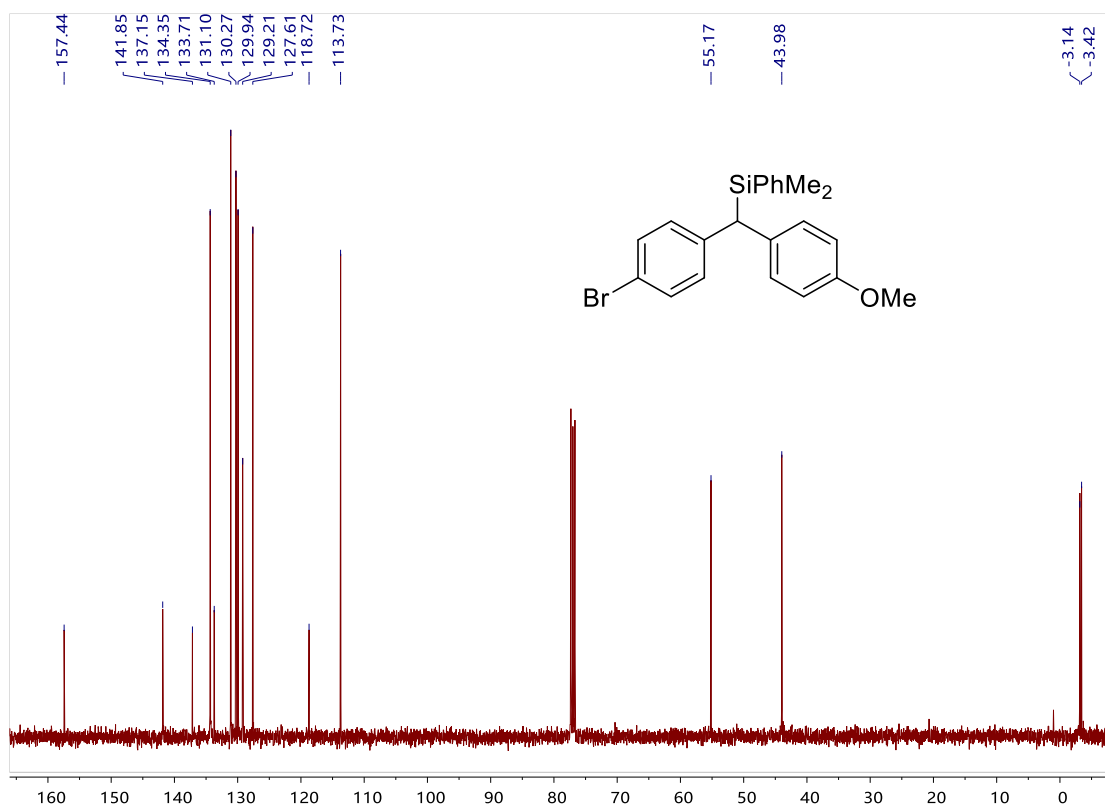
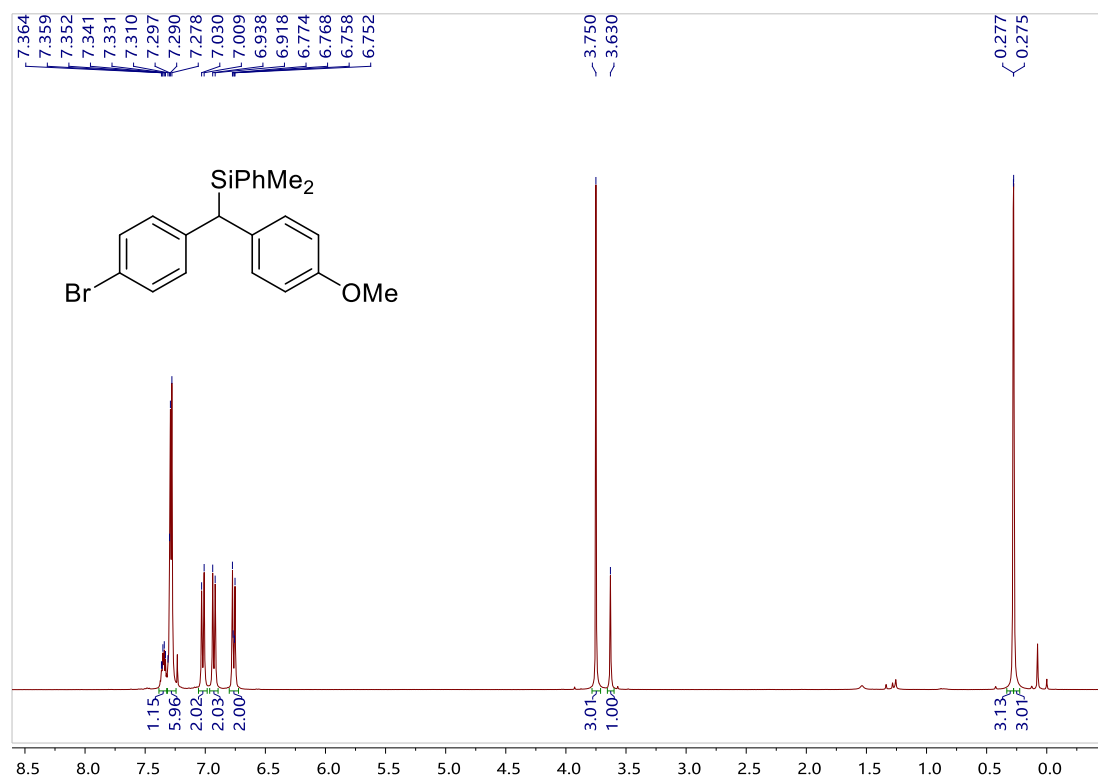
**(R)-((4-chlorophenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P25)**



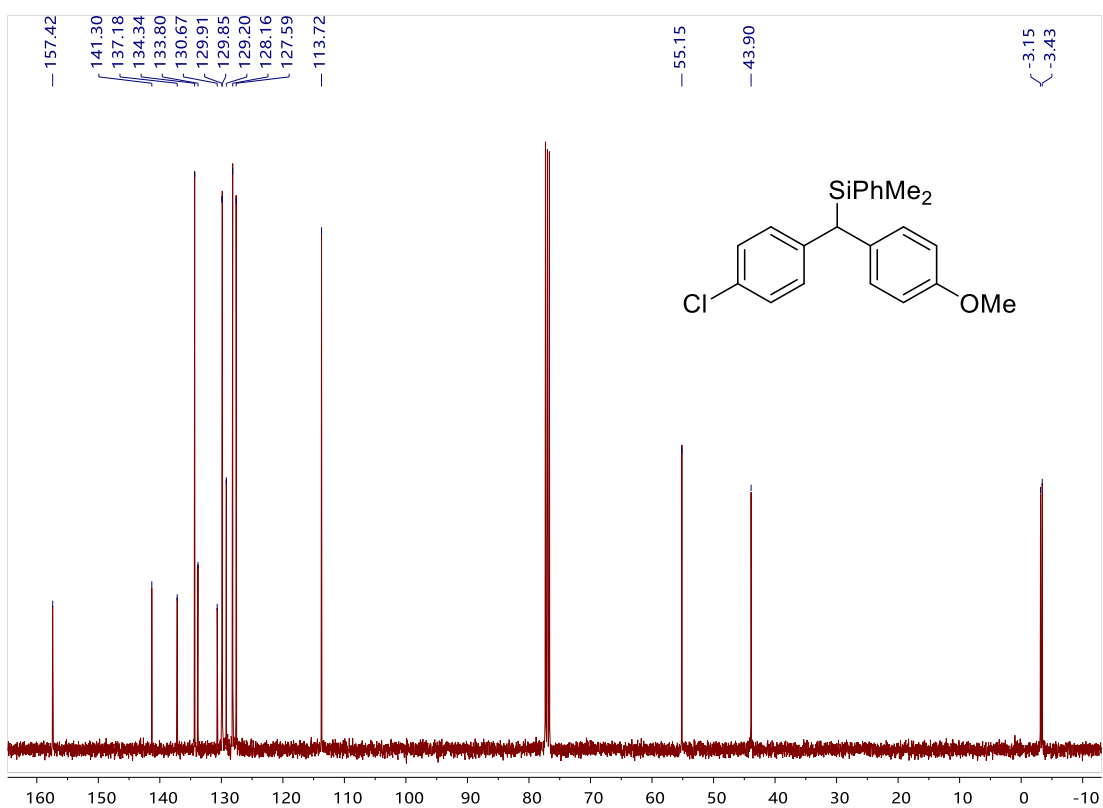
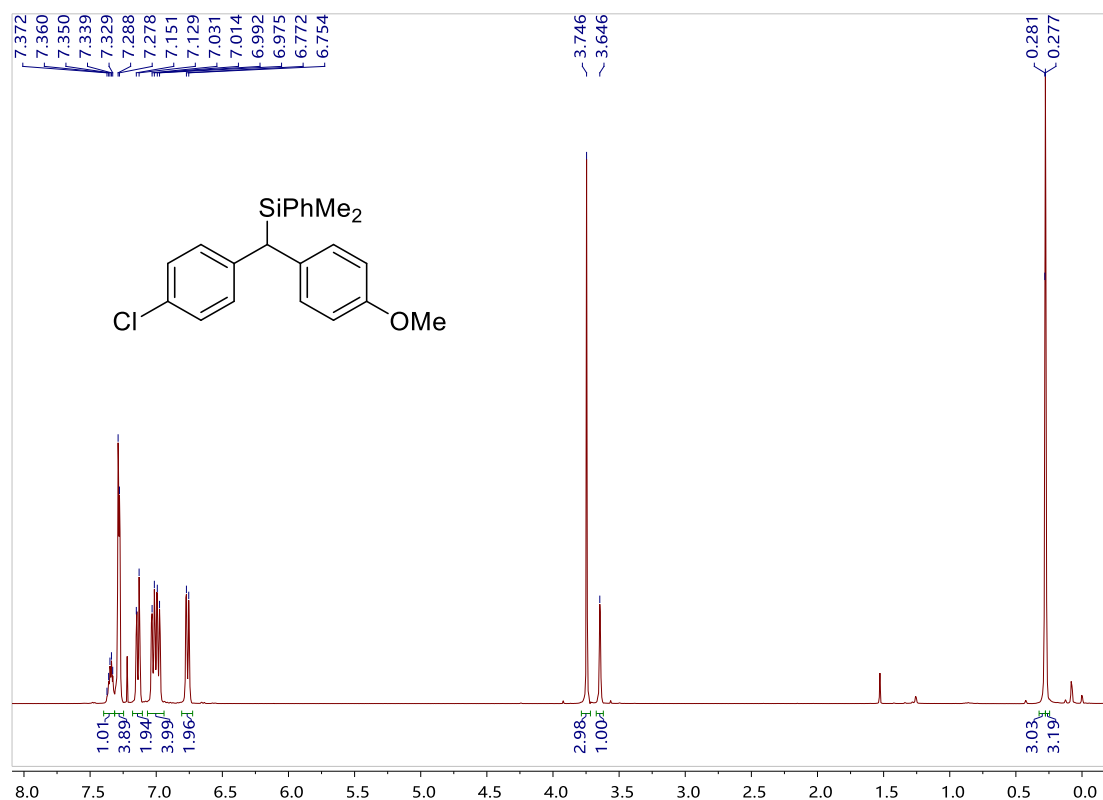
**(-)-((4-methoxyphenyl)(4-(trifluoromethoxy)phenyl)methyl)dimethyl(phenyl)silane (P26)**



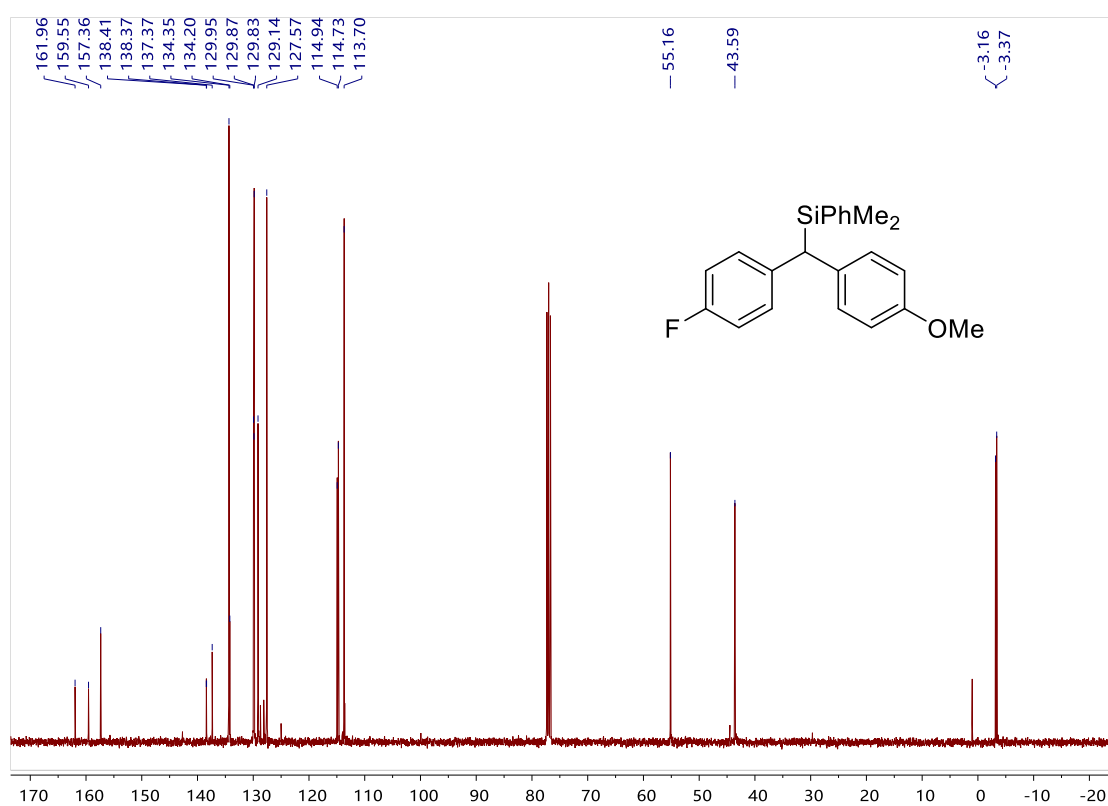
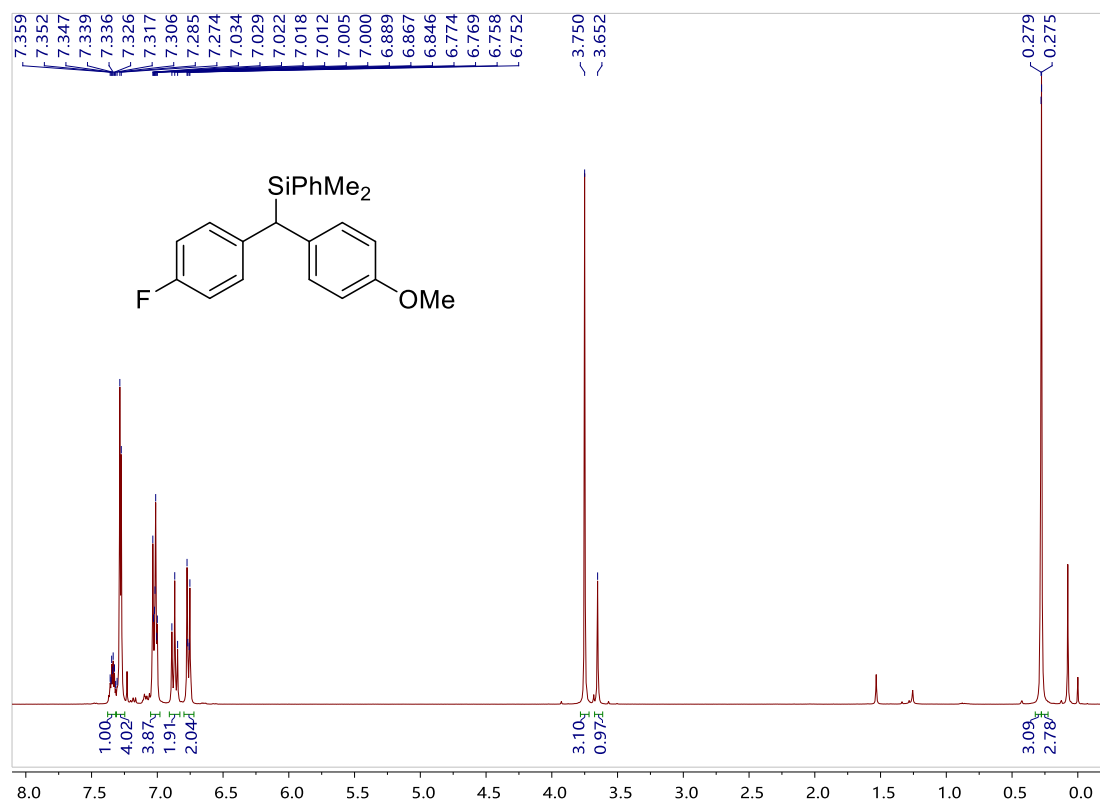
**(-)-((4-bromophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P27)**



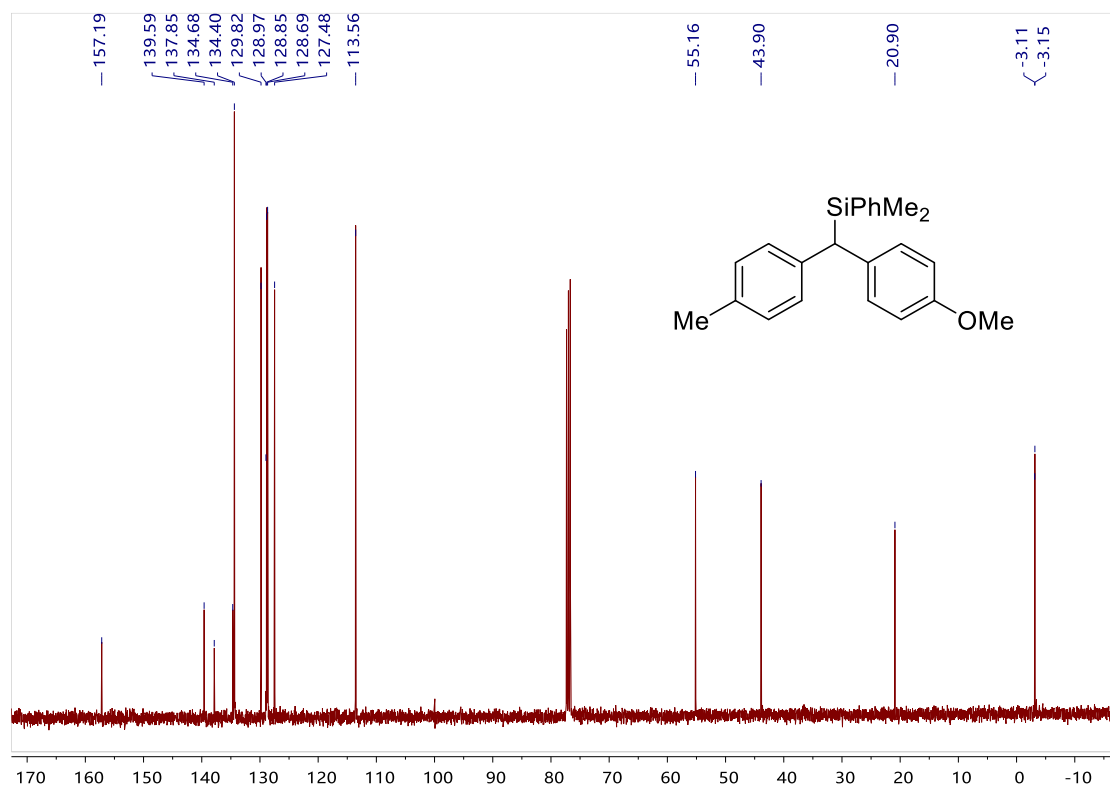
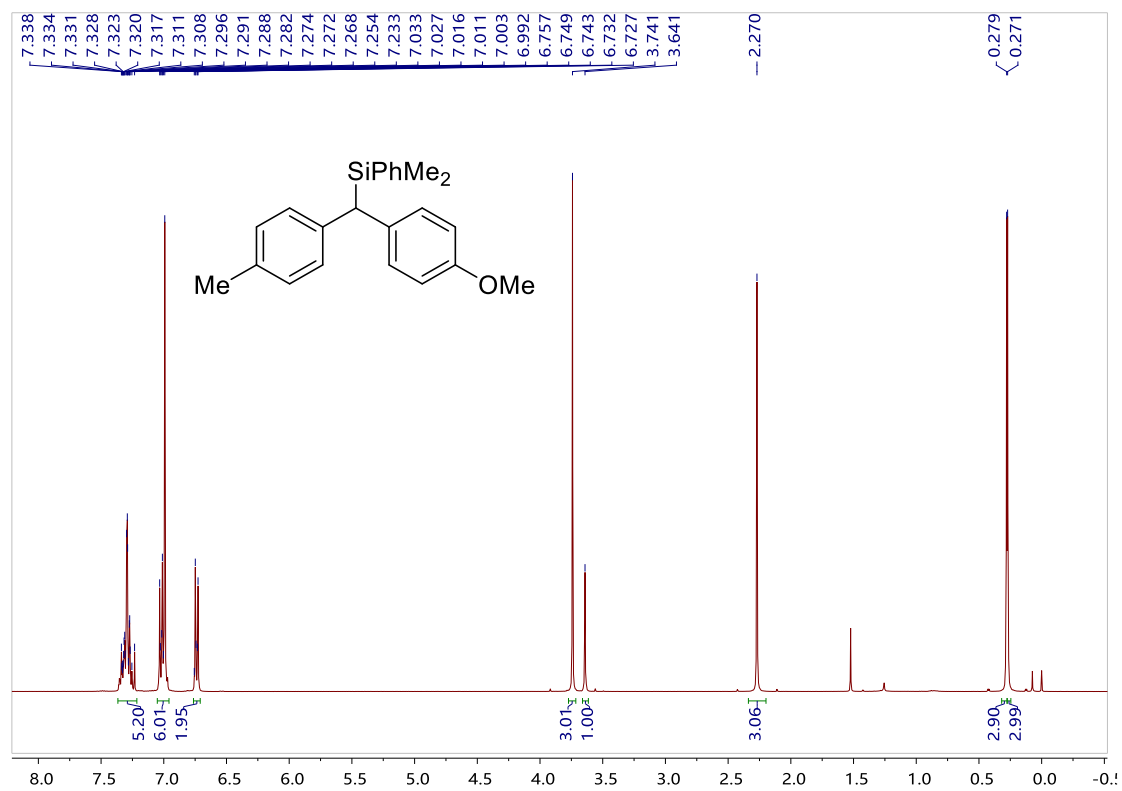
**(-)-((4-chlorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P28)**



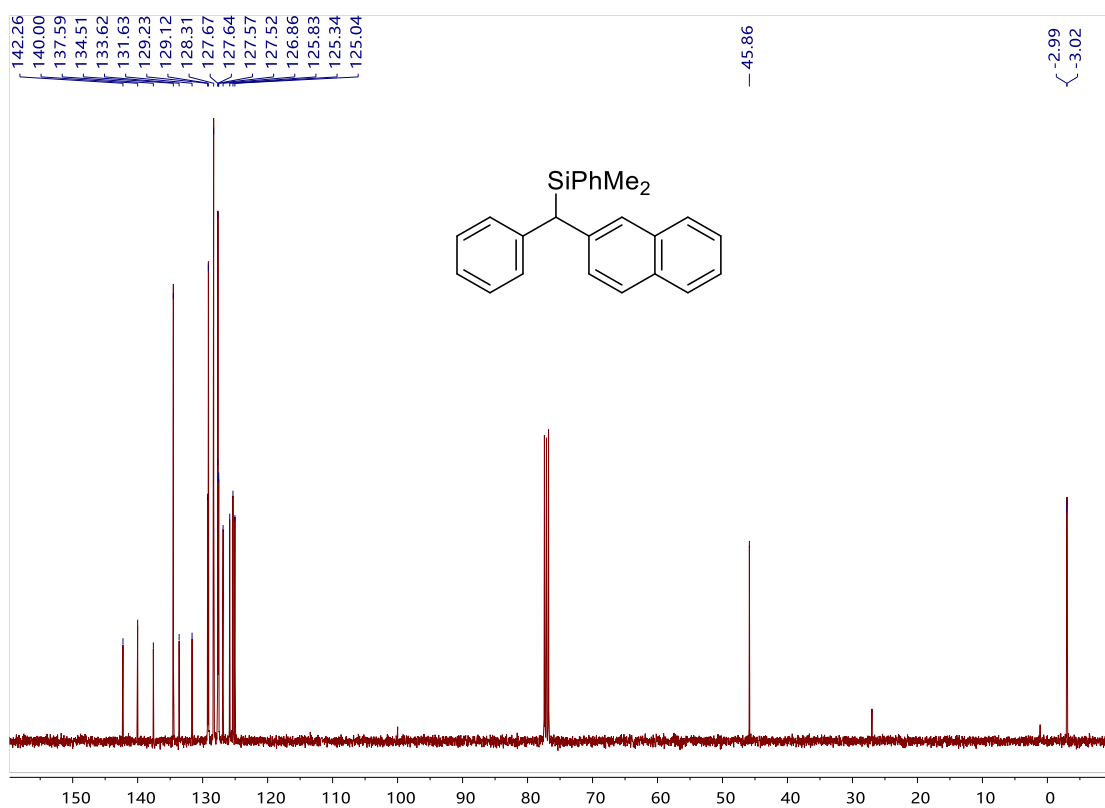
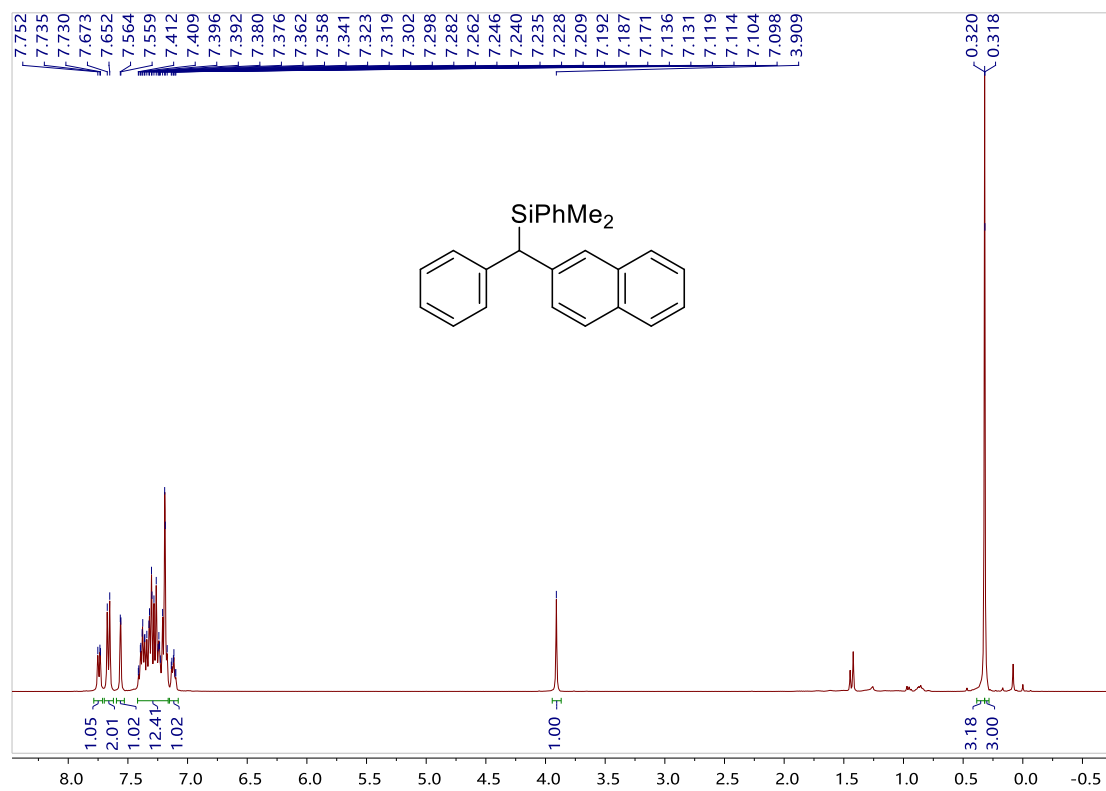
**(R)-((4-fluorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P29)**



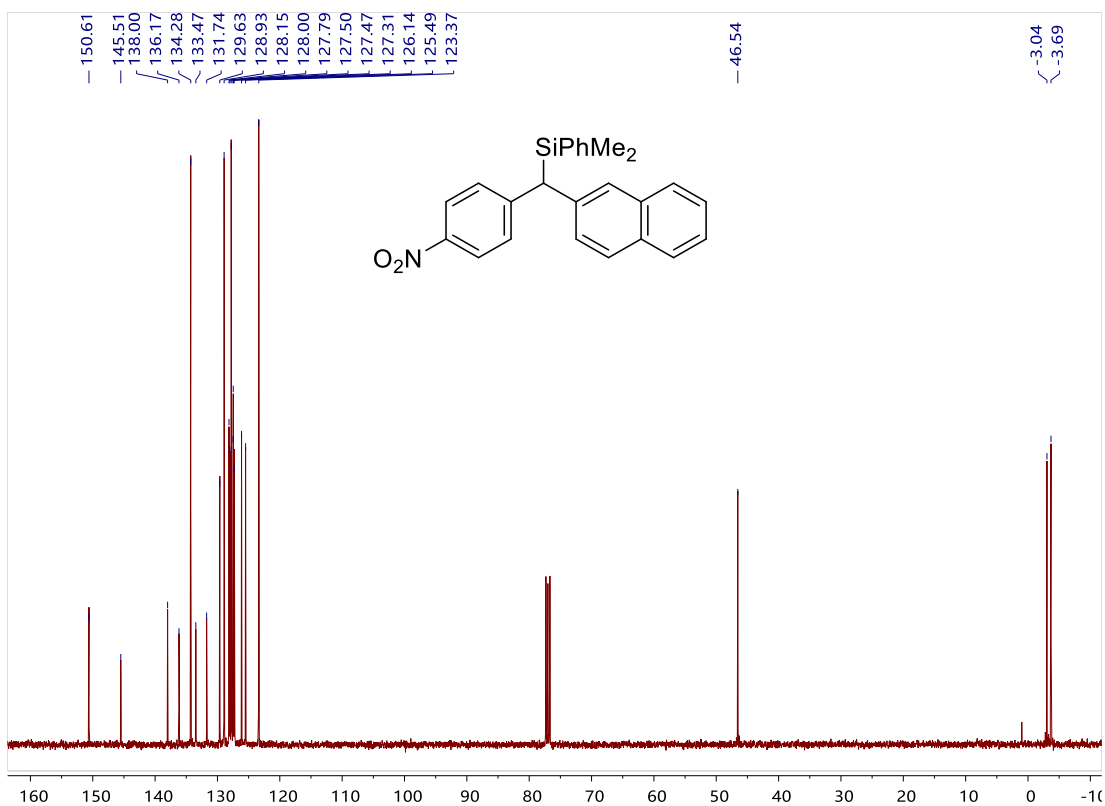
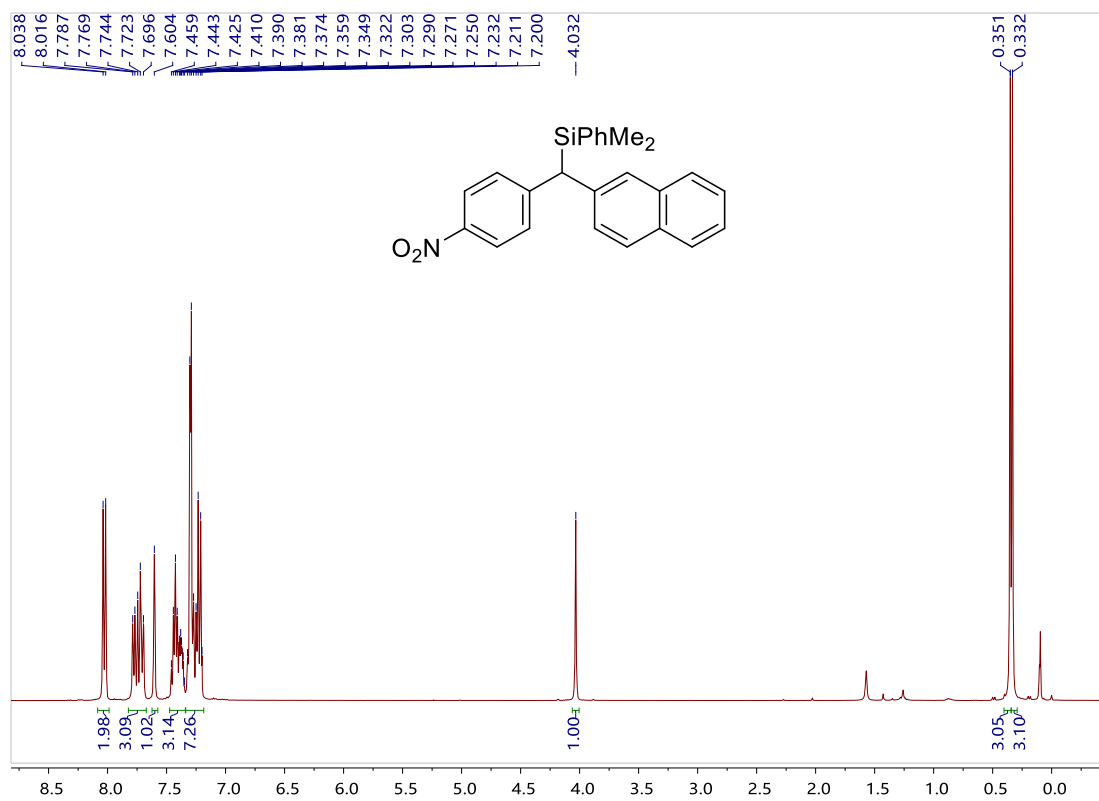
**(-)-((4-methoxyphenyl)(p-tolyl)methyl)dimethyl(phenyl)silane (P30)**



**(+)-dimethyl(naphthalen-2-yl(phenyl)methyl)(phenyl)silane (P31)**

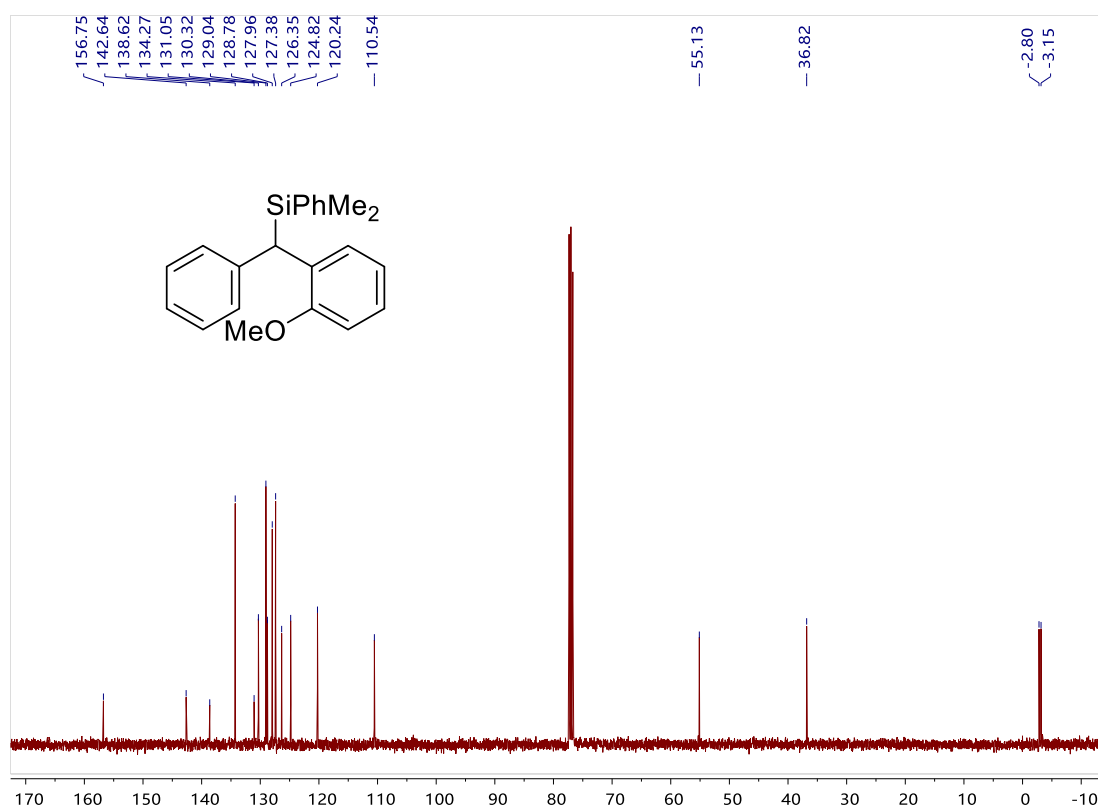
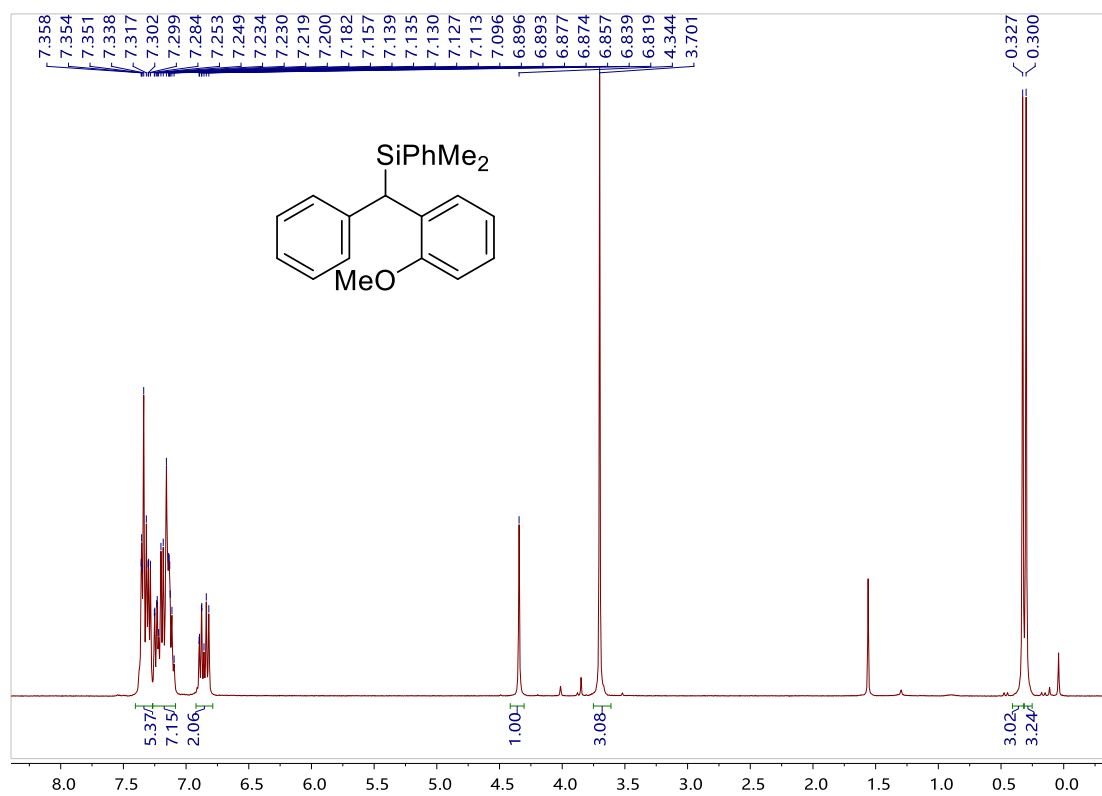


**(-)-dimethyl(naphthalen-2-yl(4-nitrophenyl)methyl)(phenyl)silane (P32)**

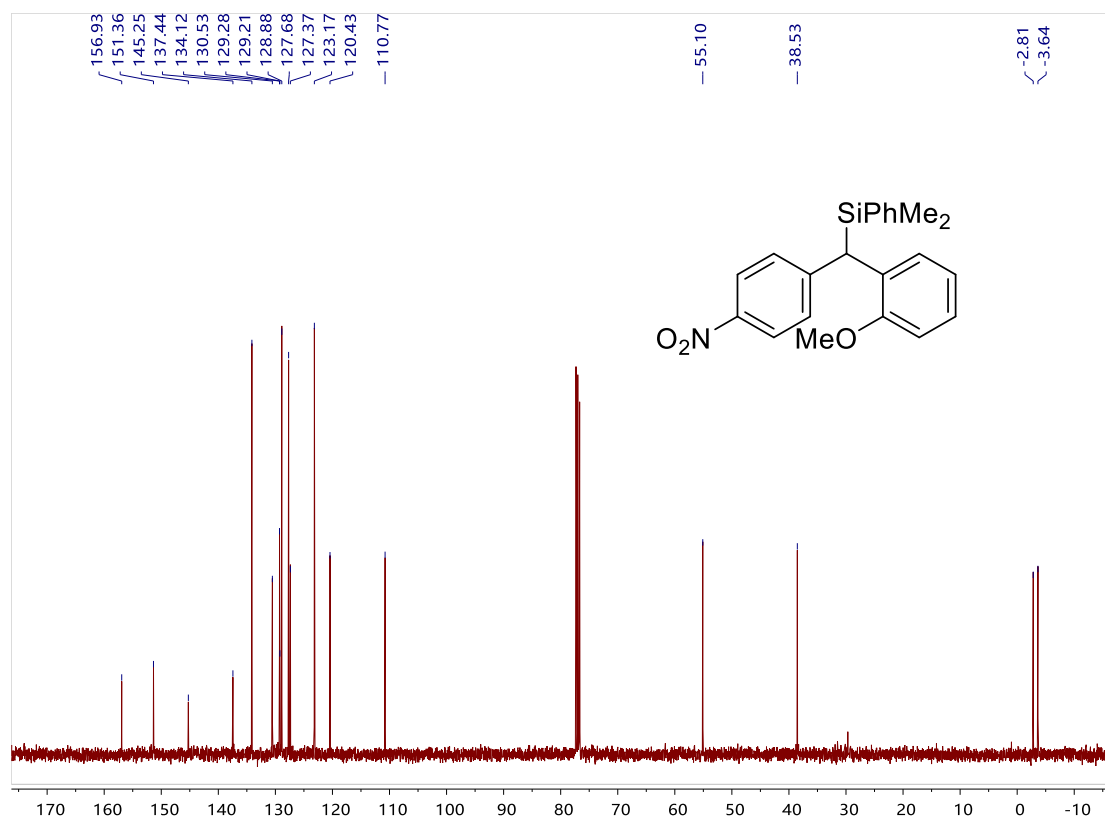
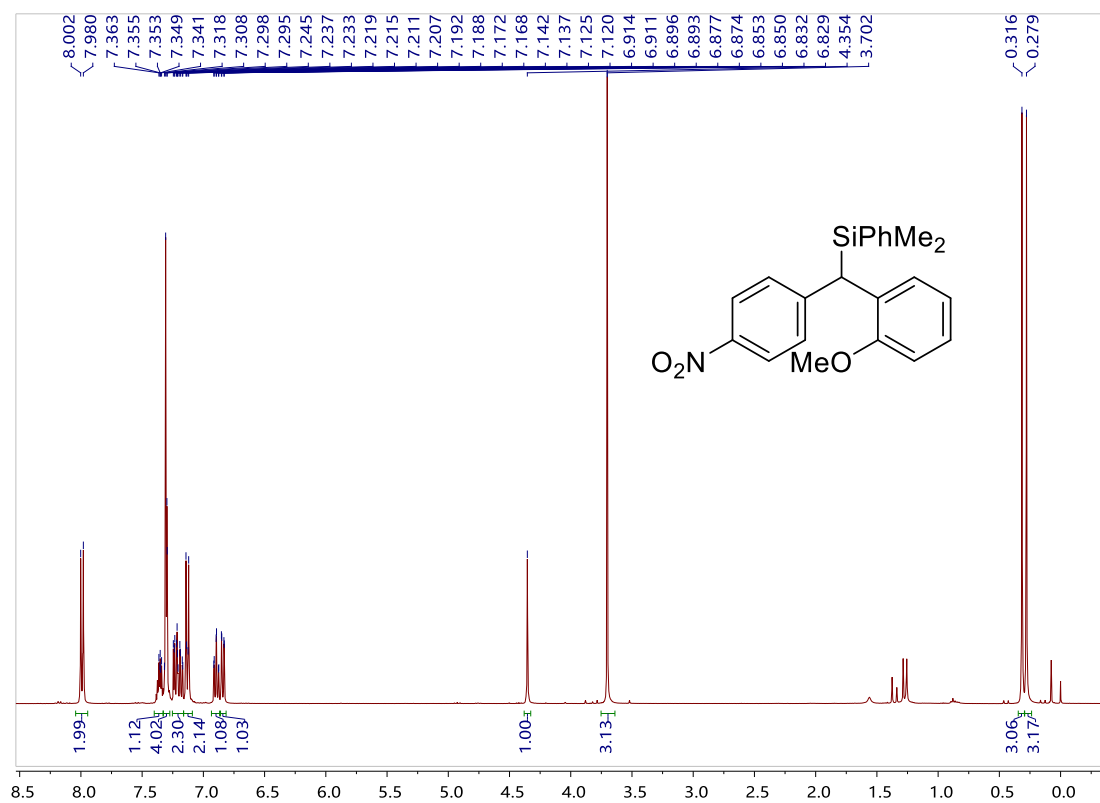




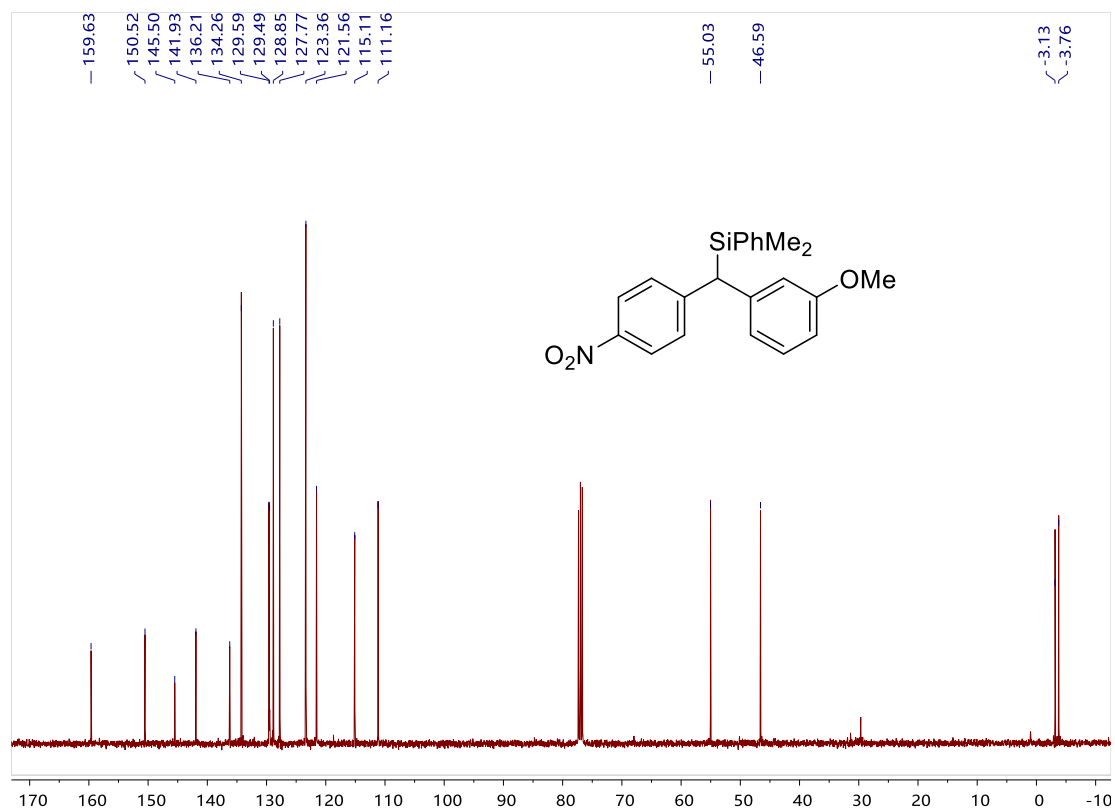
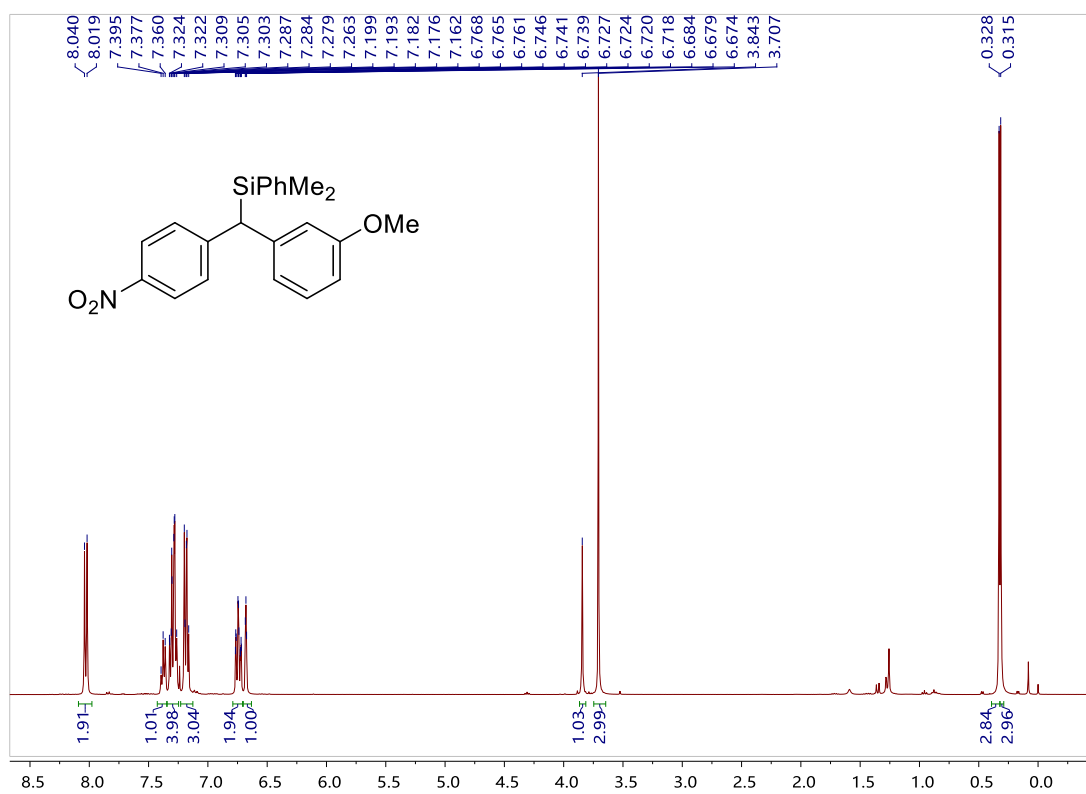
**(-)-((2-methoxyphenyl)(phenyl)methyl)dimethyl(phenyl)silane (P33)**



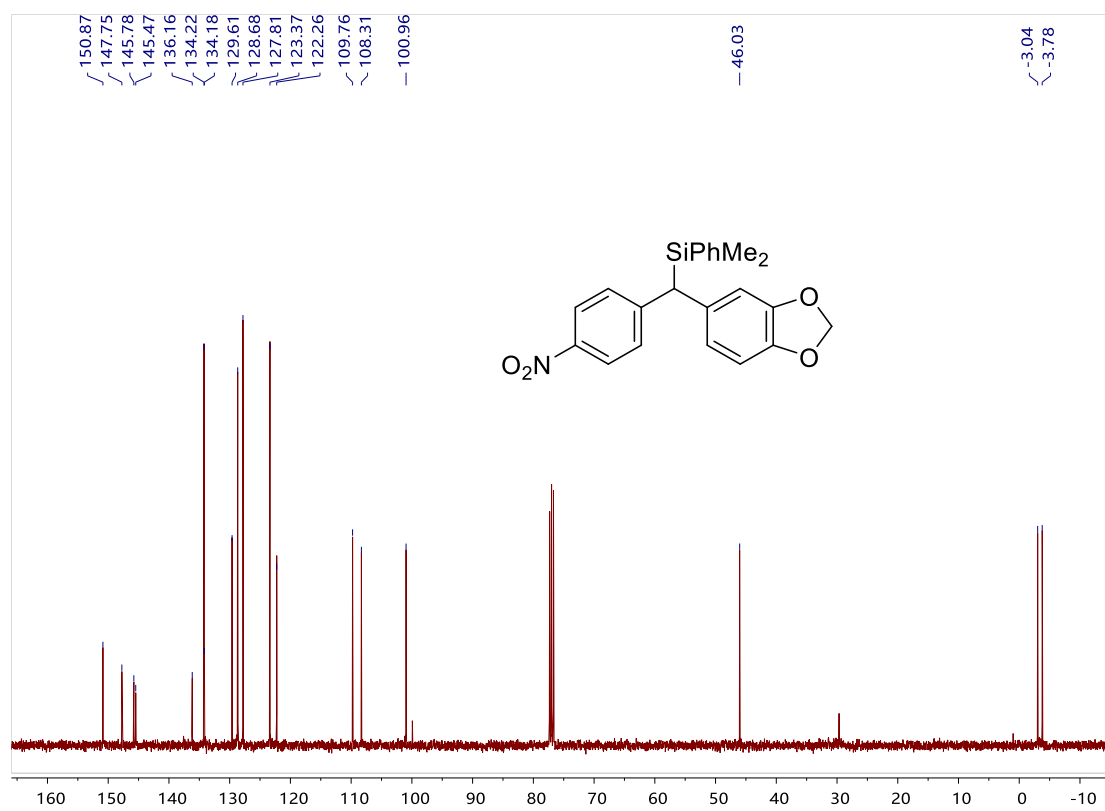
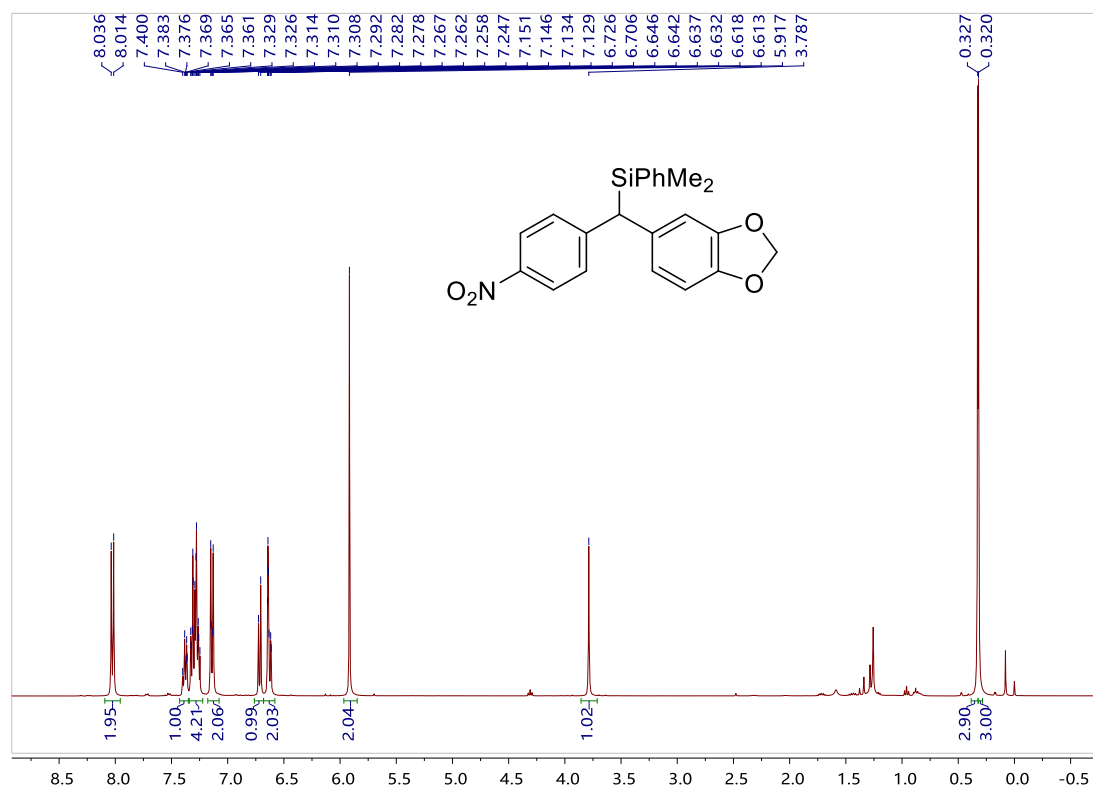
**(-)-((2-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P34)**



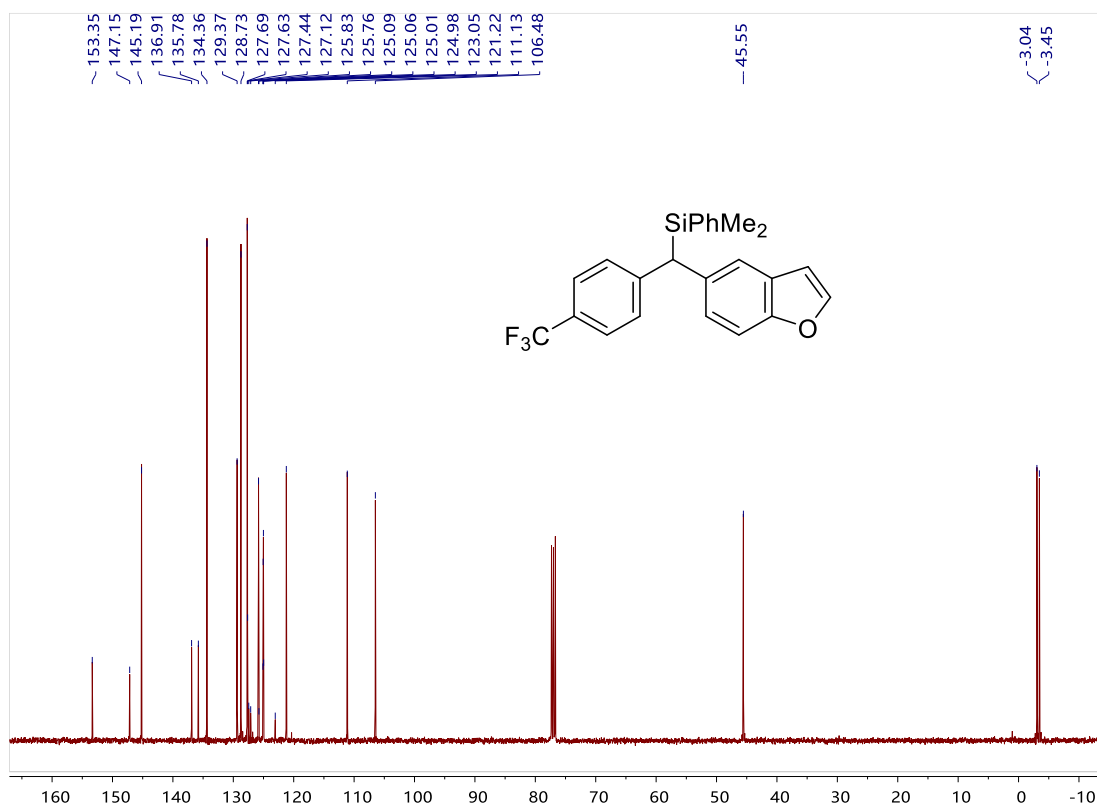
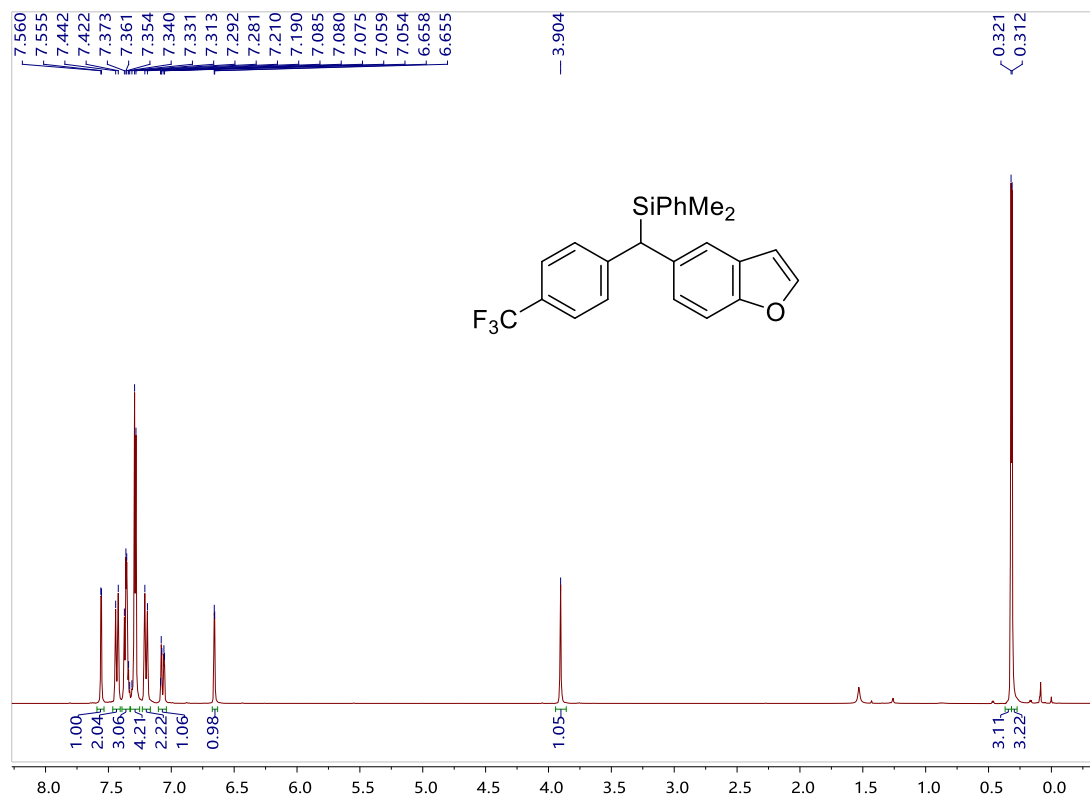
**(-)-((3-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P35)**



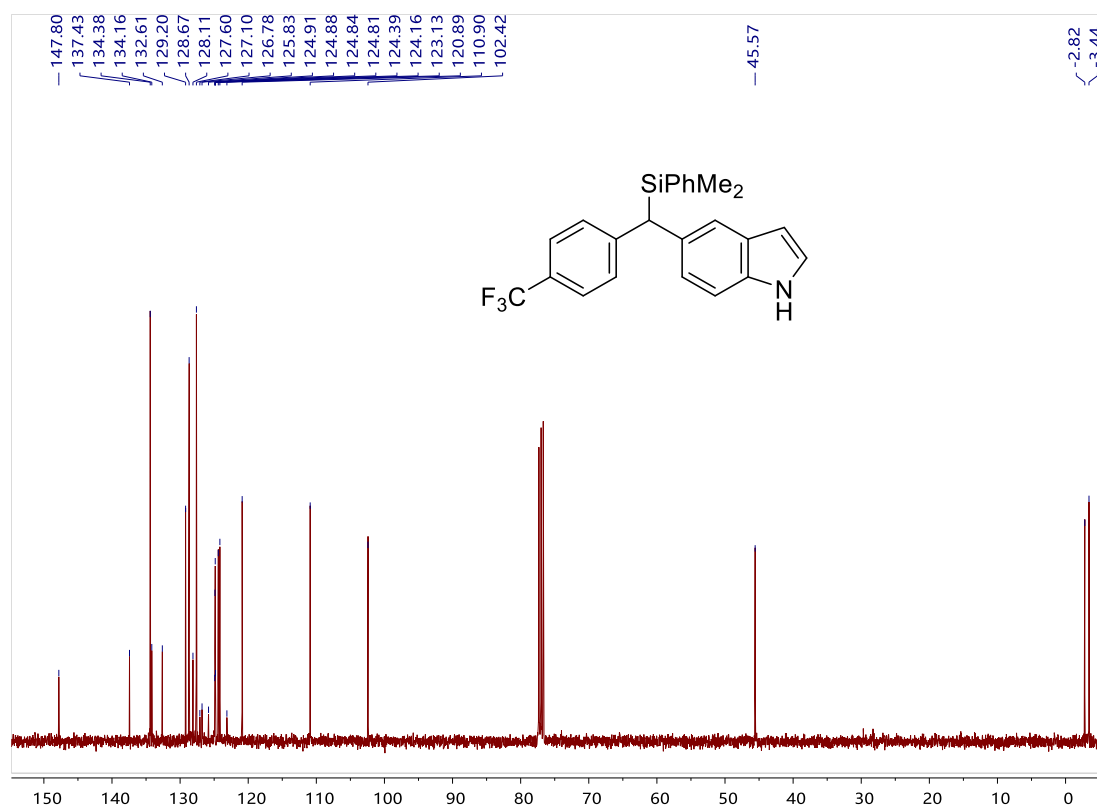
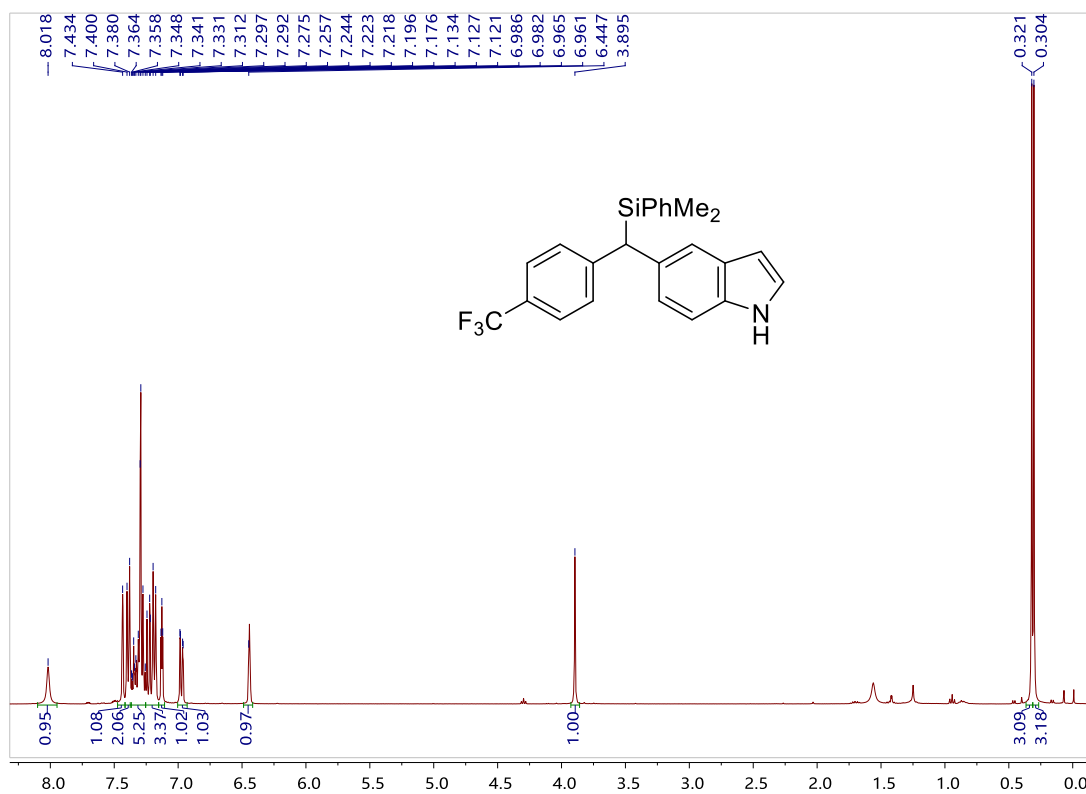
**(-)-(benzo[d][1,3]dioxol-5-yl(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P36)**



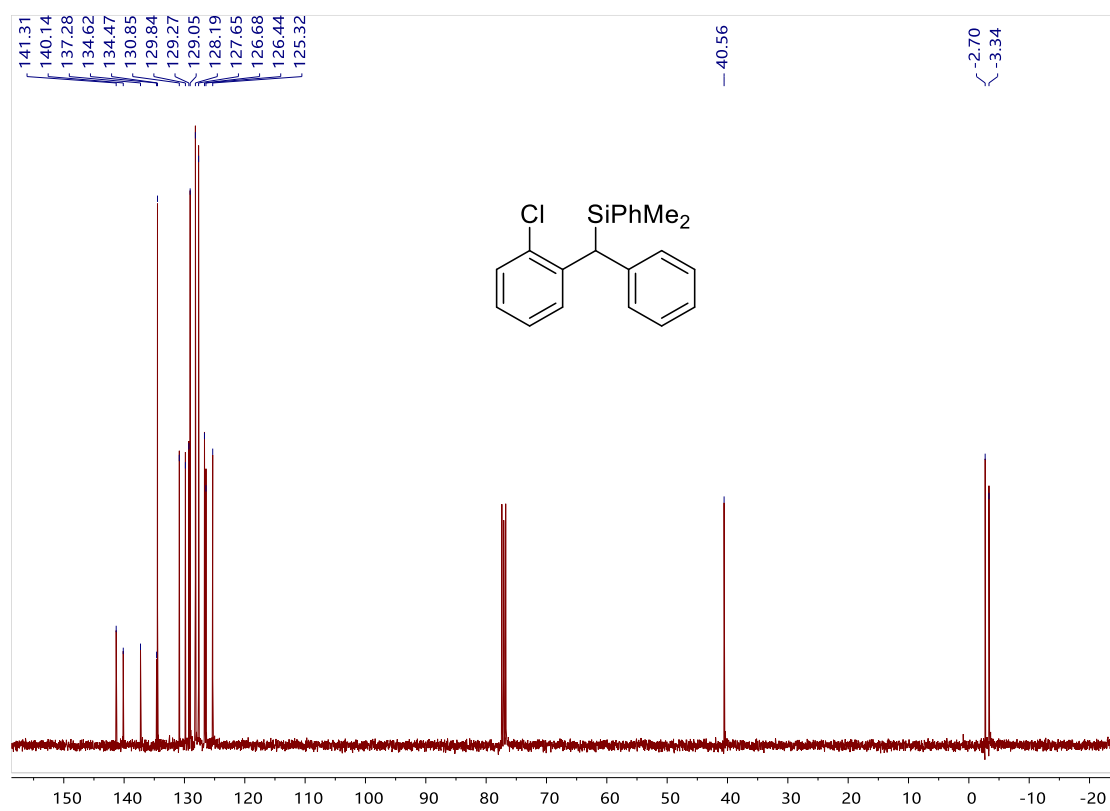
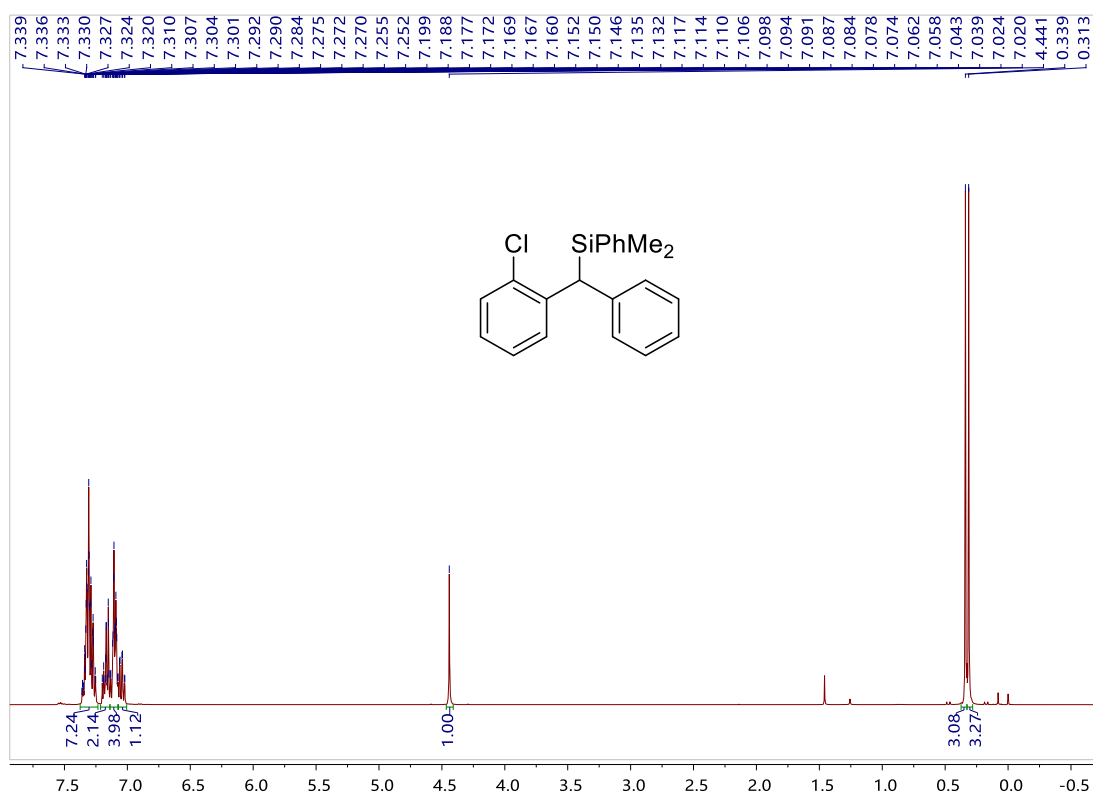
**(-)-(benzofuran-5-yl(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P37)**



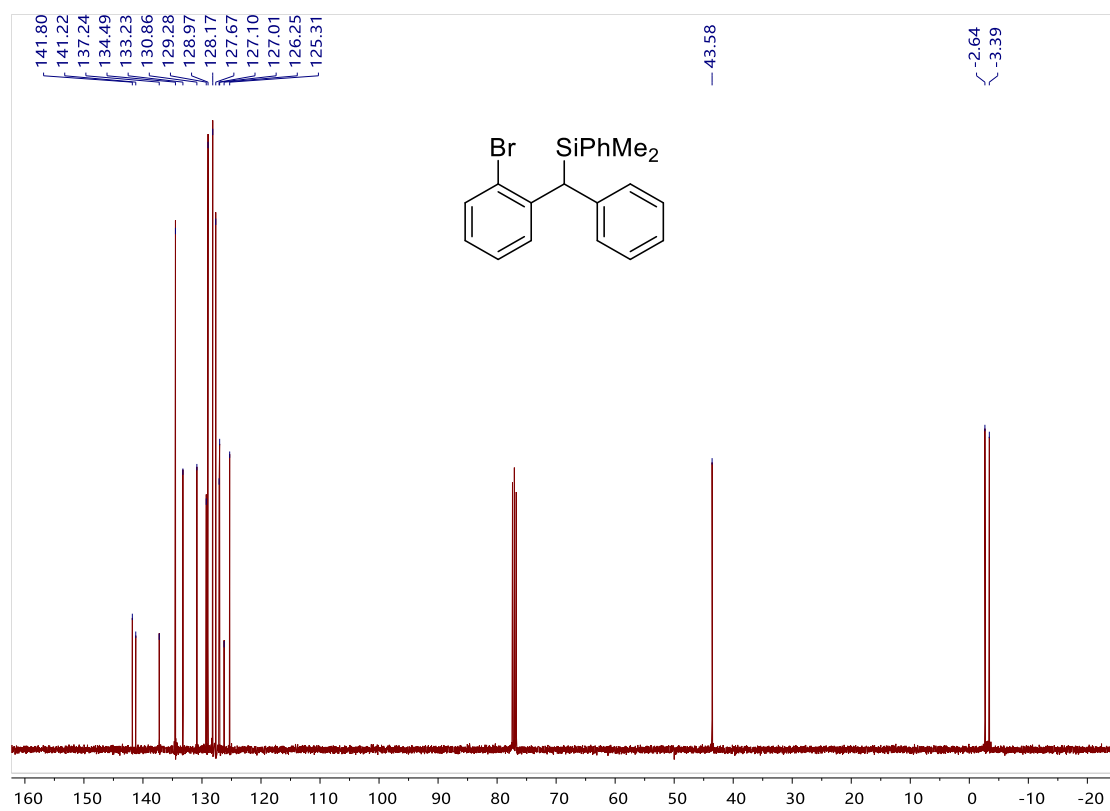
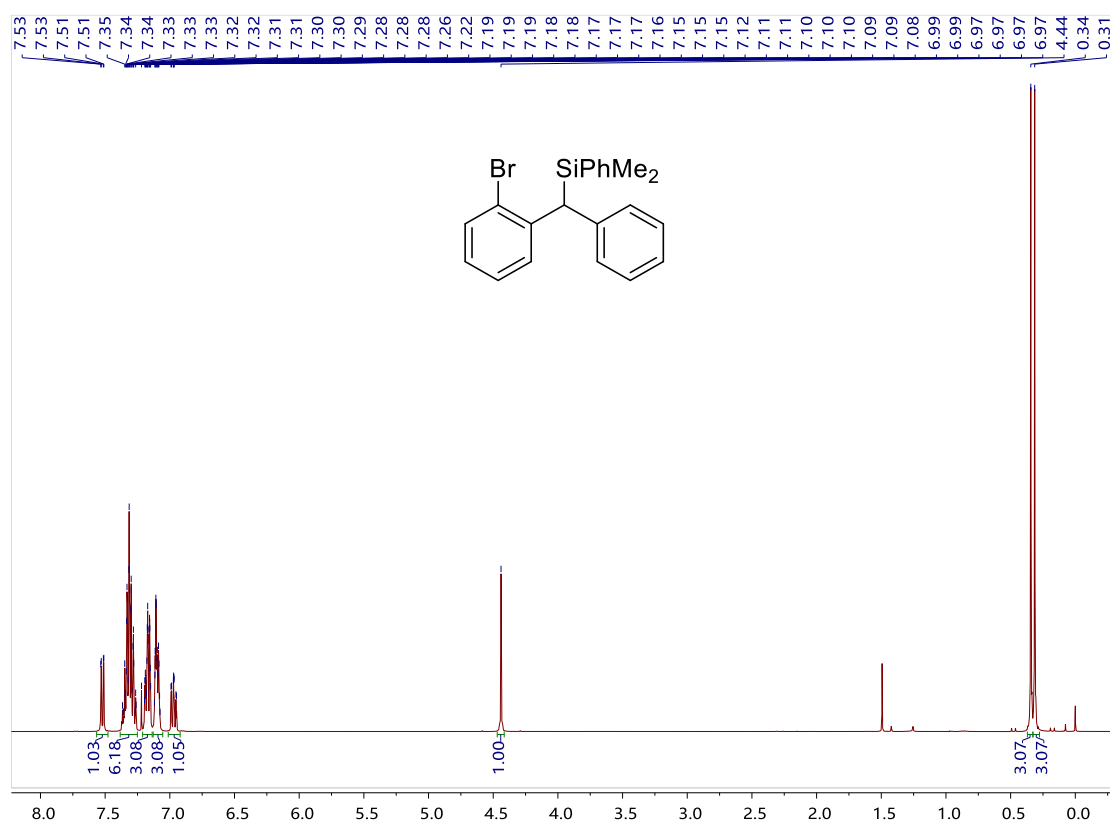
**(-)-5-((dimethyl(phenyl)silyl)(4-(trifluoromethyl)phenyl)methyl)-1H-indole (P38)**



**(+)-(2-chlorophenyl)(phenyl)methyl dimethyl(phenyl)silane (P39)**

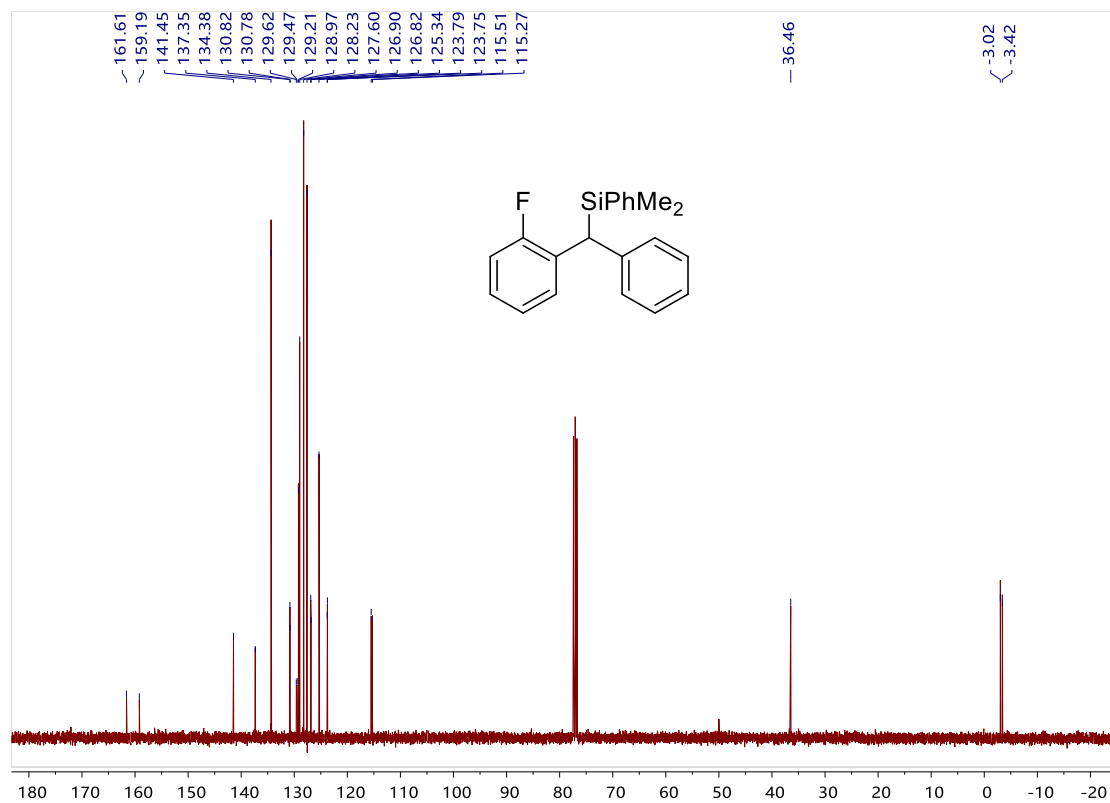
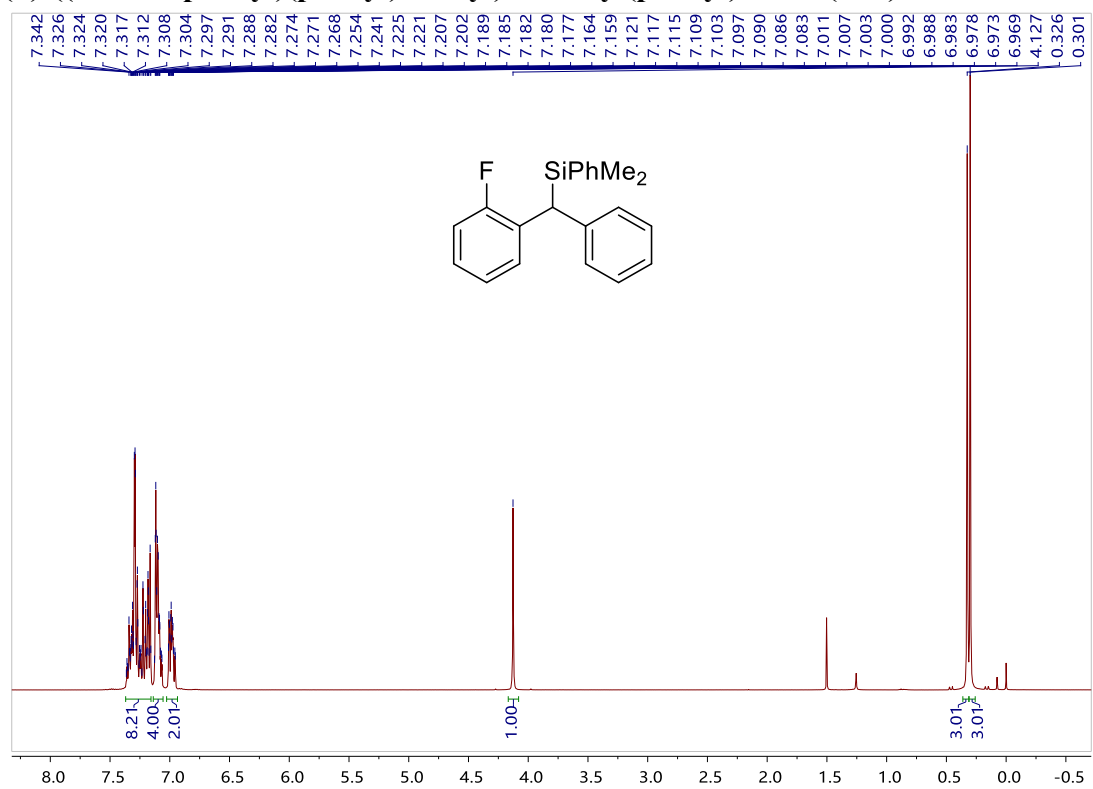


**(+)-(2-bromophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P40)**

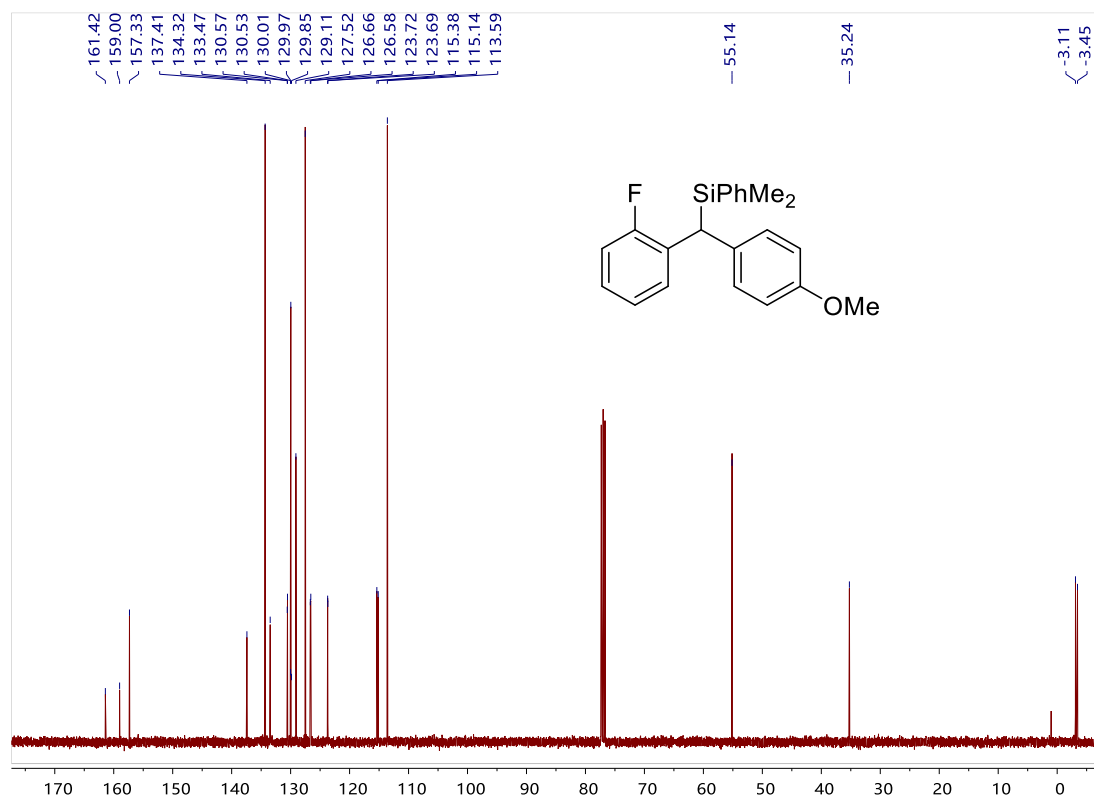
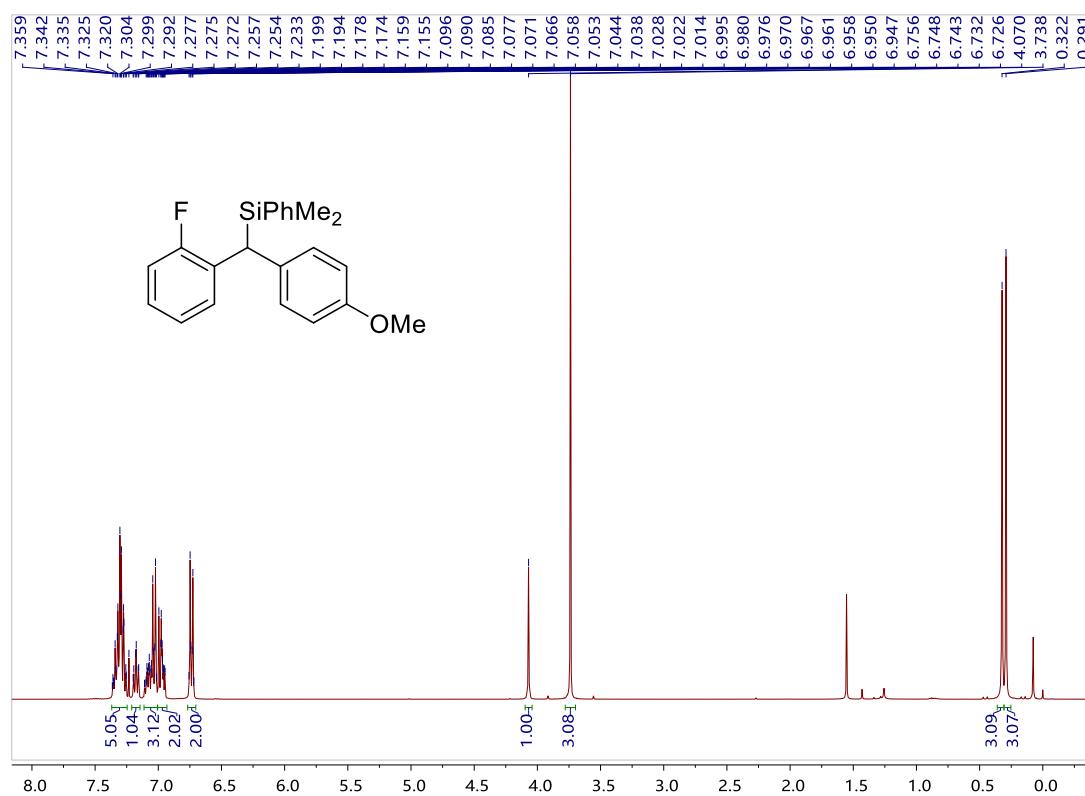




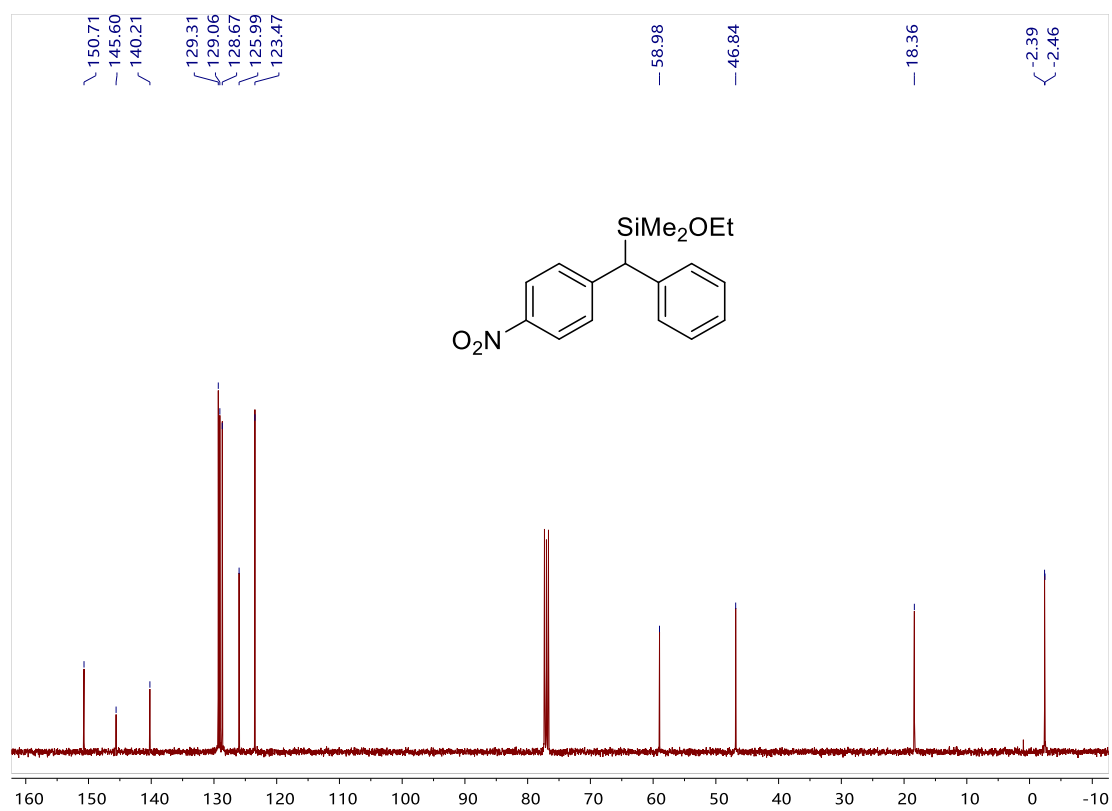
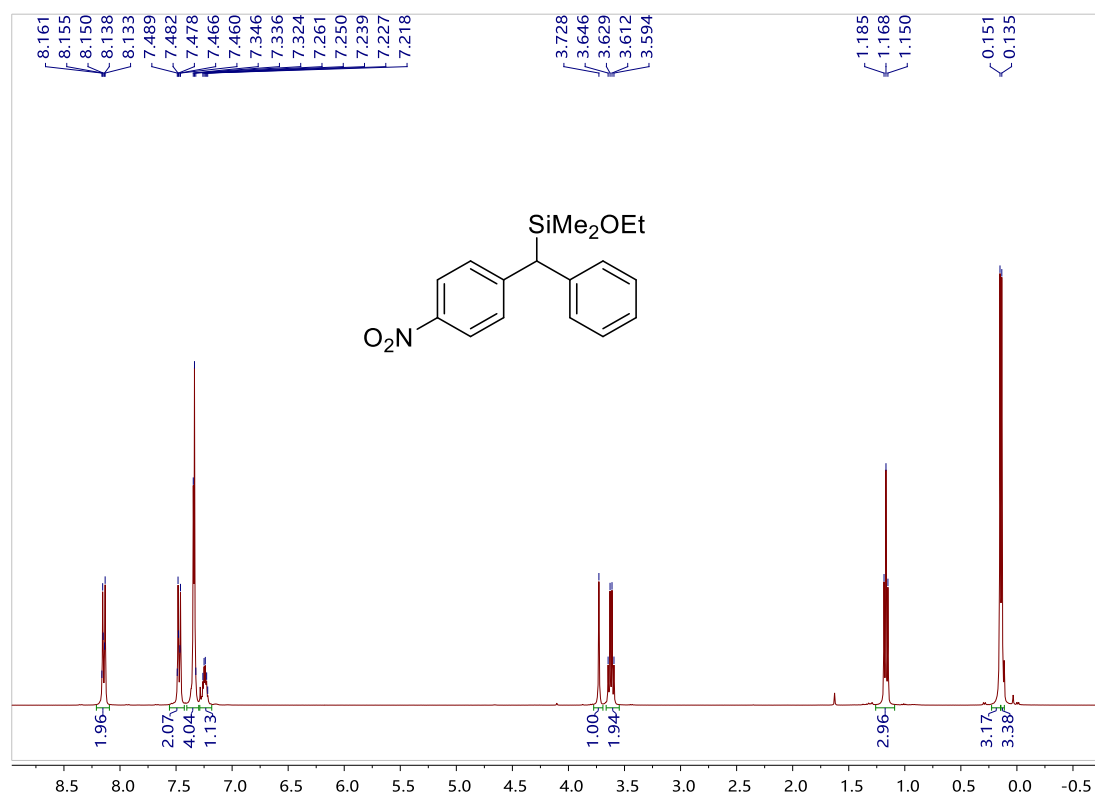
**(+)-(2-fluorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P41)**



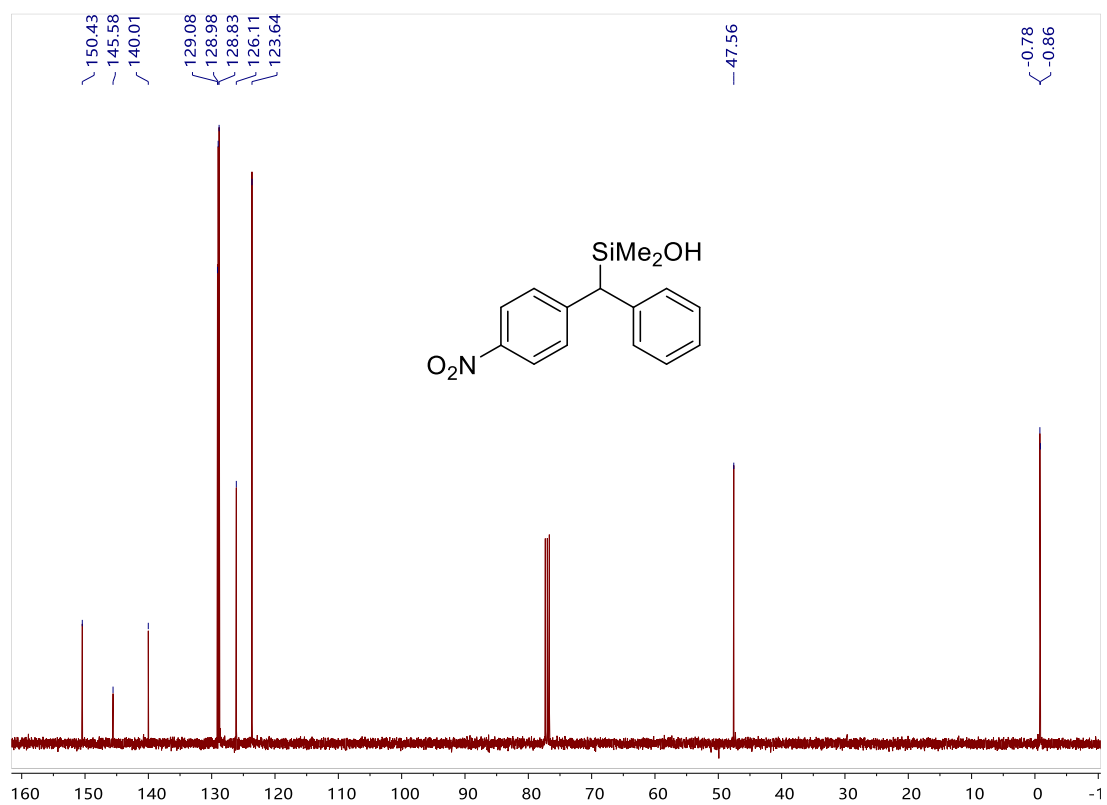
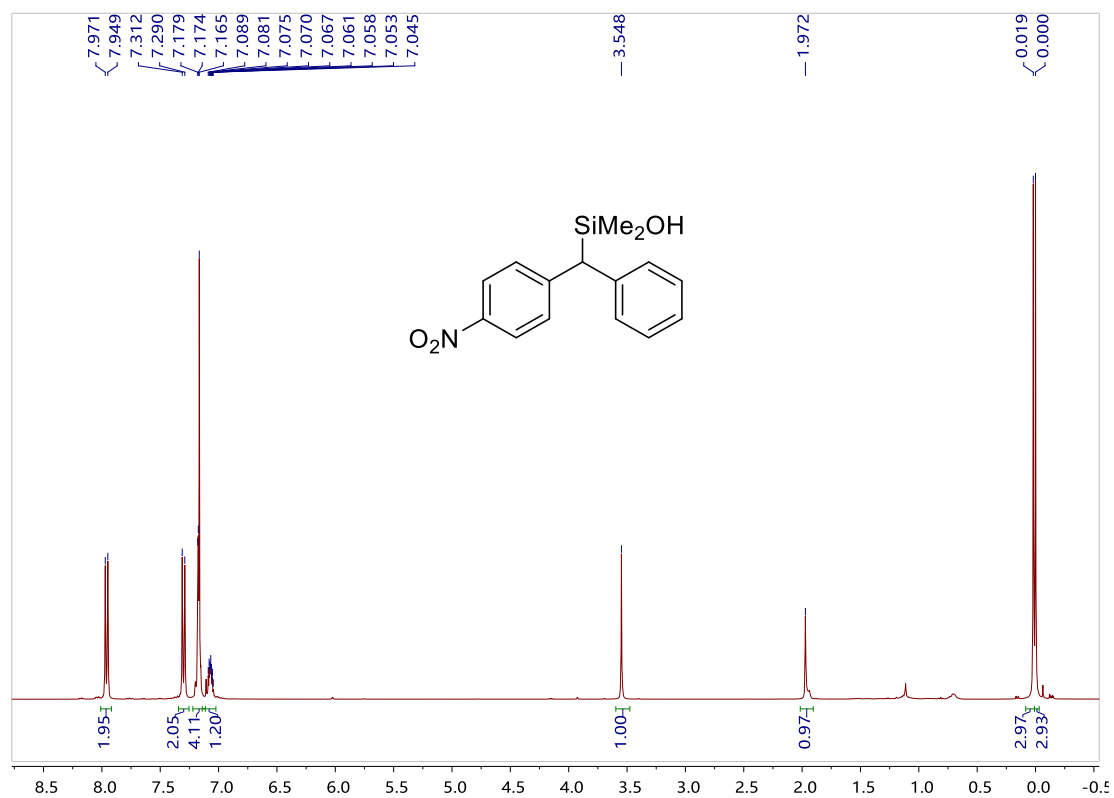
**(-)-((2-fluorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P42)**



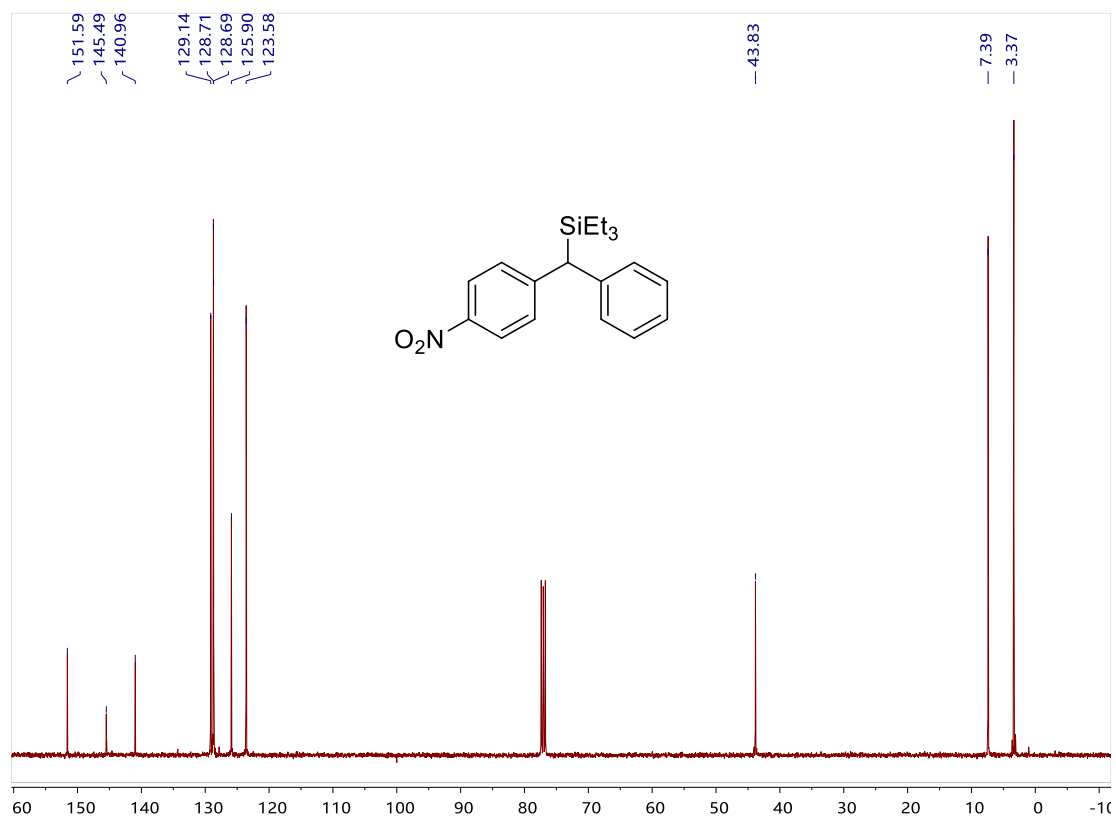
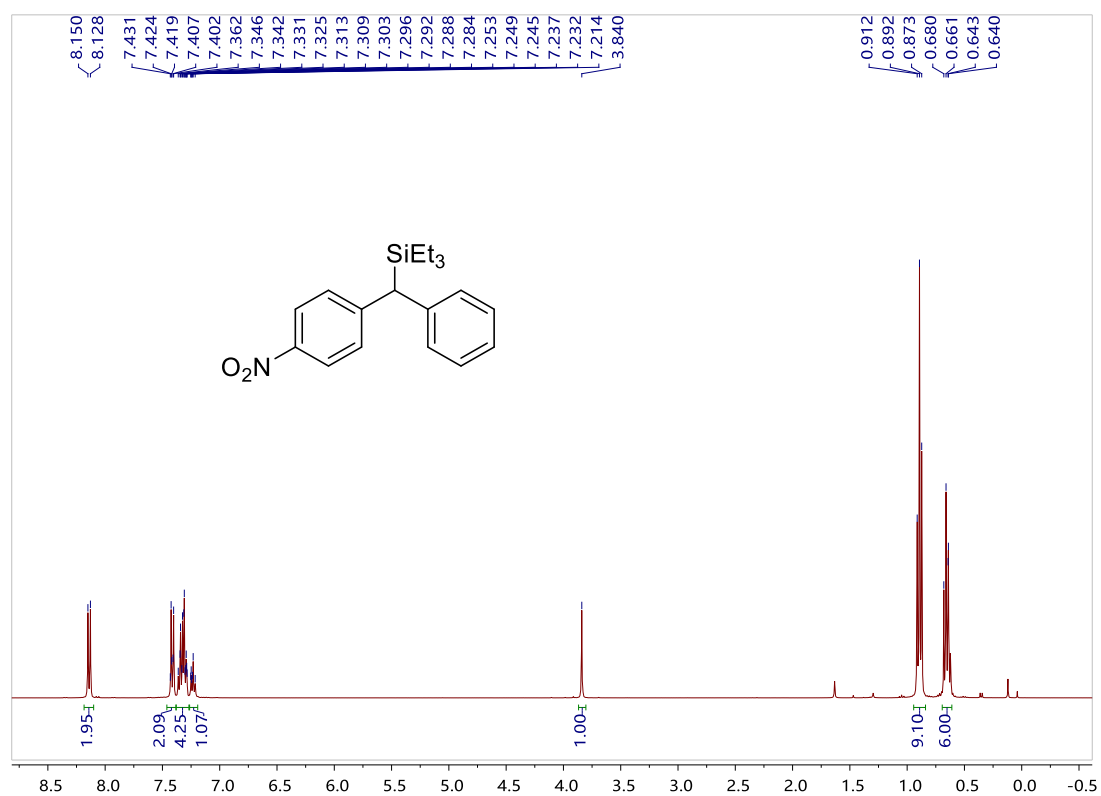
**(-)-ethoxydimethyl((4-nitrophenyl)(phenyl)methyl)silane (P43)**



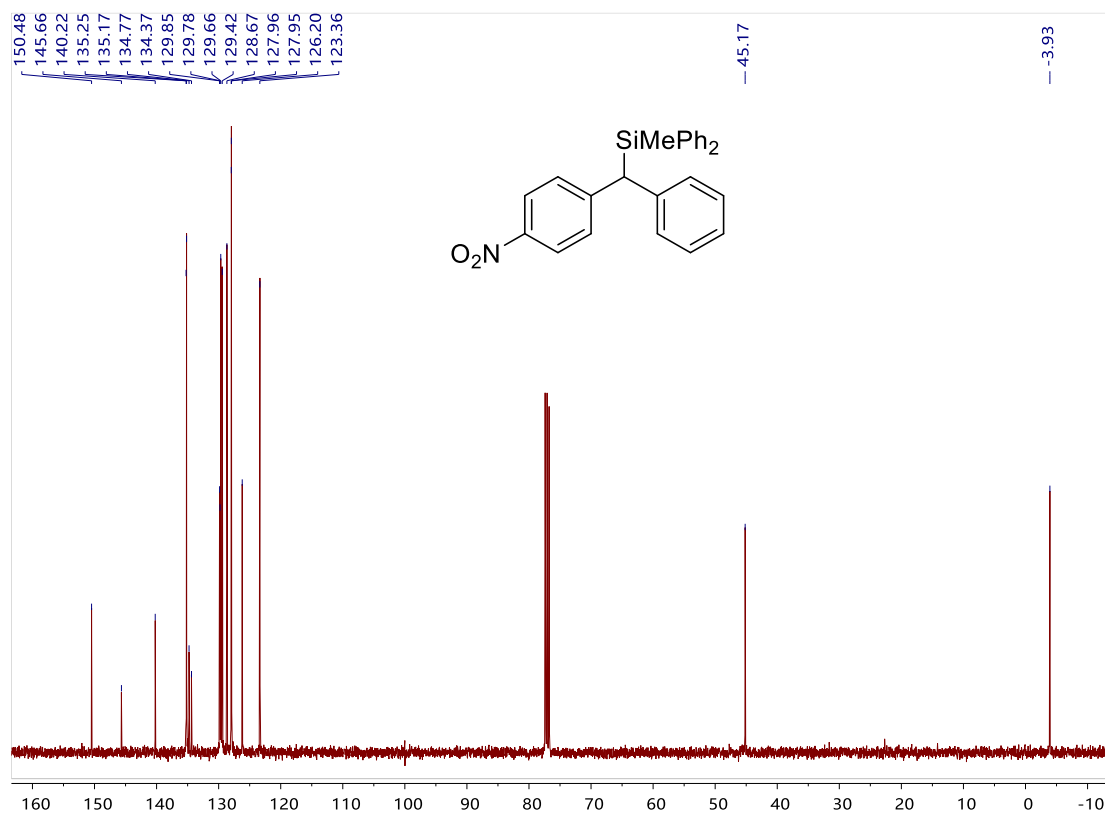
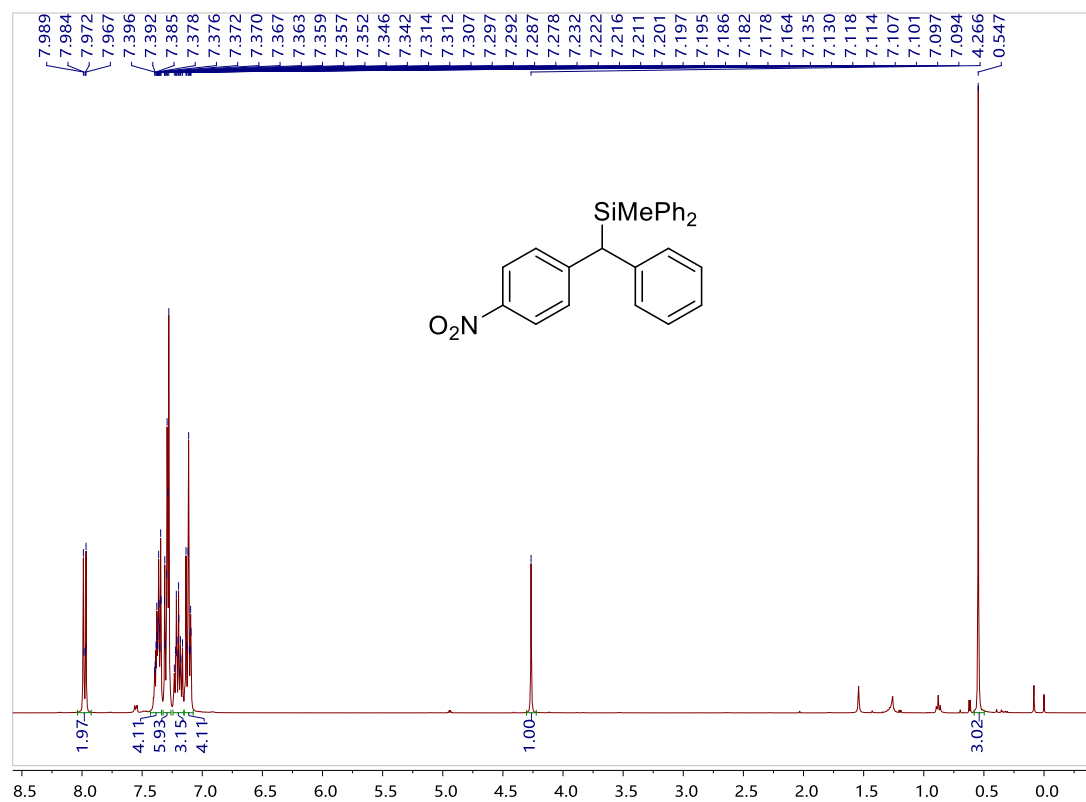
**(-)-dimethyl((4-nitrophenyl)(phenyl)methyl)silanol (P44)**



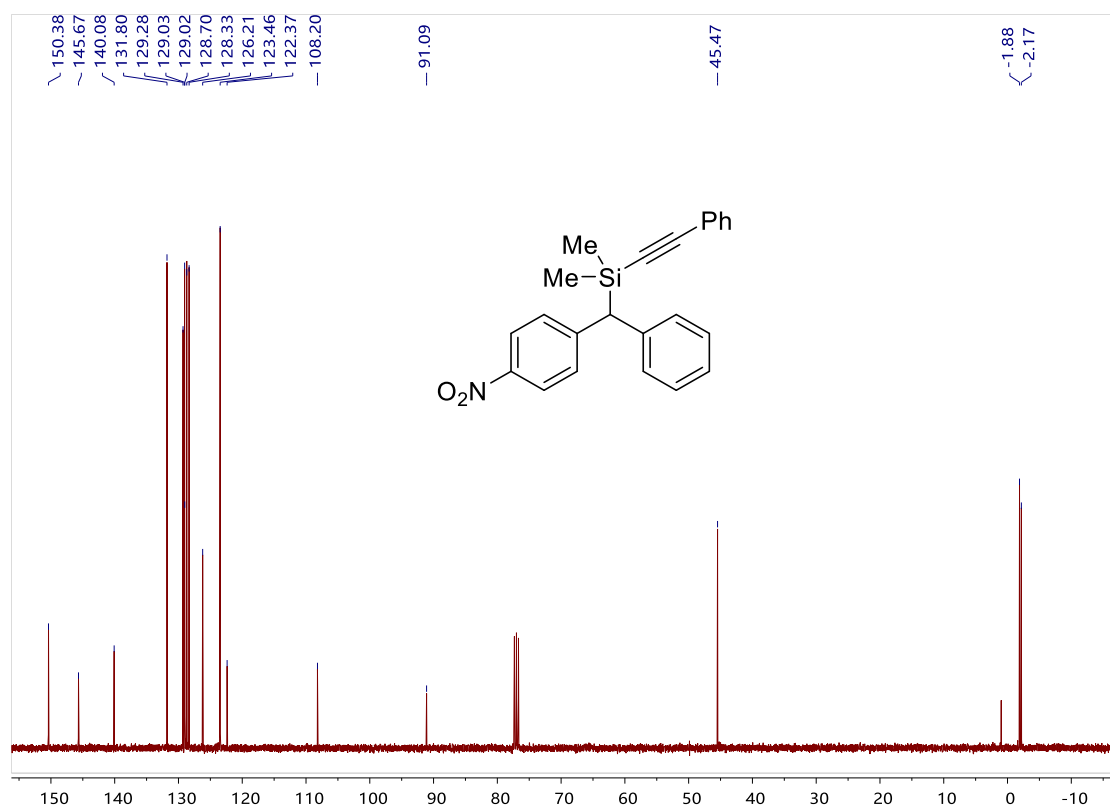
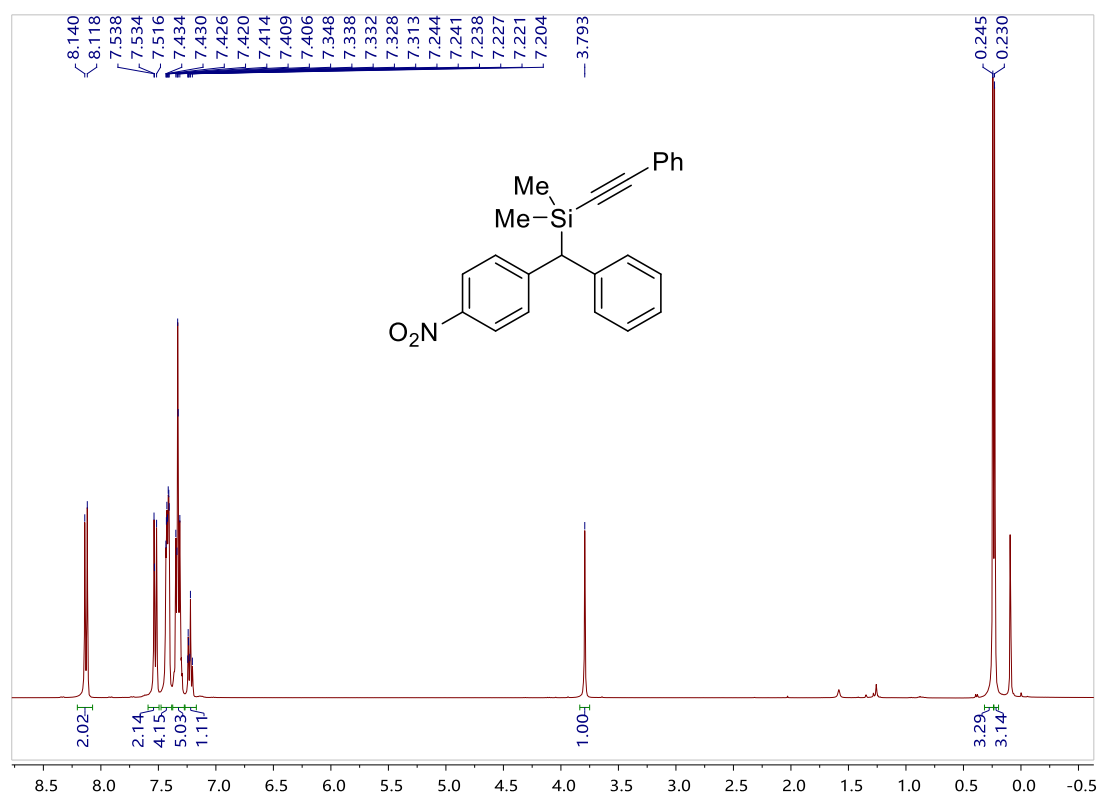
**(-)-triethyl((4-nitrophenyl)(phenyl)methyl)silane (P45)**



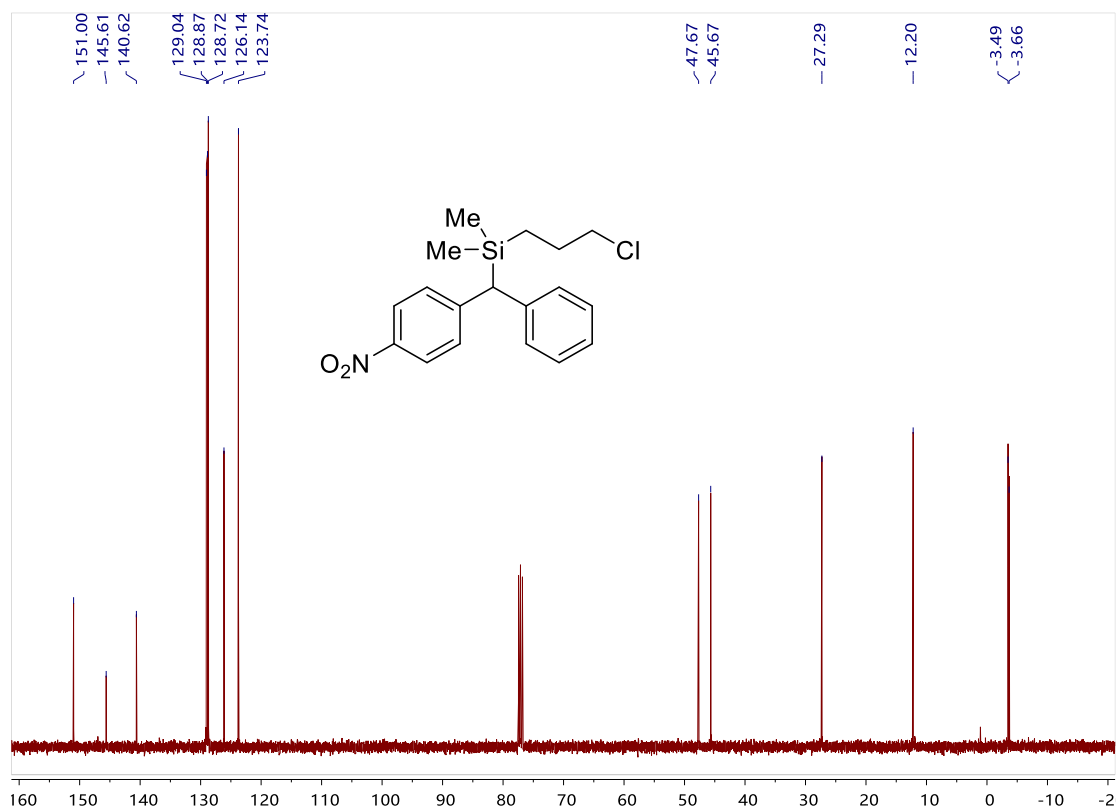
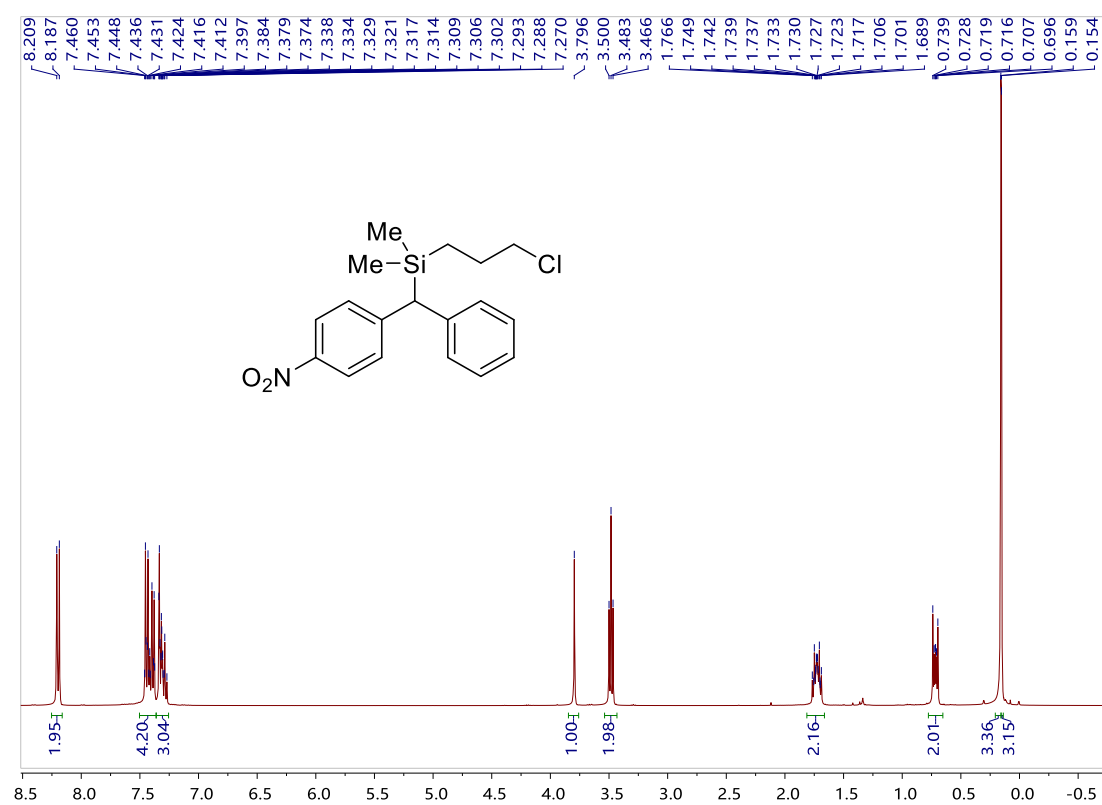
**(-)-methyl((4-nitrophenyl)(phenyl)methyl)diphenylsilane (P46)**



**(S)-dimethyl((4-nitrophenyl)(phenyl)methyl)(phenylethynyl)silane (P47)**

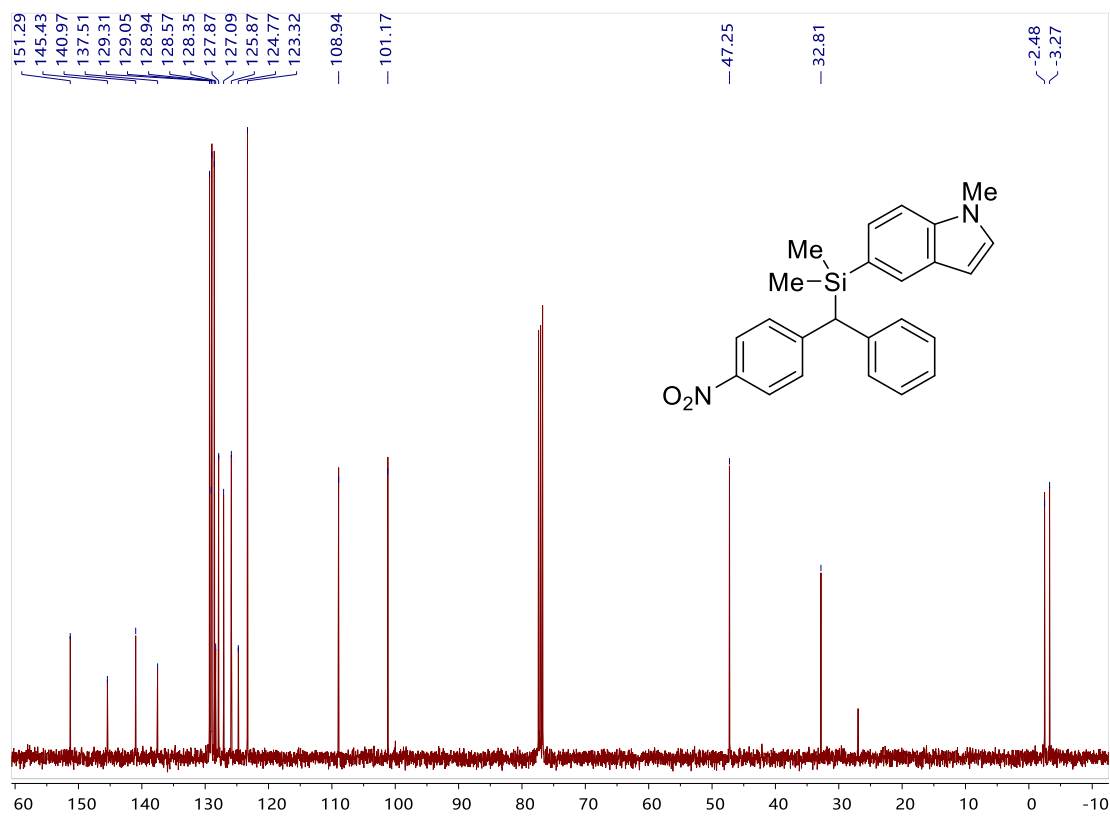
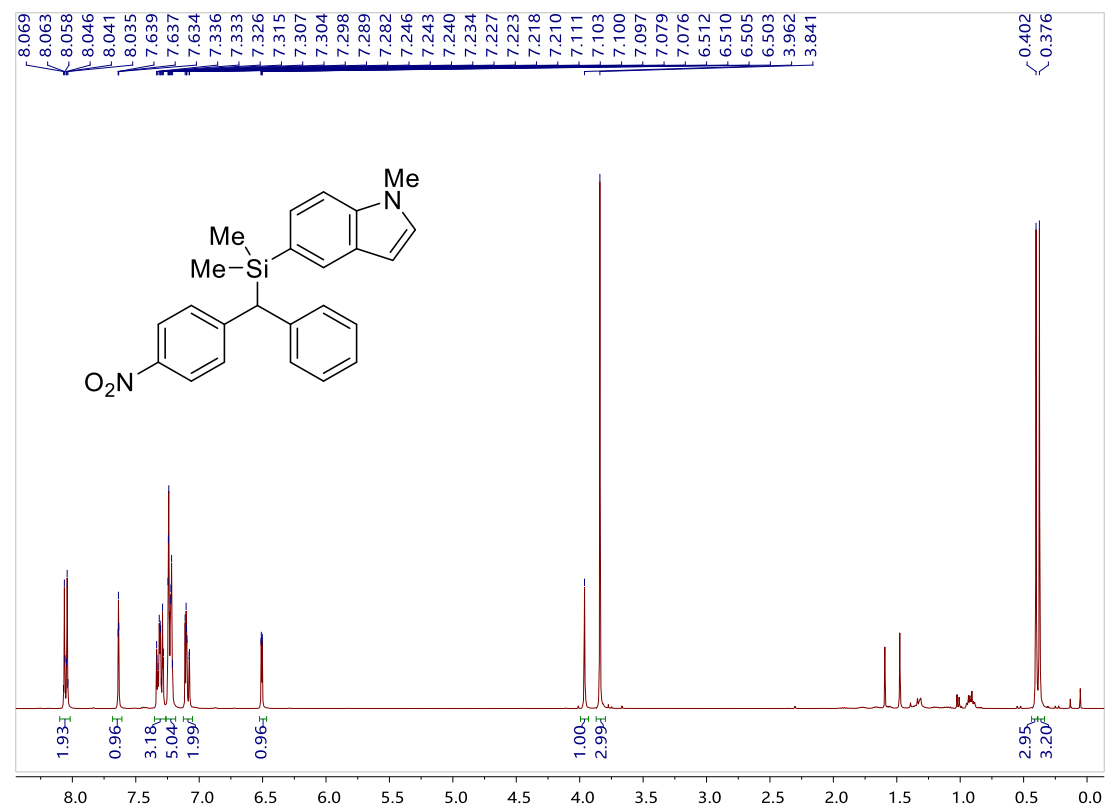


**(-)-(3-chloropropyl)dimethyl((4-nitrophenyl)(phenyl)methyl)silane (P48)**



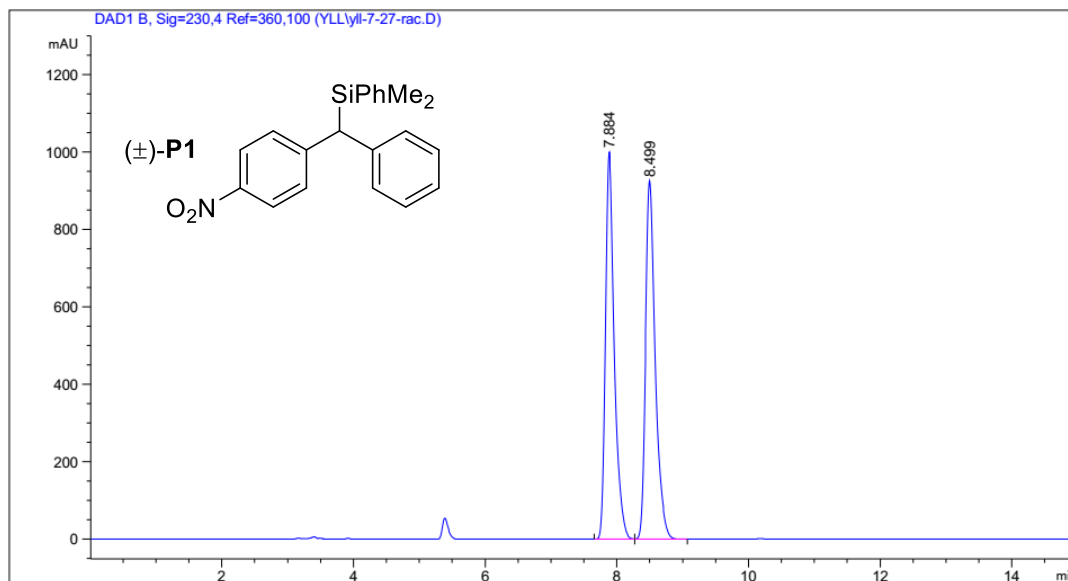


**(-)-5-(dimethyl((4-nitrophenyl)(phenyl)methyl)silyl)-1-methyl-1H-indole (P49)**

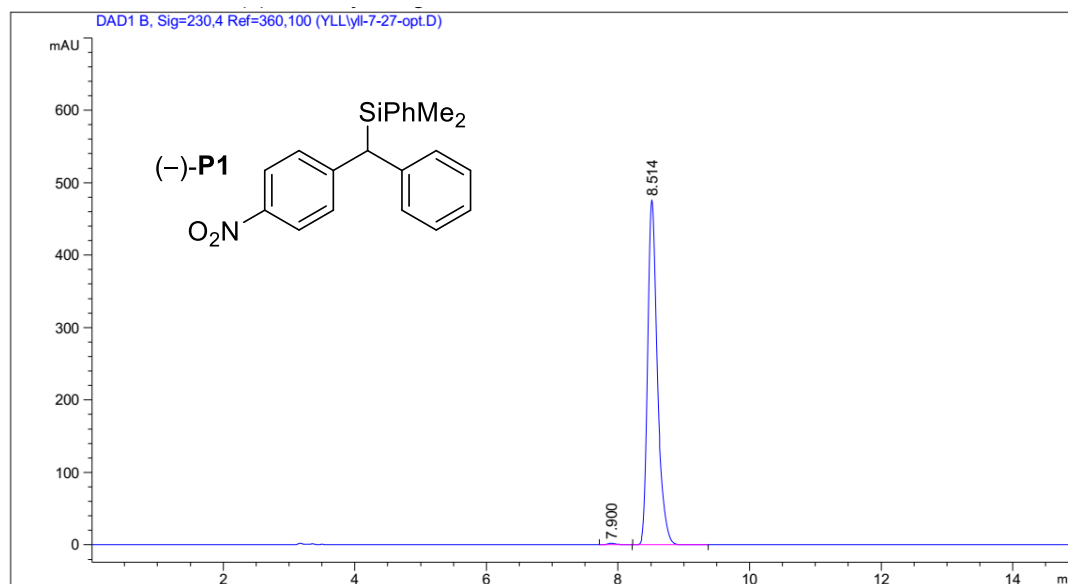


# 11 HPLC charts

## (-)-dimethyl((4-nitrophenyl)(phenyl)methyl)(phenyl)silane (P1)

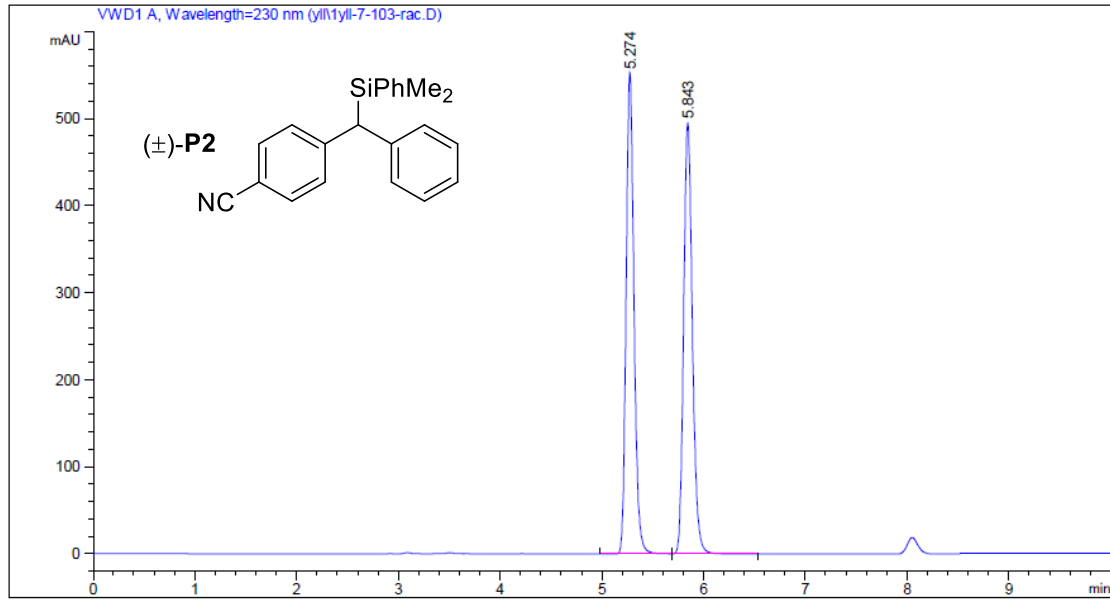


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.884	BB	0.1415	9391.26465	1000.48071	49.8194
2	8.499	BB	0.1534	9459.35254	924.58362	50.1806

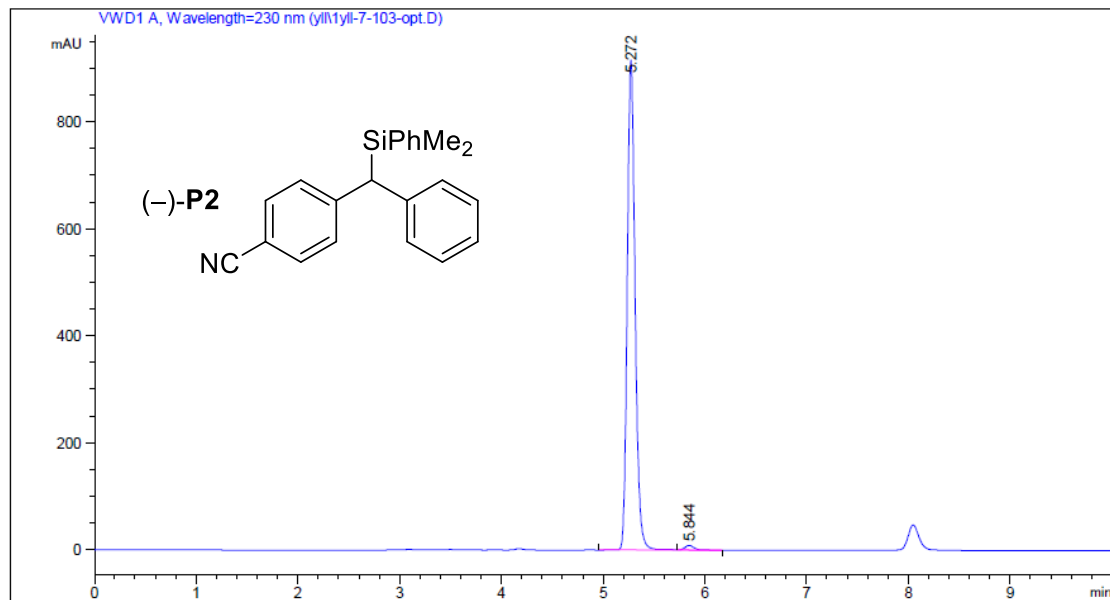


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.900	BB	0.1368	17.17072	1.87579	0.3543
2	8.514	BB	0.1525	4829.15332	475.51886	99.6457

**(±)-4-((dimethyl(phenyl)silyl)(phenyl)methyl)benzonitrile (P2)**

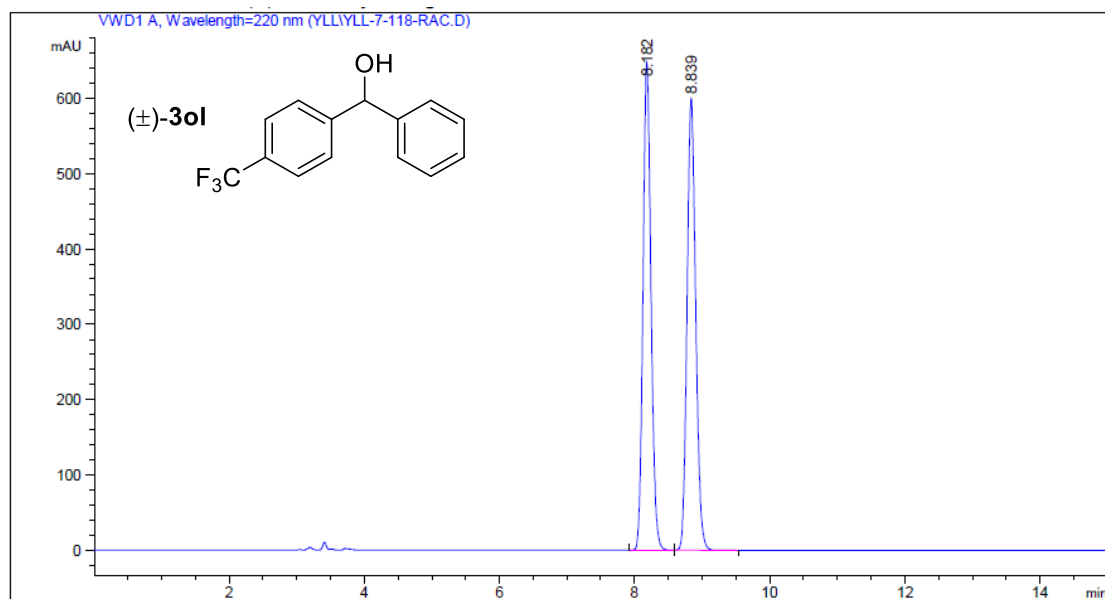


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.274	BB	0.0824	2962.58374	554.17719	50.0190
2	5.843	BB	0.0916	2960.33765	496.05014	49.9810

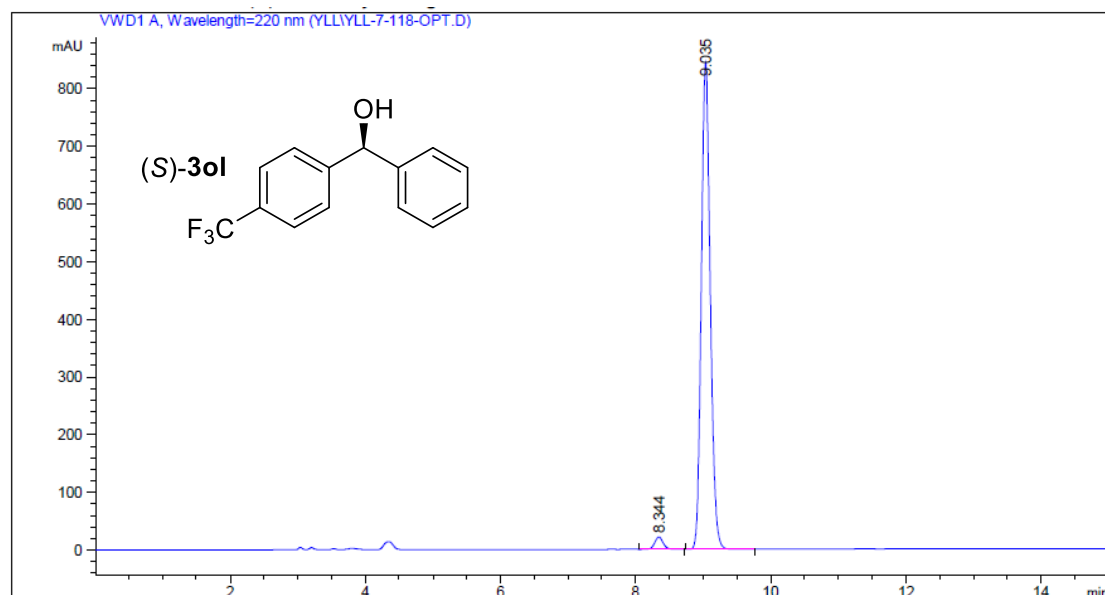


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.272	BV R	0.0824	4903.74463	916.12579	98.9345
2	5.844	VB E	0.0938	52.81038	8.58474	1.0655

### (S)-phenyl(4-(trifluoromethyl)phenyl)methanol (3ol)

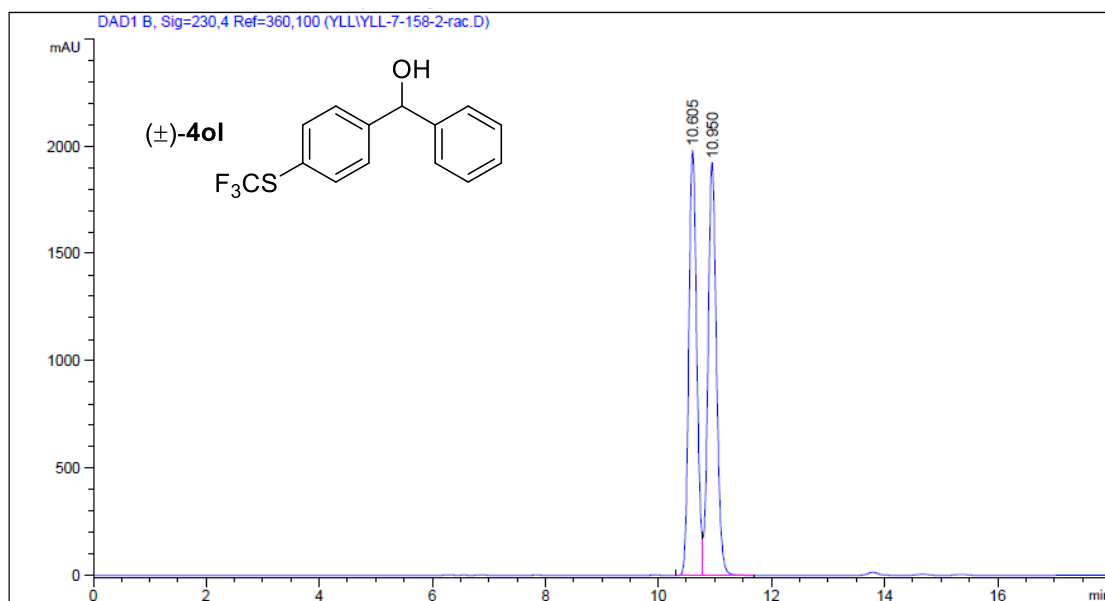


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.182	BB	0.1269	5324.54932	647.81824	49.8895
2	8.839	BB	0.1368	5348.13574	601.20770	50.1105

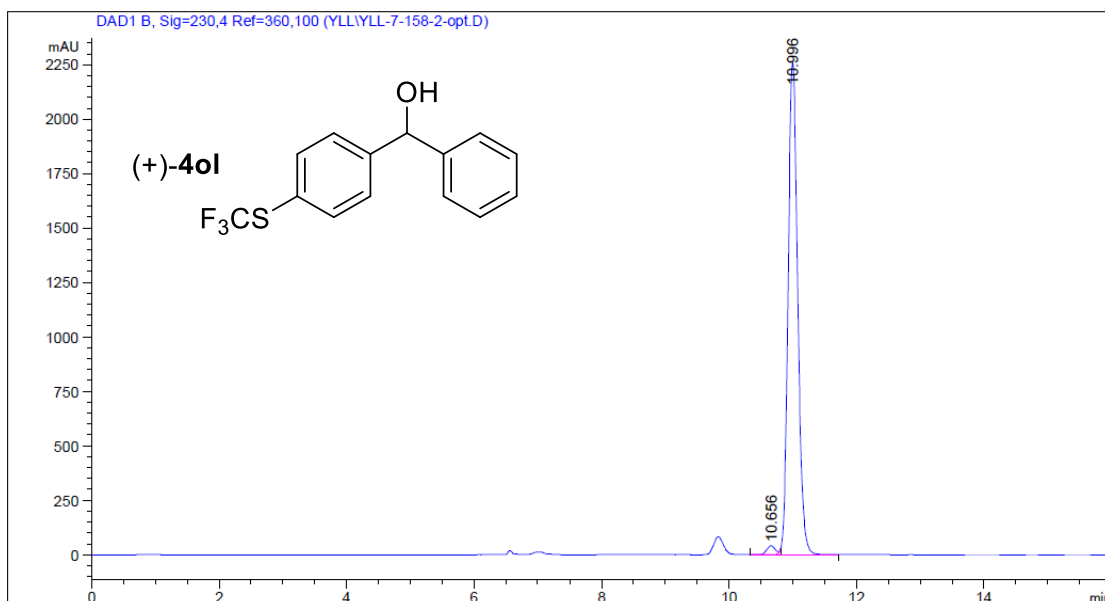


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.344	VB	0.1329	187.76241	21.49597	2.3596
2	9.035	BB	0.1423	7769.53711	844.38702	97.6404

**(+)-phenyl(4-((trifluoromethyl)thio)phenyl)methanol (4ol)**

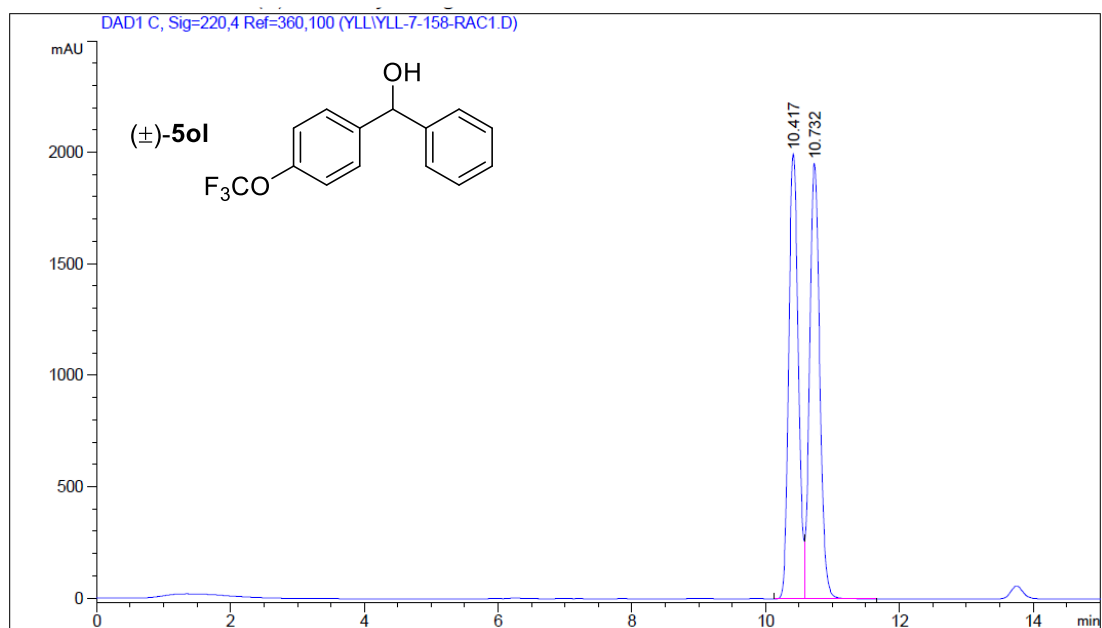


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.605	BV	0.1523	1.94086e4	1981.42847	49.3397
2	10.950	VB	0.1609	1.99280e4	1923.48218	50.6603

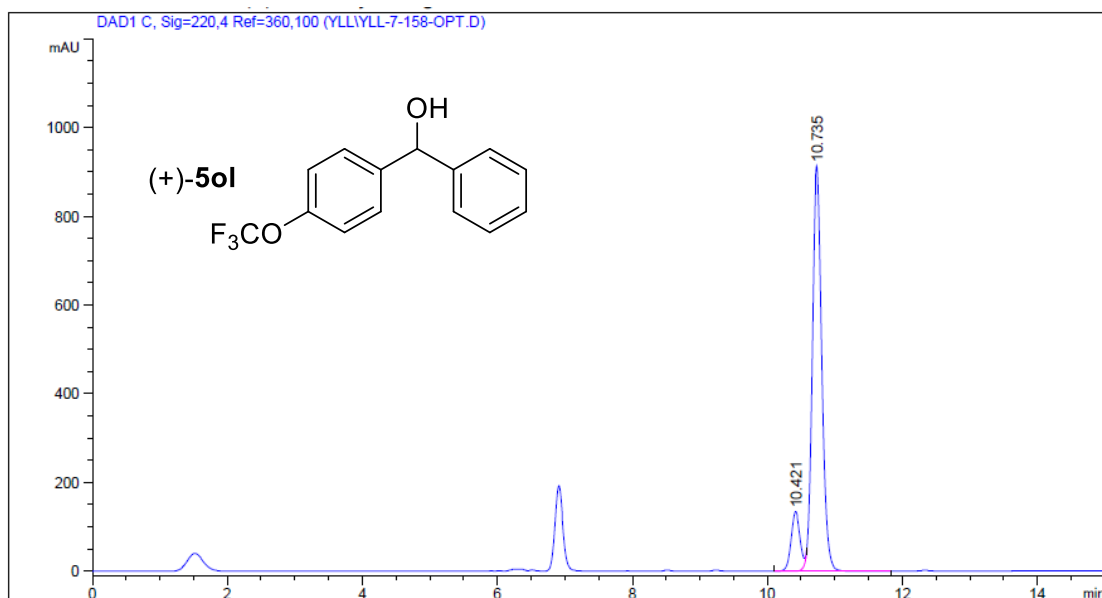


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.656	BV E	0.1433	377.80048	41.05914	1.5817
2	10.996	VB R	0.1615	2.35073e4	2257.79102	98.4183

**(+)-phenyl(4-(trifluoromethoxy)phenyl)methanol (5ol)**

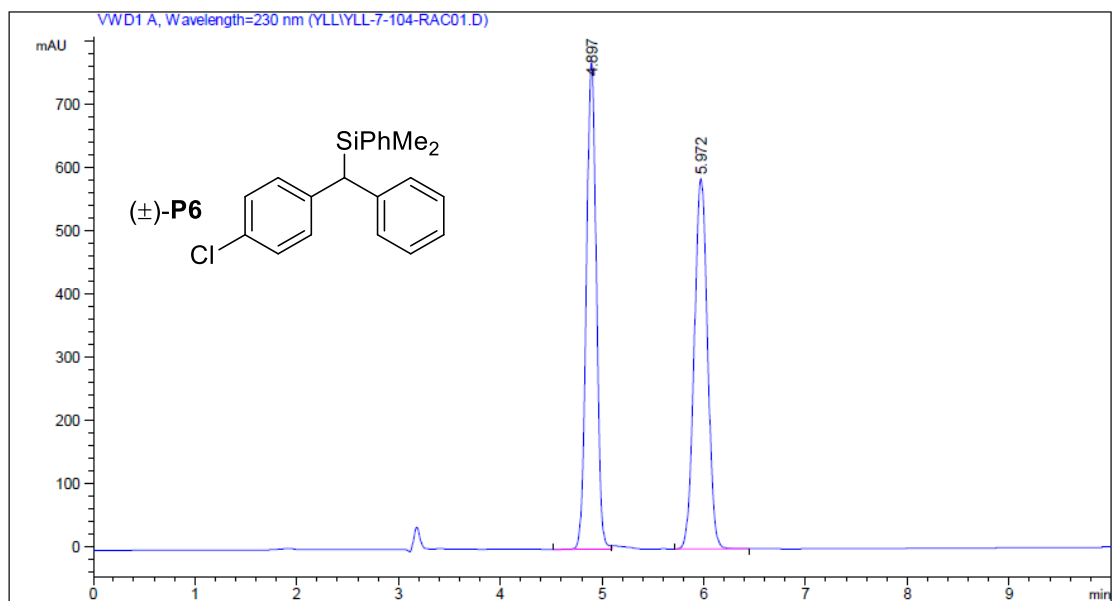


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.417	BV	0.1555	1.97606e4	1995.17517	48.9958
2	10.732	VB	0.1630	2.05706e4	1951.90979	51.0042

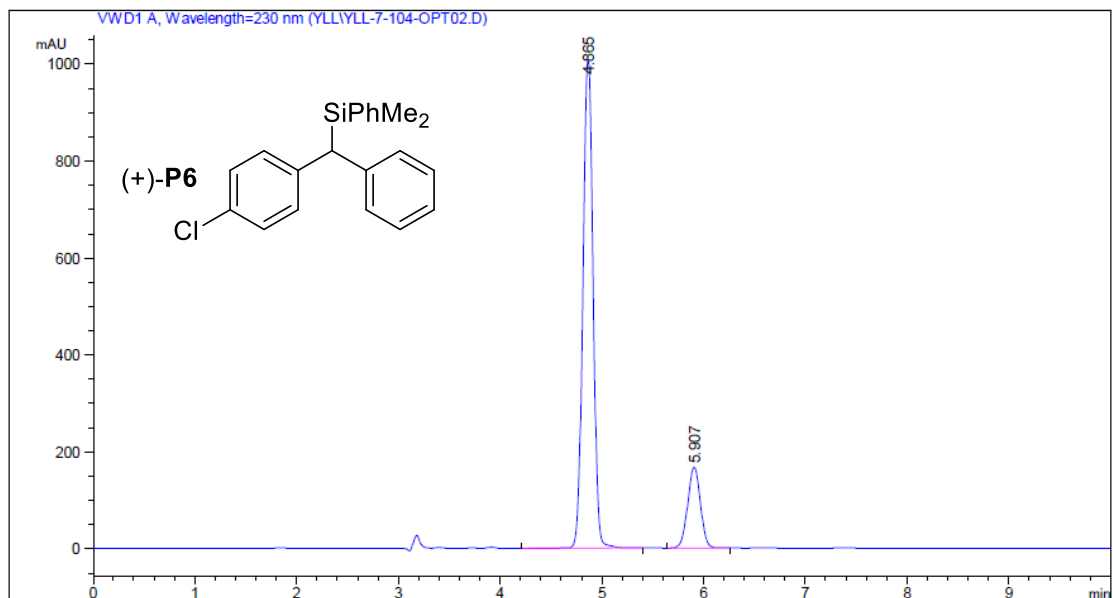


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.421	BV E	0.1421	1221.75281	134.36794	11.9457
2	10.735	VB R	0.1530	9005.83691	913.92816	88.0543

**(+)-((4-chlorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P6)**

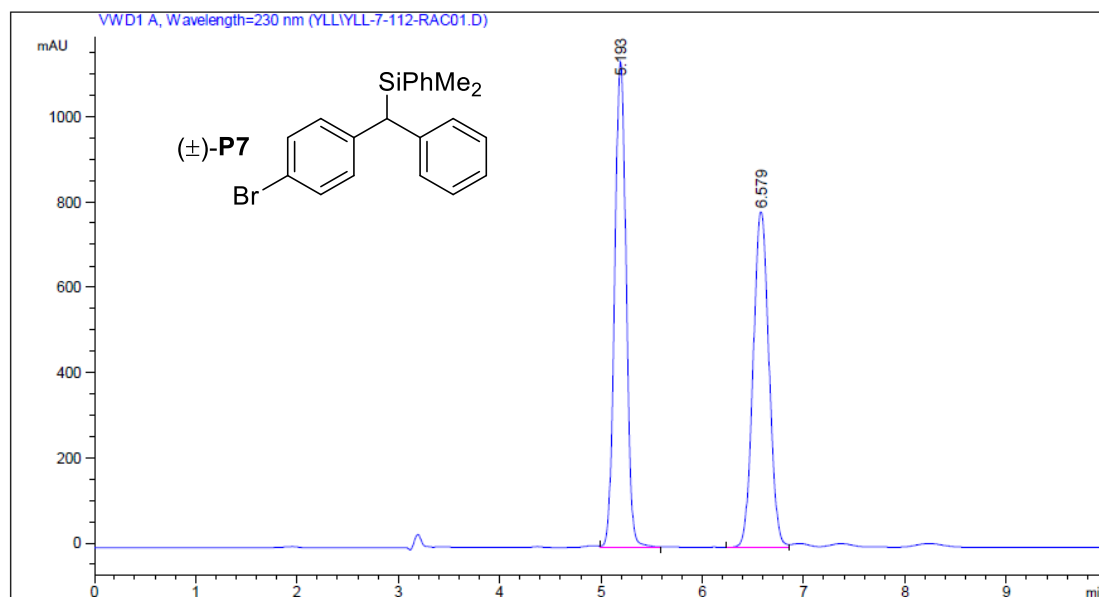


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	4.897	BV	0.1074	5259.89600	769.83411	49.8150
2	5.972	BB	0.1406	5298.95996	585.14197	50.1850

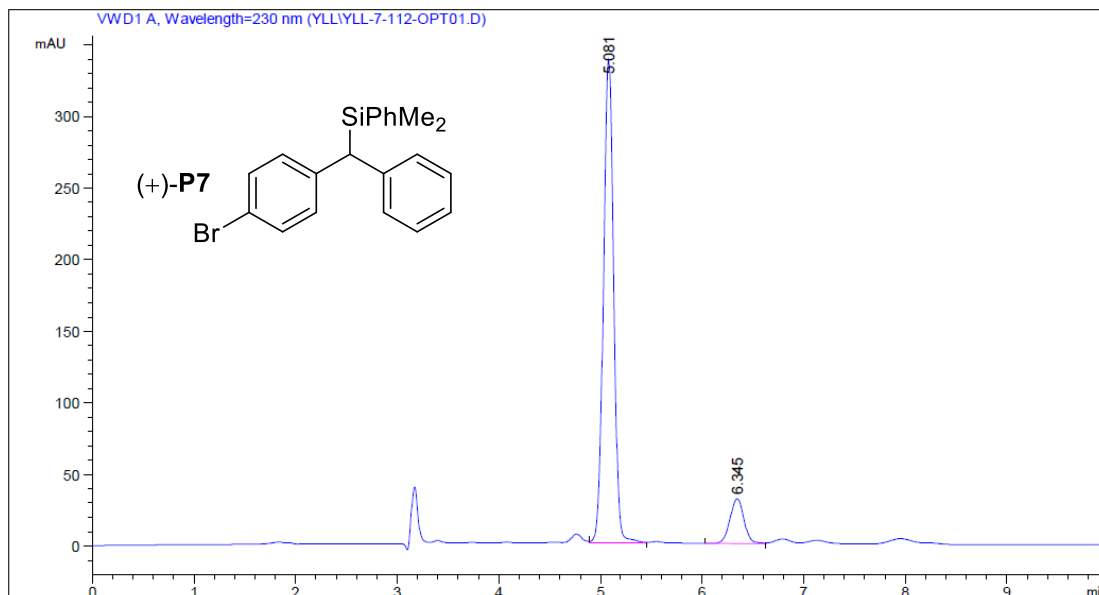


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	4.865	BB	0.1099	6973.50684	1006.67804	82.7506
2	5.907	BB	0.1354	1453.63513	166.44370	17.2494

**(+)-(4-bromophenyl)(phenyl)methyl)dimethyl(phenyl)silane(P7)**



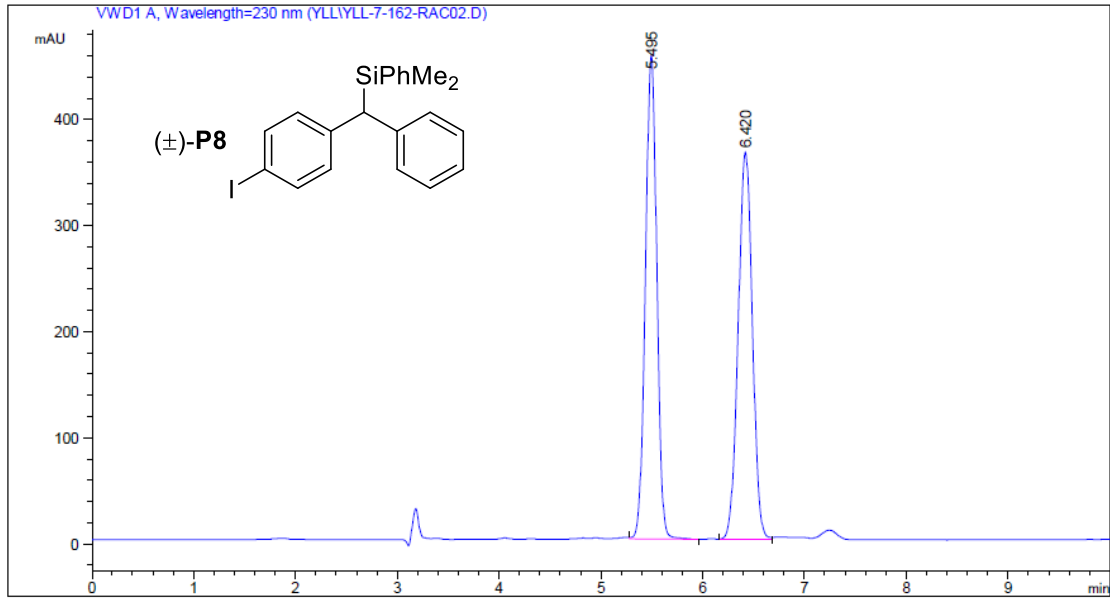
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.193	VV	0.1256	8985.88184	1137.94080	51.3349
2	6.579	BV	0.1700	8518.55469	786.77460	48.6651



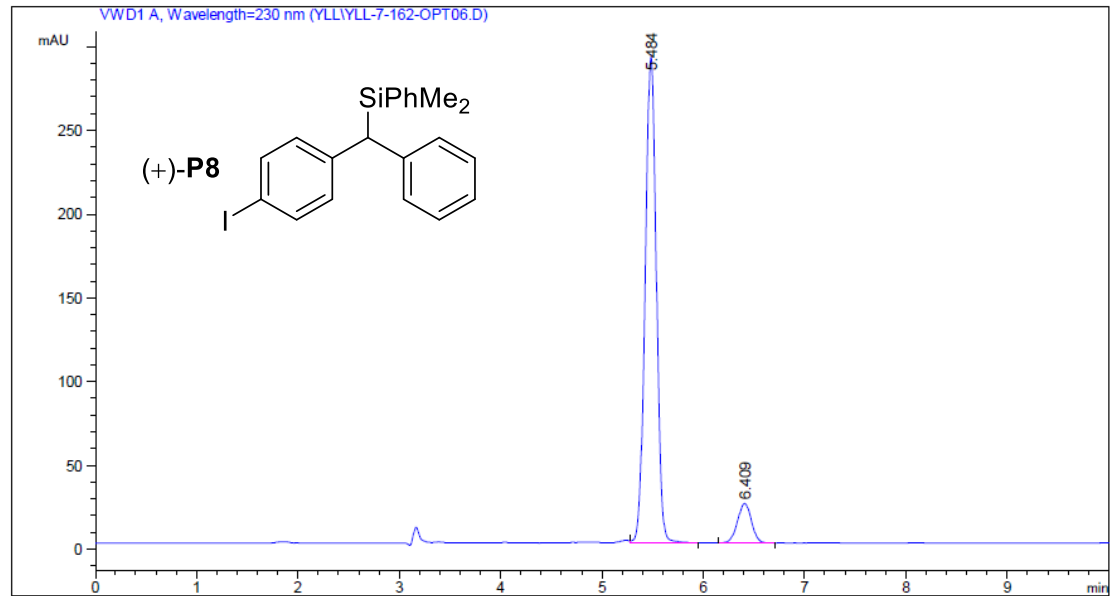
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.081	VV	0.1091	2355.06641	337.25253	88.7117
2	6.345	BV	0.1483	299.67465	31.23787	11.2883



**(+)-((4-iodophenyl)(phenyl)methyl)dimethyl(phenyl)silane(P8)**

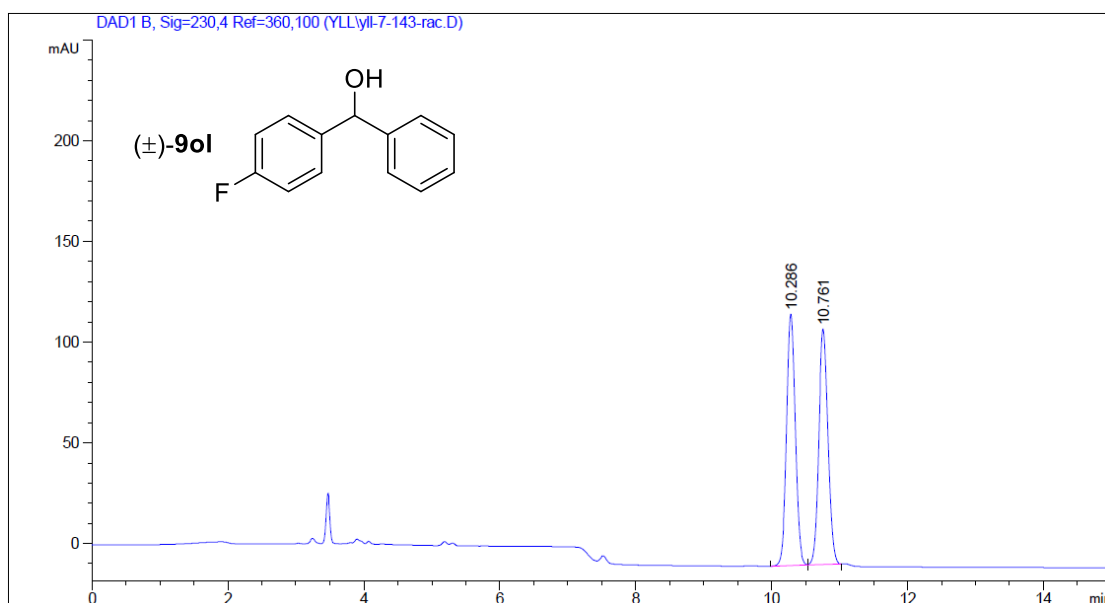


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.495	VB	0.1215	3555.15918	456.12347	50.0768
2	6.420	BV	0.1526	3544.25317	364.98331	49.9232

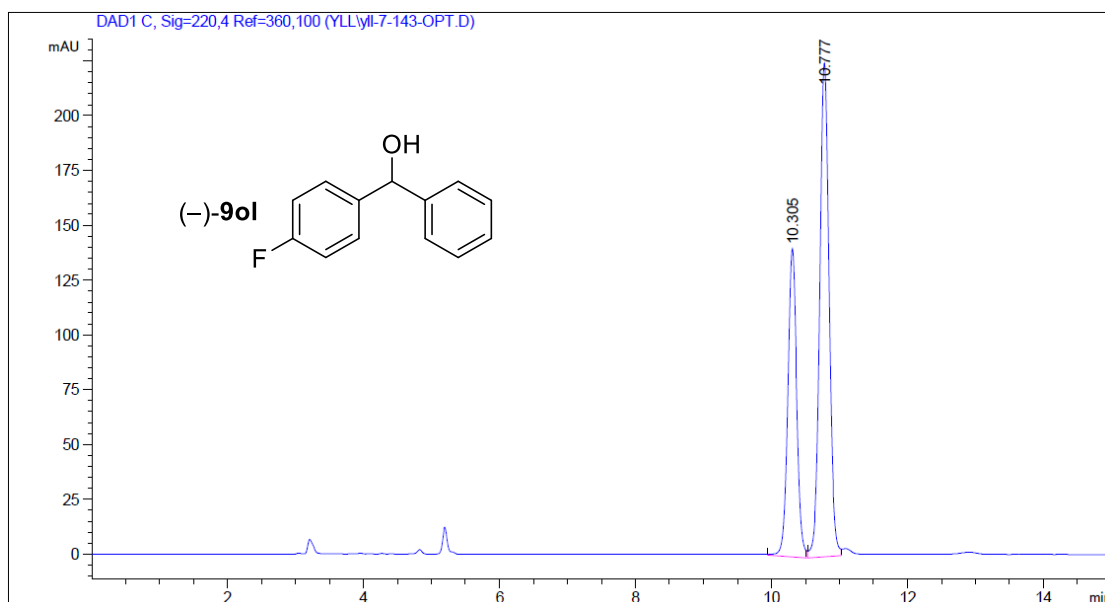


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.484	VB	0.1201	2228.09668	290.34891	90.8103
2	6.409	VB	0.1498	225.47635	23.49924	9.1897

**(-)-(4-fluorophenyl)(phenyl)methanol (9ol)**

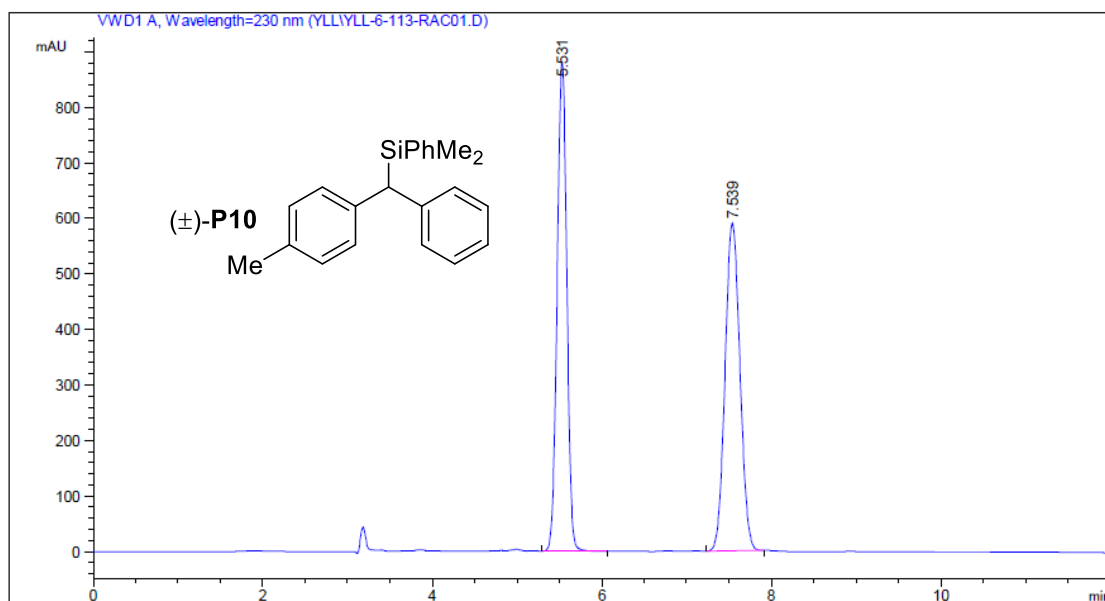


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.286	BV	0.1380	1113.85730	124.97284	50.2722
2	10.761	VB	0.1458	1101.79492	117.02339	49.7278

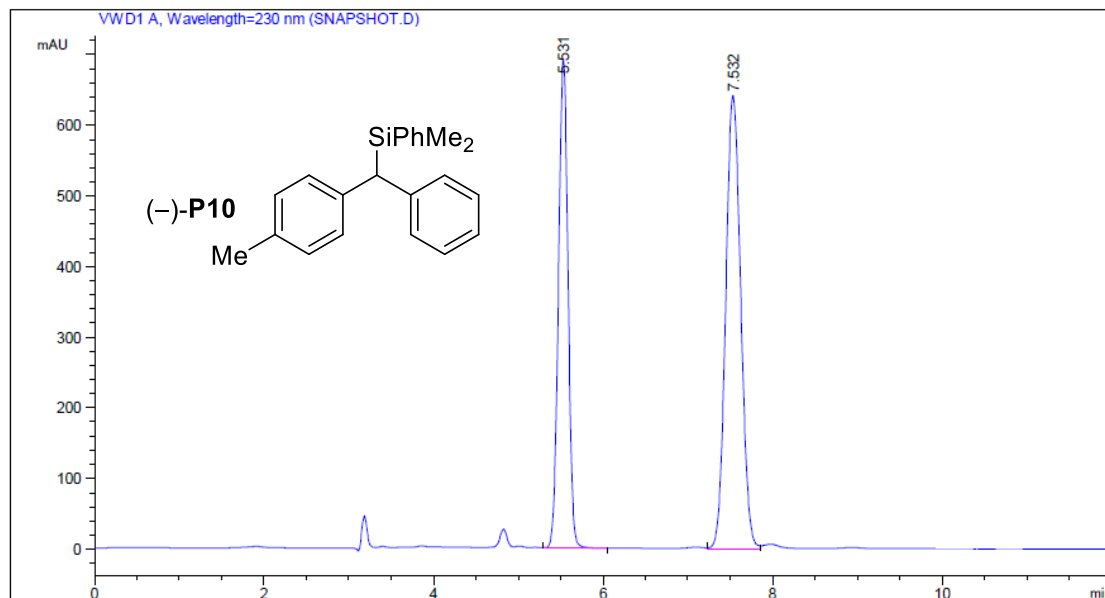


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.305	MM	0.1493	1253.72351	139.94191	37.6304
2	10.777	MM	0.1550	2077.95142	223.37556	62.3696

**(-)-dimethyl(phenyl)(phenyl(p-tolyl)methyl)silane(P10)**

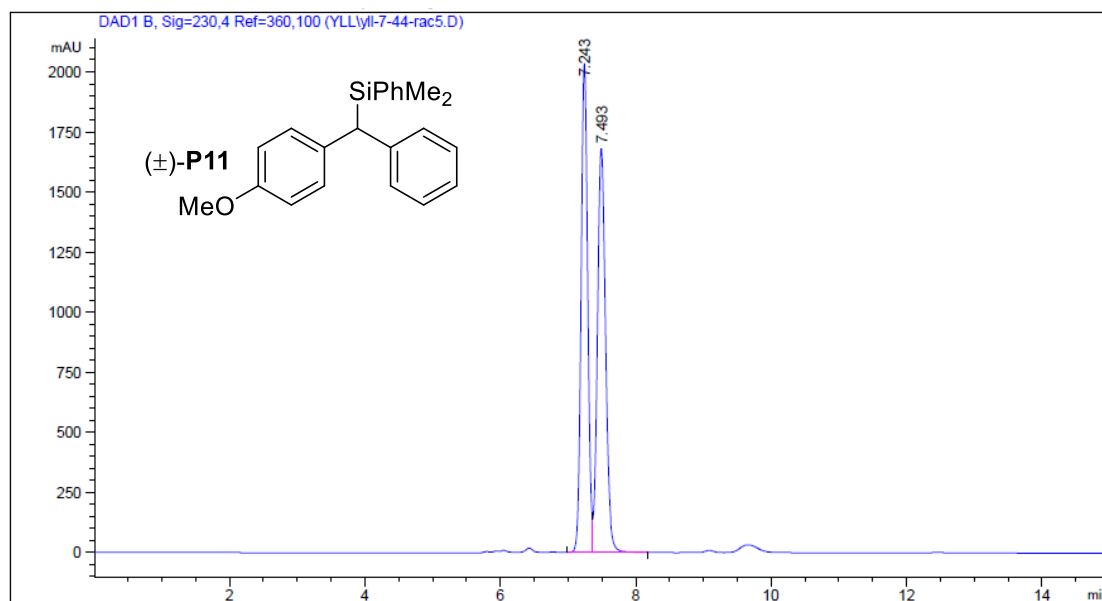


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.531	BB	0.1245	6970.30371	879.49323	49.2414
2	7.539	BB	0.1915	7185.07373	590.46796	50.7586

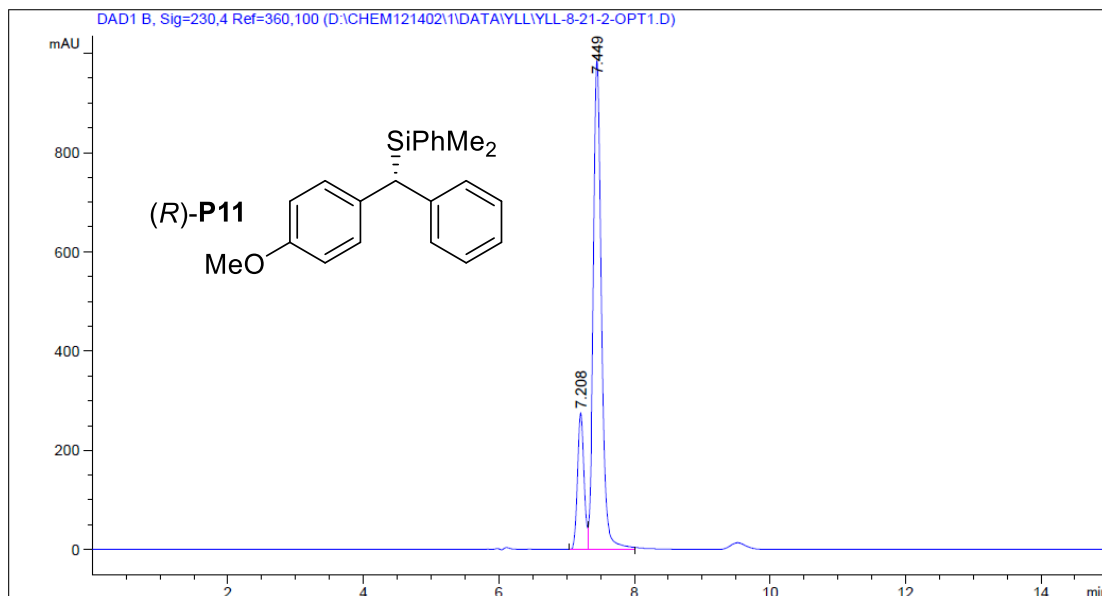


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.531	BB	0.1236	5420.60791	690.65948	40.7653
2	7.532	VV	0.1927	7876.52051	641.58459	59.2347

**(R)-((4-methoxyphenyl)(phenyl)methyl)dimethyl(phenyl)silane(P11)**

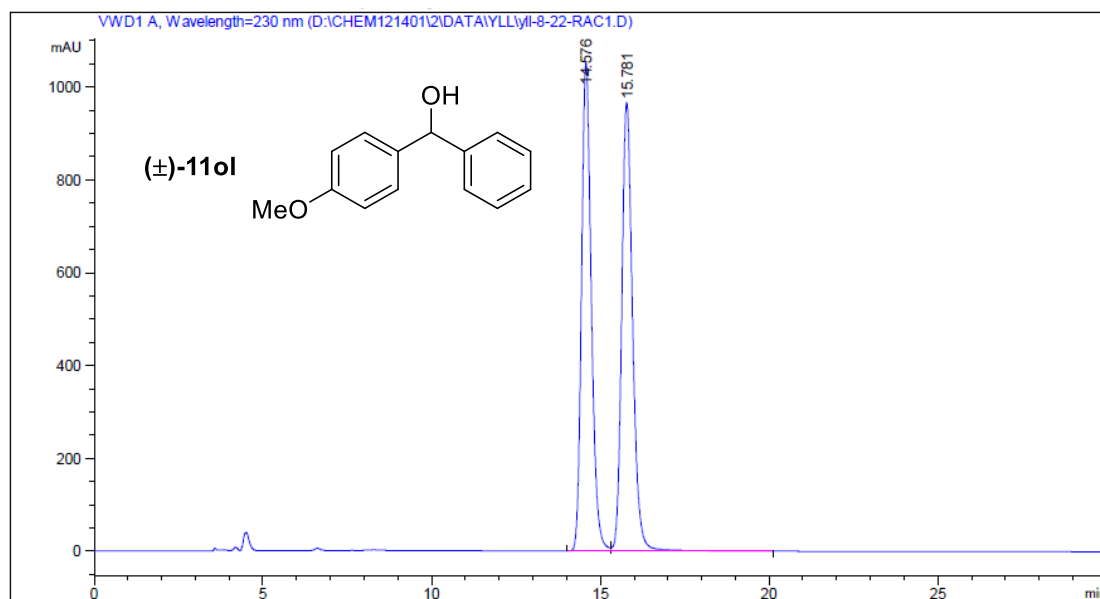


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.243	BV	0.1032	1.34772e4	2036.60693	49.3621
2	7.493	VB	0.1278	1.38256e4	1684.16943	50.6379

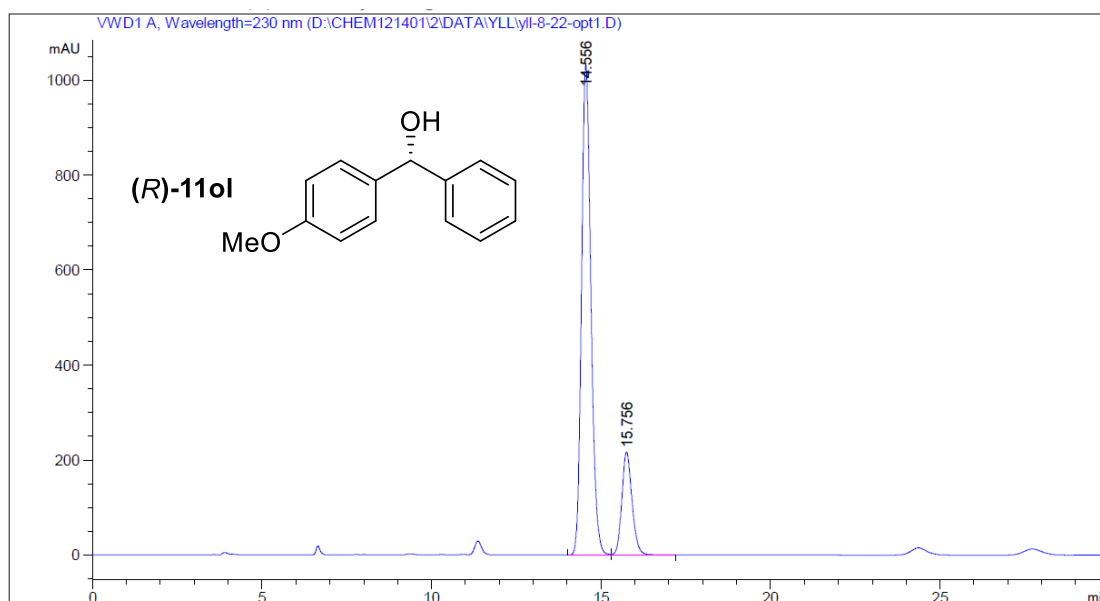


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.208	MM R	0.1093	1807.13354	275.68298	18.1668
2	7.449	MM R	0.1377	8140.31836	985.46405	81.8332

### (R)-(4-methoxyphenyl)(phenyl)methanol (11ol)

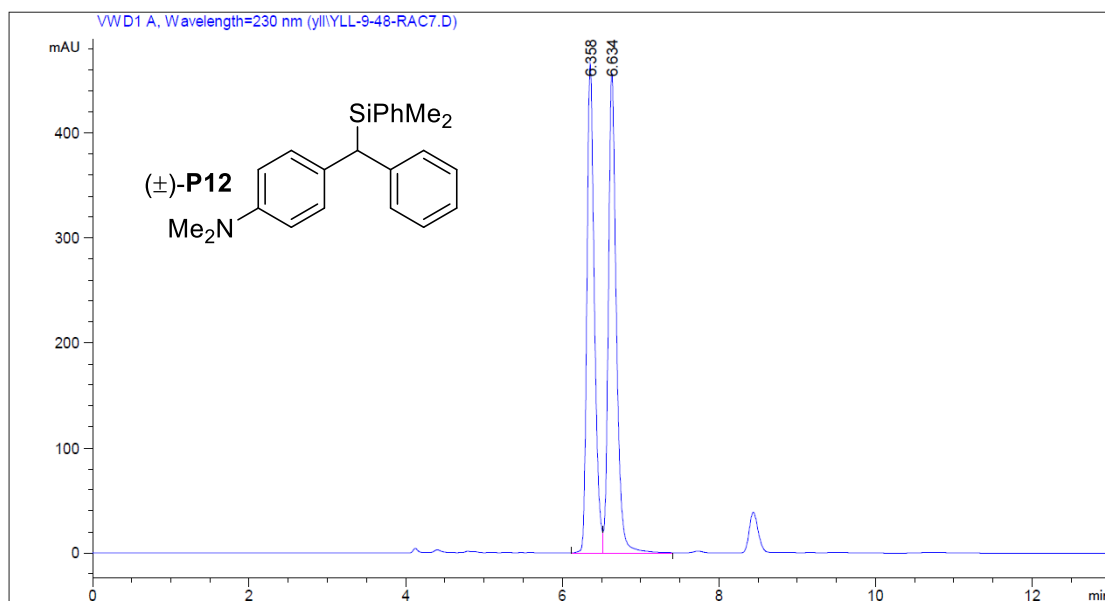


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.576	BV	0.3092	2.12109e4	1051.93665	49.4662
2	15.781	VB	0.3425	2.16687e4	966.84375	50.5338

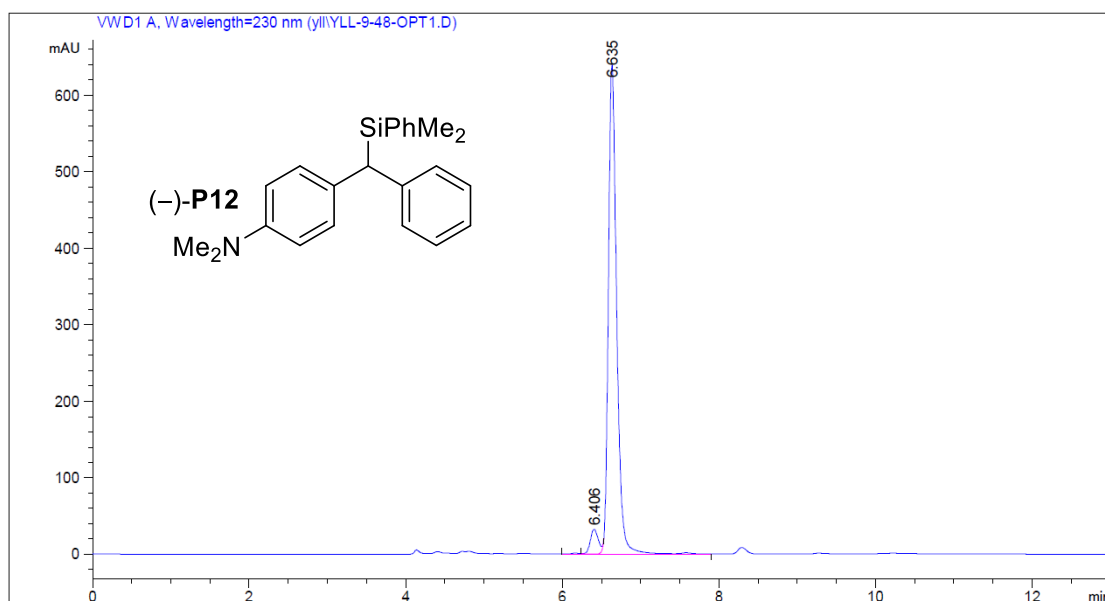


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.556	BV	0.2954	1.98531e4	1032.32886	81.3567
2	15.756	VB	0.3218	4549.43555	216.83577	18.6433

**(-)-4-((dimethyl(phenyl)silyl)(phenyl)methyl)-*N,N*-dimethylaniline(P12)**

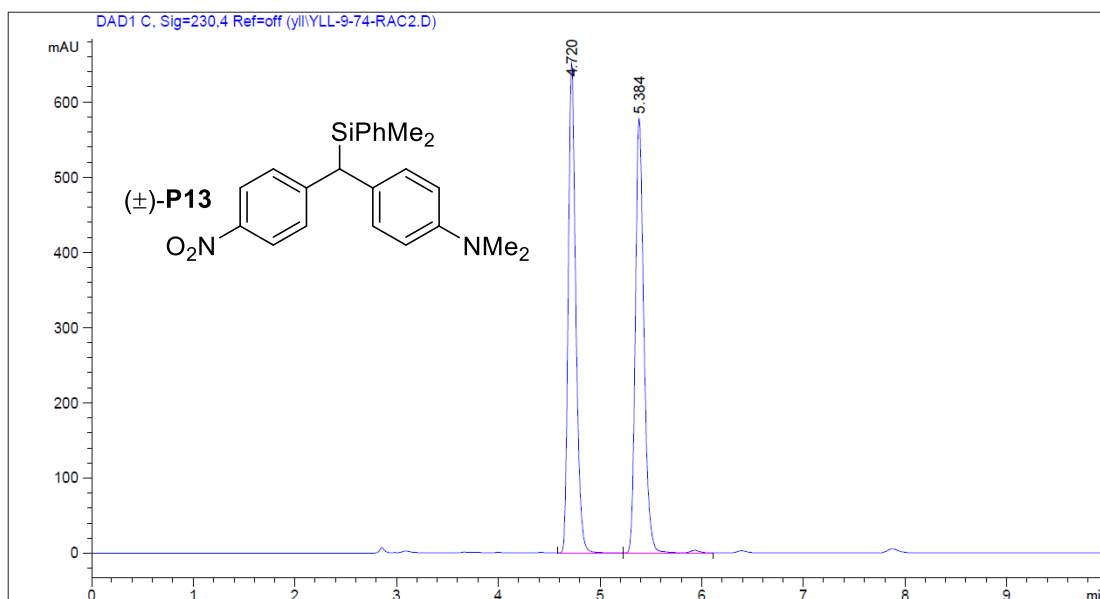


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.358	BV	0.1002	3085.69482	466.49731	48.8293
2	6.634	VB	0.1066	3233.65454	456.96005	51.1707

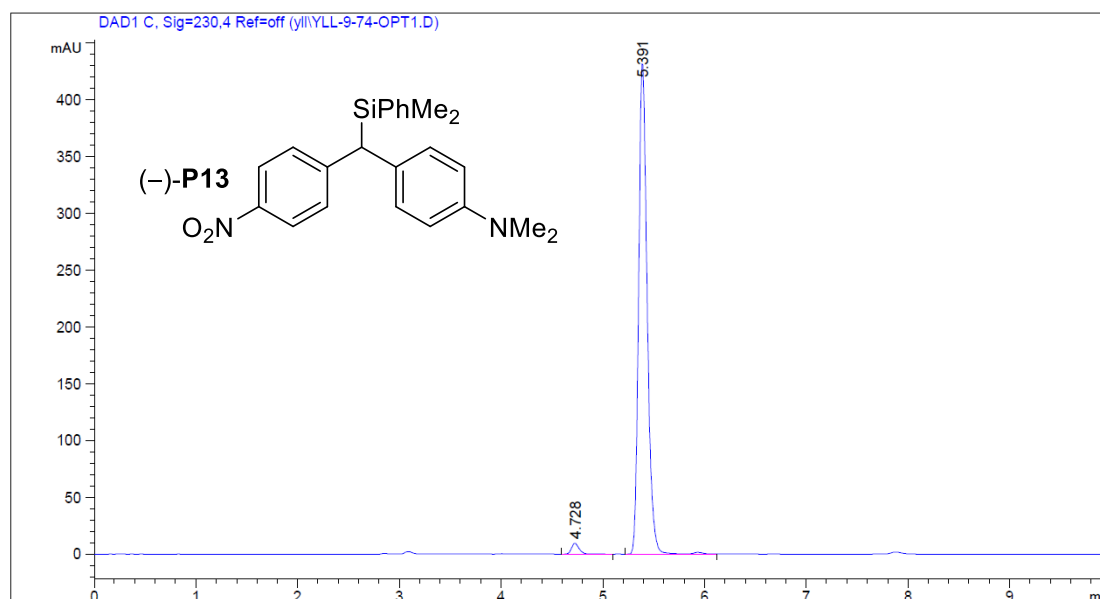


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.406	VV E	0.1085	229.75182	32.48794	4.6298
2	6.635	VV R	0.1112	4732.71436	640.24054	95.3702

**(-)-4-((dimethyl(phenyl)silyl)(4-nitrophenyl)methyl)-*N,N*-dimethylaniline (P13)**

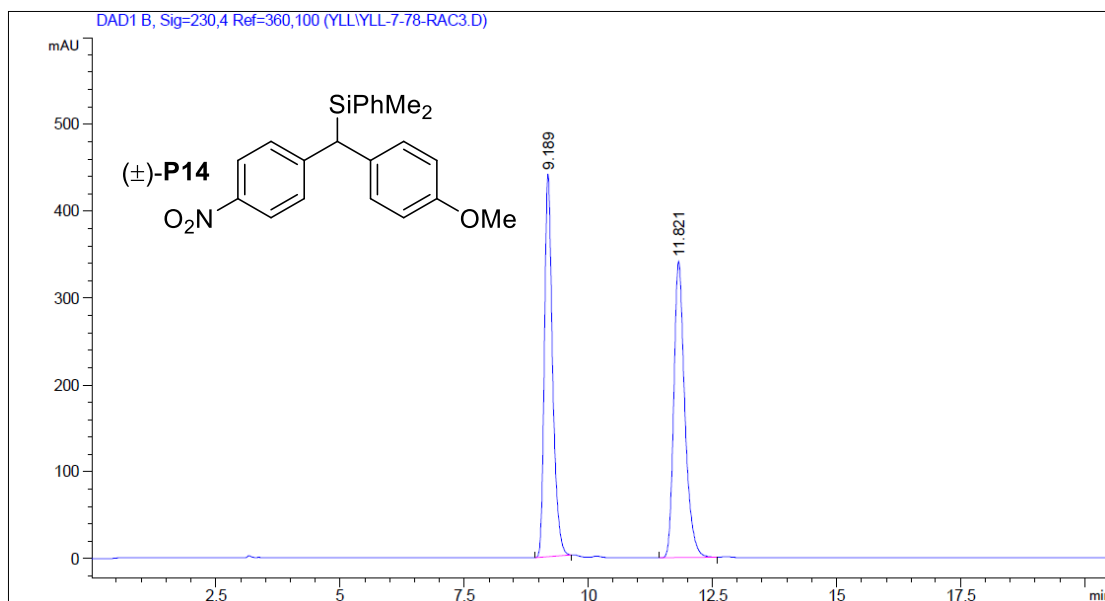


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.720	BB	0.0783	3369.67798	652.43787	49.7842
2	5.384	BV R	0.0881	3398.88452	578.78180	50.2158

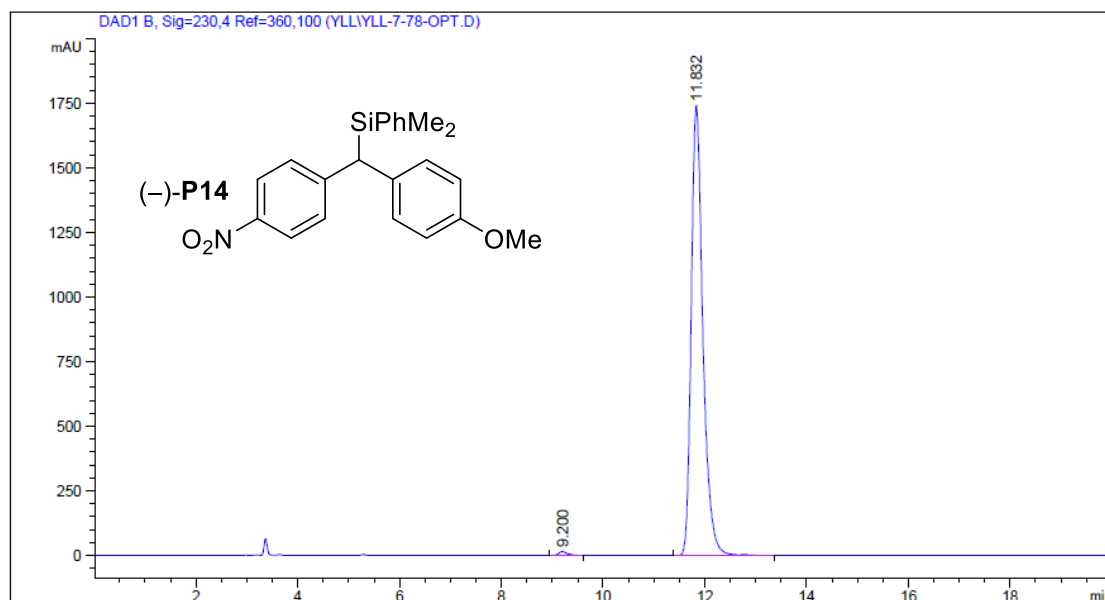


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.728	BB	0.0780	50.42667	9.81020	1.9557
2	5.391	BV R	0.0879	2528.08081	432.93674	98.0443

**(-)-((4-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P14)**



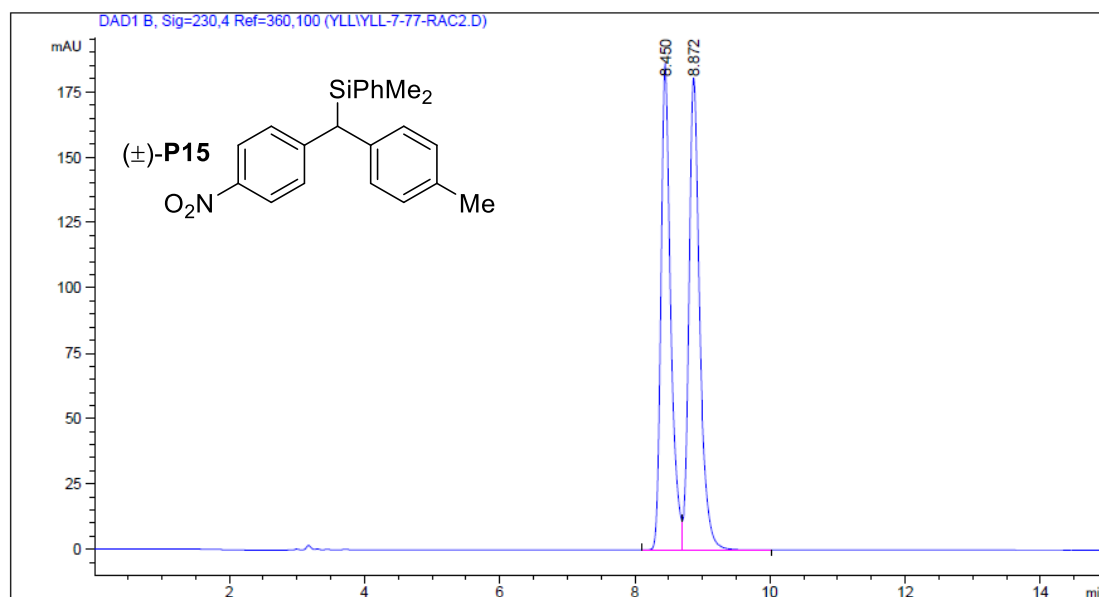
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.189	BB	0.1741	5064.55615	440.47961	48.9347
2	11.821	BB	0.2347	5285.05859	341.13690	51.0653



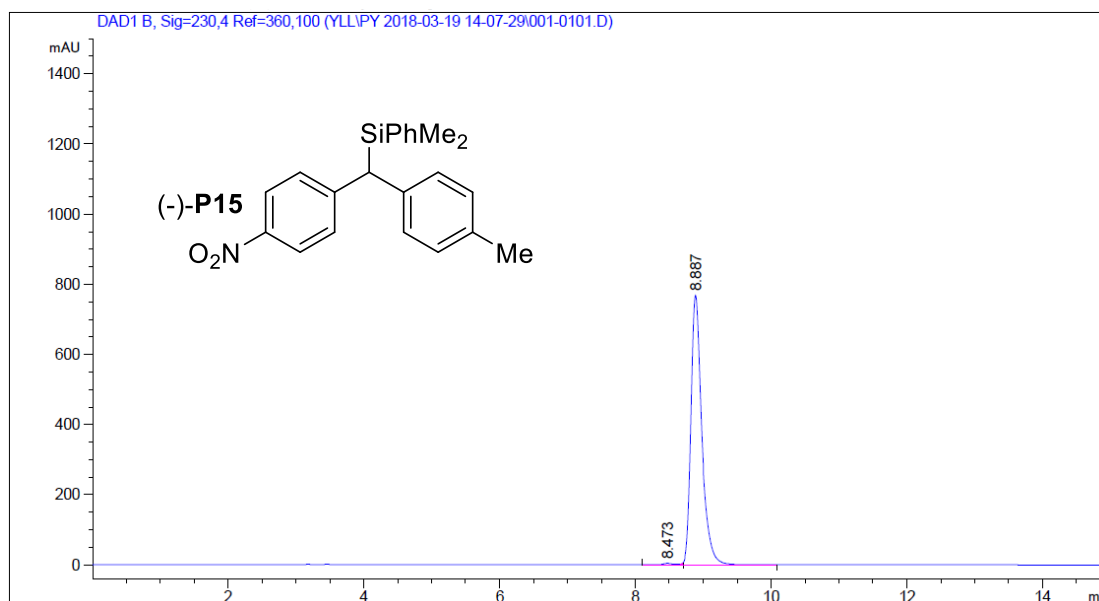
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.200	BB	0.1764	182.35788	15.36962	0.6539
2	11.832	BV R	0.2395	2.77069e4	1740.64185	99.3461



**(±)-dimethyl((4-nitrophenyl)(*p*-tolyl)methyl)(phenyl)silane (P15)**

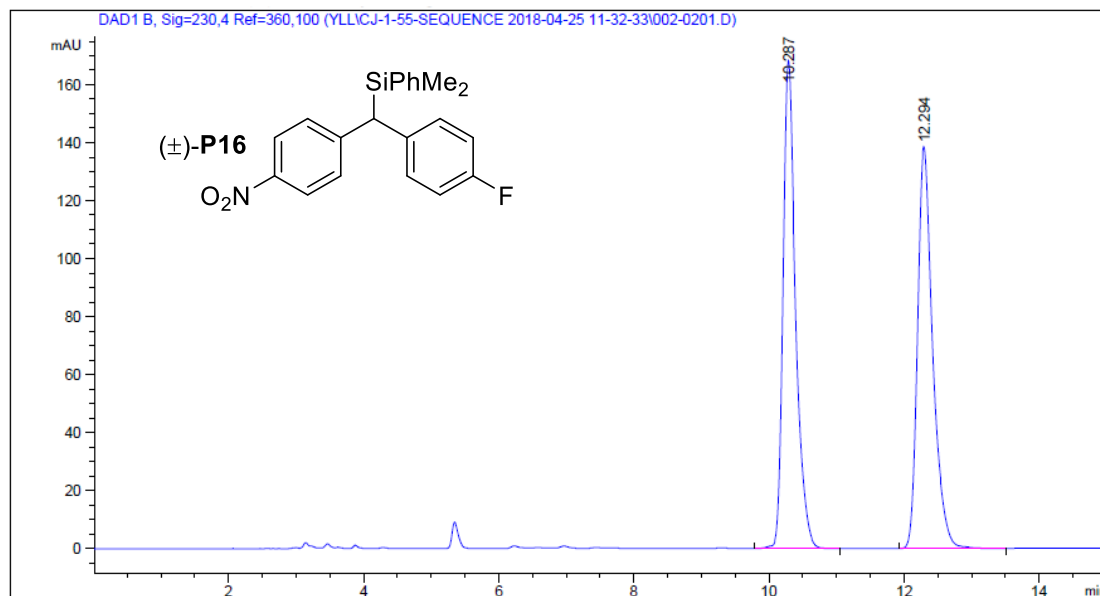


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.450	BV	0.1528	1897.40149	186.39929	48.7708
2	8.872	VB	0.1647	1993.04749	180.66096	51.2292

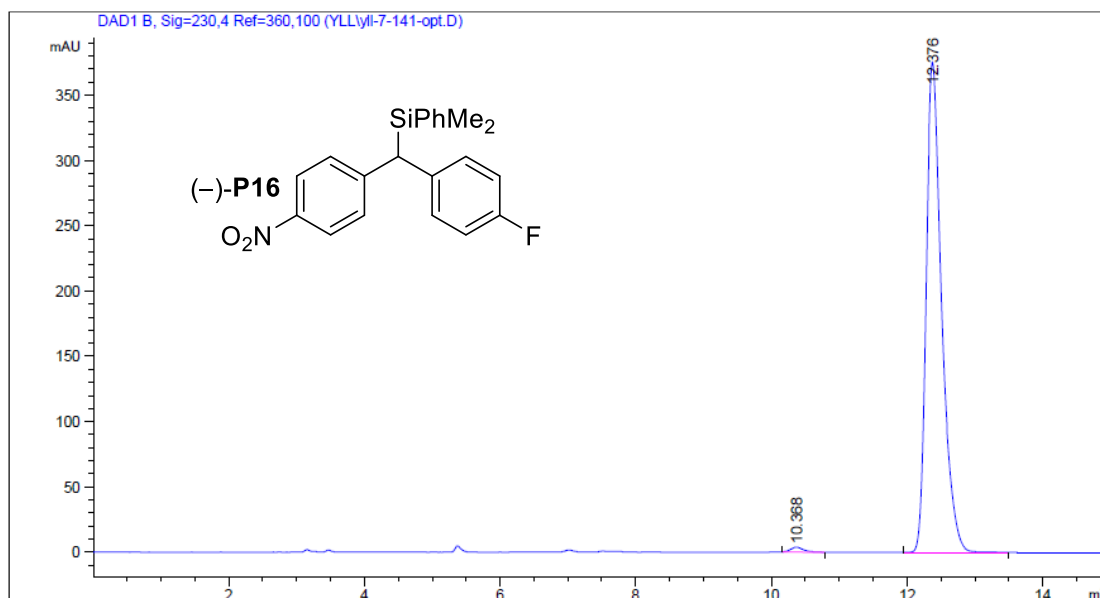


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.473	BV E	0.1626	45.82573	4.15760	0.5366
2	8.887	VB R	0.1648	8493.77637	769.12256	99.4634

**(-)-((4-fluorophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P16)**

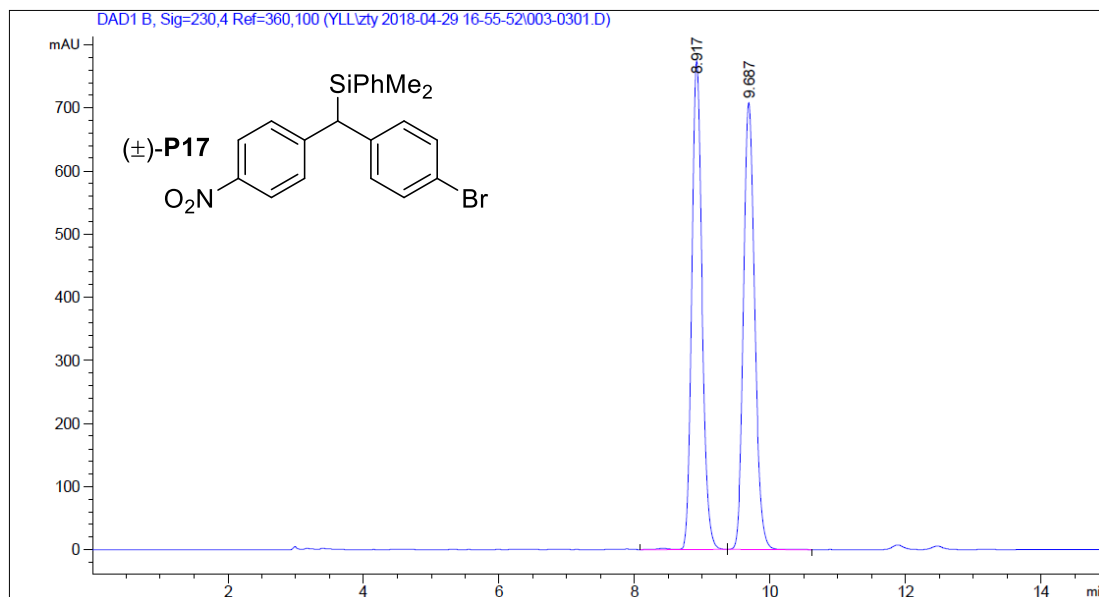


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.287	BB	0.1917	2158.41650	168.17952	49.9793
2	12.294	BB	0.2338	2160.20557	138.59587	50.0207

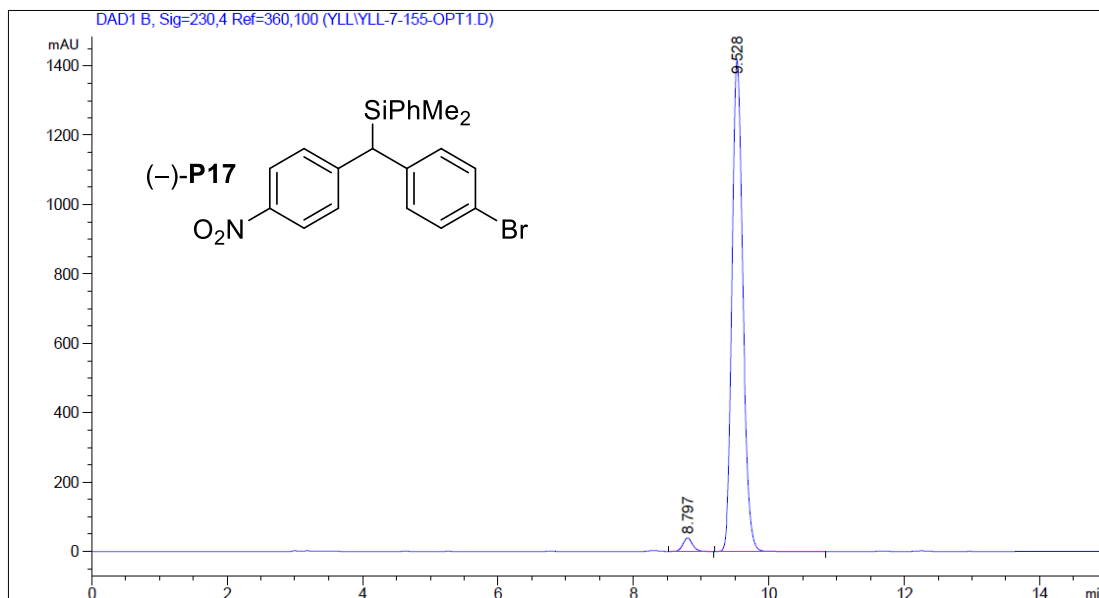


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.368	BB	0.1870	45.44220	3.65537	0.7593
2	12.376	BB	0.2386	5939.28223	375.29282	99.2407

**(±)-((4-bromophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P17)**

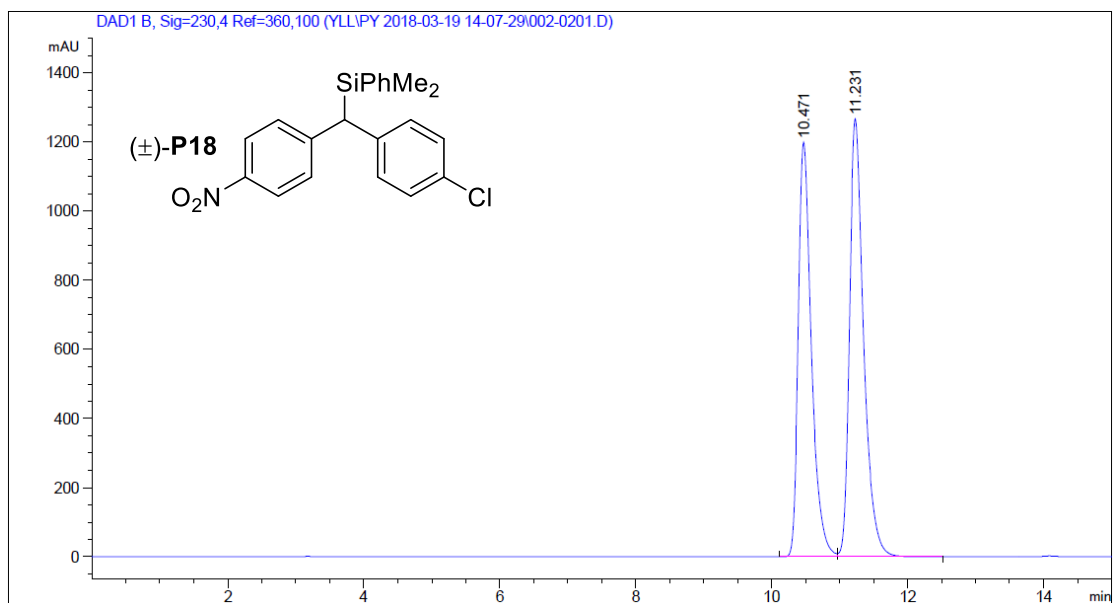


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.917	VB R	0.1597	8104.49512	774.54321	50.0027
2	9.687	BB	0.1775	8103.61816	708.22925	49.9973

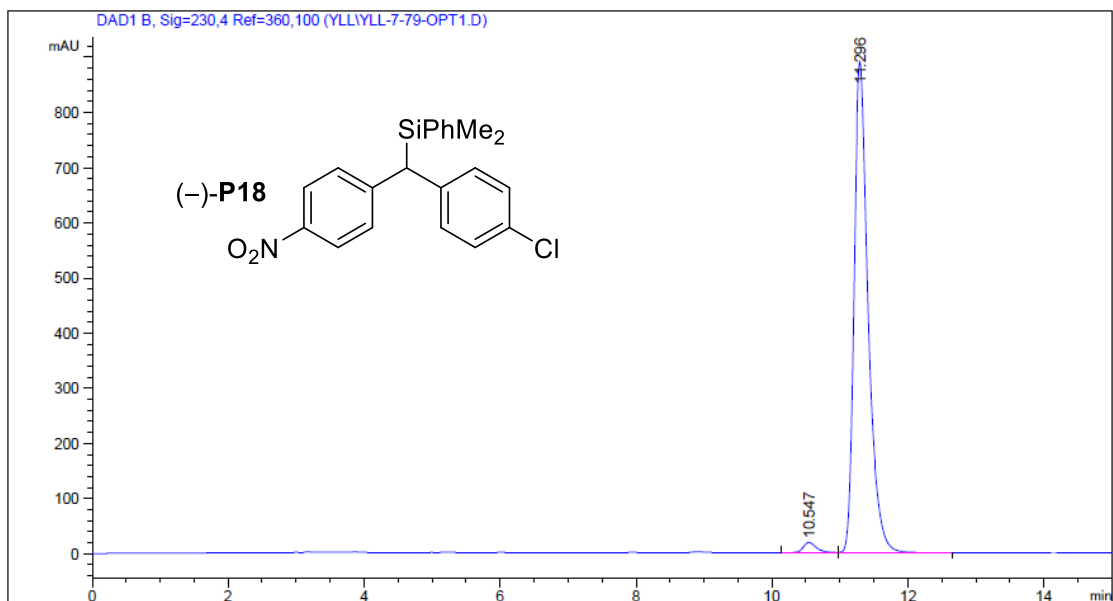


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.797	BB	0.1555	388.27914	38.56146	2.4112
2	9.528	BB	0.1715	1.57149e4	1415.55640	97.5888

**(-)-((4-chlorophenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P18)**

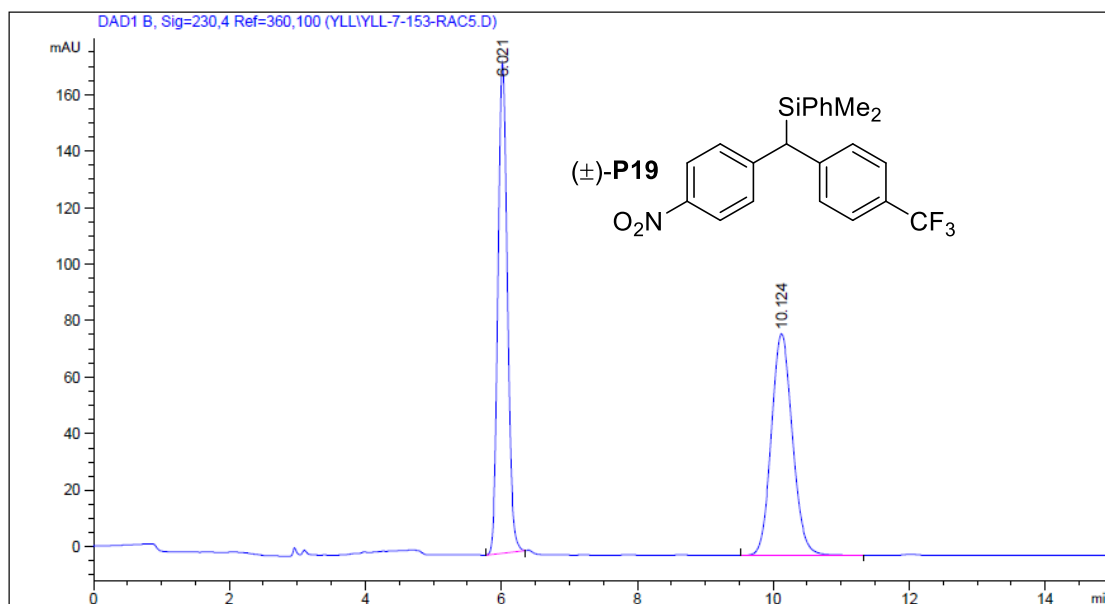


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.471	BV	0.2015	1.59805e4	1198.82263	46.6315
2	11.231	VB	0.2185	1.82892e4	1266.28638	53.3685

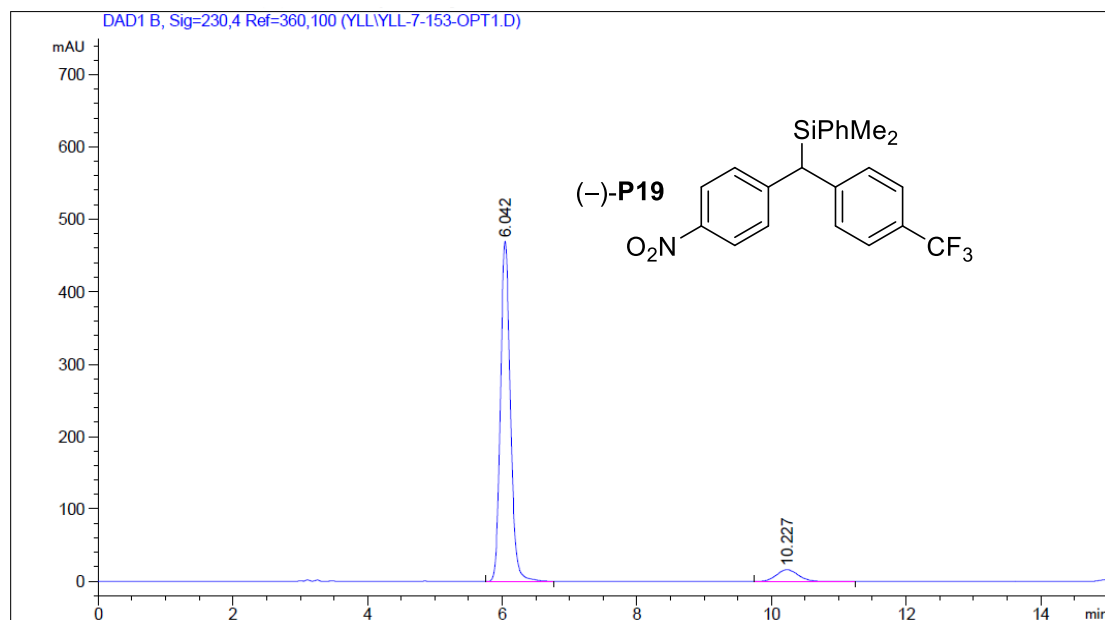


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.547	BV	0.1972	240.45412	18.31021	1.8518
2	11.296	VB	0.2172	1.27444e4	889.21930	98.1482

**(-)-dimethyl((4-nitrophenyl)(4-(trifluoromethyl)phenyl)methyl)(phenyl)silane  
(P19)**

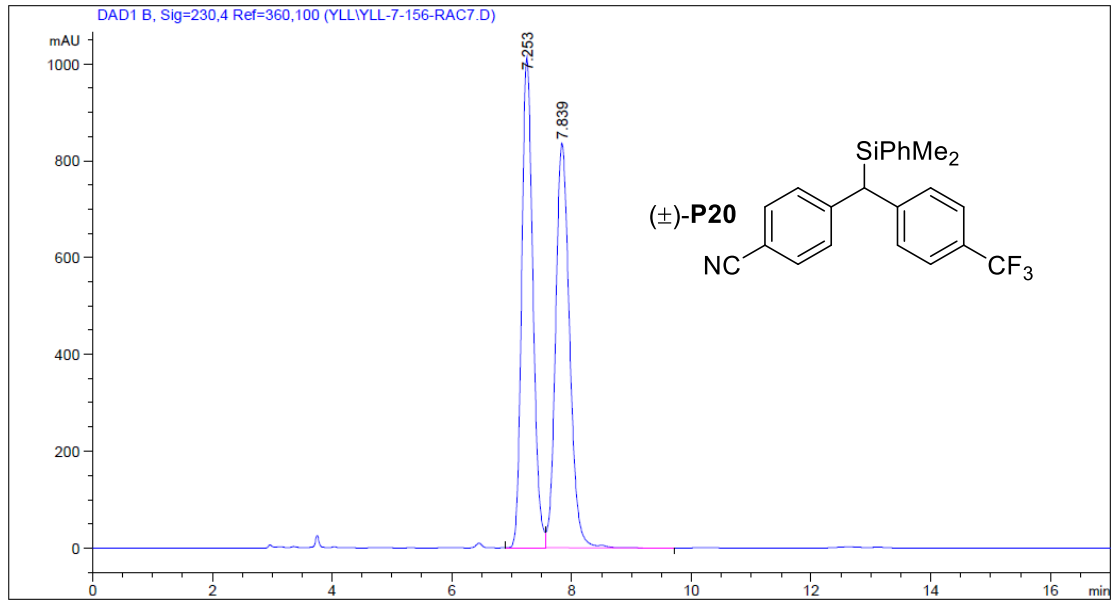


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.021	BB	0.1473	1654.47278	173.38531	49.5287
2	10.124	BB	0.3330	1685.95752	78.36142	50.4713

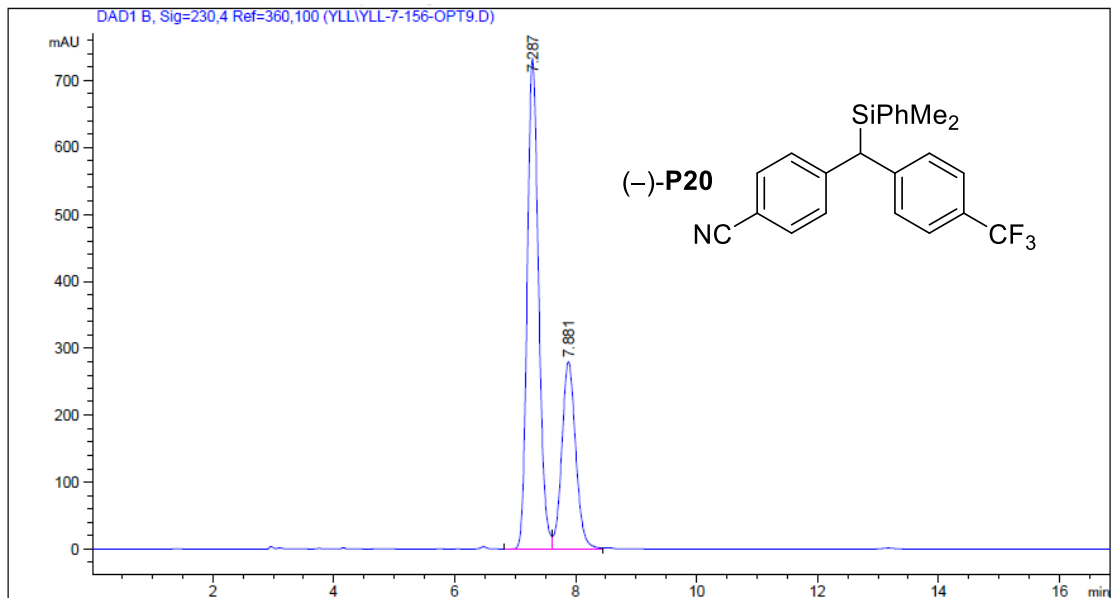


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.042	BB	0.1576	4813.60352	469.43262	93.0040
2	10.227	BB	0.3485	362.09146	16.09033	6.9960

**(-)-4-((dimethyl(phenyl)silyl)(4-(trifluoromethyl)phenyl)methyl)benzonitrile (P20)**

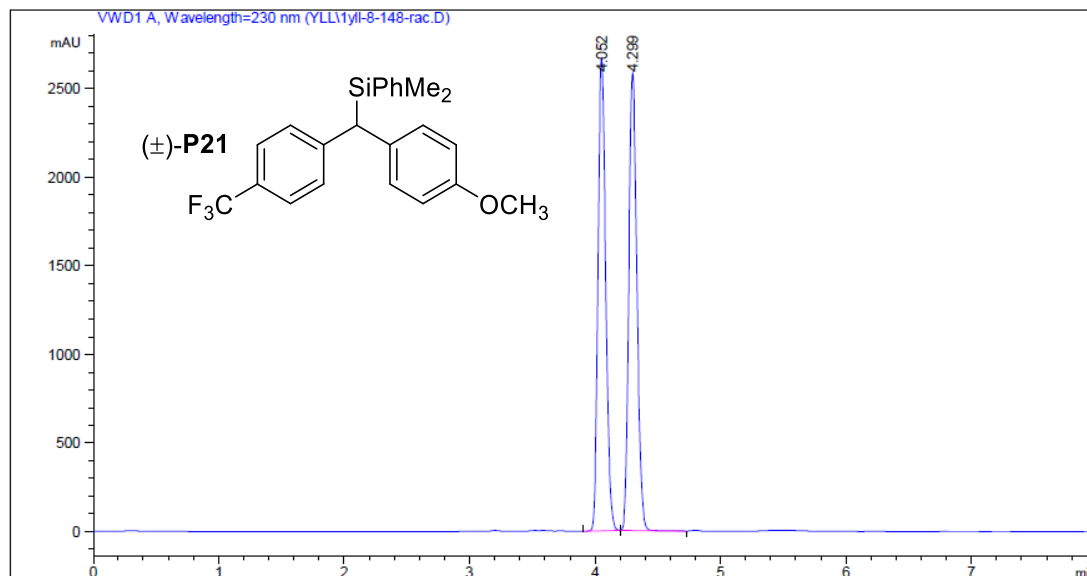


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.253	BV	0.2014	1.31635e4	1014.54059	49.2358
2	7.839	VV R	0.2508	1.35722e4	836.18707	50.7642

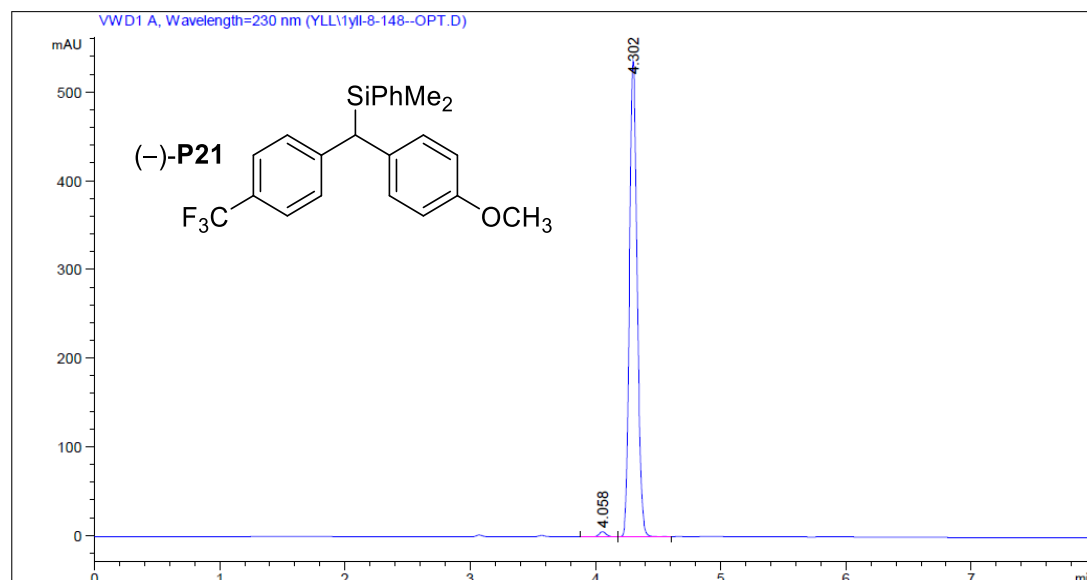


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.287	BV	0.2020	9547.83203	732.70526	68.0938
2	7.881	VV	0.2465	4473.75439	279.81241	31.9062

**(-)-((4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane  
(P21)**

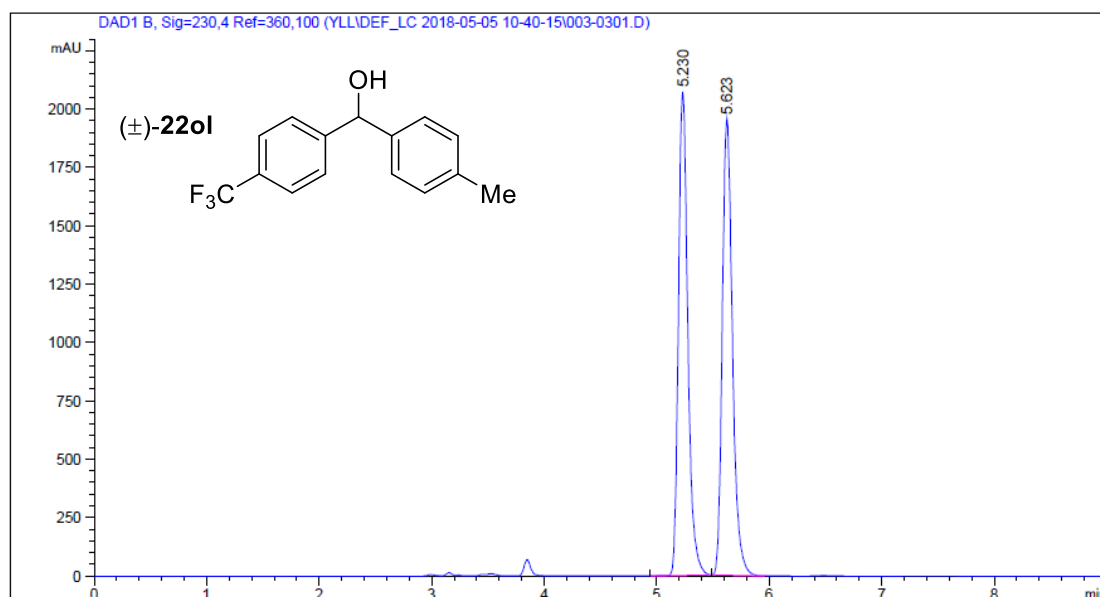


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.052	BB	0.0668	1.13849e4	2668.55908	49.5405
2	4.299	BV R	0.0704	1.15962e4	2582.93677	50.4595

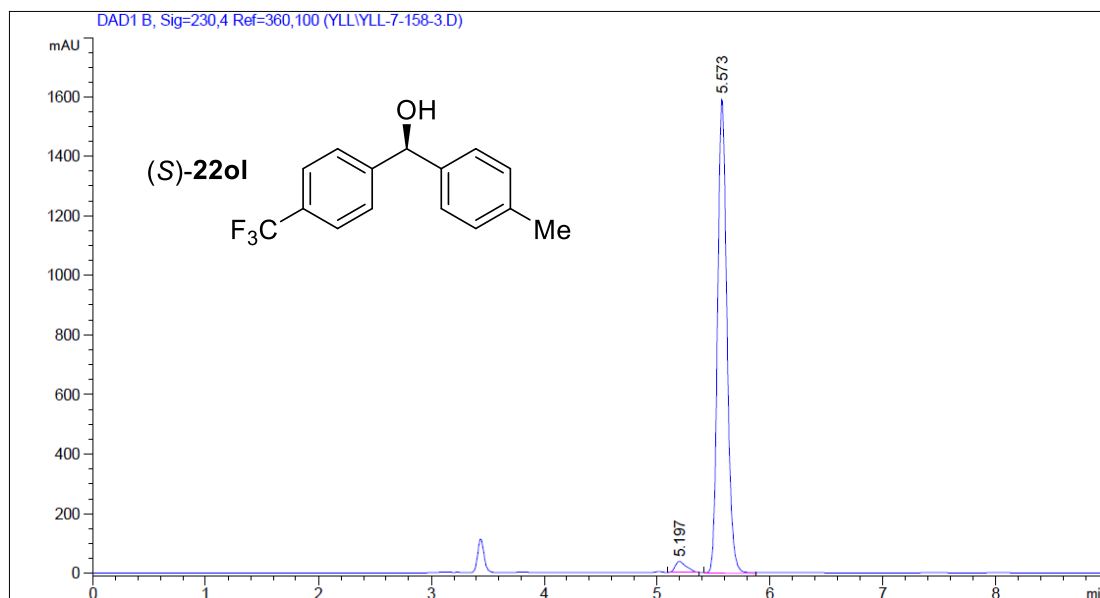


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.058	VB R	0.0630	23.90394	5.81219	1.0325
2	4.302	BV R	0.0657	2291.19360	537.48883	98.9675

**(S)-p-tolyl(4-(trifluoromethyl)phenyl)methanol (22ol)**



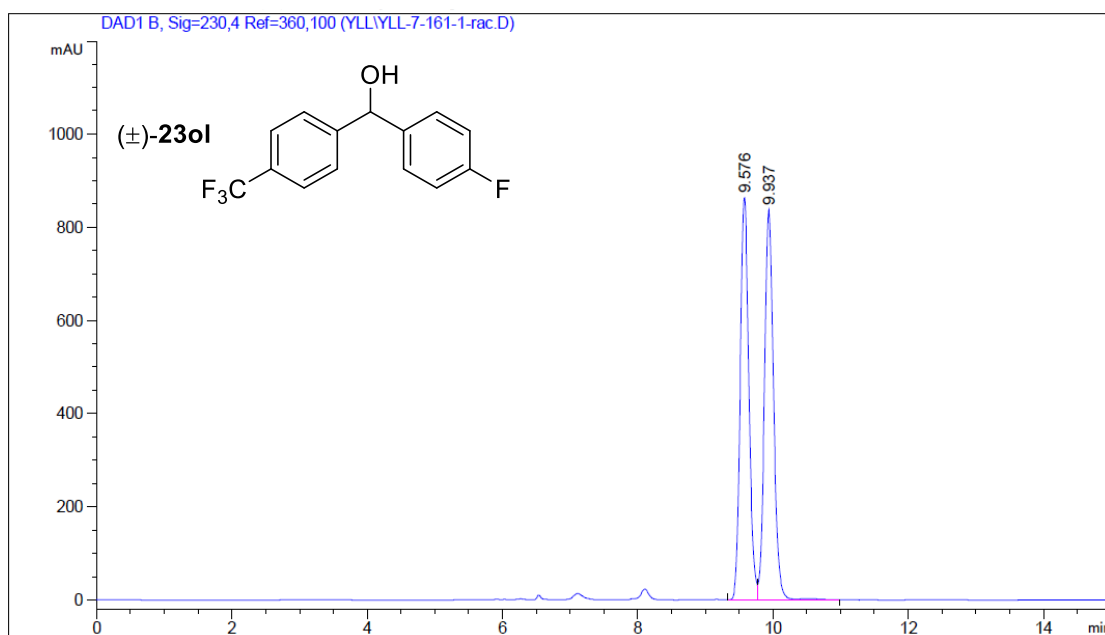
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.230	VB R	0.0897	1.20373e4	2072.35522	49.5194
2	5.623	BB	0.0971	1.22710e4	1957.53320	50.4806



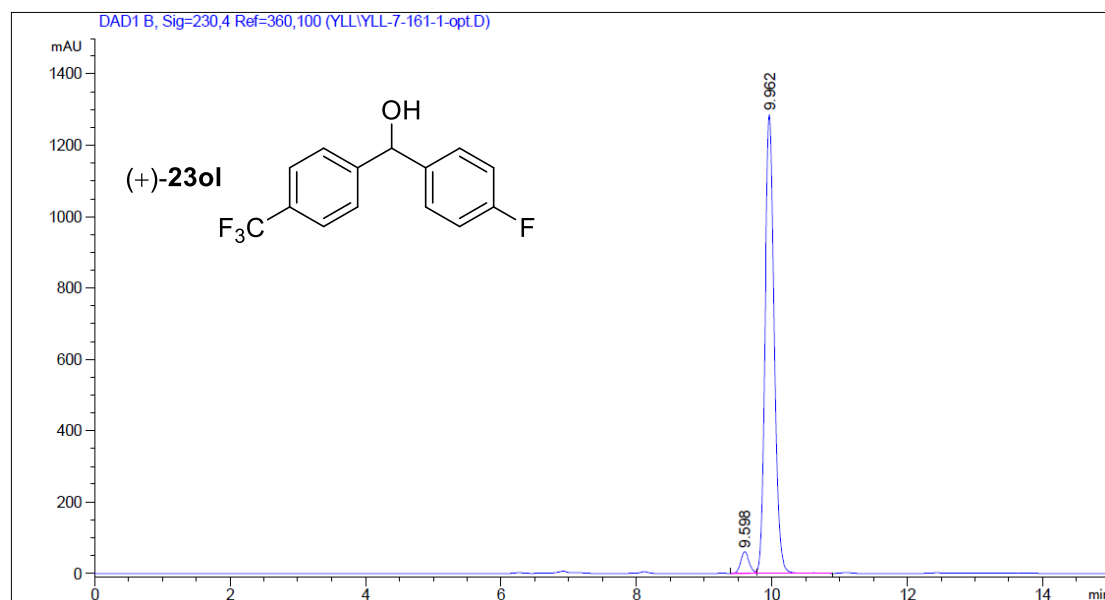
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.197	MM	0.1152	263.77548	38.14873	2.7977
2	5.573	MM	0.0956	9164.50293	1597.35803	97.2023



**(+)-(4-fluorophenyl)(4-(trifluoromethyl)phenyl)methanol (23ol)**

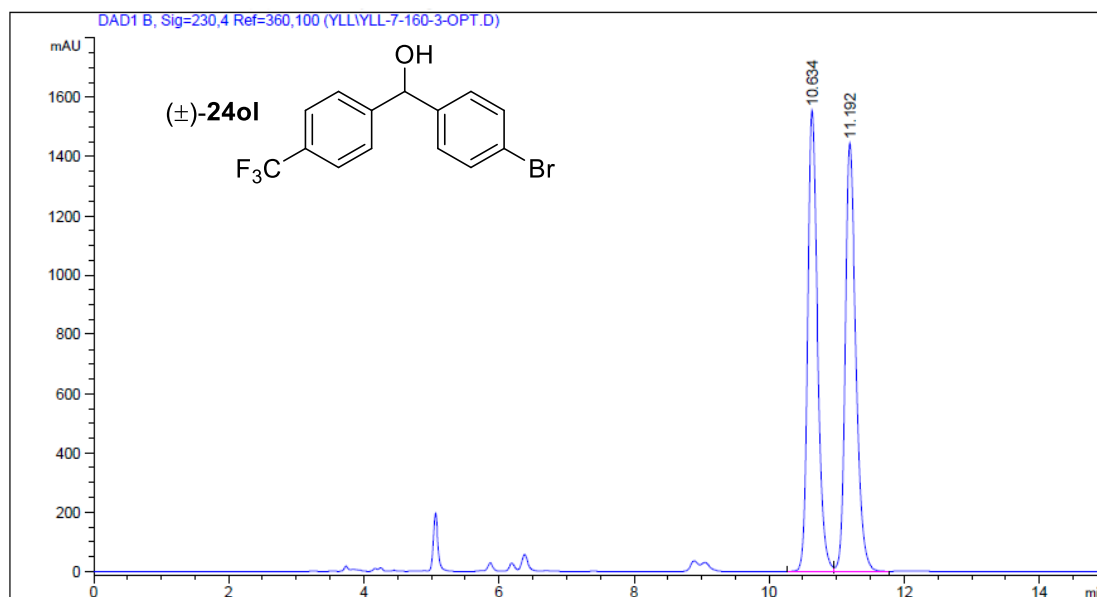


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.576	BV	0.1375	7670.19043	864.59674	49.3906
2	9.937	WV R	0.1445	7859.46191	838.10309	50.6094

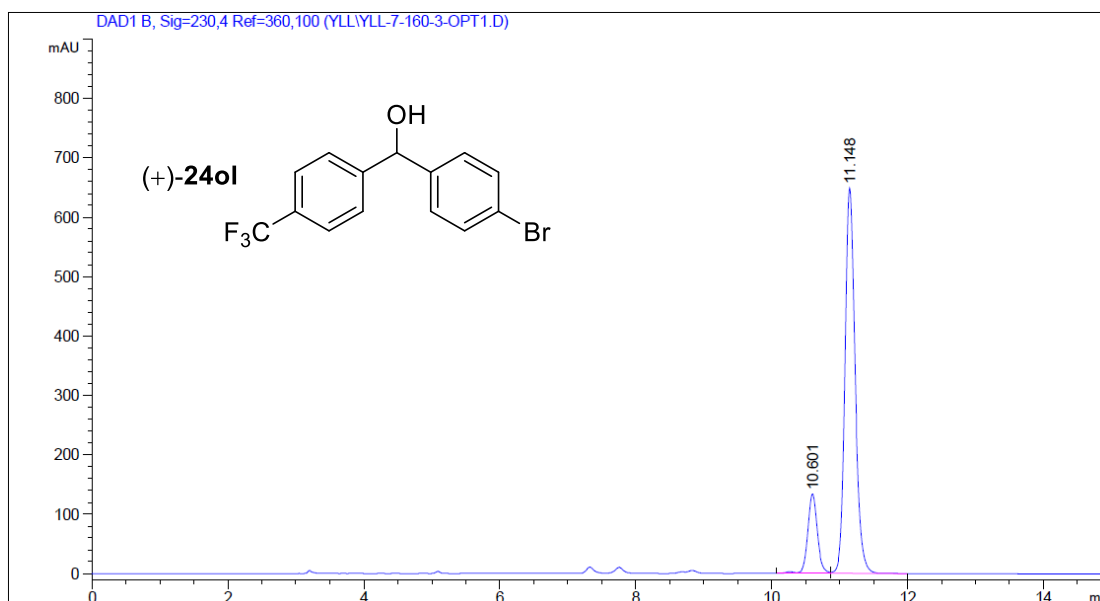


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.598	BV E	0.1316	521.79059	61.12857	4.1336
2	9.962	WV R	0.1456	1.21013e4	1285.75964	95.8664

**(+)-(4-bromophenyl)(4-(trifluoromethyl)phenyl)methanol (24ol)**

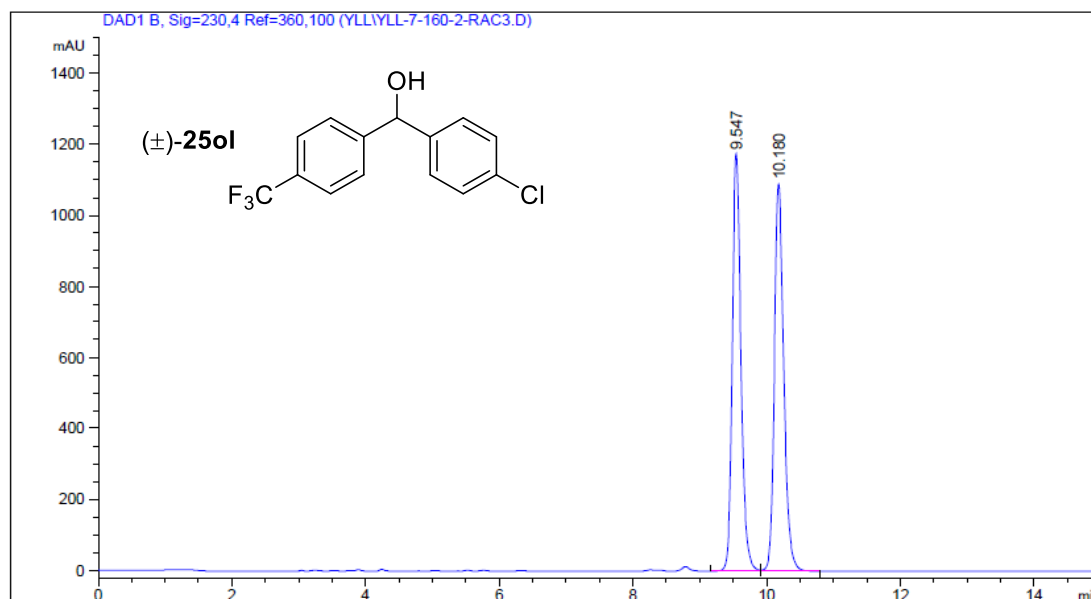


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.634	BV	0.1536	1.56828e4	1556.05774	49.8757
2	11.192	VB	0.1672	1.57610e4	1445.61450	50.1243

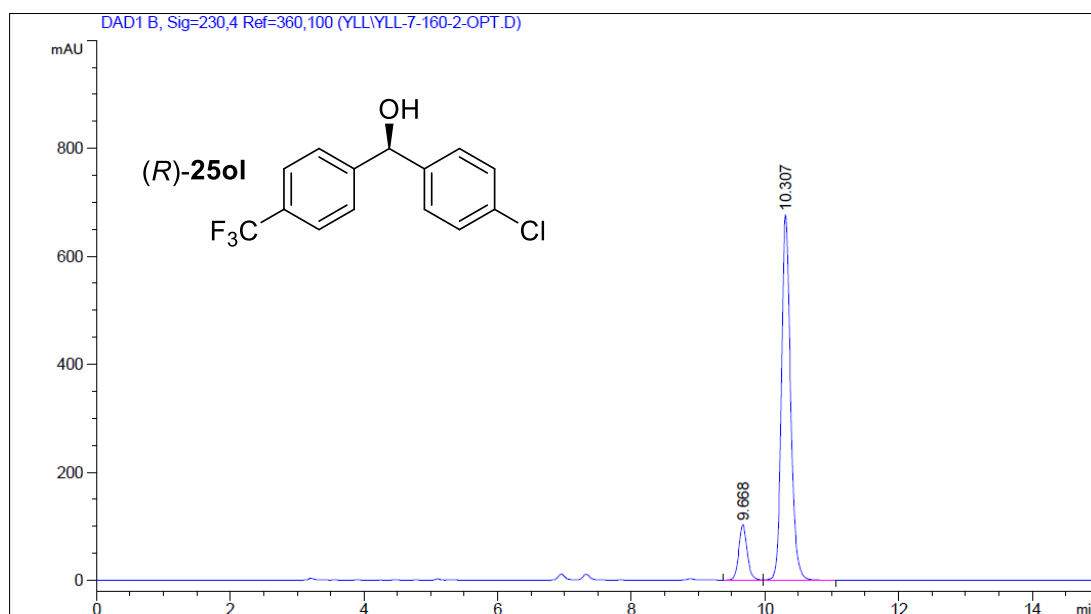


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.601	VV R	0.1461	1307.80090	133.72392	16.3181
2	11.148	VB	0.1566	6706.64014	648.90692	83.6819

**(R)-(4-chlorophenyl)(4-(trifluoromethyl)phenyl)methanol (25ol)**

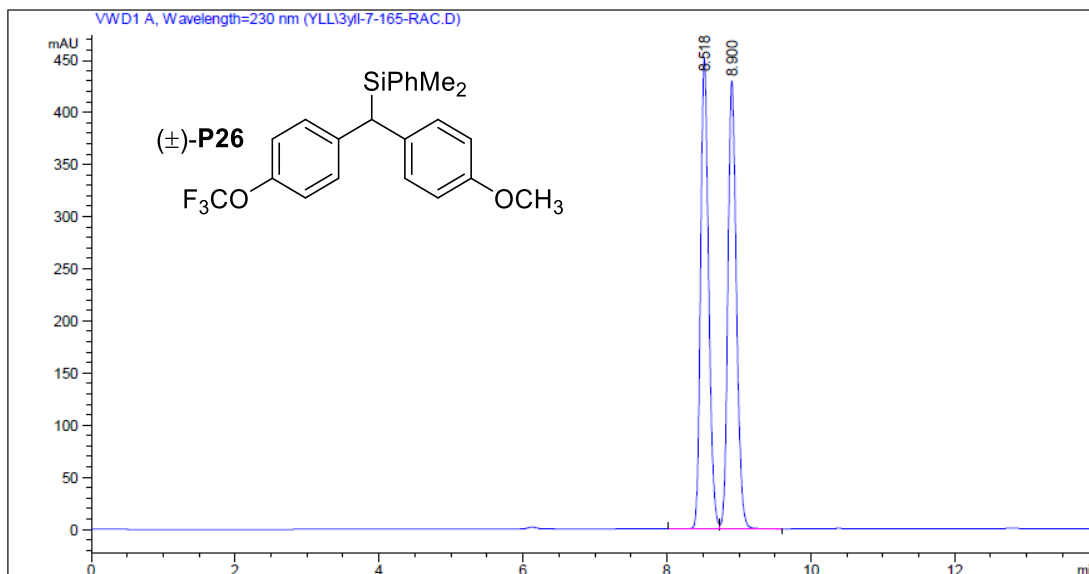


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.547	BV	0.1370	1.05914e4	1176.46558	49.9035
2	10.180	VB	0.1476	1.06323e4	1091.90283	50.0965

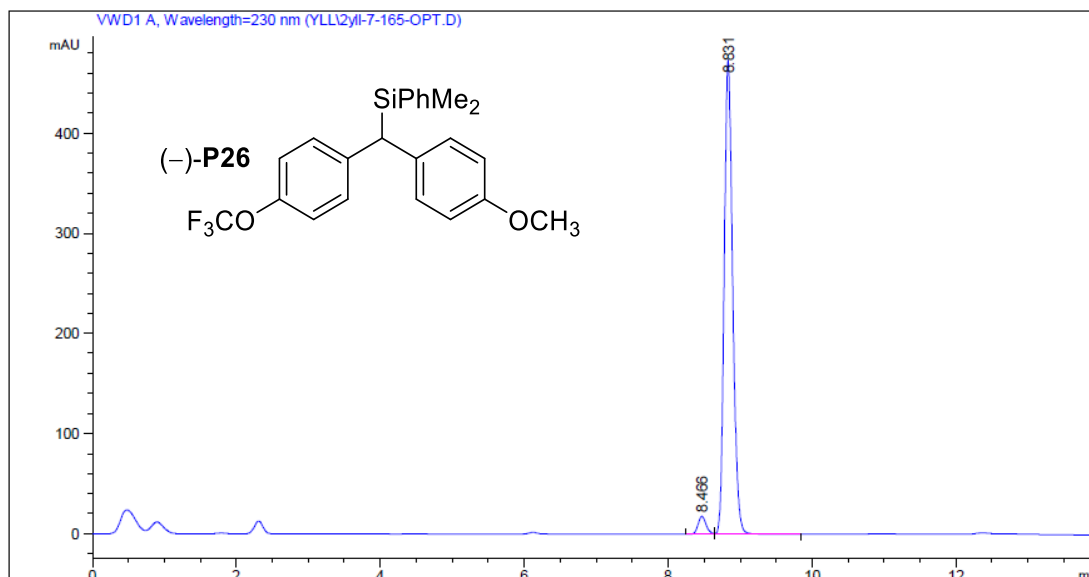


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.668	BV	0.1347	900.07404	102.25128	12.2302
2	10.307	VB	0.1473	6459.37695	676.79004	87.7698

**(-)-((4-methoxyphenyl)(4-(trifluoromethoxy)phenyl)methyl)dimethyl(phenyl)silane (P26)**

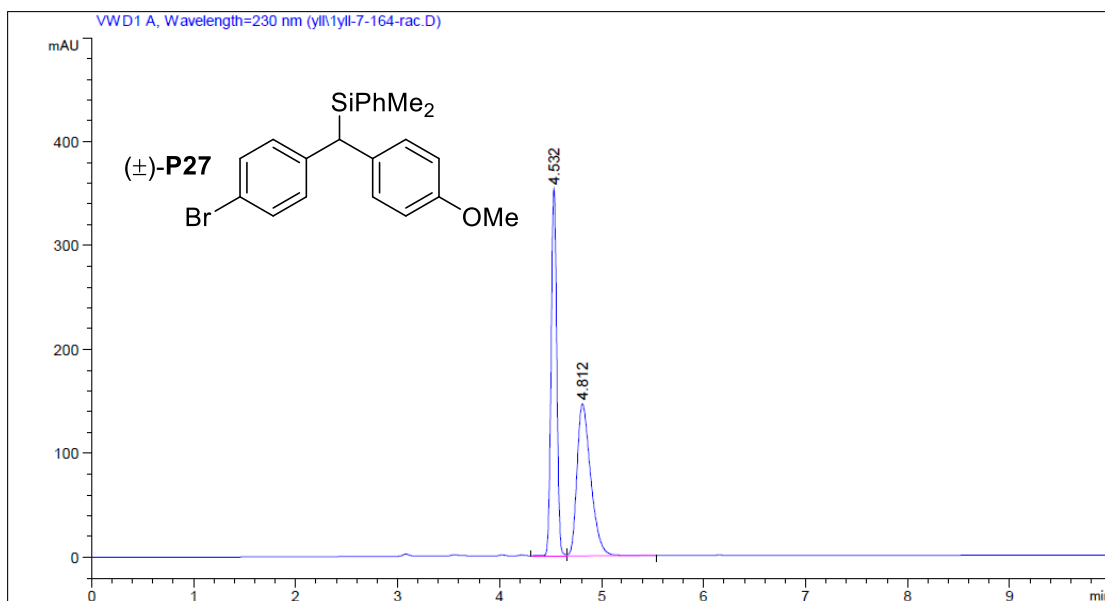


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.518	VV R	0.1202	3523.65503	450.88245	49.8832
2	8.900	VB	0.1261	3540.16187	429.95889	50.1168

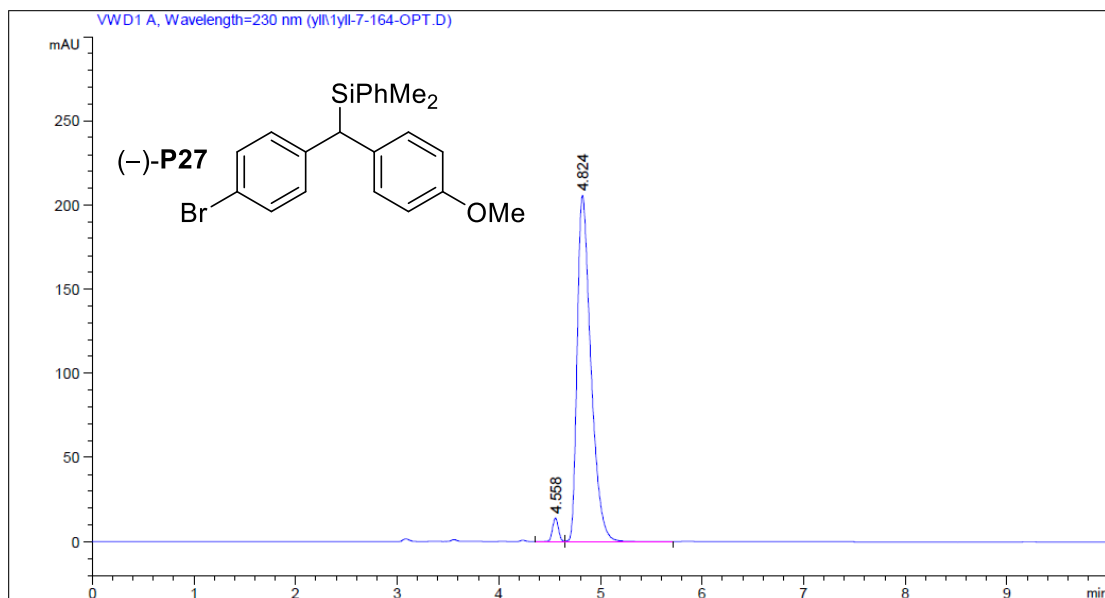


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.466	BV	0.1192	138.66765	17.93404	3.4646
2	8.831	VB	0.1252	3863.77832	473.34445	96.5354

**(-)-((4-bromophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P27)**

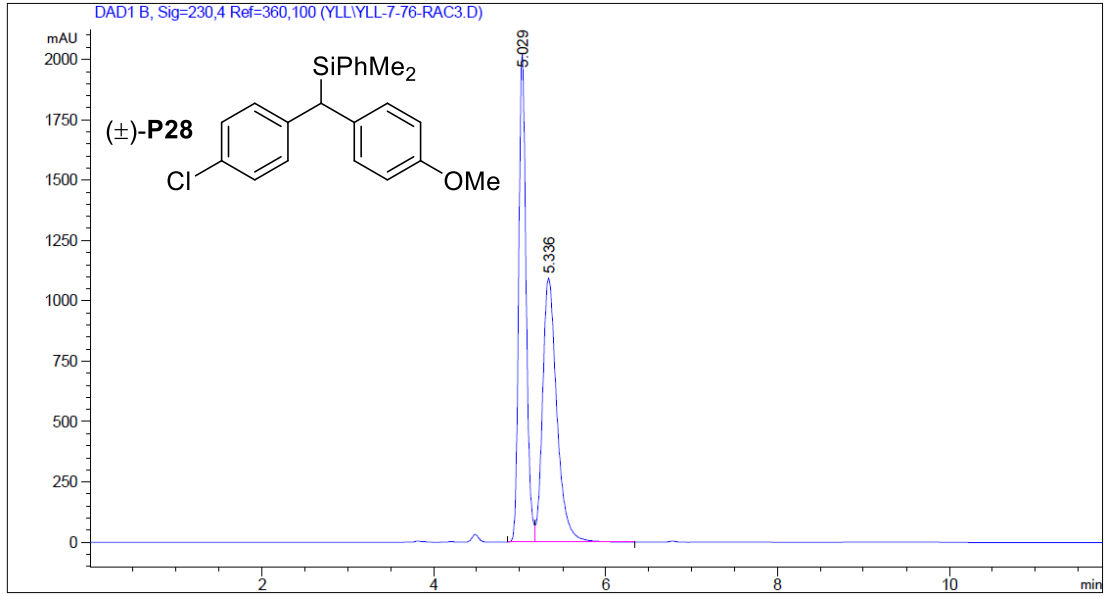


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.532	VV R	0.0600	1359.99036	352.87143	49.8513
2	4.812	VB	0.1422	1368.10400	146.21945	50.1487

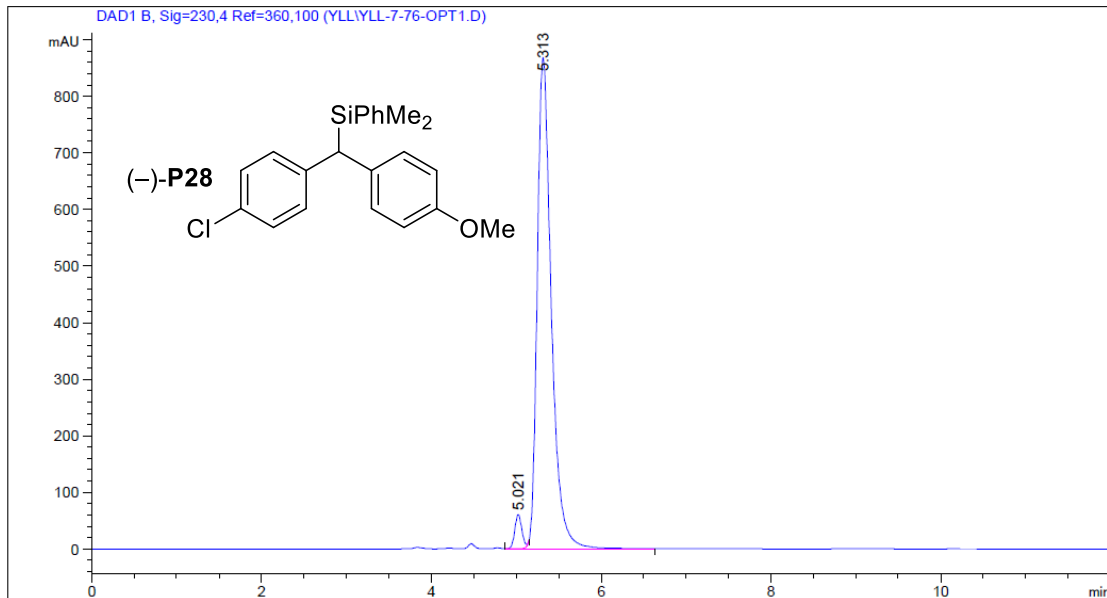


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.558	BV	0.0638	58.09558	14.18501	2.9280
2	4.824	VB	0.1422	1926.04944	205.72449	97.0720

**(-)-((4-chlorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P28)**

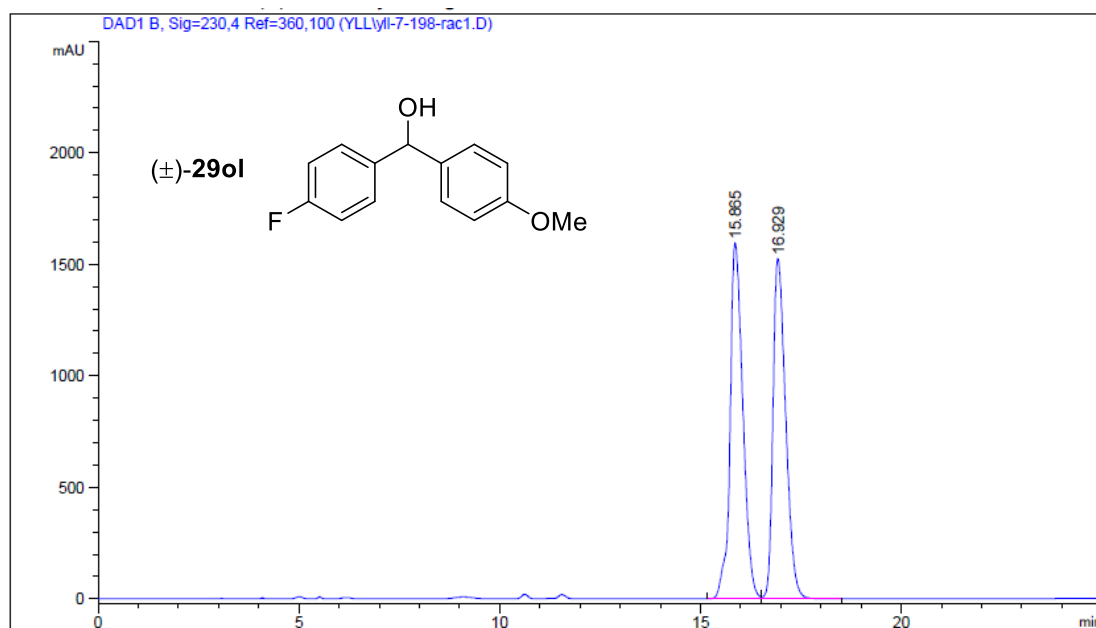


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.029	BV	0.0920	1.21203e4	2021.40930	49.0235
2	5.336	VB	0.1744	1.26032e4	1093.84204	50.9765

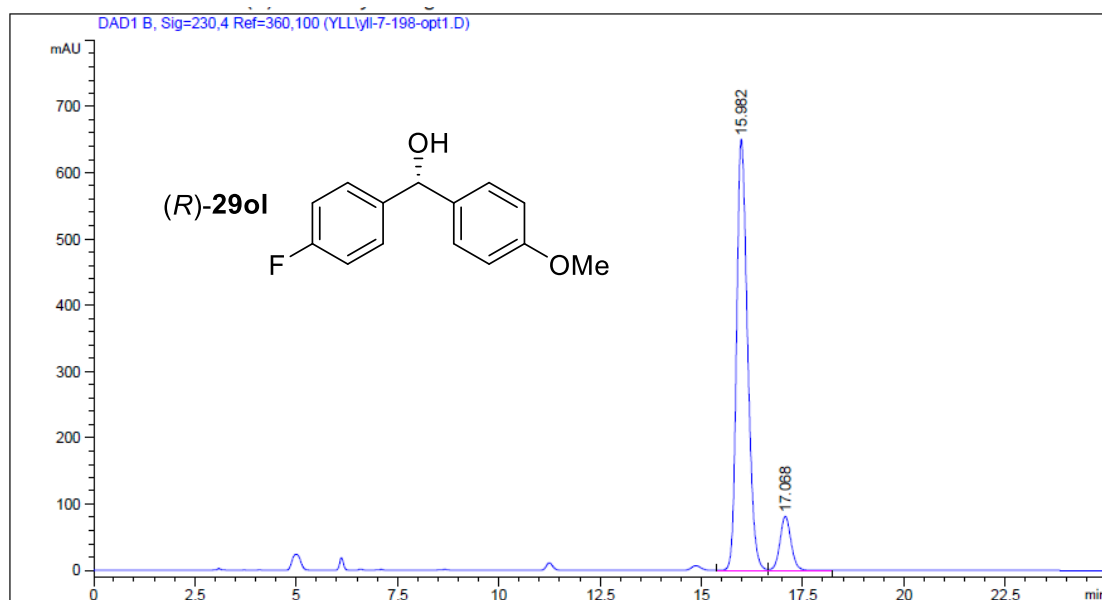


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.021	BV E	0.0894	350.57162	60.70612	3.3890
2	5.313	VB R	0.1743	9993.88184	868.28357	96.6110

### (R)-(4-fluorophenyl)(4-methoxyphenyl)methanol (29ol)

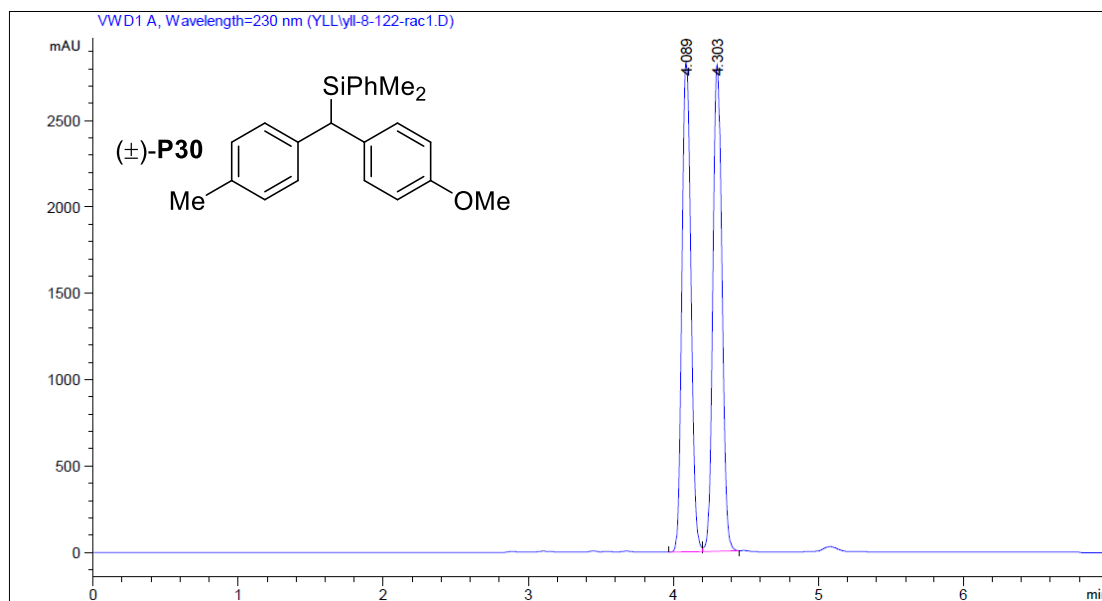


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.865	BV	0.3401	3.52569e4	1593.43994	51.3376
2	16.929	VB	0.3417	3.34197e4	1524.66736	48.6624

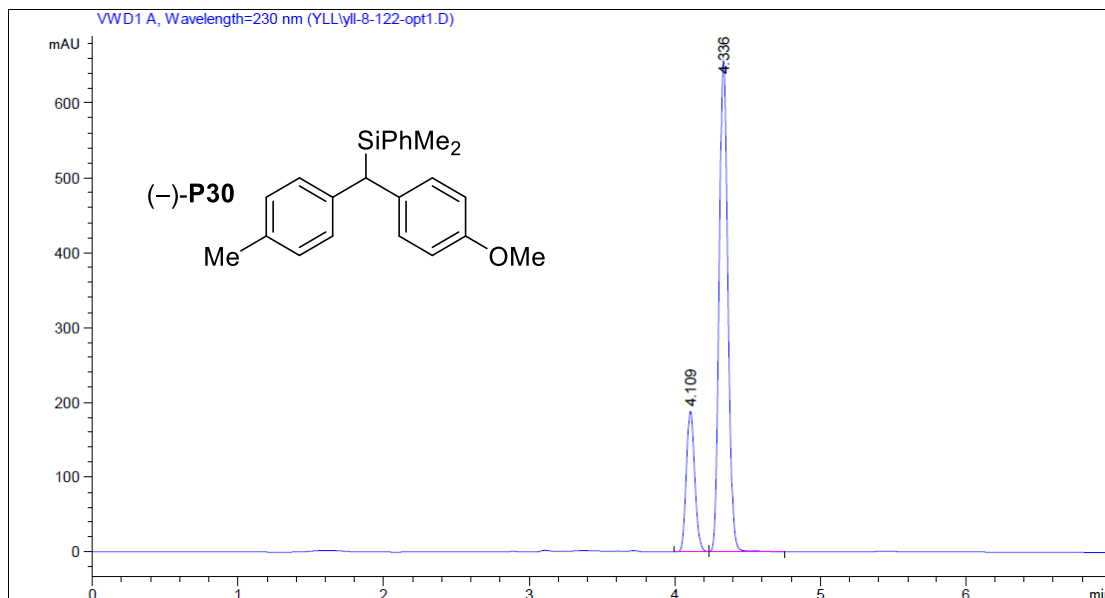


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.982	BV	0.2889	1.22105e4	650.81470	88.7221
2	17.068	VB	0.2941	1552.14087	81.53400	11.2779

**(-)-((4-methoxyphenyl)(p-tolyl)methyl)dimethyl(phenyl)silane (P30)**



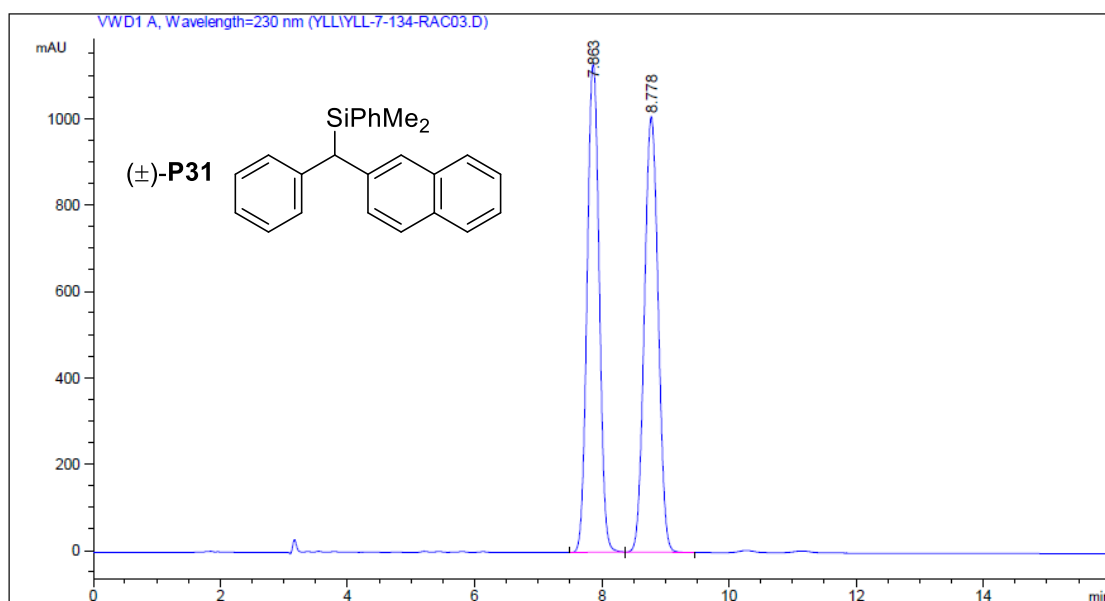
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.089	BV	0.0685	1.22602e4	2834.38892	49.8050
2	4.303	VB	0.0702	1.23562e4	2817.98047	50.1950



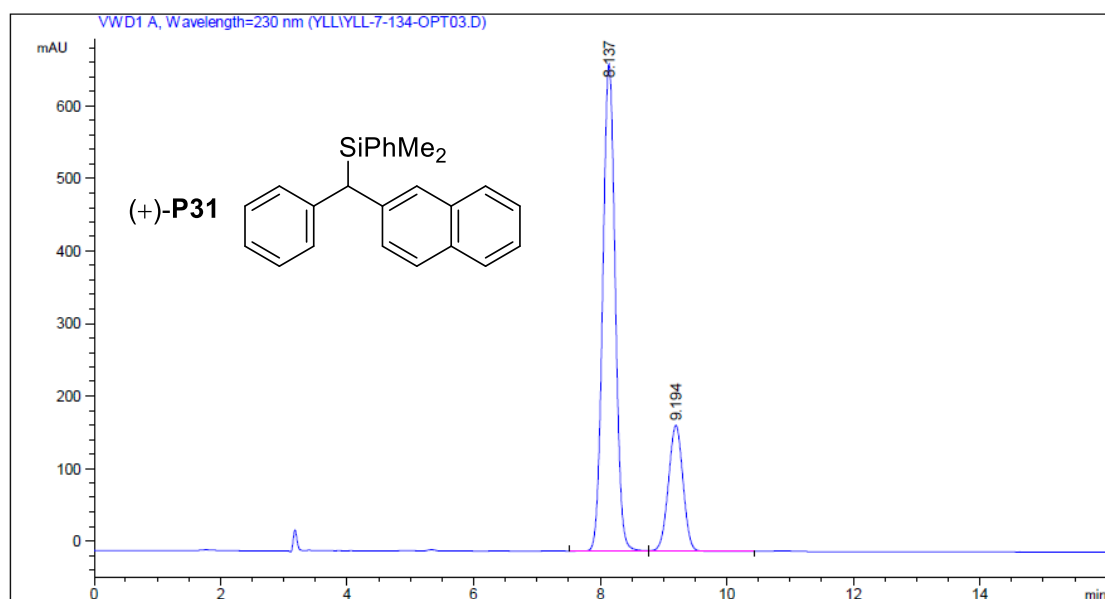
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.109	BV	0.0622	761.56470	188.30223	21.7014
2	4.336	VV R	0.0648	2747.73022	656.86603	78.2986



**(+)-dimethyl(naphthalen-2-yl(phenyl)methyl)(phenyl)silane (P31)**

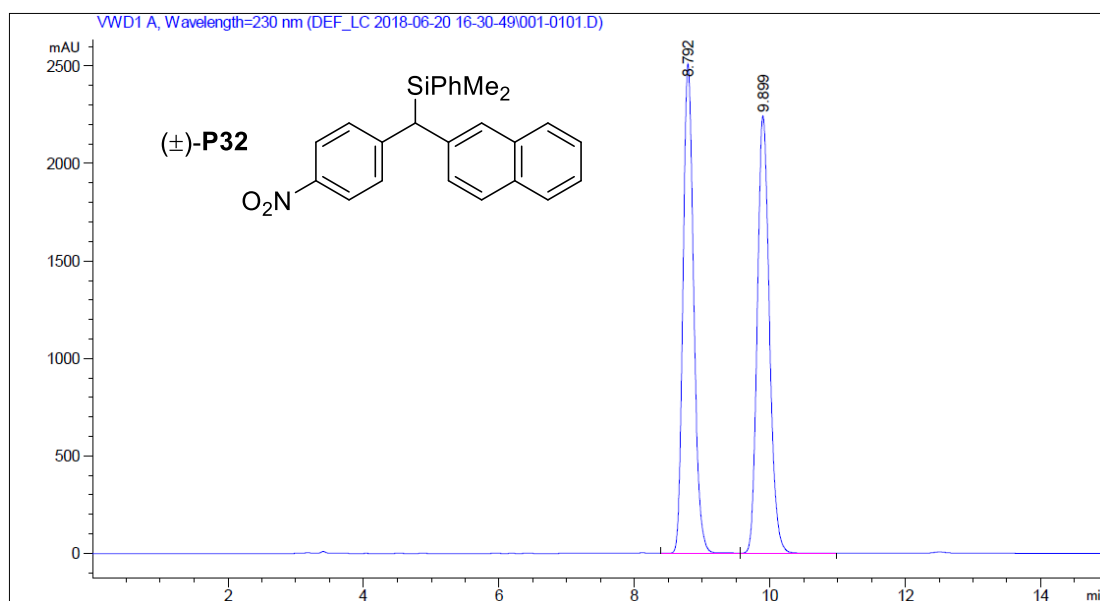


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.863	BB	0.2086	1.48551e4	1130.39685	49.3667
2	8.778	BB	0.2390	1.52362e4	1007.95526	50.6333

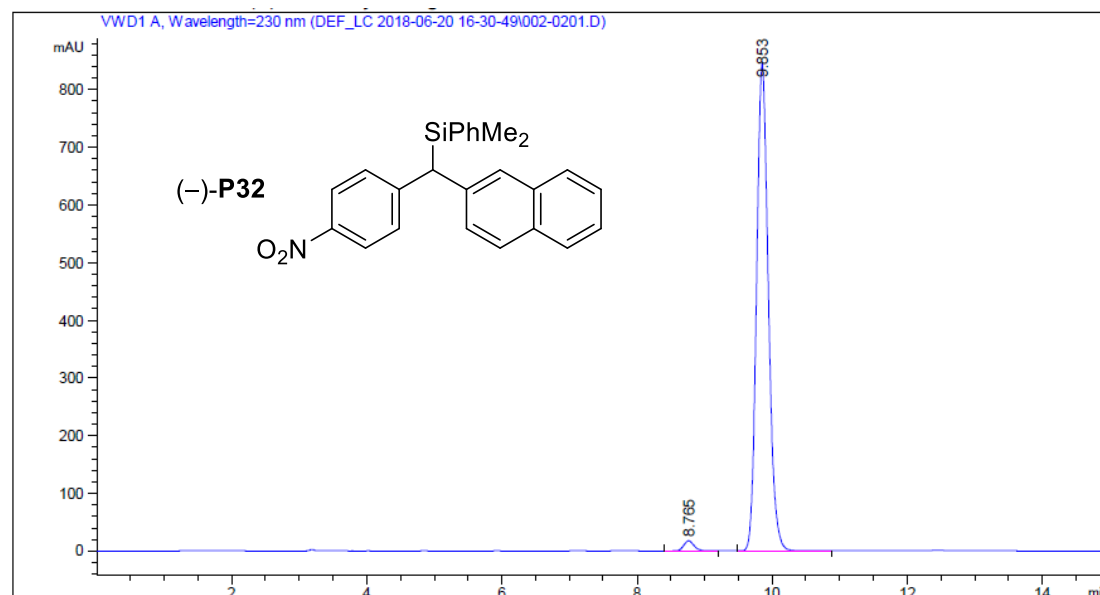


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.137	BV	0.2148	9183.89648	671.81177	76.6400
2	9.194	VV	0.2520	2799.26709	173.80780	23.3600

**(±)-dimethyl(naphthalen-2-yl(4-nitrophenyl)methyl)(phenyl)silane (P32)**

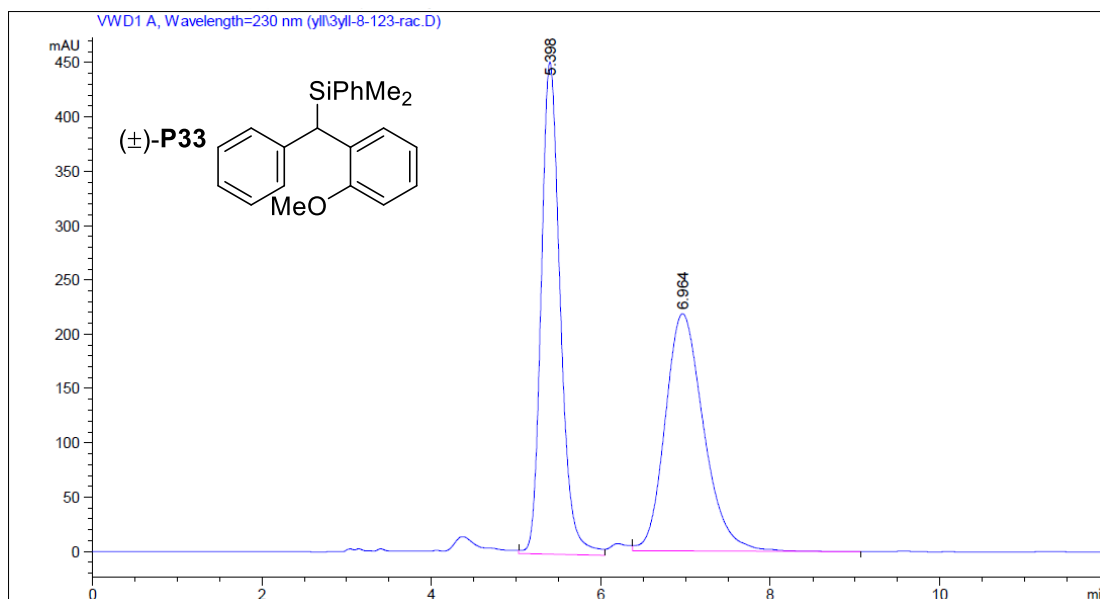


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.792	BV R	0.1709	2.75522e4	2510.41724	49.6952
2	9.899	VB	0.1932	2.78902e4	2241.60596	50.3048

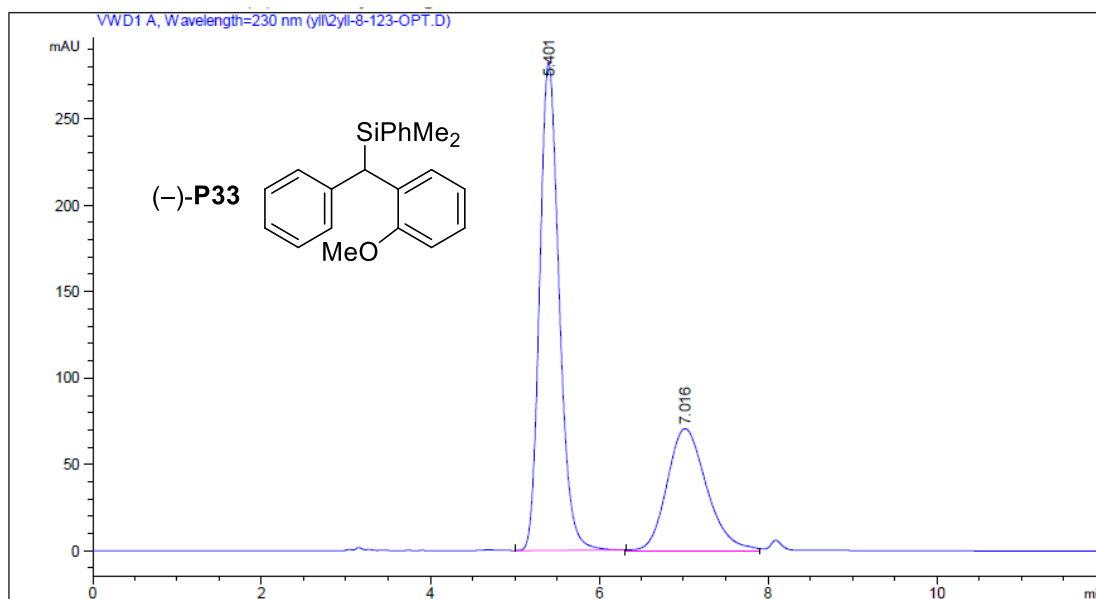


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.765	BB	0.1617	185.69287	17.66323	1.7822
2	9.853	BB	0.1862	1.02334e4	845.73407	98.2178

**(-)-((2-methoxyphenyl)(phenyl)methyl)dimethyl(phenyl)silane (P33)**

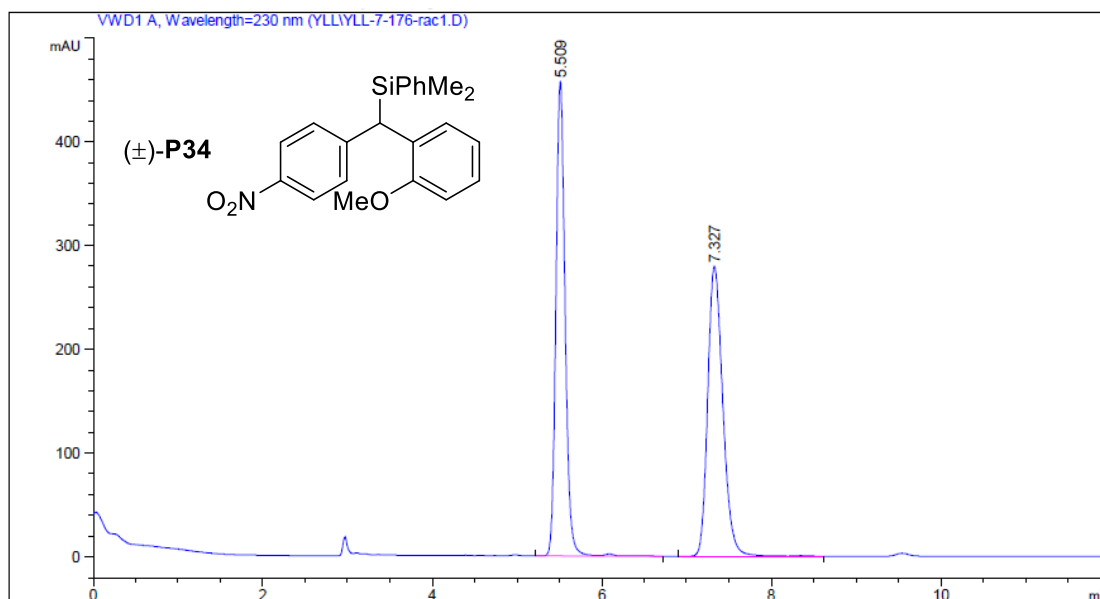


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.398	MM R	0.2610	7094.85986	452.97665	50.6621
2	6.964	VB	0.4860	6909.41553	218.45155	49.3379

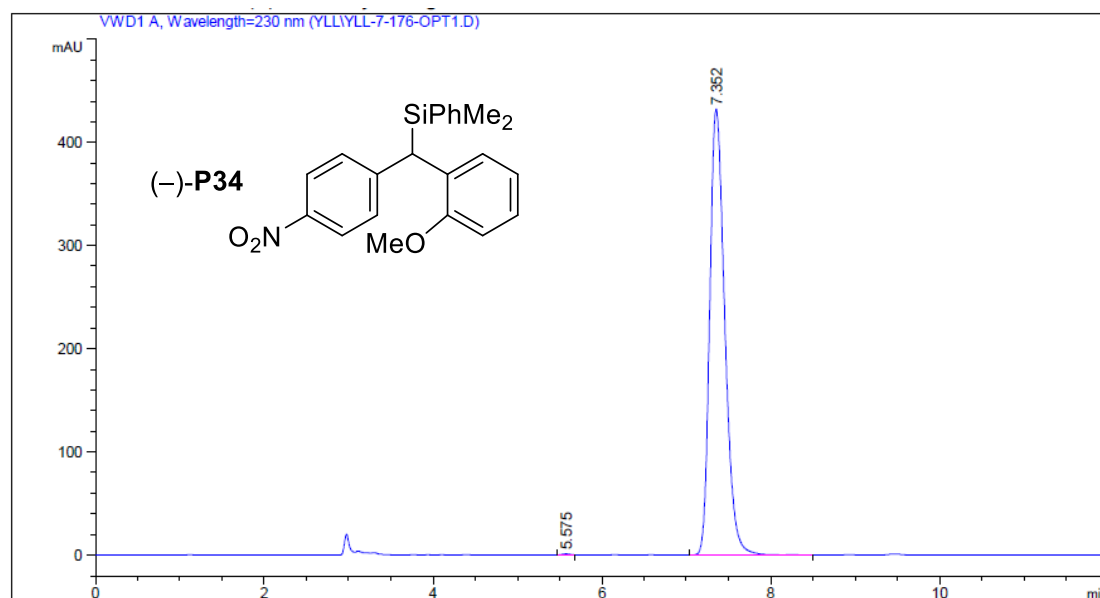


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.401	BB	0.2479	4520.97510	282.20248	66.2424
2	7.016	MM R	0.5431	2303.92505	70.69916	33.7576

**(-)-((2-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P34)**

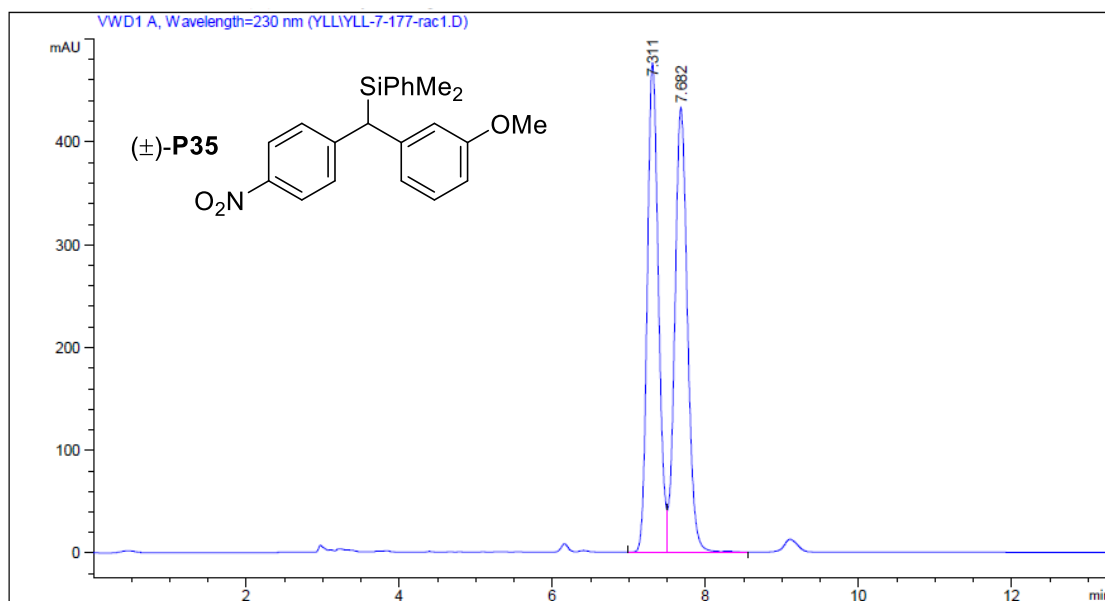


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.509	BV R	0.1154	3442.39453	457.50986	49.8911
2	7.327	BV R	0.1913	3457.41748	279.46399	50.1089

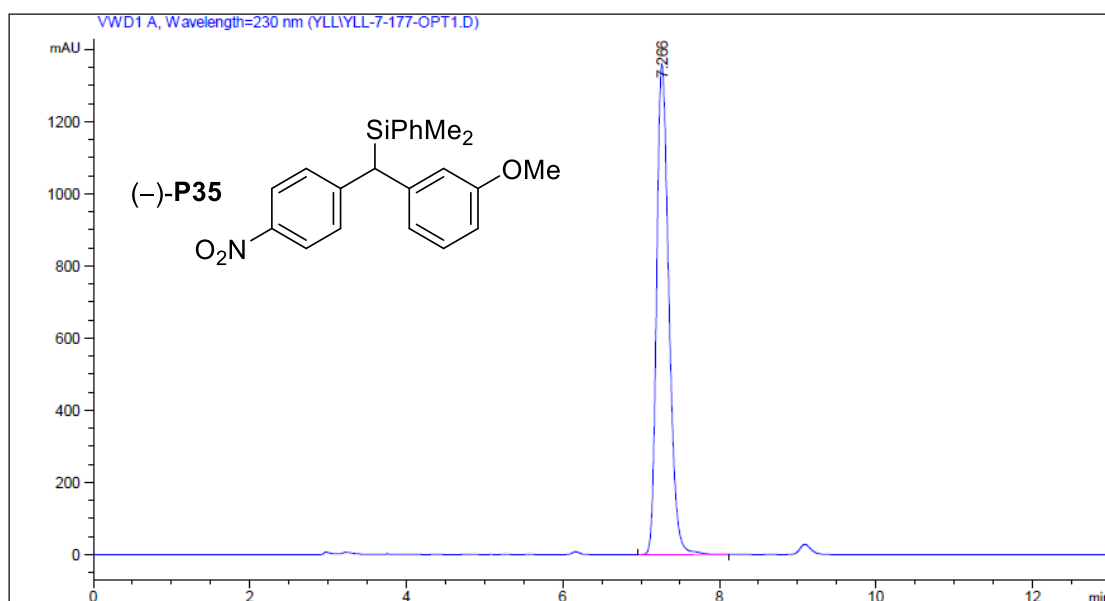


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.575	MM R	0.1152	8.24817	1.19348	0.1539
2	7.352	BV R	0.1914	5349.62695	432.19373	99.8461

**(-)-((3-methoxyphenyl)(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P35)**

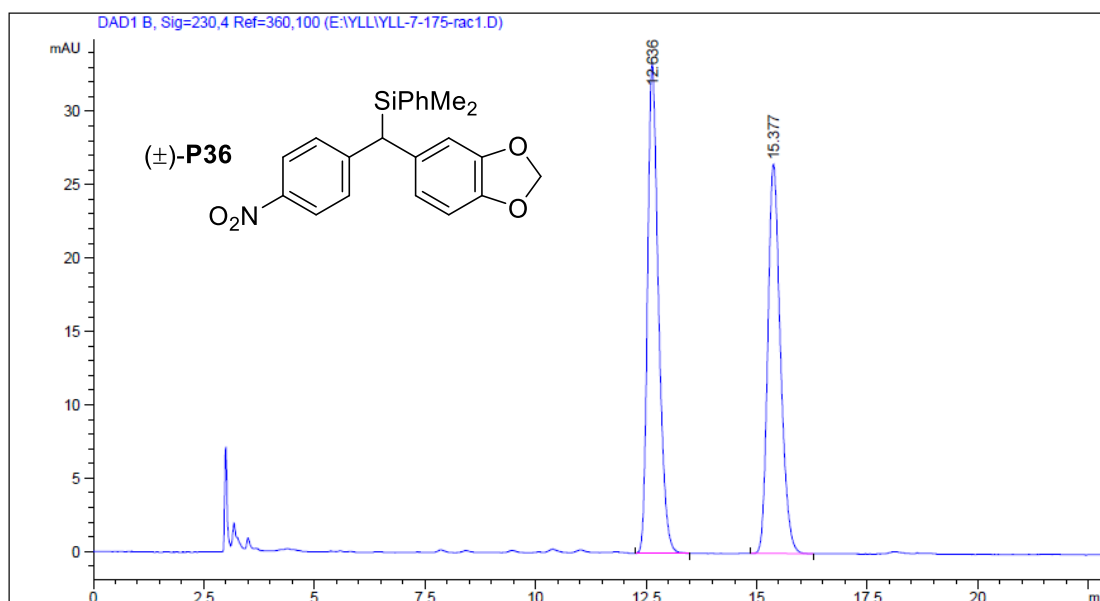


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.311	BV	0.1567	4798.25781	475.71945	49.3391
2	7.682	W R	0.1759	4926.80518	432.35315	50.6609

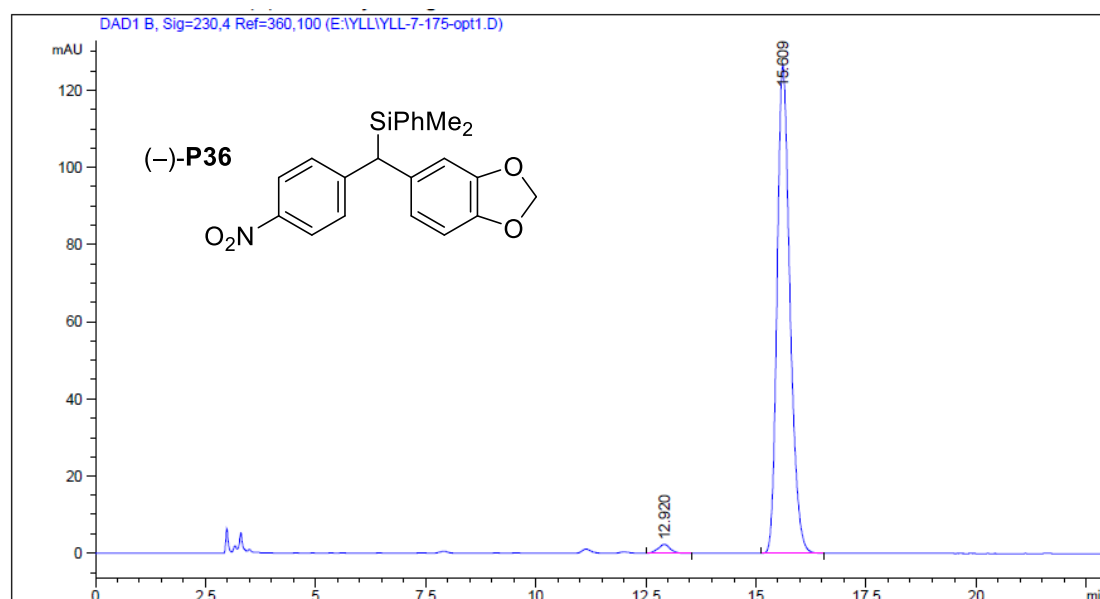


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.266	BB	0.1680	1.47855e4	1358.65503	100.0000

**(-)-(benzo[d][1,3]dioxol-5-yl(4-nitrophenyl)methyl)dimethyl(phenyl)silane (P36)**

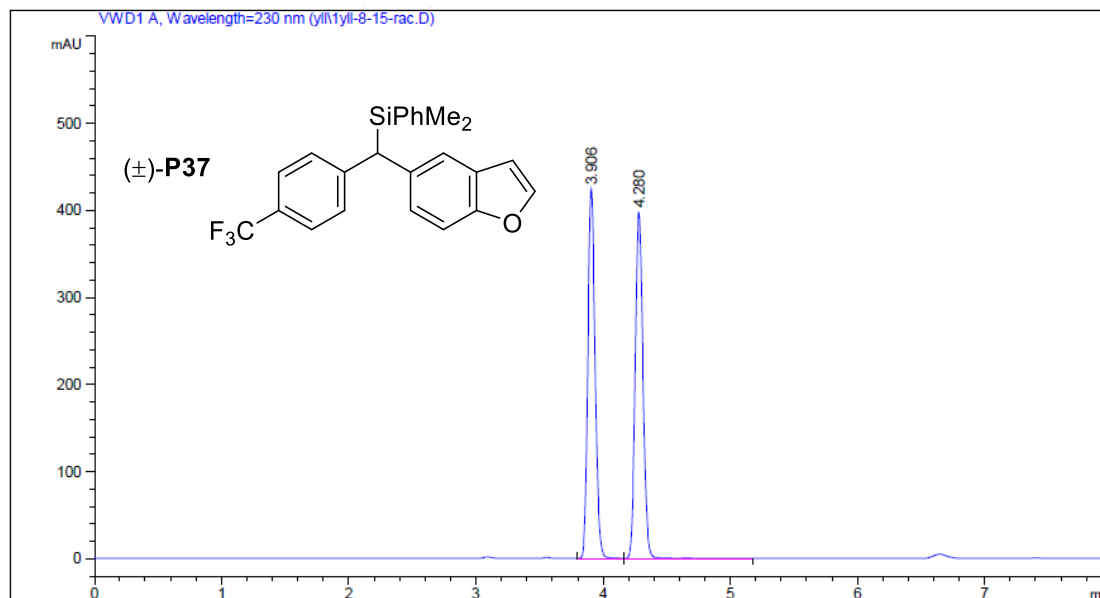


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.636	BB	0.2578	571.31885	33.36778	52.0230
2	15.377	BB	0.3015	526.88531	26.55358	47.9770

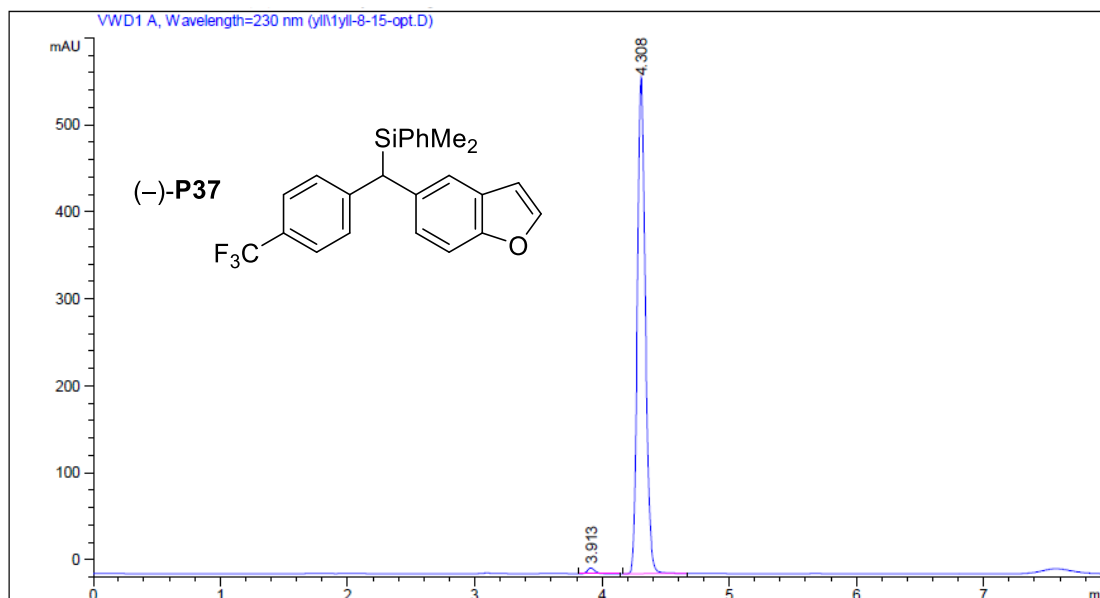


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.920	BB	0.2783	44.61031	2.32023	1.7066
2	15.609	BB	0.3110	2569.42700	126.50528	98.2934

**(-)-(benzofuran-5-yl(4-(trifluoromethyl)phenyl)methyl)dimethyl(phenyl)silane (P37)**

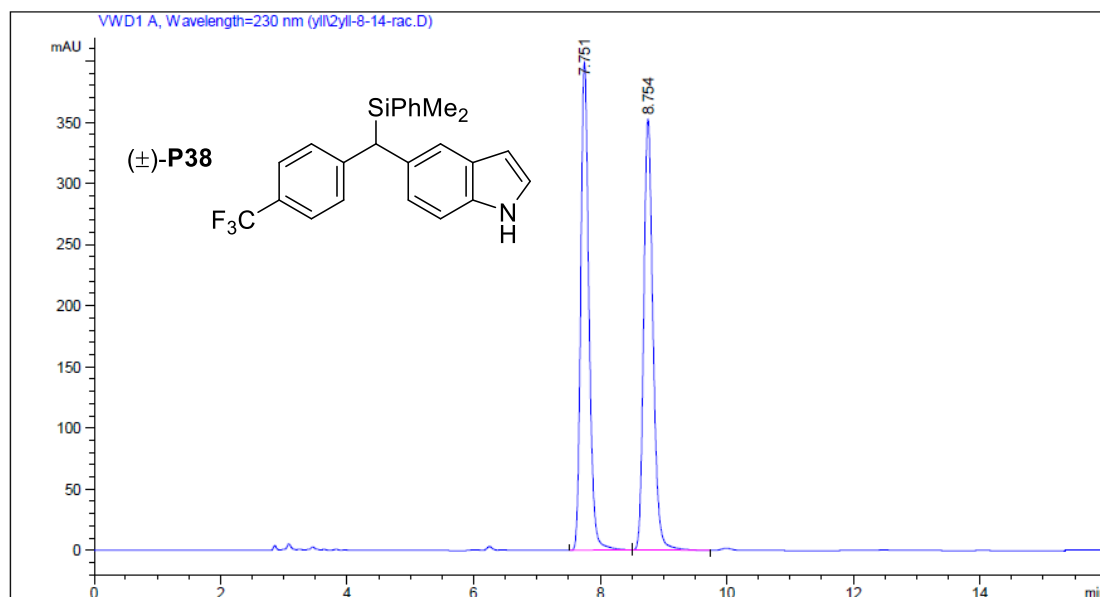


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.906	BB	0.0612	1680.84277	424.35303	49.8552
2	4.280	BV R	0.0656	1690.60938	397.66409	50.1448

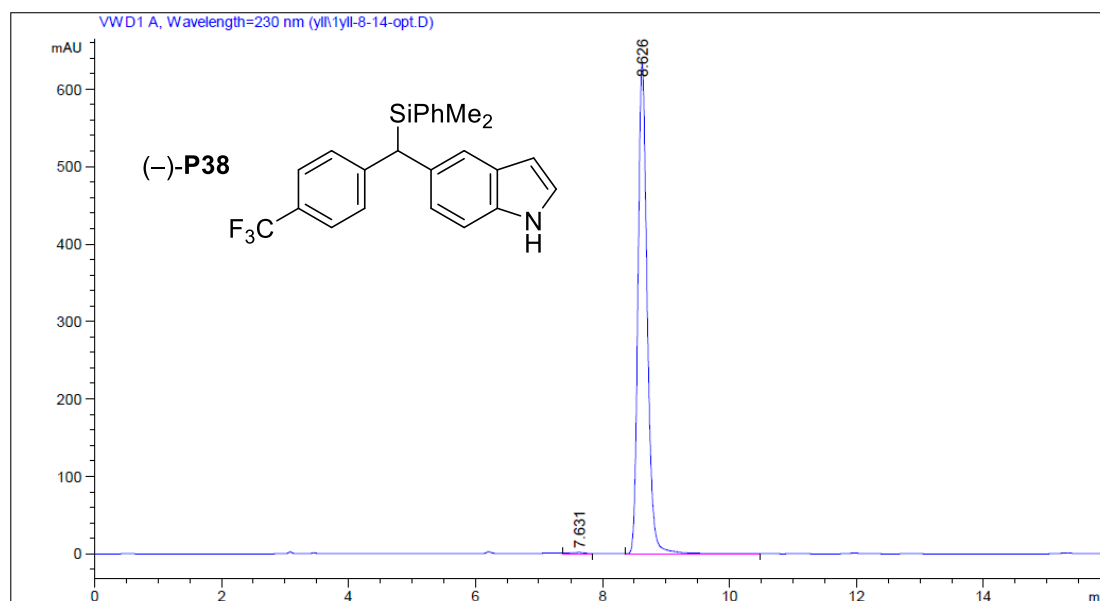


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.913	BB	0.0626	26.55536	6.51217	1.0468
2	4.308	BB	0.0683	2510.27686	571.30750	98.9532

**(-)-5-((dimethyl(phenyl)silyl)(4-(trifluoromethyl)phenyl)methyl)-1H-indole (P38)**



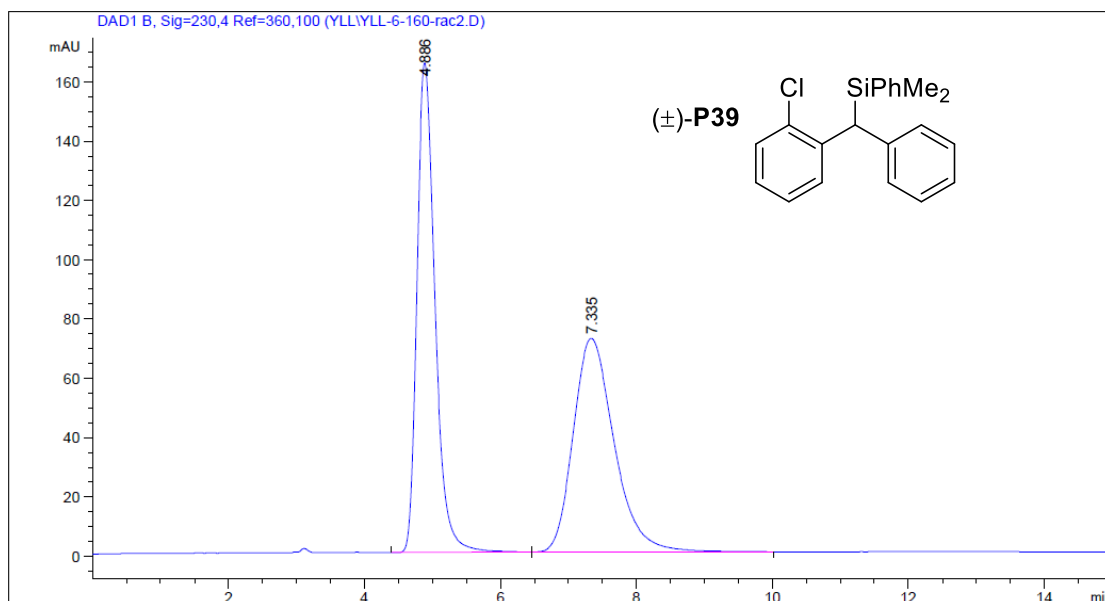
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.751	BB	0.1384	3603.27295	398.88898	49.9711
2	8.754	BB	0.1564	3607.43628	352.39386	50.0289



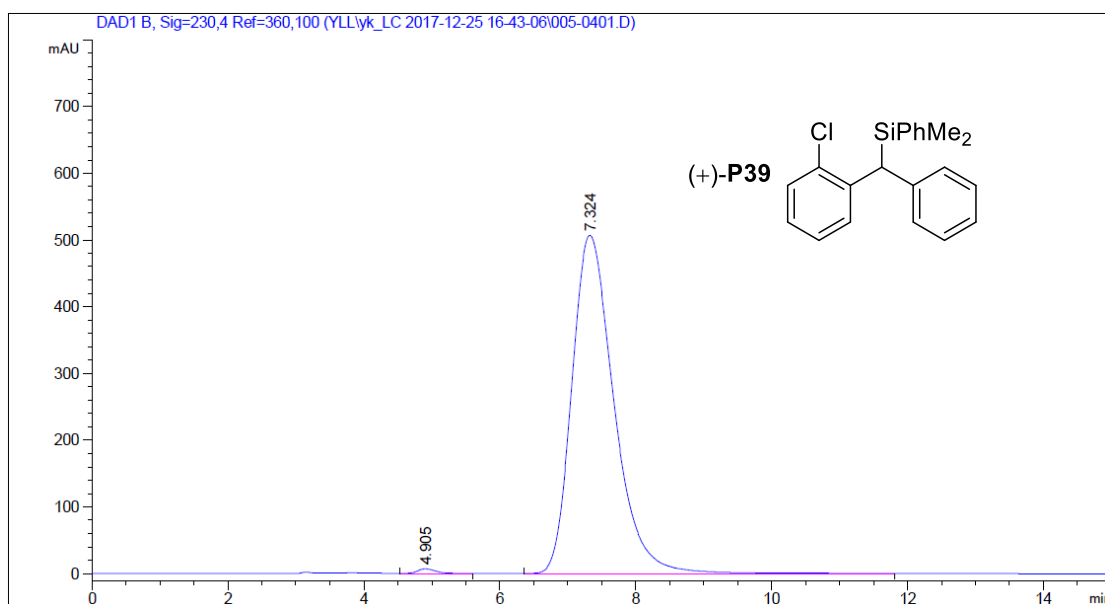
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.631	VV	0.2250	31.20424	1.88625	0.4846
2	8.626	BB	0.1541	6408.09033	632.78662	99.5154



**(+)-((2-chlorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P39)**

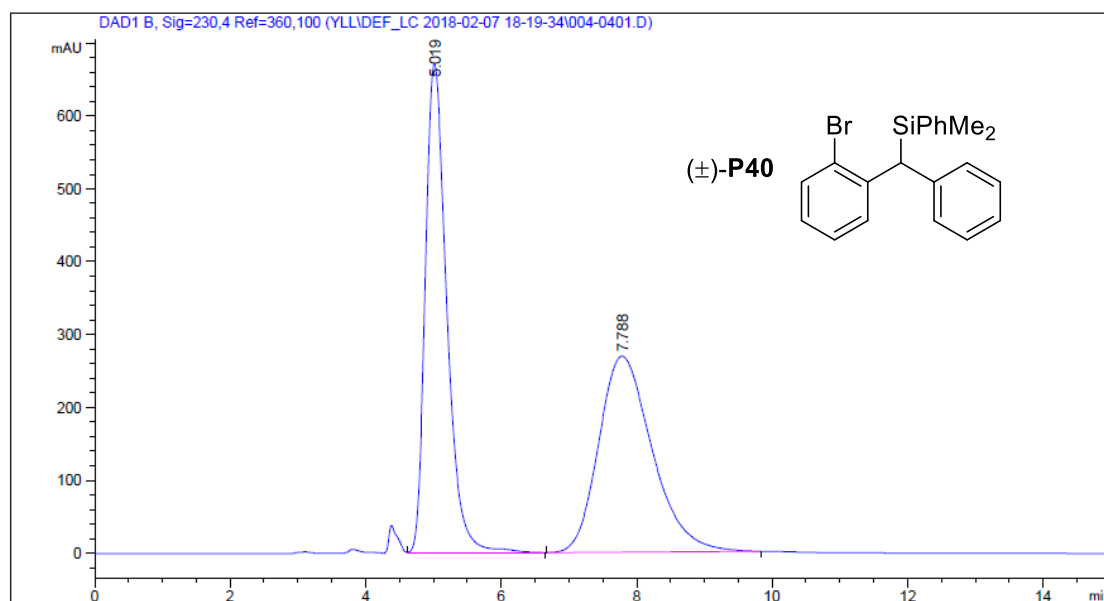


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.886	BB	0.2820	3030.58008	165.19821	50.1470
2	7.335	BB	0.6439	3012.80908	72.04922	49.8530

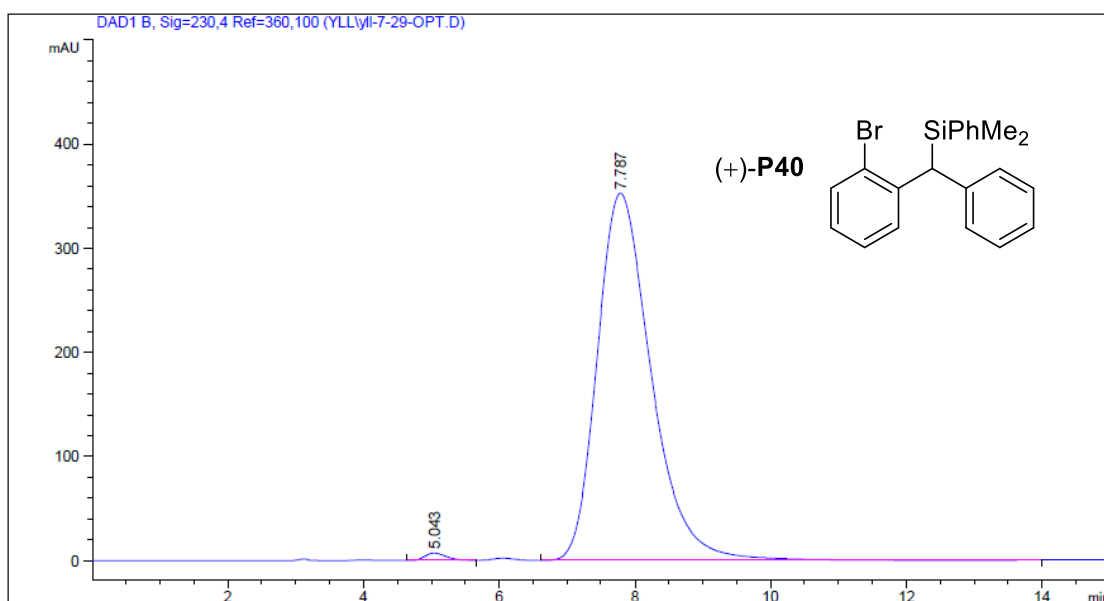


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.905	BB	0.2906	126.85776	6.77139	0.5797
2	7.324	BB	0.6587	2.17549e4	506.89182	99.4203

**(+)-((2-bromophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P40)**

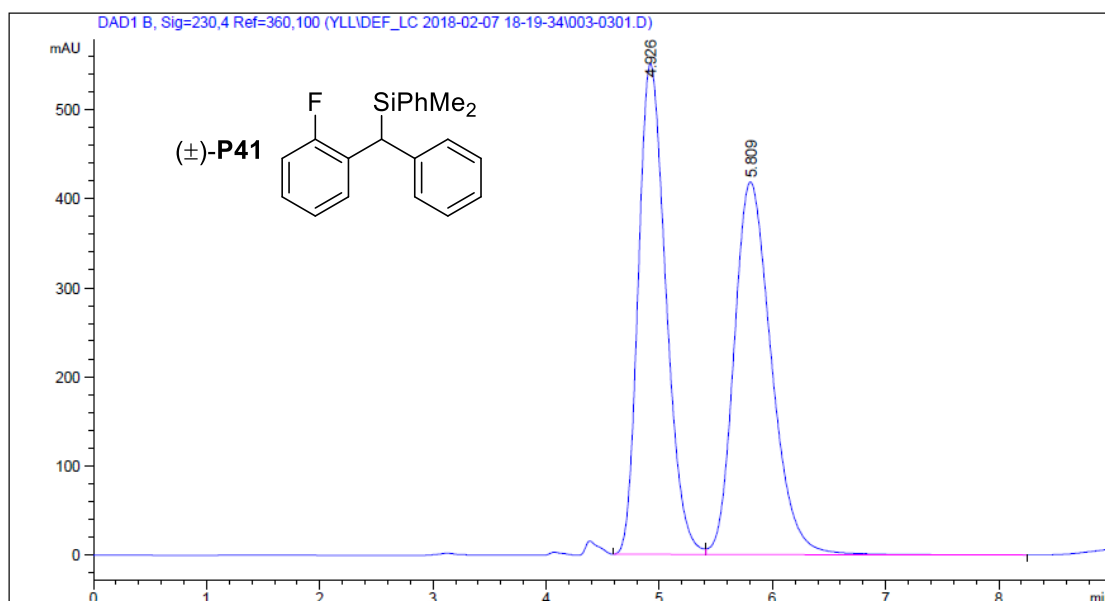


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.019	VB	0.3358	1.47142e4	670.96149	49.9892
2	7.788	BB	0.8426	1.47205e4	268.93268	50.0108

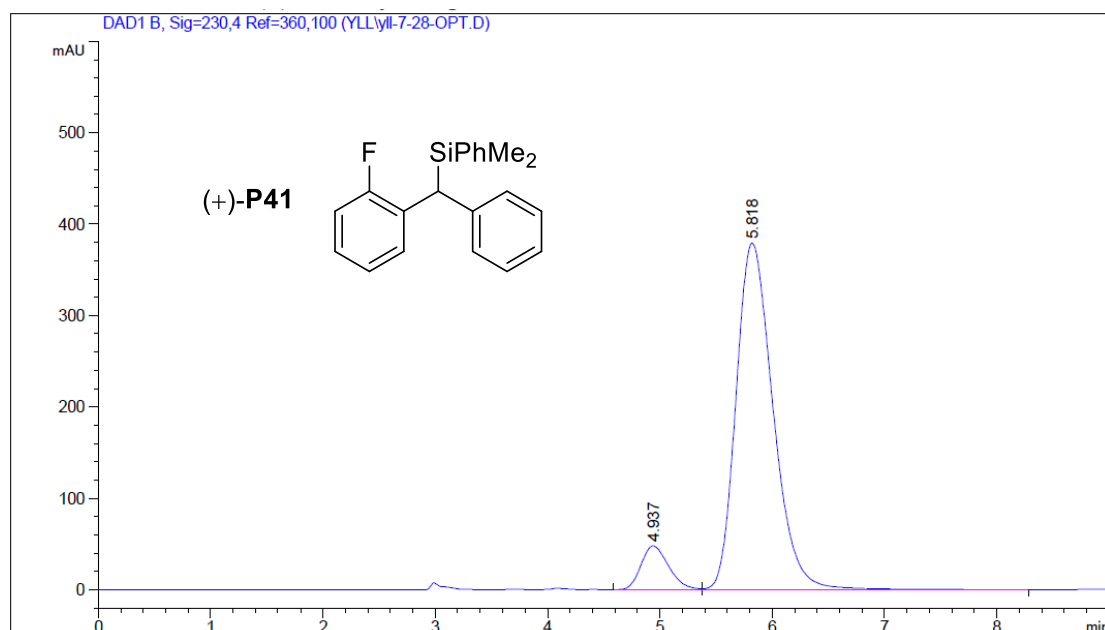


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.043	BB	0.3281	150.01660	7.05356	0.7617
2	7.787	BB	0.8484	1.95446e4	352.74164	99.2383

**(+)-(2-fluorophenyl)(phenyl)methyl)dimethyl(phenyl)silane (P41)**

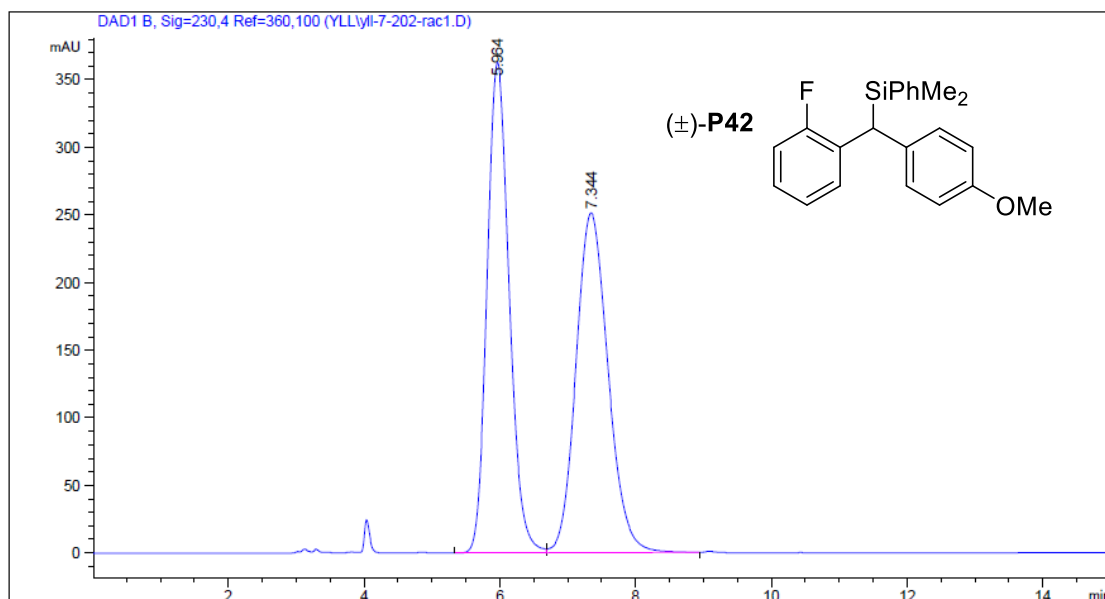


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.926	BV	0.2636	9324.99609	550.56226	49.4119
2	5.809	VB	0.3523	9546.98633	418.22757	50.5881

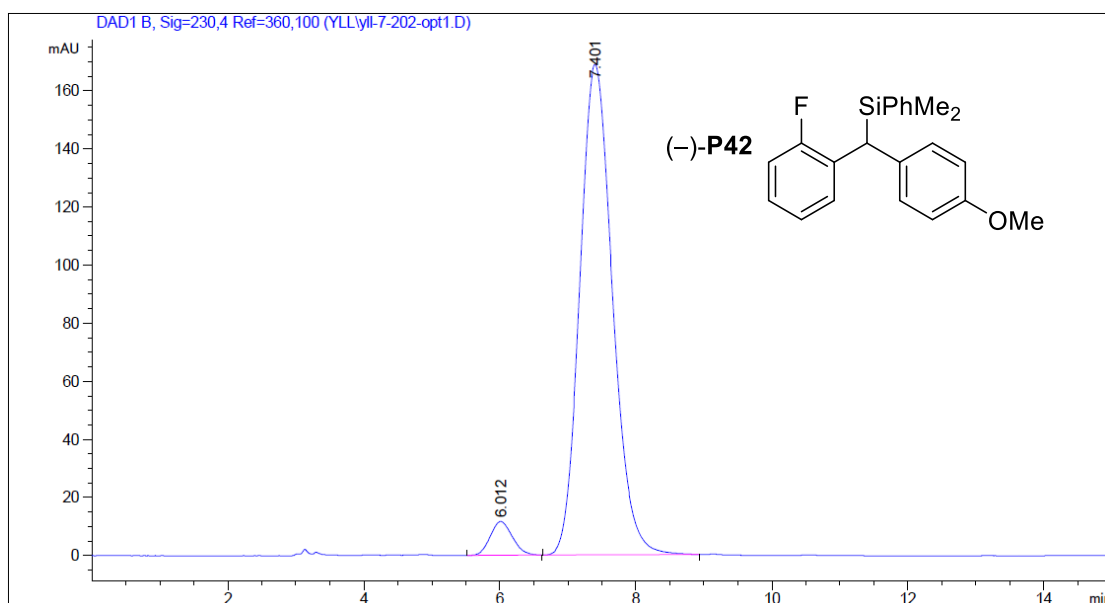


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.937	BV	0.2651	814.47949	47.73455	8.5900
2	5.818	VB	0.3547	8667.27051	379.11499	91.4100

**(-)-((2-fluorophenyl)(4-methoxyphenyl)methyl)dimethyl(phenyl)silane (P42)**

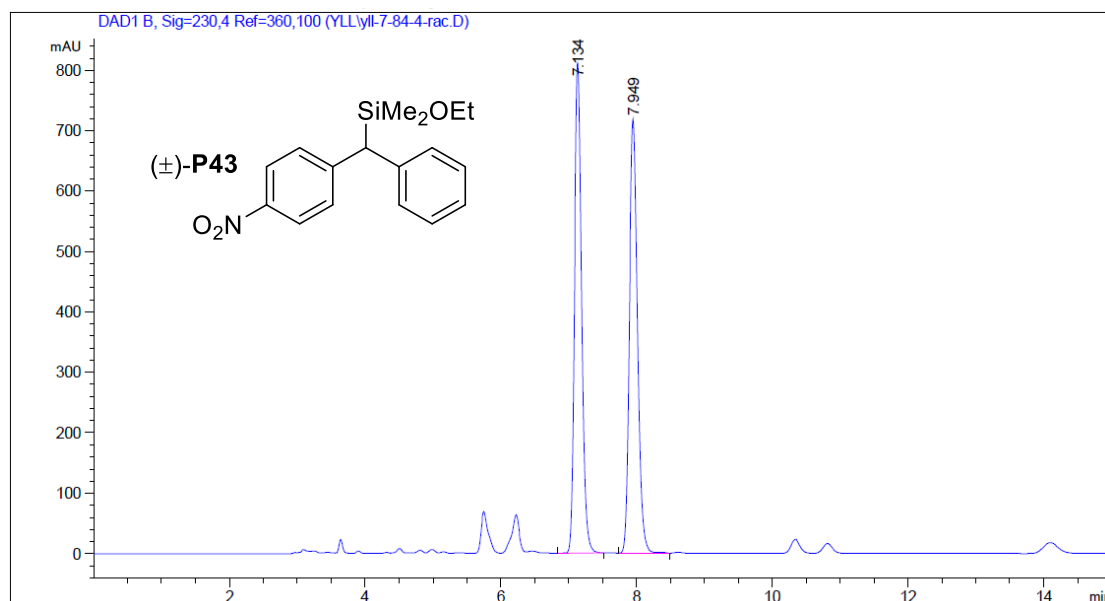


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.964	BV	0.3516	8189.85205	362.46072	49.8209
2	7.344	VB	0.5072	8248.73535	251.15915	50.1791

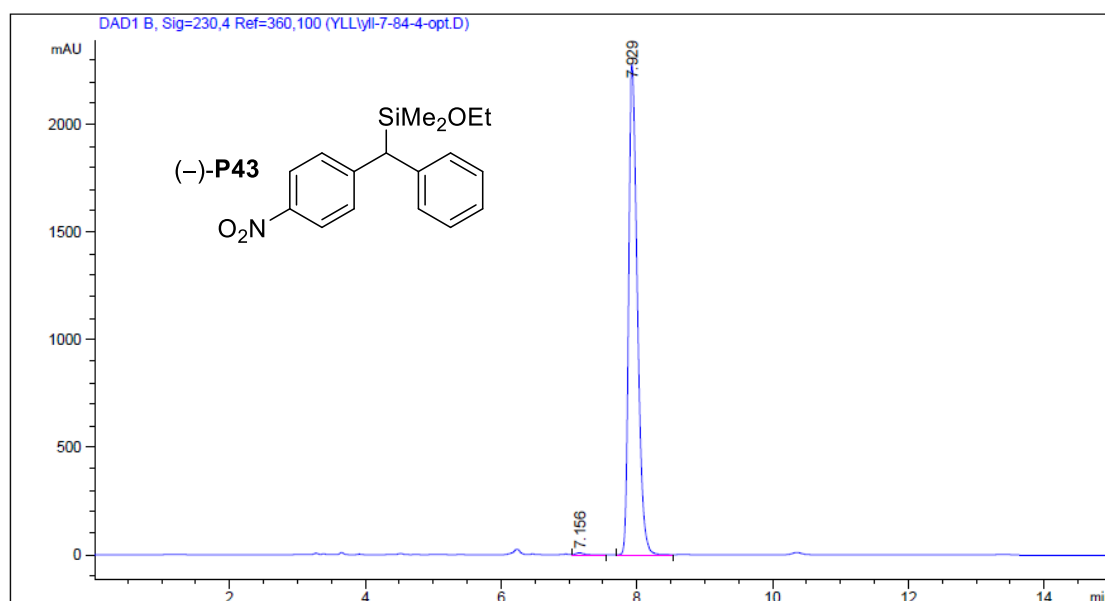


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.012	BB	0.3514	262.69489	11.63375	4.4591
2	7.401	BB	0.5169	5628.56982	168.84630	95.5409

**(-)-ethoxydimethyl((4-nitrophenyl)(phenyl)methyl)silane (P43)**

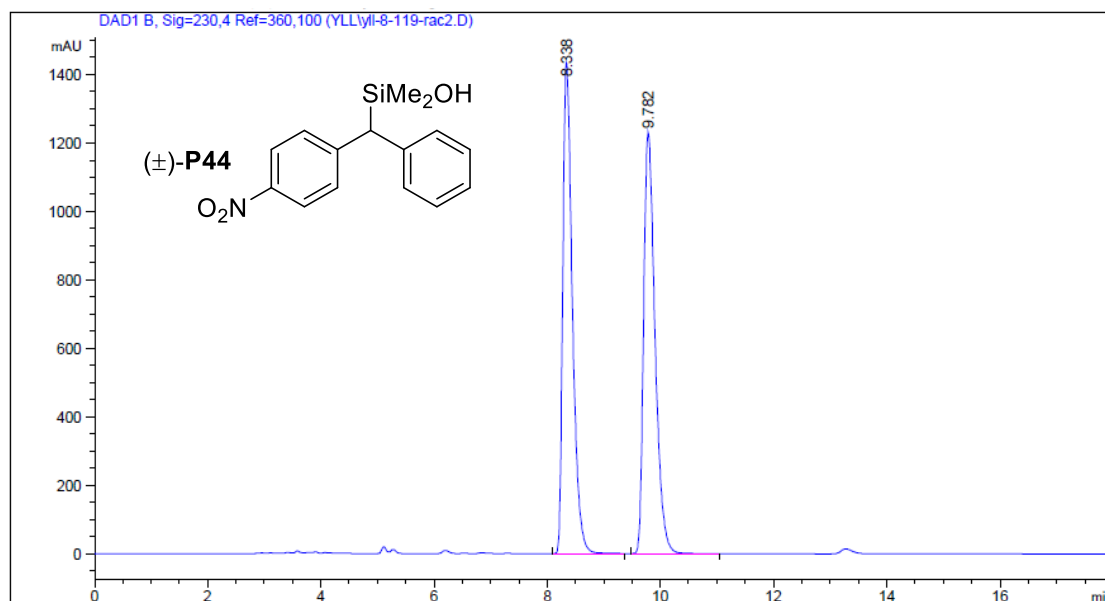


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.134	BB	0.1134	5948.02246	813.01306	49.8775
2	7.949	BV R	0.1268	5977.24170	718.74768	50.1225

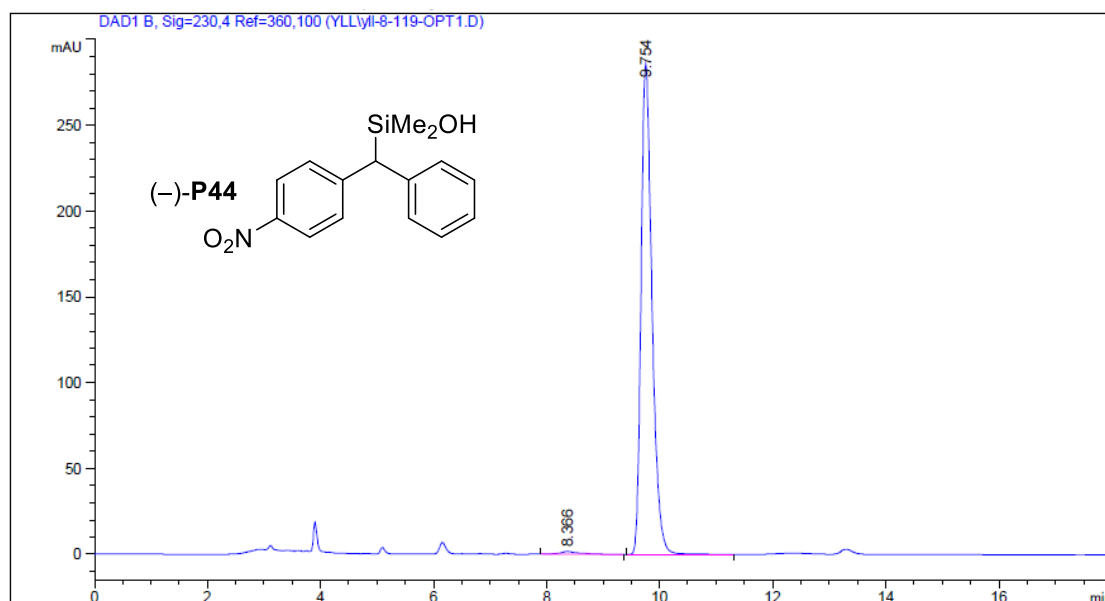


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.156	VB	0.1155	65.06393	8.67079	0.3149
2	7.929	BB	0.1414	2.05963e4	2280.07861	99.6851

**(-)-dimethyl((4-nitrophenyl)(phenyl)methyl)silanol (P44)**

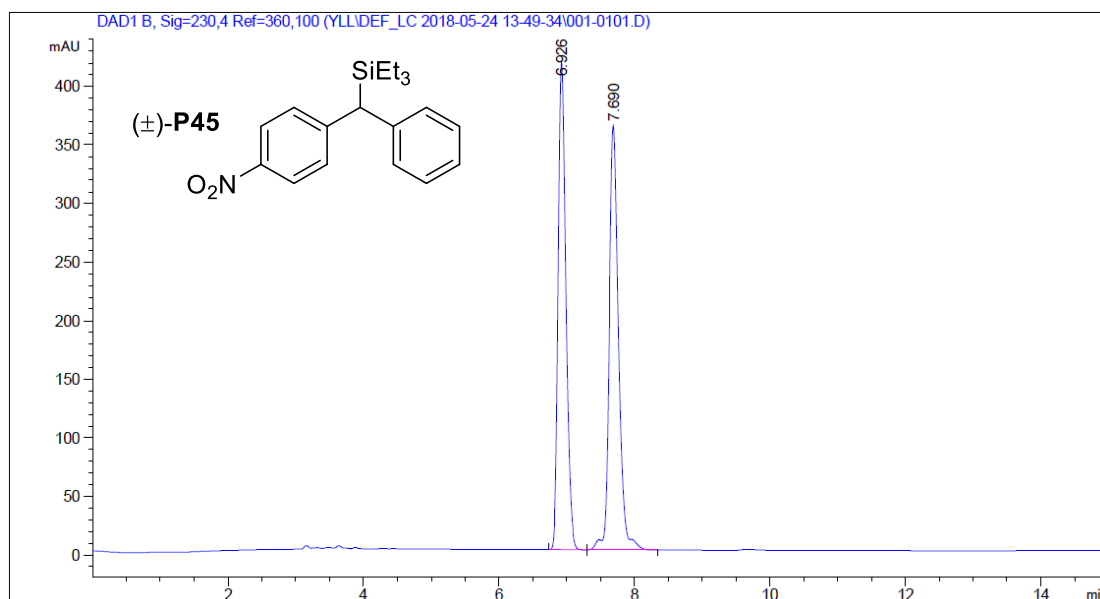


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.338	BB	0.1791	1.68506e4	1434.42700	49.5677
2	9.782	BB	0.2125	1.71445e4	1230.78857	50.4323

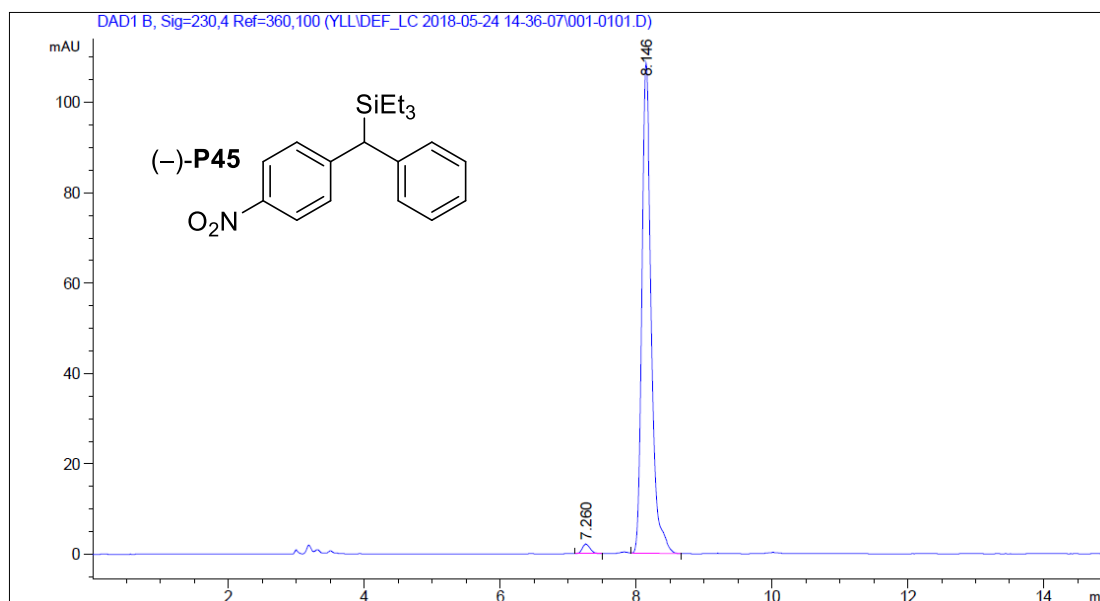


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.366	BB	0.3299	40.96298	1.67182	1.0580
2	9.754	BB	0.2043	3830.69189	285.99307	98.9420

**(-)-triethyl((4-nitrophenyl)(phenyl)methyl)silane (P45)**

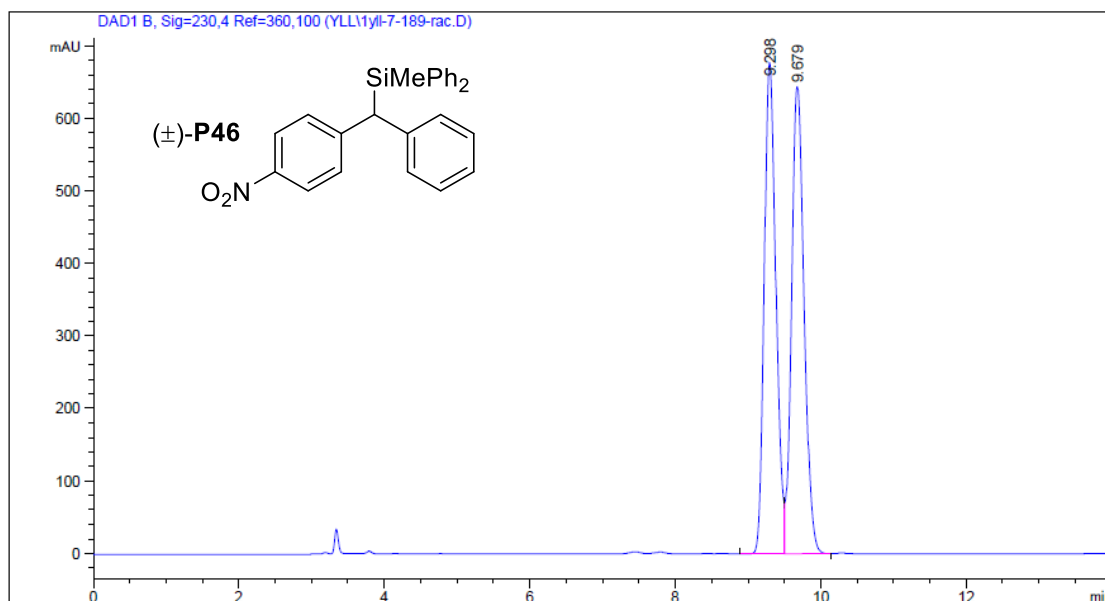


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.926	BB	0.1202	3285.98608	415.79910	48.8113
2	7.690	VB R	0.1414	3446.03125	362.25903	51.1887

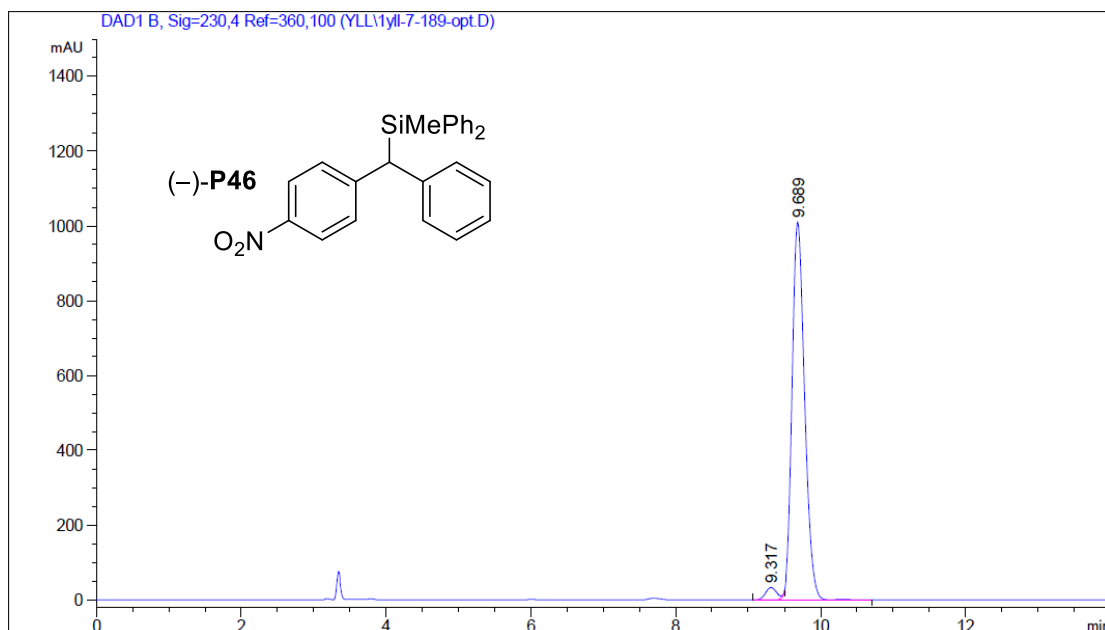


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.260	BB	0.1235	17.13815	2.13925	1.6231
2	8.146	BB	0.1457	1038.77844	108.49282	98.3769

**(-)-methyl((4-nitrophenyl)(phenyl)methyl)diphenylsilane (P46)**



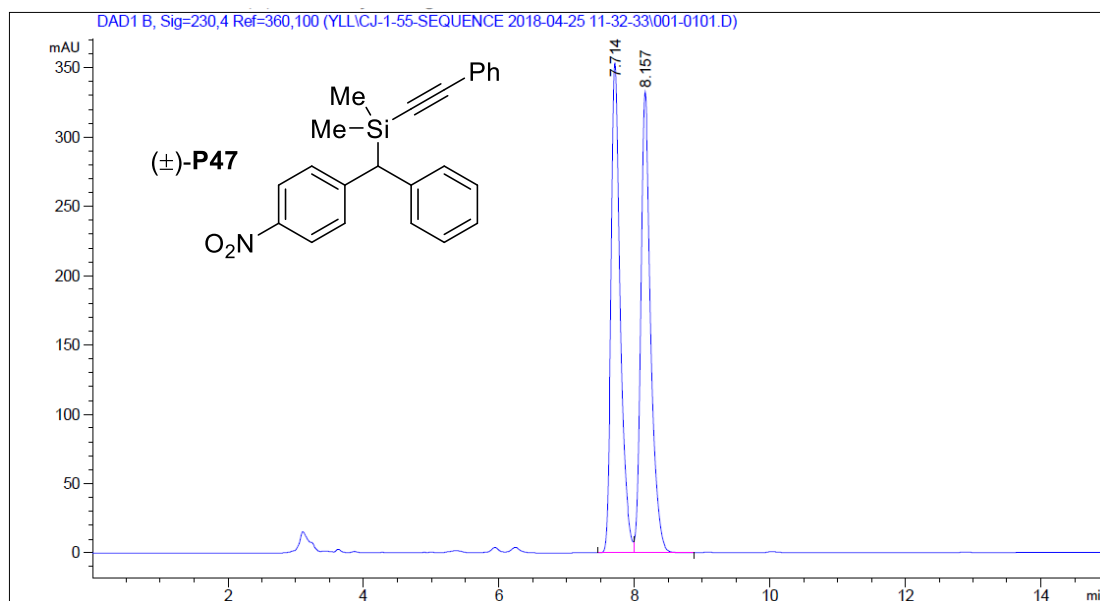
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.298	BV	0.1722	7561.35645	677.59052	49.5505
2	9.679	VB	0.1834	7698.55176	644.09003	50.4495



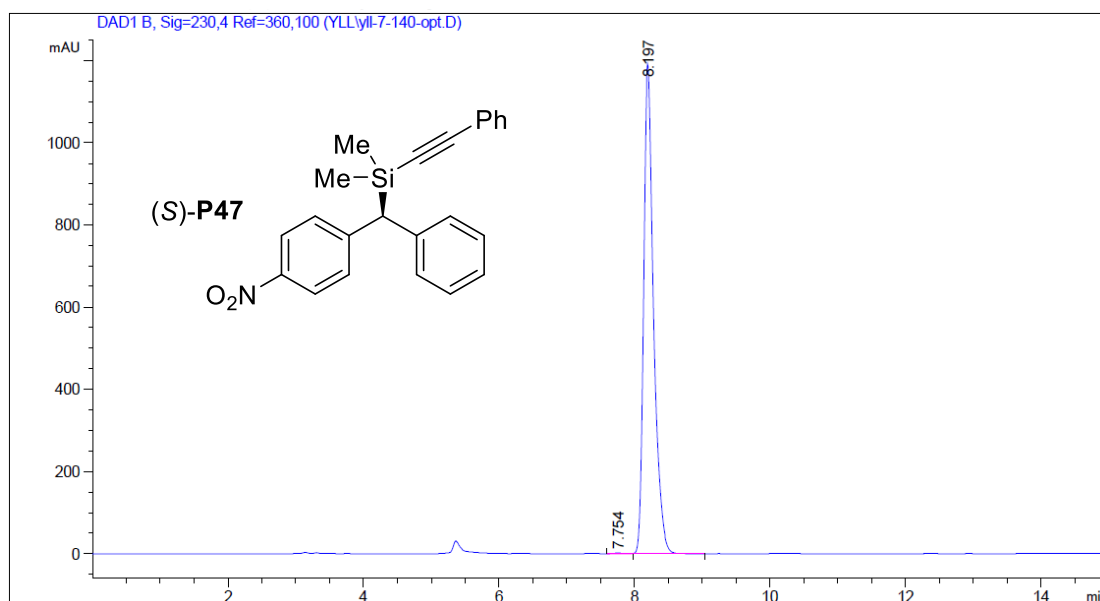
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.317	BV E	0.1645	346.02747	32.94694	2.7699
2	9.689	VV R	0.1860	1.21463e4	1009.95319	97.2301



### (S)-dimethyl((4-nitrophenyl)(phenyl)methyl)(phenylethynyl)silane (P47)

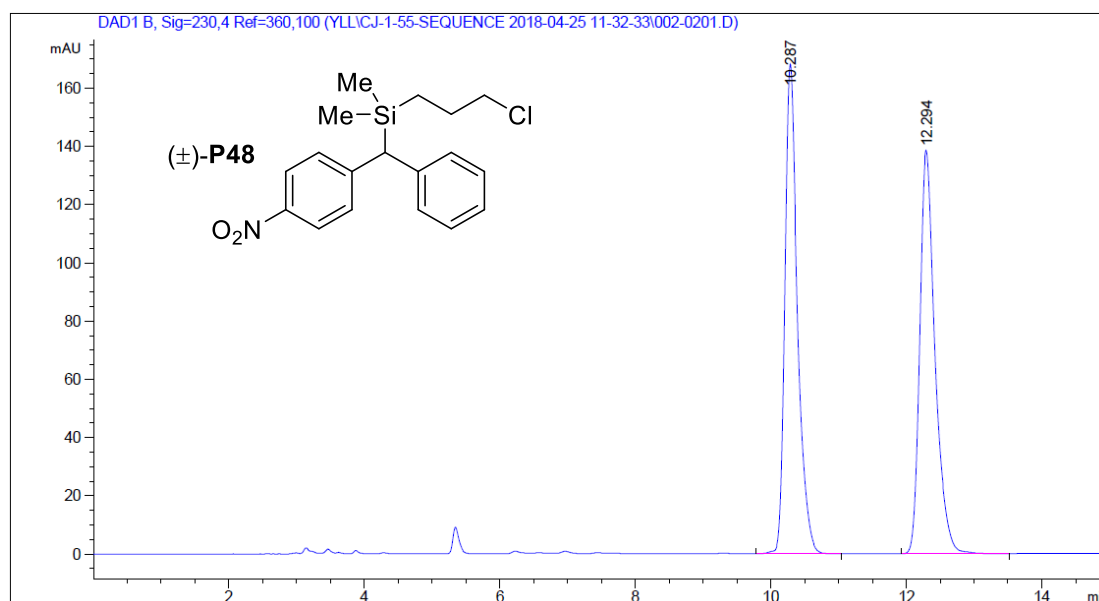


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.714	BV	0.1424	3348.23242	353.75223	49.7646
2	8.157	VB	0.1526	3379.90283	332.56125	50.2354

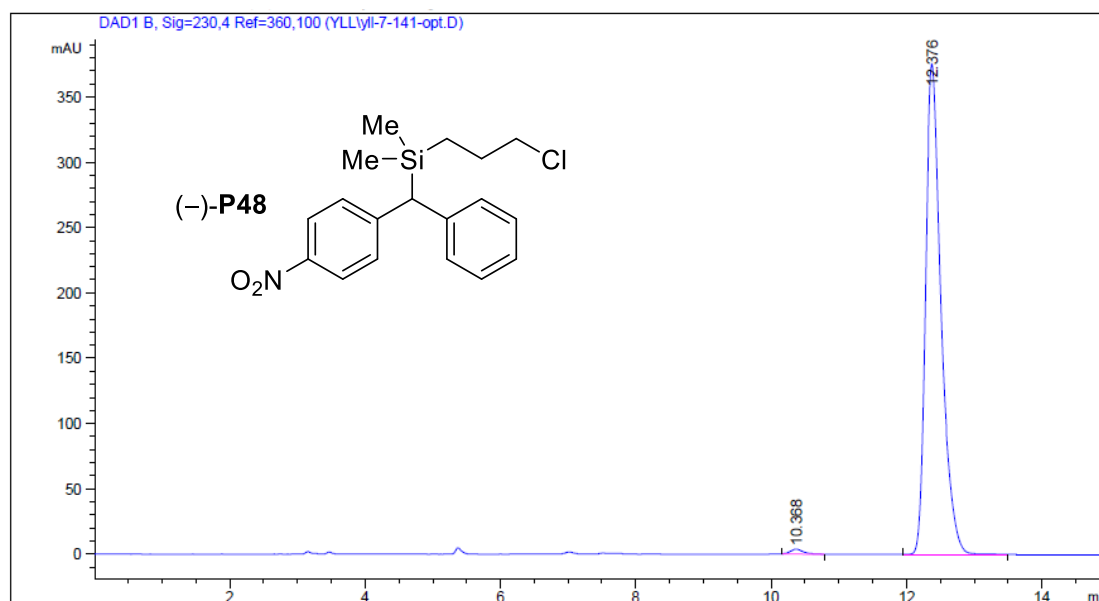


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.754	BV E	0.1407	14.67232	1.57428	0.1201
2	8.197	VB R	0.1534	1.22005e4	1191.80066	99.8799

**(-)-(3-chloropropyl)dimethyl((4-nitrophenyl)(phenyl)methyl)silane (P48)**

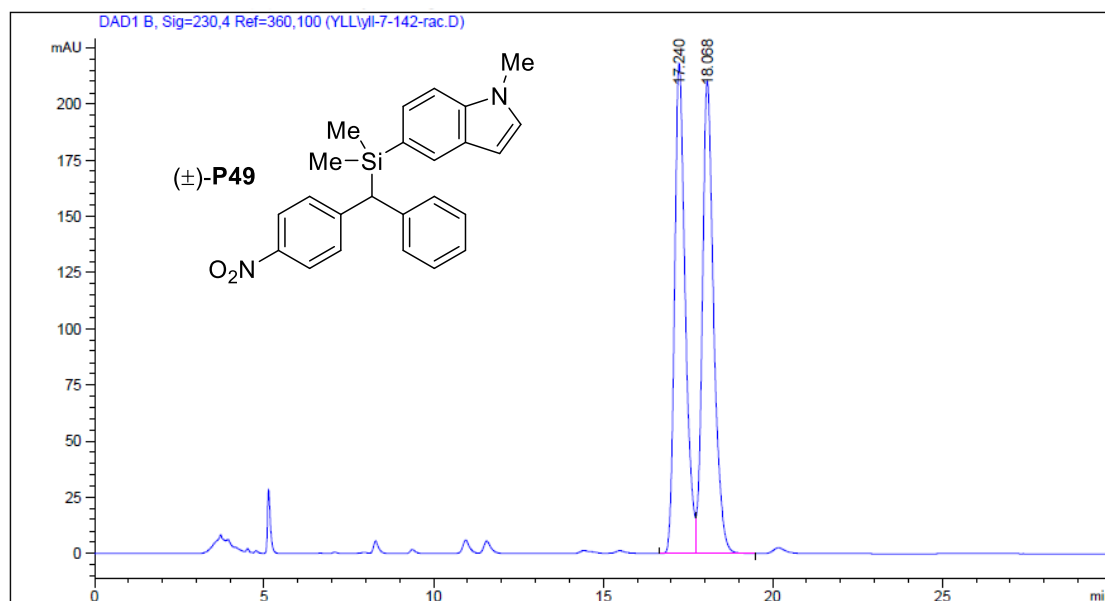


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.287	BB	0.1917	2158.41650	168.17952	49.9793
2	12.294	BB	0.2338	2160.20557	138.59587	50.0207

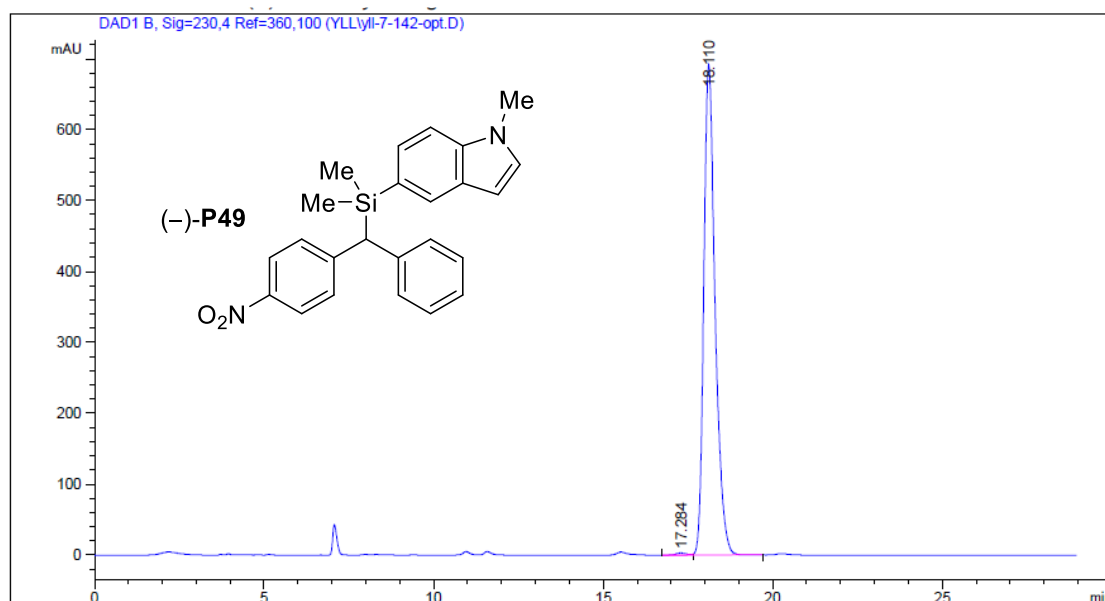


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.368	BB	0.1870	45.44220	3.65537	0.7593
2	12.376	BB	0.2386	5939.28223	375.29282	99.2407

**(-)-5-(dimethyl((4-nitrophenyl)(phenyl)methyl)silyl)-1-methyl-1H-indole (P49)**



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.240	BV	0.3287	4762.49121	218.17859	49.3869
2	18.068	VB	0.3486	4880.74023	210.43614	50.6131



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.284	BV E	0.3091	58.51109	2.78512	0.3637
2	18.110	VB R	0.3484	1.60278e4	691.61871	99.6363

## 12. Computational details

### Dirhodium-Tetraformate Catalyst

Conformations of each species were generated using Maestro with the OPLS3 force field. Conformational searches were conducted by restraining the position of the rhodium and rhodium-bound atoms. Geometry optimizations and frequency calculations were performed with Gaussian09 at the B3LYP-D3/6-31G(d)-LANL2DZ(Rh,I) level of theory before single point energy corrections at the M06/6-311++G(d,p)-SDD(Rh,I)/SMD(DCM) level of theory. Free energies were corrected with Truhlar's rigid-rotor harmonic oscillator treatment<sup>23,24</sup> through Goodvibes<sup>25</sup>.

### Computed Energies (Hartree)

Structure	Electronic Energy	Zero Point Energy	Enthalpy	Free Energy	Quazi-Harmonic Free Energy
TS-1 (R=Br)	-4653.6958	0.454312	-4653.2026	-4653.313	-4653.3048
TS-2 (R=Br)	-4653.6959	0.45421	-4653.2026	-4653.3141	-4653.3049
TS-1 (R=CF <sub>3</sub> )	-2417.3084	0.469088	-2416.7981	-2416.9143	-2416.9041
TS-2 (R=CF <sub>3</sub> )	-2417.3105	0.469279	-2416.8	-2416.9162	-2416.9059
TS-1 (R=Cl)	-2539.8707	0.454748	-2539.3773	-2539.4866	-2539.4786
TS-2 (R=Cl)	-2539.8701	0.454802	-2539.3767	-2539.4869	-2539.4778
TS-1 (R=CN)	-2172.4855	0.463051	-2171.9833	-2172.0937	-2172.0857
TS-2 (R=CN)	-2172.4885	0.462981	-2171.9862	-2172.0972	-2172.0887
TS-1 (R=F)	-2179.5172	0.456153	-2179.0229	-2179.1306	-2179.1232
TS-2 (R=F)	-2179.5162	0.456112	-2179.0218	-2179.1299	-2179.1221
TS-1 (R=I)	-2091.0628	0.453815	-2090.5699	-2090.681	-2090.6728
TS-2 (R=I)	-2091.0615	0.453516	-2090.5687	-2090.681	-2090.6721
TS-1 (R=Me)	-2119.5715	0.491766	-2119.0405	-2119.1513	-2119.1428
TS-2 (R=Me)	-2119.5704	0.491862	-2119.0393	-2119.1503	-2119.1416
TS-1 (R=NMe <sub>2</sub> )	-2214.1929	0.537649	-2213.6134	-2213.7297	-2213.7206
TS-2 (R=NMe <sub>2</sub> )	-2214.1878	0.537483	-2213.6084	-2213.7247	-2213.7158
TS-1 (R=NO <sub>2</sub> )	-2284.744	0.467082	-2284.2369	-2284.3494	-2284.3407
TS-2 (R=NO <sub>2</sub> )	-2284.7474	0.467329	-2284.2402	-2284.3529	-2284.3438
TS-1 (R=OCF <sub>3</sub> )	-2492.52	0.473789	-2492.0047	-2492.1196	-2492.1117
TS-2 (R=OCF <sub>3</sub> )	-2492.5183	0.473769	-2492.0027	-2492.1201	-2492.1099
TS-1 (R=OMe)	-2194.7734	0.496911	-2194.2364	-2194.3487	-2194.3403
TS-2 (R=OMe)	-2194.7707	0.496603	-2194.2341	-2194.3462	-2194.3378
TS-1 (R=SCF <sub>3</sub> )	-2815.4781	0.470362	-2814.9651	-2815.083	-2815.074
TS-2 (R=SCF <sub>3</sub> )	-2815.4801	0.469987	-2814.9673	-2815.0878	-2815.0762

### Cartesian Coordinates

**TS-1 (R=Br)**

Rh	-3.93328	-0.78749	-0.34488
Rh	-1.55776	-0.22373	0.18343
O	-4.44838	0.17503	1.42185
O	-2.27301	0.67891	1.90977
O	-3.65253	-2.55628	0.71237
O	-1.48797	-2.02974	1.21823
O	-1.02775	-1.15770	-1.60970
O	-3.19732	-1.69648	-2.08145
O	-1.86192	1.53234	-0.90381
O	-4.04080	1.02926	-1.35812
C	0.41693	0.26004	0.65212
C	0.54676	1.41763	1.55495
C	0.07745	2.70006	1.20812
C	1.02512	1.21544	2.86772
C	0.12234	3.74535	2.12196
H	-0.32964	2.85806	0.21787
C	1.03116	2.25857	3.79239
H	1.36025	0.22823	3.16816
C	0.59520	3.53077	3.42087
H	-0.22318	4.73187	1.82460
H	1.38698	2.07533	4.80258
H	0.61803	4.34780	4.13680
C	1.53577	-0.70809	0.62724
C	1.34567	-2.04363	0.21783
C	2.85629	-0.28702	0.91083
C	2.41622	-2.92780	0.12508
H	0.35246	-2.38793	-0.02643
C	3.93606	-1.15610	0.80389
H	3.04051	0.74499	1.18614
C	3.70480	-2.47781	0.41577
H	2.25561	-3.95527	-0.18171
H	4.94419	-0.81499	1.01242
C	-3.52611	0.67019	2.12363
H	-3.83775	1.16851	3.05418
C	-3.01190	1.74799	-1.40800
H	-3.10217	2.69399	-1.96421
C	-2.53190	-2.75916	1.24550
H	-2.42396	-3.69466	1.81550
C	-1.96358	-1.66712	-2.31272
H	-1.62919	-2.14285	-3.24817
Si	1.37909	1.31672	-2.08093
H	0.62597	0.91701	-0.77247
C	2.13922	-0.27906	-2.71288

H	1.34103	-1.01555	-2.84667
H	2.64085	-0.11937	-3.67525
H	2.86485	-0.70004	-2.01057
C	0.11694	2.04769	-3.26428
H	-0.34118	2.95376	-2.85738
H	0.58655	2.29320	-4.22484
H	-0.68110	1.31939	-3.43522
C	2.64251	2.56137	-1.48049
C	2.26772	3.89272	-1.21543
C	3.96903	2.18278	-1.19667
C	3.17674	4.80851	-0.68631
H	1.25141	4.22107	-1.42050
C	4.88302	3.09584	-0.66809
H	4.29312	1.16264	-1.38535
C	4.48674	4.41000	-0.40920
H	2.86417	5.83010	-0.48693
H	5.90285	2.78320	-0.45889
H	5.19588	5.12118	0.00609
Br	5.17718	-3.67961	0.26550

**TS-2 (R=Br)**

Rh	-3.76317	1.00933	-0.51813
Rh	-1.52215	0.15390	0.18734
O	-3.05732	2.91377	-0.07470
O	-1.00963	2.12876	0.56902
O	-4.36650	0.77686	1.45791
O	-2.30520	0.04269	2.11202
O	-2.20971	-1.76487	-0.27700
O	-4.26114	-0.98403	-0.90938
O	-0.95243	0.36543	-1.81356
O	-2.98683	1.18565	-2.44243
C	0.34986	-0.53978	0.78269
C	1.41980	0.46447	0.64988
C	1.77697	1.03083	-0.58934
C	2.02204	0.98718	1.81382
C	2.72511	2.04130	-0.67299
H	1.29569	0.67292	-1.48972
C	2.94514	2.02793	1.74354
H	1.74236	0.59405	2.78531
C	3.30362	2.53720	0.49739
H	3.00965	2.45017	-1.63624
H	3.38851	2.43053	2.64742
C	0.56913	-1.63888	1.74609
C	-0.51117	-2.35388	2.30491

C	1.88224	-2.07157	2.05285
C	-0.28549	-3.42881	3.16095
H	-1.52120	-2.05811	2.06692
C	2.10300	-3.15731	2.89421
H	2.72818	-1.56926	1.59780
C	1.01774	-3.83585	3.45763
H	-1.13125	-3.95886	3.58982
H	3.11949	-3.47735	3.10629
C	-1.87836	3.03219	0.35347
H	-1.54139	4.05639	0.57431
C	-1.79913	0.83047	-2.64423
H	-1.42876	0.92540	-3.67683
C	-3.52109	0.37383	2.29651
H	-3.86734	0.28895	3.33794
C	-3.40370	-1.87993	-0.71270
H	-3.71142	-2.91160	-0.94537
Si	0.91562	-2.55422	-1.49982
H	0.49851	-1.36837	-0.58248
C	0.31469	-4.09767	-0.61477
H	-0.76322	-4.00803	-0.44943
H	0.50969	-4.99572	-1.21379
H	0.78980	-4.22205	0.36297
C	0.09079	-2.29159	-3.16714
H	0.43150	-1.36960	-3.64735
H	0.29665	-3.13349	-3.83945
H	-0.99037	-2.21030	-3.02098
C	2.78282	-2.41161	-1.55190
C	3.41066	-1.45189	-2.36916
C	3.59770	-3.18977	-0.70681
C	4.79343	-1.27153	-2.34200
H	2.81306	-0.83190	-3.03347
C	4.98226	-3.01497	-0.67753
H	3.14700	-3.93624	-0.05835
C	5.58171	-2.05240	-1.49293
H	5.25612	-0.52163	-2.97801
H	5.59278	-3.62771	-0.01915
H	6.65893	-1.91099	-1.46754
H	1.18790	-4.68225	4.11783
Br	4.60232	3.93276	0.38584

**TS-1 (R=CF3)**

Rh	-3.96278	-0.69943	-0.34293
Rh	-1.57644	-0.17551	0.17754
O	-4.47079	0.38240	1.35586

O	-2.28742	0.86452	1.82831
O	-3.74731	-2.40496	0.82581
O	-1.57728	-1.90699	1.33554
O	-1.05651	-1.25173	-1.53448
O	-3.23892	-1.73246	-2.01158
O	-1.81149	1.50239	-1.04152
O	-4.00675	1.05324	-1.46937
C	0.40083	0.29085	0.64918
C	0.54881	1.49152	1.48969
C	0.05837	2.75047	1.08600
C	1.06451	1.36651	2.79781
C	0.11998	3.84537	1.93805
H	-0.37756	2.84869	0.09960
C	1.08826	2.46013	3.66228
H	1.41624	0.40072	3.14478
C	0.63220	3.70654	3.23282
H	-0.24510	4.81088	1.59790
H	1.47359	2.33632	4.67058
H	0.66807	4.56227	3.90144
C	1.50543	-0.69953	0.68276
C	1.28449	-2.05858	0.38609
C	2.83560	-0.27527	0.91218
C	2.34503	-2.95953	0.34351
H	0.28035	-2.40435	0.19478
C	3.89643	-1.16952	0.85063
H	3.03659	0.77142	1.10549
C	3.64976	-2.51653	0.56950
H	2.16192	-4.00658	0.12765
H	4.91208	-0.82558	1.01720
C	-3.54189	0.90024	2.03174
H	-3.84756	1.46596	2.92496
C	-2.95141	1.72679	-1.56535
H	-3.00316	2.63440	-2.18649
C	-2.64203	-2.60408	1.39110
H	-2.57038	-3.50306	2.02212
C	-2.00094	-1.76730	-2.22075
H	-1.67165	-2.31536	-3.11751
Si	1.47399	1.17028	-2.11499
H	0.66866	0.87305	-0.81158
C	2.03860	-0.50666	-2.74165
H	2.72171	-0.99376	-2.03877
H	1.16335	-1.15277	-2.85555
H	2.54516	-0.41718	-3.71053
C	0.31195	2.06487	-3.28977



H	-0.04162	3.00621	-2.85786
H	0.81739	2.28503	-4.23813
H	-0.56244	1.43877	-3.48851
C	2.89019	2.23790	-1.51362
C	2.65342	3.54444	-1.04402
C	4.20461	1.73836	-1.43567
C	3.68382	4.31841	-0.51058
H	1.65040	3.96135	-1.08241
C	5.24100	2.51185	-0.91029
H	4.42202	0.73069	-1.77995
C	4.98028	3.80196	-0.44217
H	3.47606	5.32072	-0.14572
H	6.24910	2.10814	-0.86311
H	5.78428	4.40318	-0.02591
C	4.81183	-3.46439	0.43758
F	4.44348	-4.75005	0.61615
F	5.78538	-3.18672	1.33327
F	5.37323	-3.37557	-0.79198

**TS-2 (R=CF3)**

Rh	-3.74901	0.95642	-0.56219
Rh	-1.50850	0.15496	0.19742
O	-3.10439	2.87663	-0.09143
O	-1.05461	2.13930	0.60040
O	-4.39817	0.70025	1.39716
O	-2.33722	0.01121	2.09962
O	-2.13831	-1.77845	-0.28911
O	-4.19051	-1.04506	-0.97304
O	-0.89249	0.39082	-1.78599
O	-2.93073	1.16206	-2.46331
C	0.35102	-0.48940	0.83708
C	1.41065	0.52401	0.69104
C	1.83811	1.01046	-0.55854
C	1.93088	1.12577	1.85719
C	2.78338	2.02311	-0.64117
H	1.41731	0.58987	-1.46079
C	2.84945	2.16708	1.77225
H	1.58981	0.78805	2.82995
C	3.29060	2.60738	0.52324
H	3.12149	2.37318	-1.61071
H	3.22830	2.63389	2.67548
C	0.58212	-1.57752	1.80031
C	-0.48825	-2.33968	2.31785
C	1.90101	-1.95321	2.15788

C	-0.24956	-3.40532	3.18089
H	-1.49980	-2.08746	2.03976
C	2.13503	-3.02900	3.00757
H	2.74103	-1.41325	1.73608
C	1.05820	-3.75497	3.52757
H	-1.08689	-3.97308	3.57650
H	3.15475	-3.30514	3.26139
H	1.23935	-4.59437	4.19371
C	-1.93995	3.02251	0.36615
H	-1.63349	4.05335	0.59957
C	-1.72904	0.83839	-2.63590
H	-1.33497	0.94855	-3.65801
C	-3.56553	0.31168	2.25490
H	-3.93582	0.21099	3.28651
C	-3.31785	-1.92118	-0.75533
H	-3.59472	-2.95935	-0.99709
Si	0.98162	-2.54047	-1.47326
H	0.53948	-1.37235	-0.57005
C	0.47208	-4.10097	-0.55875
H	-0.61090	-4.08150	-0.40194
H	0.73087	-4.99820	-1.13409
H	0.94657	-4.17169	0.42499
C	0.11276	-2.33629	-3.12730
H	0.40609	-1.40680	-3.62412
H	0.33262	-3.17631	-3.79711
H	-0.96721	-2.29264	-2.95663
C	2.84104	-2.32213	-1.57401
C	3.41801	-1.45194	-2.51880
C	3.69700	-2.93718	-0.63989
C	4.79017	-1.20043	-2.52891
H	2.78900	-0.95954	-3.25726
C	5.07047	-2.68800	-0.64451
H	3.28718	-3.61475	0.10443
C	5.61895	-1.81615	-1.58780
H	5.21315	-0.52366	-3.26663
H	5.71257	-3.17379	0.08584
H	6.68738	-1.61772	-1.59041
C	4.35722	3.66182	0.43234
F	4.29415	4.53433	1.46315
F	5.59760	3.11520	0.45749
F	4.26779	4.37393	-0.71351
<b>TS-1 (R=Cl)</b>			
Rh	-3.82494	0.45926	0.27539

Rh	-1.39078	0.09345	-0.14102
O	-4.19974	-0.92804	-1.22086
O	-1.97374	-1.24010	-1.62715
O	-3.73645	1.96808	-1.15253
O	-1.50592	1.64024	-1.52479
O	-1.03265	1.45156	1.40744
O	-3.25905	1.82404	1.75066
O	-1.48336	-1.41952	1.29430
O	-3.71135	-1.09111	1.67008
C	0.64887	-0.23550	-0.54339
C	0.87894	-1.48003	-1.31062
C	0.55461	-2.74797	-0.78748
C	1.28568	-1.40491	-2.65813
C	0.68750	-3.89587	-1.55930
H	0.17322	-2.81538	0.22463
C	1.38742	-2.55644	-3.43929
H	1.49455	-0.43691	-3.10080
C	1.10761	-3.80786	-2.89151
H	0.44694	-4.86363	-1.12696
H	1.69452	-2.47053	-4.47812
H	1.20323	-4.70528	-3.49649
C	1.63091	0.86411	-0.71153
C	1.28385	2.20325	-0.43060
C	2.96983	0.60041	-1.08357
C	2.21731	3.22920	-0.53537
H	0.27491	2.43972	-0.13026
C	3.91320	1.61618	-1.18881
H	3.28690	-0.41897	-1.26511
C	3.52736	2.92755	-0.91297
H	1.93606	4.25533	-0.32449
H	4.93922	1.39054	-1.45620
C	-3.21405	-1.43975	-1.81655
H	-3.44881	-2.16304	-2.61236
C	-2.60554	-1.65752	1.85156
H	-2.58882	-2.47124	2.59396
C	-2.63307	2.20254	-1.71033
H	-2.62837	3.00509	-2.46367
C	-2.03539	1.99647	1.97559
H	-1.78073	2.71330	2.77224
Si	1.75952	-0.94180	2.18870
H	0.93620	-0.68447	0.85778
C	1.54902	0.64873	3.15654
H	0.49799	0.77822	3.42682
H	2.15868	0.64447	4.06858

H	1.83616	1.50988	2.54427
C	1.05506	-2.47489	3.01483
H	1.16643	-3.35797	2.37720
H	1.58513	-2.66909	3.95576
H	-0.00831	-2.33594	3.22261
C	3.50051	-1.20005	1.56261
C	3.81113	-2.31818	0.76211
C	4.50929	-0.24594	1.78763
C	5.07803	-2.46760	0.19842
H	3.05001	-3.06432	0.54858
C	5.78312	-0.39959	1.23791
H	4.29688	0.63776	2.38412
C	6.06661	-1.50754	0.43642
H	5.29465	-3.32960	-0.42691
H	6.54784	0.34985	1.42363
H	7.05430	-1.62394	-0.00197
Cl	4.71333	4.21562	-1.02397

**TS-2 (R=Cl)**

Rh	-3.71007	0.38278	-0.51247
Rh	-1.33811	0.03063	0.19067
O	-3.44087	2.39153	-0.06168
O	-1.28635	2.06206	0.62695
O	-4.24390	0.02283	1.46324
O	-2.07771	-0.30723	2.10779
O	-1.57569	-1.97734	-0.33567
O	-3.76323	-1.67152	-0.91759
O	-0.82406	0.42349	-1.79518
O	-2.99207	0.72454	-2.43942
C	0.64714	-0.25160	0.77912
C	1.45165	0.98300	0.74200
C	1.64456	1.71987	-0.44344
C	1.93005	1.53584	1.94843
C	2.32176	2.93115	-0.43709
H	1.24574	1.33437	-1.37302
C	2.57798	2.76865	1.97156
H	1.76665	1.00814	2.88175
C	2.78447	3.45099	0.77442
H	2.48377	3.47901	-1.35918
H	2.92795	3.19060	2.90753
C	1.10247	-1.32964	1.68656
C	0.20508	-2.28807	2.20089
C	2.47945	-1.48553	1.97613
C	0.66359	-3.33799	2.99335

H	-0.84724	-2.20070	1.97836
C	2.93566	-2.54641	2.75216
H	3.19407	-0.78564	1.55837
C	2.02635	-3.47462	3.26902
H	-0.04560	-4.06012	3.38814
H	3.99904	-2.65206	2.94930
H	2.37975	-4.30315	3.87721
C	-2.32613	2.75723	0.39868
H	-2.22709	3.82669	0.63922
C	-1.75222	0.67407	-2.63177
H	-1.40747	0.86538	-3.65983
C	-3.33451	-0.22479	2.29577
H	-3.65659	-0.39815	3.33399
C	-2.72019	-2.35175	-0.75780
H	-2.78877	-3.42083	-1.01396
Si	1.69325	-1.90347	-1.59166
H	0.99236	-0.91325	-0.60057
C	1.43145	-3.60078	-0.83557
H	0.35671	-3.76220	-0.70830
H	1.83594	-4.38695	-1.48498
H	1.89854	-3.68754	0.15000
C	0.87942	-1.70579	-3.27333
H	1.01263	-0.69415	-3.66774
H	1.30464	-2.41914	-3.99020
H	-0.19461	-1.89080	-3.18257
C	3.47628	-1.33340	-1.56720
C	3.86940	-0.18435	-2.28036
C	4.44466	-1.98019	-0.77540
C	5.17323	0.30454	-2.20243
H	3.14779	0.34025	-2.90197
C	5.75189	-1.49724	-0.69708
H	4.17458	-2.86679	-0.20793
C	6.11669	-0.35125	-1.40764
H	5.45307	1.19648	-2.75657
H	6.48498	-2.01290	-0.08211
H	7.13248	0.02958	-1.34306
Cl	3.63463	4.98767	0.78653

**TS-1 (R=CN)**

Rh	-3.78567	0.41460	0.29895
Rh	-1.35479	0.08459	-0.15954
O	-4.16294	-1.01716	-1.15455
O	-1.93911	-1.31308	-1.58387
O	-3.76361	1.88315	-1.17159

O	-1.54119	1.57438	-1.59851
O	-0.98892	1.49911	1.33292
O	-3.21417	1.82557	1.72678
O	-1.38603	-1.37415	1.33256
O	-3.61535	-1.08980	1.73359
C	0.66370	-0.19423	-0.61031
C	0.94447	-1.45324	-1.32640
C	0.62906	-2.70832	-0.76488
C	1.40156	-1.41865	-2.66033
C	0.82090	-3.88029	-1.48518
H	0.21884	-2.74502	0.23731
C	1.55541	-2.59593	-3.39282
H	1.60633	-0.46377	-3.13243
C	1.28583	-3.83138	-2.80500
H	0.59061	-4.83720	-1.02436
H	1.89619	-2.54309	-4.42316
H	1.42420	-4.74863	-3.37064
C	1.62022	0.92637	-0.79721
C	1.22389	2.26666	-0.59548
C	2.97741	0.68032	-1.11302
C	2.13090	3.31037	-0.72613
H	0.19929	2.48567	-0.34142
C	3.89283	1.71653	-1.23837
H	3.32629	-0.33730	-1.23123
C	3.47288	3.04229	-1.04706
H	1.80905	4.33583	-0.57628
H	4.93249	1.50204	-1.46013
C	-3.17994	-1.53477	-1.74867
H	-3.41608	-2.28577	-2.51772
C	-2.49280	-1.62144	1.91675
H	-2.44253	-2.40769	2.68634
C	-2.68227	2.11424	-1.77042
H	-2.71135	2.88908	-2.55141
C	-1.98965	2.03238	1.91597
H	-1.73158	2.77241	2.68964
Si	1.84015	-0.81719	2.19673
H	1.03131	-0.60495	0.87348
C	1.57222	0.75882	3.17735
H	1.81391	1.63526	2.56716
H	0.51895	0.84077	3.45885
H	2.18837	0.77947	4.08459
C	1.20562	-2.37928	3.02792
H	1.33460	-3.25389	2.38167
H	1.75788	-2.56295	3.95788

H	0.14175	-2.27969	3.25621
C	3.59710	-1.01021	1.58215
C	3.95234	-2.12475	0.79495
C	4.56587	-0.01183	1.78949
C	5.22187	-2.22805	0.22637
H	3.22279	-2.90629	0.59624
C	5.84241	-0.11756	1.23376
H	4.32004	0.86850	2.37844
C	6.16933	-1.22273	0.44495
H	5.47290	-3.08903	-0.38747
H	6.57579	0.66573	1.40617
H	7.15885	-1.30232	0.00256
C	4.41636	4.11550	-1.16056
N	5.18650	4.98295	-1.24766

**TS-2 (R=CN)**

Rh	-3.66398	0.35024	-0.55560
Rh	-1.30454	0.04792	0.20460
O	-3.45393	2.35803	-0.07226
O	-1.31579	2.07052	0.68051
O	-4.23999	-0.05204	1.40024
O	-2.08425	-0.35233	2.09196
O	-1.47759	-1.95402	-0.36624
O	-3.65884	-1.69623	-0.99174
O	-0.74972	0.49917	-1.75694
O	-2.90863	0.73441	-2.45684
C	0.65086	-0.19361	0.84815
C	1.43486	1.05189	0.82433
C	1.69762	1.76387	-0.36291
C	1.82319	1.63062	2.05267
C	2.35784	2.98135	-0.33220
H	1.36885	1.35176	-1.30716
C	2.45314	2.86825	2.09238
H	1.60490	1.11195	2.97976
C	2.74102	3.54725	0.89777
H	2.57627	3.50788	-1.25561
H	2.73675	3.30673	3.04368
C	1.12262	-1.27752	1.72383
C	0.24753	-2.28464	2.18580
C	2.49789	-1.38870	2.04783
C	0.72456	-3.33788	2.96116
H	-0.80076	-2.22917	1.93581
C	2.97220	-2.45270	2.80689
H	3.19587	-0.65088	1.66875

C	2.08404	-3.42878	3.27146
H	0.03441	-4.09789	3.31615
H	4.03244	-2.52470	3.03306
H	2.45249	-4.25995	3.86684
C	-2.36448	2.74485	0.42788
H	-2.29848	3.81269	0.68522
C	-1.66271	0.72863	-2.61595
H	-1.29719	0.94502	-3.63146
C	-3.34743	-0.29861	2.25055
H	-3.69065	-0.49961	3.27671
C	-2.60193	-2.35166	-0.82067
H	-2.63563	-3.41722	-1.09667
Si	1.79062	-1.82103	-1.59880
H	1.06998	-0.87067	-0.61863
C	1.61073	-3.53235	-0.84675
H	0.54474	-3.74641	-0.72141
H	2.05297	-4.29834	-1.49529
H	2.07916	-3.60051	0.13996
C	0.95889	-1.66411	-3.27743
H	1.05038	-0.64941	-3.67632
H	1.39975	-2.36306	-3.99853
H	-0.10769	-1.88674	-3.17652
C	3.55261	-1.18060	-1.59172
C	3.91518	-0.07028	-2.37866
C	4.52716	-1.72142	-0.73093
C	5.19391	0.48241	-2.30644
H	3.18979	0.37260	-3.05770
C	5.80868	-1.17285	-0.65541
H	4.28318	-2.57785	-0.10773
C	6.14283	-0.06719	-1.44077
H	5.45043	1.34102	-2.92133
H	6.54639	-1.60743	0.01433
H	7.13847	0.36395	-1.37995
C	3.42273	4.80622	0.92964
N	3.98099	5.82695	0.95282

**TS-1 (R=F)**

Rh	3.73687	-0.30999	0.25442
Rh	1.28553	-0.04762	-0.14191
O	4.03234	1.19533	-1.14120
O	1.78992	1.44601	-1.49913
O	3.73063	-1.71136	-1.28410
O	1.49473	-1.44047	-1.66934
O	1.00005	-1.55307	1.27563



O	3.24107	-1.80204	1.63197
O	1.28587	1.32090	1.43889
O	3.53829	1.12084	1.76041
C	-0.77012	0.18531	-0.52987
C	-1.07303	1.52117	-1.09232
C	-0.91536	2.70437	-0.34453
C	-1.37198	1.64271	-2.46488
C	-1.10561	3.95178	-0.92825
H	-0.61274	2.63470	0.69292
C	-1.53402	2.89687	-3.05315
H	-1.44719	0.74953	-3.07583
C	-1.41996	4.05695	-2.28735
H	-0.99432	4.84820	-0.32368
H	-1.75613	2.96245	-4.11492
H	-1.56191	5.03260	-2.74389
C	-1.65084	-0.94221	-0.90820
C	-1.22776	-2.28077	-0.73772
C	-2.96874	-0.72639	-1.37878
C	-2.06052	-3.34722	-1.05563
H	-0.23962	-2.47880	-0.35181
C	-3.80918	-1.78386	-1.70563
H	-3.34960	0.28355	-1.46461
C	-3.33795	-3.08183	-1.54204
H	-1.73753	-4.37606	-0.93661
H	-4.82236	-1.61744	-2.05385
C	3.01829	1.71245	-1.68271
H	3.21317	2.50827	-2.41781
C	2.39737	1.58733	2.00354
H	2.33627	2.32763	2.81706
C	2.64724	-1.93725	-1.88299
H	2.68825	-2.66647	-2.70666
C	2.02934	-2.06927	1.82311
H	1.81184	-2.85467	2.56435
Si	-1.99055	0.33362	2.22912
H	-1.09746	0.36337	0.91880
C	-1.64862	-1.34459	2.99058
H	-0.61566	-1.38837	3.34392
H	-2.32586	-1.54280	3.83069
H	-1.77285	-2.13424	2.24285
C	-1.46431	1.79685	3.28364
H	-1.76624	2.74655	2.83017
H	-1.92680	1.73317	4.27650
H	-0.37666	1.79964	3.39314
C	-3.72941	0.48380	1.56275

C	-4.15818	1.67363	0.94010
C	-4.61197	-0.61138	1.57704
C	-5.41726	1.75944	0.34626
H	-3.49441	2.53313	0.89144
C	-5.87760	-0.52543	0.99525
H	-4.30403	-1.54969	2.03154
C	-6.27956	0.65894	0.37421
H	-5.72606	2.68162	-0.13872
H	-6.54356	-1.38398	1.01599
H	-7.26128	0.72548	-0.08745
F	-4.14695	-4.11259	-1.84706

**TS-2 (R=F)**

Rh	-3.64522	0.21224	-0.51415
Rh	-1.25541	0.00515	0.19359
O	-3.60357	2.12900	0.28123
O	-1.41537	1.94713	0.91621
O	-4.15850	-0.54252	1.35478
O	-1.97747	-0.67823	2.02013
O	-1.28060	-1.92379	-0.61052
O	-3.46279	-1.73703	-1.26186
O	-0.76486	0.73187	-1.70512
O	-2.94845	0.96394	-2.32678
C	0.74652	-0.15373	0.78791
C	1.42353	1.15066	0.91342
C	1.57071	2.02979	-0.17897
C	1.80957	1.61132	2.19096
C	2.11570	3.29594	-0.01683
H	1.24114	1.70972	-1.15850
C	2.32202	2.89387	2.37127
H	1.67612	0.96885	3.05431
C	2.48086	3.71302	1.26067
H	2.25184	3.96825	-0.85740
H	2.60364	3.25969	3.35291
C	1.29129	-1.27847	1.58812
C	0.49181	-2.38237	1.94805
C	2.66702	-1.32059	1.91735
C	1.03862	-3.46306	2.63649
H	-0.55511	-2.38546	1.68688
C	3.21371	-2.40959	2.58958
H	3.31204	-0.50466	1.61187
C	2.39787	-3.48378	2.95804
H	0.40200	-4.29881	2.91324
H	4.27527	-2.42254	2.82162

H	2.82147	-4.33434	3.48564
C	-2.53103	2.54440	0.79617
H	-2.55176	3.56769	1.20117
C	-1.70744	1.04594	-2.50279
H	-1.37669	1.43687	-3.47771
C	-3.23672	-0.79106	2.17322
H	-3.54802	-1.16019	3.16251
C	-2.36446	-2.33392	-1.14554
H	-2.31546	-3.35364	-1.55934
Si	1.95745	-1.41916	-1.71283
H	1.15724	-0.61605	-0.62269
C	1.87095	-3.20769	-1.15347
H	0.81822	-3.48545	-1.04534
H	2.34068	-3.86984	-1.89138
H	2.35708	-3.36306	-0.18580
C	1.11398	-1.11501	-3.36284
H	1.14313	-0.05796	-3.64204
H	1.59773	-1.70092	-4.15427
H	0.06396	-1.41209	-3.29103
C	3.67212	-0.67725	-1.60674
C	3.95462	0.56245	-2.21219
C	4.69305	-1.29178	-0.85601
C	5.20353	1.16715	-2.07278
H	3.18879	1.06608	-2.79735
C	5.94552	-0.69196	-0.71593
H	4.50750	-2.24567	-0.36959
C	6.20115	0.54044	-1.32197
H	5.39865	2.12599	-2.54554
H	6.72084	-1.18408	-0.13439
H	7.17437	1.01100	-1.21010
F	3.00053	4.94613	1.42234

**TS-1 (R=I)**

Rh	-4.08969	-1.32670	-0.27159
Rh	-1.86270	-0.27437	0.14209
O	-4.78298	-0.29104	1.38913
O	-2.73925	0.65056	1.78612
O	-3.47325	-2.87540	0.97068
O	-1.43592	-1.91239	1.34833
O	-1.19078	-1.28507	-1.55993
O	-3.21734	-2.27670	-1.91460
O	-2.48631	1.27603	-1.10659
O	-4.52696	0.32150	-1.47673
C	-0.00036	0.61312	0.53069

C	-0.10359	1.79395	1.41414
C	-0.83066	2.94238	1.04048
C	0.39972	1.72703	2.72941
C	-1.00037	3.99988	1.92556
H	-1.27687	2.98178	0.05350
C	0.19866	2.77732	3.62524
H	0.92391	0.83570	3.05713
C	-0.48541	3.92461	3.22500
H	-1.55030	4.88206	1.60826
H	0.58713	2.69706	4.63690
C	1.27680	-0.14153	0.54510
C	1.33453	-1.49491	0.15147
C	2.49426	0.49693	0.87333
C	2.54393	-2.18370	0.10549
H	0.42595	-2.01068	-0.11889
C	3.71015	-0.17819	0.82547
H	2.49668	1.54791	1.13627
C	3.72511	-1.51802	0.44004
H	2.56110	-3.22593	-0.19401
H	4.62828	0.34726	1.06099
C	-3.96918	0.43446	2.02139
H	-4.36933	0.96032	2.90173
C	-3.65549	1.21541	-1.61198
H	-3.92435	2.06799	-2.25555
C	-2.32711	-2.81147	1.48582
H	-2.04252	-3.64385	2.14743
C	-2.01160	-2.04136	-2.17633
H	-1.59451	-2.55129	-3.05916
Si	0.72046	1.85065	-2.15346
H	0.06224	1.25890	-0.84464
C	1.07895	0.34208	-3.20654
H	0.14161	-0.14654	-3.48376
H	1.62938	0.61207	-4.11619
H	1.67101	-0.38482	-2.64059
C	-0.50079	3.06988	-2.89631
H	-0.08207	3.51641	-3.80680
H	-1.43630	2.56171	-3.14173
H	-0.72820	3.87988	-2.19541
C	2.27408	2.67582	-1.52079
C	2.19438	3.79274	-0.66470
C	3.54709	2.14519	-1.79906
C	3.34227	4.34814	-0.09955
H	1.22664	4.21771	-0.41164
C	4.69970	2.70722	-1.24786

H	3.64238	1.27098	-2.43784
C	4.59760	3.80544	-0.39112
H	3.25906	5.20081	0.56900
H	5.67305	2.28101	-1.47601
H	5.49247	4.23783	0.04877
H	-0.62676	4.74867	3.91887
I	5.59637	-2.55695	0.33173

**TS-2 (R=I)**

Rh	3.79873	-1.59503	-0.26927
Rh	1.71720	-0.28520	0.16279
O	2.67664	-3.31494	0.04511
O	0.77709	-2.11481	0.46334
O	4.17730	-1.47784	1.77115
O	2.26436	-0.29371	2.16803
O	2.84370	1.43412	-0.21061
O	4.75852	0.23682	-0.55396
O	1.35038	-0.39872	-1.88805
O	3.24699	-1.60631	-2.28461
C	-0.04479	0.78214	0.56350
C	-1.25535	-0.05546	0.43067
C	-1.60704	-0.66745	-0.78857
C	-2.00542	-0.39260	1.57387
C	-2.69331	-1.52818	-0.88080
H	-1.00409	-0.47444	-1.66827
C	-3.07869	-1.28104	1.50045
H	-1.73274	0.02384	2.53744
C	-3.42949	-1.82814	0.26908
H	-2.95291	-1.97174	-1.83591
H	-3.63421	-1.52941	2.39805
C	-0.11035	1.94260	1.48058
C	1.06028	2.48596	2.05451
C	-1.34062	2.58788	1.75331
C	0.99508	3.59954	2.88722
H	2.01361	2.02579	1.84771
C	-1.40006	3.70632	2.57937
H	-2.24976	2.22575	1.28835
C	-0.23245	4.21314	3.15381
H	1.90709	3.99275	3.32782
H	-2.35612	4.18990	2.75695
H	-0.27662	5.08652	3.79937
C	1.45745	-3.18117	0.33518
H	0.89215	-4.11075	0.50184
C	2.18449	-1.02750	-2.61984

H	1.92783	-1.05585	-3.69066
C	3.34405	-0.88042	2.50047
H	3.56997	-0.85276	3.57741
C	4.08378	1.29337	-0.47105
H	4.62725	2.23507	-0.64767
Si	-0.28249	2.62845	-1.85837
H	-0.02208	1.48952	-0.80573
C	1.09244	3.86259	-1.53919
H	2.05827	3.39925	-1.75672
H	0.97693	4.76356	-2.15406
H	1.10185	4.15531	-0.48385
C	-0.26378	1.84040	-3.56448
H	-0.43402	2.60260	-4.33503
H	0.69870	1.35566	-3.74531
H	-1.04871	1.08266	-3.65933
C	-1.96879	3.28245	-1.38126
C	-3.11400	2.46886	-1.49490
C	-2.11909	4.55631	-0.80315
C	-4.35606	2.90521	-1.03400
H	-3.03520	1.47302	-1.92284
C	-3.36302	5.00383	-0.35535
H	-1.25345	5.20276	-0.68318
C	-4.48192	4.17515	-0.46271
H	-5.22361	2.25624	-1.11789
H	-3.45654	5.99218	0.08711
H	-5.44925	4.51642	-0.10347
I	-5.10917	-3.15399	0.13384

**TS-1 (R=Me)**

Rh	-3.74813	0.28567	0.25942
Rh	-1.29244	0.05363	-0.14038
O	-4.02927	-1.18506	-1.17553
O	-1.78482	-1.39992	-1.54518
O	-3.75008	1.72938	-1.23881
O	-1.50928	1.49494	-1.62146
O	-1.02226	1.51103	1.32963
O	-3.26664	1.74656	1.67481
O	-1.28619	-1.36834	1.39050
O	-3.53858	-1.18711	1.72484
C	0.76813	-0.15054	-0.52888
C	1.07949	-1.45973	-1.14744
C	0.91820	-2.67534	-0.45437
C	1.39290	-1.51925	-2.52051
C	1.11610	-3.89513	-1.09141

H	0.60778	-2.65184	0.58323
C	1.56338	-2.74555	-3.16272
H	1.47510	-0.59893	-3.08860
C	1.44324	-3.93892	-2.45091
H	1.00109	-4.81803	-0.52871
H	1.79732	-2.76320	-4.22388
H	1.59120	-4.89306	-2.94922
C	1.64462	0.99720	-0.85643
C	1.21514	2.32671	-0.64804
C	2.97063	0.80955	-1.31103
C	2.05511	3.40067	-0.91737
H	0.22099	2.50900	-0.26955
C	3.80264	1.89007	-1.58054
H	3.36151	-0.19465	-1.42368
C	3.35960	3.20613	-1.39682
H	1.69317	4.41306	-0.75264
H	4.82047	1.70597	-1.91494
C	-3.01043	-1.67434	-1.73393
H	-3.19818	-2.45048	-2.49174
C	-2.39517	-1.65729	1.94870
H	-2.32885	-2.42421	2.73692
C	-2.66582	1.98555	-1.82448
H	-2.71120	2.74039	-2.62467
C	-2.05665	2.00994	1.88258
H	-1.84668	2.77522	2.64688
Si	1.98657	-0.39082	2.20987
H	1.08701	-0.39076	0.90172
C	1.70689	1.30517	2.95642
H	0.66997	1.39724	3.28769
H	2.37650	1.47935	3.80787
H	1.88111	2.08244	2.20518
C	1.40228	-1.82835	3.26902
H	1.63783	-2.79017	2.80174
H	1.89159	-1.79908	4.25062
H	0.31925	-1.77091	3.40419
C	3.71991	-0.60864	1.54856
C	4.11084	-1.81501	0.93327
C	4.63978	0.45560	1.56165
C	5.36867	-1.94672	0.34534
H	3.41942	-2.65225	0.88599
C	5.90456	0.32311	0.98719
H	4.36137	1.40709	2.00740
C	6.26851	-0.87690	0.37301
H	5.64684	-2.88077	-0.13536

H	6.59956	1.15845	1.00774
H	7.24931	-0.97932	-0.08411
C	4.25101	4.38011	-1.71678
H	4.09057	4.71967	-2.74895
H	4.04474	5.23245	-1.06034
H	5.31050	4.11977	-1.62063

**TS-2 (R=Me)**

Rh	-3.65570	0.22153	-0.50499
Rh	-1.26200	0.00937	0.19214
O	-3.60325	2.14283	0.27932
O	-1.41198	1.95620	0.90313
O	-4.16129	-0.52104	1.37162
O	-1.97744	-0.65750	2.02797
O	-1.29966	-1.92543	-0.59972
O	-3.48388	-1.73337	-1.24278
O	-0.77921	0.71723	-1.71520
O	-2.96508	0.96093	-2.32544
C	0.74467	-0.15279	0.77646
C	1.42775	1.14969	0.87822
C	1.59461	2.00603	-0.22849
C	1.80455	1.63938	2.14550
C	2.14742	3.26881	-0.07775
H	1.27274	1.66945	-1.20549
C	2.32452	2.92406	2.29054
H	1.65613	1.02015	3.02394
C	2.52320	3.75663	1.18434
H	2.28316	3.89844	-0.95464
H	2.58794	3.28017	3.28378
C	1.28349	-1.26854	1.59530
C	0.48200	-2.36903	1.96082
C	2.65605	-1.30574	1.93667
C	1.02371	-3.44200	2.66522
H	-0.56245	-2.37669	1.68996
C	3.19781	-2.38686	2.62580
H	3.30194	-0.49129	1.62948
C	2.38018	-3.45799	2.99866
H	0.38538	-4.27544	2.94518
H	4.25733	-2.39589	2.86739
H	2.80003	-4.30247	3.53898
C	-2.52564	2.55647	0.78580
H	-2.54024	3.58222	1.18518
C	-1.72413	1.03297	-2.50858
H	-1.39645	1.41591	-3.48784



C	-3.23596	-0.76603	2.18737
H	-3.54381	-1.12752	3.18068
C	-2.38745	-2.33389	-1.12766
H	-2.34451	-3.35625	-1.53588
Si	1.94234	-1.45518	-1.69705
H	1.14209	-0.63339	-0.61789
C	1.82595	-3.23867	-1.12754
H	0.76892	-3.50127	-1.02468
H	2.29238	-3.91173	-1.85770
H	2.30317	-3.39358	-0.15535
C	1.11118	-1.14310	-3.35168
H	1.15427	-0.08646	-3.63076
H	1.59101	-1.73542	-4.14072
H	0.05722	-1.42659	-3.28346
C	3.66950	-0.74377	-1.58565
C	3.98065	0.48465	-2.19973
C	4.67422	-1.37399	-0.82611
C	5.24209	1.06284	-2.06112
H	3.22751	1.00071	-2.79005
C	5.93896	-0.80048	-0.68645
H	4.46604	-2.31891	-0.33164
C	6.22349	0.42072	-1.30207
H	5.45927	2.01344	-2.54097
H	6.70117	-1.30438	-0.09769
H	7.20665	0.87054	-1.19107
C	3.13708	5.12775	1.32898
H	4.18737	5.12596	1.00725
H	2.61319	5.86685	0.71164
H	3.11148	5.47395	2.36729

**TS-1 (R=NMe<sub>2</sub>)**

Rh	3.86914	0.45365	-0.28972
Rh	1.43032	0.15007	0.16302
O	4.22164	-0.48642	1.52737
O	1.98982	-0.74277	1.95169
O	3.72241	2.27785	0.70099
O	1.49558	1.99324	1.12876
O	1.06367	1.04921	-1.69551
O	3.29144	1.36662	-2.08779
O	1.58473	-1.68103	-0.82979
O	3.81387	-1.40507	-1.23836
C	-0.64577	-0.14042	0.52834
C	-0.86177	-1.26722	1.46858
C	-0.63870	-2.60958	1.11375

C	-1.16199	-0.98219	2.81622
C	-0.74521	-3.62815	2.05491
H	-0.35545	-2.84653	0.09604
C	-1.24836	-2.00266	3.76137
H	-1.30119	0.04963	3.12147
C	-1.05267	-3.33263	3.38579
H	-0.58353	-4.65849	1.74841
H	-1.47244	-1.75412	4.79558
H	-1.13301	-4.12883	4.12097
C	-1.60837	0.97861	0.57015
C	-1.28944	2.25919	0.07036
C	-2.94289	0.78502	0.99466
C	-2.22191	3.28164	0.02122
H	-0.29104	2.44796	-0.29548
C	-3.89261	1.79245	0.94112
H	-3.24626	-0.19290	1.35244
C	-3.55591	3.08399	0.45973
H	-1.91094	4.24240	-0.37086
H	-4.89987	1.57368	1.27519
C	3.22777	-0.85535	2.21082
H	3.45527	-1.34597	3.16980
C	2.72180	-2.02506	-1.28747
H	2.73857	-3.00088	-1.79878
C	2.60624	2.61071	1.17899
H	2.57537	3.57200	1.71555
C	2.07146	1.44431	-2.37168
H	1.82314	1.91527	-3.33662
Si	-1.61932	-1.07264	-2.06342
H	-0.79828	-0.68908	-0.70465
C	-2.17183	0.59831	-2.70274
H	-1.29575	1.24840	-2.78069
H	-2.62555	0.48724	-3.69598
H	-2.89250	1.08393	-2.03921
C	-0.39143	-1.94199	-3.18271
H	-0.02281	-2.87024	-2.73907
H	-0.85515	-2.16951	-4.15120
H	0.46861	-1.28644	-3.34232
C	-3.00808	-2.15931	-1.46105
C	-2.84212	-3.55316	-1.34593
C	-4.23367	-1.60305	-1.04449
C	-3.85650	-4.36055	-0.83320
H	-1.90839	-4.01612	-1.65567
C	-5.24990	-2.40774	-0.52861
H	-4.39315	-0.53070	-1.11092

C	-5.06187	-3.78753	-0.42020
H	-3.70653	-5.43364	-0.75075
H	-6.18729	-1.95905	-0.21012
H	-5.85153	-4.41455	-0.01475
N	-4.48573	4.09845	0.41398
C	-4.13332	5.38121	-0.17438
H	-3.29437	5.84635	0.35844
H	-3.85464	5.28707	-1.23424
H	-4.98779	6.05629	-0.10543
C	-5.86900	3.83400	0.77527
H	-6.32933	3.07643	0.12355
H	-5.95097	3.48567	1.81288
H	-6.44740	4.75489	0.68633

**TS-2 (R=NMe2)**

Rh	-3.73489	0.70346	-0.47286
Rh	-1.40409	0.06189	0.17394
O	-3.21978	2.66363	-0.00417
O	-1.09765	2.06925	0.61084
O	-4.26795	0.38840	1.51181
O	-2.13650	-0.17585	2.11002
O	-1.89122	-1.90609	-0.34596
O	-4.03572	-1.32946	-0.88648
O	-0.89040	0.38304	-1.82798
O	-3.01282	0.98533	-2.41167
C	0.58735	-0.47539	0.69425
C	1.51371	0.66500	0.63854
C	1.73945	1.39285	-0.54775
C	2.09905	1.18168	1.81338
C	2.52534	2.53003	-0.57612
H	1.27101	1.05496	-1.46406
C	2.85715	2.34416	1.80760
H	1.91922	0.68583	2.76139
C	3.11486	3.04424	0.60622
H	2.67292	3.03000	-1.52593
H	3.24698	2.70592	2.75125
C	0.90373	-1.55896	1.67904
C	-0.10082	-2.37804	2.22632
C	2.24716	-1.86715	1.98849
C	0.22354	-3.44110	3.06842
H	-1.13458	-2.17969	1.98845
C	2.57091	-2.93831	2.81825
H	3.04185	-1.27532	1.54845
C	1.55710	-3.72896	3.36626

H	-0.57108	-4.05442	3.48479
H	3.61386	-3.15806	3.03195
H	1.80552	-4.56518	4.01474
C	-2.05365	2.88442	0.42322
H	-1.82050	3.93184	0.67106
C	-1.79614	0.76939	-2.63569
H	-1.45487	0.92770	-3.67122
C	-3.37103	0.04321	2.32412
H	-3.68841	-0.09280	3.36978
C	-3.08233	-2.13424	-0.74379
H	-3.29007	-3.18676	-0.99534
Si	1.31937	-2.26218	-1.53288
H	0.74228	-1.12753	-0.51757
C	0.88215	-3.88510	-0.70592
H	-0.19099	-3.88266	-0.49382
H	1.11269	-4.72687	-1.37136
H	1.41099	-4.02855	0.24023
C	0.44869	-2.00729	-3.17455
H	0.67852	-1.03208	-3.61113
H	0.74927	-2.79191	-3.88092
H	-0.63195	-2.05966	-3.01950
C	3.14479	-1.87999	-1.57686
C	3.63471	-0.80391	-2.34211
C	4.06356	-2.60582	-0.79357
C	4.98653	-0.46289	-2.32467
H	2.95324	-0.21888	-2.95434
C	5.41784	-2.27070	-0.77726
H	3.71779	-3.43561	-0.18346
C	5.88042	-1.19590	-1.54054
H	5.34205	0.37547	-2.91768
H	6.11122	-2.84510	-0.16847
H	6.93413	-0.93013	-1.52398
N	3.90932	4.17744	0.58216
C	4.35351	4.76491	1.83516
H	3.51455	5.09281	2.46895
H	4.95523	4.05098	2.41044
H	4.98283	5.63155	1.62375
C	3.96384	4.98742	-0.62390
H	4.37228	4.41463	-1.46575
H	2.97468	5.36994	-0.91989
H	4.62446	5.83985	-0.45499

**TS-1 (R=NO2)**

Rh	-3.89264	0.50421	0.29590
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Rh	-1.47446	0.09826	-0.16360
O	-4.31707	-0.86816	-1.20184
O	-2.10384	-1.21416	-1.64787
O	-3.81074	2.01790	-1.12437
O	-1.59411	1.65600	-1.53883
O	-1.06038	1.44039	1.38332
O	-3.27445	1.84955	1.76681
O	-1.57798	-1.42309	1.25771
O	-3.78993	-1.05340	1.67961
C	0.53684	-0.25809	-0.59924
C	0.77649	-1.48906	-1.37320
C	0.34571	-2.74779	-0.90293
C	1.31527	-1.41409	-2.67476
C	0.49563	-3.88840	-1.68019
H	-0.11401	-2.80818	0.07681
C	1.42774	-2.55681	-3.46675
H	1.61642	-0.45270	-3.07685
C	1.03652	-3.79926	-2.96883
H	0.17458	-4.85057	-1.29011
H	1.83130	-2.47273	-4.47196
H	1.14126	-4.69105	-3.58058
C	1.55882	0.81909	-0.70131
C	1.21772	2.17414	-0.50459
C	2.92049	0.49768	-0.91243
C	2.19015	3.16803	-0.53101
H	0.18782	2.44478	-0.33528
C	3.90374	1.47948	-0.92211
H	3.21513	-0.53685	-1.03512
C	3.52105	2.80495	-0.73233
H	1.93526	4.21063	-0.38716
H	4.94845	1.22985	-1.05562
C	-3.35114	-1.39205	-1.81792
H	-3.61082	-2.10552	-2.61457
C	-2.69331	-1.64425	1.83568
H	-2.67654	-2.46375	2.57092
C	-2.71554	2.23846	-1.70156
H	-2.71101	3.04419	-2.45108
C	-2.04414	1.99904	1.97248
H	-1.76343	2.70598	2.76879
Si	1.66955	-0.99304	2.18761
H	0.85574	-0.75501	0.86961
C	1.75769	0.70066	2.98823
H	2.22718	1.42160	2.31023
H	0.74568	1.05924	3.19450

H	2.33056	0.67745	3.92323
C	0.76455	-2.29778	3.19240
H	0.61491	-3.21142	2.60785
H	1.34256	-2.55552	4.08843
H	-0.21784	-1.92658	3.49486
C	3.33172	-1.58263	1.56126
C	3.43289	-2.78168	0.82742
C	4.48955	-0.79485	1.70176
C	4.63870	-3.16789	0.24202
H	2.55699	-3.40887	0.68451
C	5.70202	-1.18432	1.13007
H	4.44311	0.14383	2.24816
C	5.77551	-2.36799	0.39169
H	4.69107	-4.08801	-0.33378
H	6.58375	-0.56049	1.25031
H	6.71495	-2.66648	-0.06592
N	4.55968	3.85292	-0.72804
O	4.19421	5.01760	-0.57815
O	5.72889	3.49609	-0.87105

**TS-2 (R=NO2)**

Rh	-3.72184	0.59011	-0.55732
Rh	-1.40355	0.08209	0.20834
O	-3.31482	2.58381	-0.14434
O	-1.19682	2.11441	0.57661
O	-4.32540	0.31580	1.41282
O	-2.20064	-0.13656	2.11589
O	-1.78947	-1.91800	-0.24930
O	-3.92658	-1.45999	-0.91376
O	-0.82764	0.36698	-1.78074
O	-2.94974	0.83810	-2.47180
C	0.52576	-0.33094	0.84341
C	1.44032	0.81672	0.73230
C	1.75673	1.42255	-0.50051
C	1.91697	1.41715	1.91961
C	2.55417	2.55475	-0.55482
H	1.36083	0.99768	-1.41216
C	2.68849	2.57235	1.87691
H	1.66077	0.98159	2.87905
C	3.01281	3.11855	0.63687
H	2.82165	3.01183	-1.49928
H	3.05295	3.04188	2.78216
C	0.90147	-1.41246	1.76407
C	-0.06556	-2.28788	2.30536

C	2.26586	-1.65937	2.05944
C	0.31590	-3.34285	3.12961
H	-1.10895	-2.12831	2.08037
C	2.64256	-2.72694	2.86629
H	3.02921	-1.02738	1.61993
C	1.66623	-3.56899	3.40984
H	-0.44266	-3.99900	3.54664
H	3.69481	-2.90585	3.06890
C	-2.17982	2.87972	0.31591
H	-2.00164	3.94506	0.52550
C	-1.71556	0.67644	-2.64055
H	-1.33878	0.81287	-3.66566
C	-3.45381	0.03309	2.27326
H	-3.80766	-0.08906	3.30809
C	-2.94763	-2.21583	-0.69566
H	-3.09467	-3.28450	-0.91661
Si	1.43583	-2.21188	-1.53269
H	0.83854	-1.13614	-0.60533
C	1.07993	-3.84871	-0.68316
H	-0.00174	-3.94018	-0.54396
H	1.43378	-4.69467	-1.28476
H	1.54612	-3.90643	0.30537
C	0.60468	-2.05620	-3.21182
H	0.80050	-1.08056	-3.66663
H	0.95863	-2.83653	-3.89634
H	-0.47843	-2.15626	-3.09227
C	3.25860	-1.77398	-1.57218
C	3.72384	-0.72235	-2.38557
C	4.18689	-2.40755	-0.72386
C	5.05692	-0.31351	-2.34992
H	3.03632	-0.21044	-3.05547
C	5.52302	-2.00433	-0.68594
H	3.86394	-3.22281	-0.08159
C	5.95894	-0.95331	-1.49614
H	5.39204	0.50359	-2.98317
H	6.22364	-2.50907	-0.02564
H	6.99735	-0.63463	-1.46398
H	1.95876	-4.40192	4.04365
N	3.86009	4.31704	0.58198
O	4.23870	4.80076	1.64950
O	4.14472	4.76605	-0.52928

**TS-1 (R=OCF3)**

Rh	3.93455	-1.29279	0.36485
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Rh	1.74115	-0.22164	-0.16209
O	4.76645	-0.13028	-1.13882
O	2.76095	0.84889	-1.62592
O	3.44628	-2.74428	-1.04102
O	1.45005	-1.74953	-1.53689
O	0.91804	-1.39544	1.35725
O	2.92388	-2.37554	1.83916
O	2.22295	1.22268	1.27544
O	4.24087	0.25650	1.72968
C	-0.08139	0.68946	-0.65942
C	0.09924	1.92181	-1.45627
C	0.80554	3.03579	-0.95953
C	-0.28903	1.93595	-2.81300
C	1.06102	4.13809	-1.76579
H	1.17199	3.01189	0.05841
C	0.00269	3.02904	-3.62853
H	-0.79005	1.07188	-3.23558
C	0.66157	4.14215	-3.10688
H	1.59170	4.99207	-1.35306
H	-0.29415	3.00902	-4.67368
H	0.87319	5.00010	-3.73909
C	-1.34689	-0.05741	-0.84904
C	-1.41941	-1.44715	-0.61654
C	-2.53216	0.60775	-1.24408
C	-2.60376	-2.14707	-0.82576
H	-0.54006	-1.97924	-0.28945
C	-3.72108	-0.08096	-1.45214
H	-2.52061	1.68187	-1.38100
C	-3.73503	-1.45867	-1.25122
H	-2.65997	-3.21951	-0.67326
H	-4.62619	0.43241	-1.75215
C	4.00715	0.64991	-1.77377
H	4.47896	1.24831	-2.56798
C	3.34955	1.12938	1.86827
H	3.55316	1.92559	2.60148
C	2.35413	-2.63889	-1.65601
H	2.13641	-3.41827	-2.40206
C	1.69188	-2.18425	1.99339
H	1.20161	-2.77115	2.78592
Si	-0.86803	1.77490	2.13052
H	-0.27947	1.24263	0.76437
C	-0.27593	0.60588	3.47227
H	0.81607	0.61841	3.51151
H	-0.67687	0.90824	4.44761



H	-0.58349	-0.42142	3.26179
C	-0.26709	3.54366	2.35182
H	-0.51274	4.17268	1.49015
H	-0.72224	3.99103	3.24408
H	0.82052	3.55079	2.47611
C	-2.71196	1.67441	1.84795
C	-3.42914	2.75512	1.29848
C	-3.41111	0.47865	2.10038
C	-4.79025	2.64470	1.00986
H	-2.92074	3.69343	1.08799
C	-4.76968	0.36274	1.81210
H	-2.88603	-0.37953	2.51177
C	-5.46026	1.44524	1.26160
H	-5.32561	3.48998	0.58511
H	-5.28465	-0.57438	1.99202
H	-6.51475	1.34668	1.02031
O	-4.88792	-2.20337	-1.54472
C	-5.90211	-2.17831	-0.64917
F	-6.84603	-3.01443	-1.07473
F	-5.50495	-2.56376	0.58309
F	-6.45025	-0.94874	-0.51833

**TS-2 (R=OCF3)**

Rh	-3.59251	1.28833	-0.56148
Rh	-1.48541	0.16807	0.17581
O	-2.62720	3.09918	-0.23765
O	-0.70910	2.07186	0.46322
O	-4.19274	1.26465	1.42993
O	-2.26472	0.24346	2.10509
O	-2.43121	-1.65711	-0.20292
O	-4.37507	-0.63344	-0.83075
O	-0.90372	0.21013	-1.83036
O	-2.82806	1.23605	-2.49908
C	0.27992	-0.74207	0.80066
C	1.46202	0.12662	0.65966
C	1.88301	0.63218	-0.58639
C	2.10407	0.59876	1.82464
C	2.92225	1.54773	-0.67321
H	1.37298	0.30913	-1.48399
C	3.11906	1.54917	1.74742
H	1.77833	0.24492	2.79652
C	3.52474	2.00280	0.49832
H	3.26203	1.92688	-1.63029
H	3.60145	1.93457	2.63901

C	0.35692	-1.84006	1.78502
C	-0.80582	-2.39417	2.36047
C	1.60375	-2.43296	2.10023
C	-0.71956	-3.47388	3.23592
H	-1.76849	-1.97037	2.11903
C	1.68337	-3.52357	2.96002
H	2.50684	-2.05163	1.63729
C	0.52009	-4.04426	3.53612
H	-1.62548	-3.87989	3.67707
H	2.64984	-3.97010	3.17731
H	0.58010	-4.89474	4.21013
C	-1.44298	3.07495	0.19256
H	-0.96564	4.05234	0.35977
C	-1.69569	0.72630	-2.68456
H	-1.32805	0.71347	-3.72230
C	-3.41070	0.77049	2.28136
H	-3.75274	0.78714	3.32748
C	-3.64028	-1.62777	-0.61063
H	-4.08930	-2.61734	-0.79022
Si	0.61310	-2.85092	-1.45155
H	0.34321	-1.60996	-0.55382
C	-0.18190	-4.28836	-0.54315
H	-1.23990	-4.05605	-0.38701
H	-0.10298	-5.21511	-1.12466
H	0.26821	-4.45493	0.44009
C	-0.16086	-2.53008	-3.13327
H	0.29165	-1.66672	-3.62973
H	-0.04702	-3.40635	-3.78327
H	-1.22681	-2.31992	-3.00564
C	2.48379	-2.93555	-1.50201
C	3.21714	-2.07911	-2.34606
C	3.20537	-3.78243	-0.63872
C	4.61171	-2.06392	-2.32761
H	2.69503	-1.41071	-3.02719
C	4.60117	-3.77287	-0.61797
H	2.67353	-4.45449	0.02978
C	5.30663	-2.91062	-1.46048
H	5.15619	-1.39177	-2.98551
H	5.13818	-4.43705	0.05441
H	6.39315	-2.89850	-1.44221
O	4.59816	2.90403	0.42229
C	4.27349	4.21759	0.30837
F	5.40875	4.91546	0.28320
F	3.52166	4.64720	1.33993

F	3.58332	4.47869	-0.82134
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**TS-1 (R=OMe)**

Rh	3.77513	0.05026	-0.34073
Rh	1.32684	0.05469	0.15750
O	4.04089	-0.92749	1.47201
O	1.80014	-0.92468	1.92535
O	3.88128	1.87845	0.64719
O	1.65118	1.85892	1.14430
O	1.04756	1.01926	-1.68030
O	3.28814	1.03330	-2.12692
O	1.23205	-1.76035	-0.87063
O	3.47814	-1.78645	-1.28274
C	-0.73303	0.03671	0.59762
C	-1.09463	-1.08757	1.48994
C	-1.04600	-2.43291	1.08098
C	-1.35078	-0.81690	2.85040
C	-1.27919	-3.46365	1.98453
H	-0.80366	-2.66161	0.05127
C	-1.55656	-1.85414	3.75832
H	-1.35684	0.21170	3.19588
C	-1.53483	-3.18200	3.32971
H	-1.25547	-4.49372	1.63841
H	-1.73998	-1.61977	4.80358
H	-1.71070	-3.98941	4.03531
C	-1.56111	1.25573	0.66224
C	-1.08611	2.49443	0.18703
C	-2.90745	1.20654	1.10665
C	-1.88257	3.63511	0.19001
H	-0.07849	2.56155	-0.19463
C	-3.71453	2.33029	1.10309
H	-3.32278	0.26227	1.43953
C	-3.20495	3.56188	0.65360
H	-1.46946	4.56833	-0.17440
H	-4.74487	2.28889	1.44203
C	3.02040	-1.18298	2.16699
H	3.20070	-1.70389	3.11984
C	2.31145	-2.25206	-1.33388
H	2.19416	-3.21676	-1.85244
C	2.82956	2.33941	1.16151
H	2.92989	3.29322	1.70260
C	2.08323	1.27685	-2.38056
H	1.87735	1.78164	-3.33812
Si	-1.91319	-0.68899	-2.06477

H	-1.05548	-0.49167	-0.74368
C	-2.22139	1.05802	-2.67260
H	-1.25700	1.56015	-2.79227
H	-2.74176	1.04383	-3.63838
H	-2.81601	1.64294	-1.96478
C	-0.86073	-1.71962	-3.22721
H	-0.64850	-2.70837	-2.81107
H	-1.36105	-1.84421	-4.19565
H	0.09632	-1.21333	-3.38054
C	-3.45634	-1.55373	-1.46209
C	-3.49418	-2.95407	-1.31768
C	-4.58915	-0.81858	-1.06151
C	-4.61518	-3.59579	-0.79226
H	-2.63691	-3.55344	-1.61480
C	-5.71256	-1.45666	-0.53390
H	-4.59361	0.26382	-1.15337
C	-5.72583	-2.84644	-0.39617
H	-4.62218	-4.67743	-0.68761
H	-6.57590	-0.87042	-0.22990
H	-6.59853	-3.34435	0.01811
O	-4.06825	4.60578	0.69986
C	-3.61336	5.88650	0.27731
H	-3.32266	5.87984	-0.78120
H	-4.45824	6.56275	0.41683
H	-2.76620	6.23046	0.88447

**TS-2 (R=OMe)**

Rh	-3.70403	0.41069	-0.51099
Rh	-1.32733	0.05373	0.18061
O	-3.39721	2.43425	-0.15776
O	-1.23186	2.10506	0.50033
O	-4.21976	0.15218	1.48570
O	-2.04788	-0.15383	2.12480
O	-1.60750	-1.98099	-0.22115
O	-3.79151	-1.66322	-0.81232
O	-0.83193	0.31597	-1.83244
O	-2.99934	0.65478	-2.46033
C	0.69340	-0.24162	0.73301
C	1.50767	0.98035	0.60415
C	1.68090	1.64401	-0.63150
C	2.01965	1.61285	1.75300
C	2.36127	2.84337	-0.71616
H	1.26052	1.20362	-1.52664
C	2.67412	2.84277	1.68505

H	1.87489	1.15337	2.72482
C	2.86386	3.45934	0.44321
H	2.51187	3.33926	-1.66998
H	3.03075	3.30091	2.60017
C	1.12861	-1.23895	1.75571
C	0.21538	-2.12671	2.35531
C	2.50006	-1.39428	2.06126
C	0.65314	-3.10816	3.24350
H	-0.83525	-2.04259	2.12301
C	2.93700	-2.38538	2.93641
H	3.22717	-0.74832	1.58200
C	2.01178	-3.24515	3.53566
H	-0.07108	-3.77668	3.70102
H	3.99832	-2.48980	3.14649
H	2.34896	-4.01934	4.22001
C	-2.26556	2.80318	0.25886
H	-2.14572	3.88230	0.44144
C	-1.76458	0.55646	-2.66631
H	-1.43045	0.68944	-3.70741
C	-3.30110	-0.05210	2.32079
H	-3.61344	-0.16221	3.37087
C	-2.76247	-2.35468	-0.61516
H	-2.85585	-3.43577	-0.80627
Si	1.60796	-2.06792	-1.44326
H	0.94248	-0.96047	-0.48599
C	1.38324	-3.67852	-0.51228
H	0.31974	-3.79711	-0.28423
H	1.71052	-4.52439	-1.13013
H	1.93279	-3.70080	0.43287
C	0.67564	-2.03031	-3.07063
H	0.77910	-1.06938	-3.58069
H	1.04643	-2.82393	-3.73190
H	-0.38772	-2.19424	-2.87747
C	3.37662	-1.48583	-1.57225
C	3.72643	-0.43858	-2.44673
C	4.38542	-2.02430	-0.74972
C	5.02998	0.05382	-2.49772
H	2.97241	0.00417	-3.09295
C	5.69180	-1.53652	-0.80004
H	4.14823	-2.82834	-0.05842
C	6.01483	-0.49432	-1.67235
H	5.27690	0.86619	-3.17583
H	6.45679	-1.96772	-0.15953
H	7.03083	-0.11025	-1.70918

O	3.51040	4.64139	0.24967
C	4.02839	5.31998	1.38424
H	4.49449	6.23014	1.00227
H	3.23215	5.58895	2.09137
H	4.78379	4.71610	1.90528

**TS-1 (R=SCF3)**

Rh	4.18374	-1.07606	0.31876
Rh	1.90565	-0.17184	-0.16939
O	4.92978	0.33993	-1.00108
O	2.84920	1.17799	-1.43750
O	3.89626	-2.38836	-1.27203
O	1.83332	-1.52802	-1.74483
O	1.16402	-1.59089	1.16758
O	3.24333	-2.42608	1.60757
O	2.18249	1.09890	1.46390
O	4.28854	0.31443	1.86780
C	0.02820	0.59600	-0.64281
C	0.07534	1.98472	-1.13537
C	0.55356	3.04439	-0.33877
C	-0.21879	2.24936	-2.48924
C	0.68687	4.32445	-0.86215
H	0.82889	2.84301	0.68942
C	-0.04815	3.52807	-3.01905
H	-0.55131	1.44082	-3.13188
C	0.38897	4.57425	-2.20663
H	1.03848	5.13076	-0.22380
H	-0.26740	3.70515	-4.06841
H	0.50460	5.57402	-2.61600
C	-1.12904	-0.23982	-1.04314
C	-1.07333	-1.64704	-0.96317
C	-2.36874	0.35677	-1.36830
C	-2.21401	-2.41887	-1.15531
H	-0.14227	-2.12974	-0.71000
C	-3.50781	-0.41085	-1.58058
H	-2.45280	1.43615	-1.40333
C	-3.43870	-1.80065	-1.43750
H	-2.16524	-3.49754	-1.04524
H	-4.45435	0.07113	-1.79446
C	4.11301	1.12006	-1.55991
H	4.54317	1.86006	-2.25188
C	3.29536	1.05324	2.08354
H	3.38467	1.76036	2.92301
C	2.82570	-2.30603	-1.92631

H	2.71700	-2.99825	-2.77525
C	1.99573	-2.37259	1.73729
H	1.54446	-3.09427	2.43636
Si	-1.31893	0.85595	2.13061
H	-0.37784	0.80679	0.88124
C	-1.78167	-0.92507	2.49888
H	-2.35745	-1.36383	1.67773
H	-0.87275	-1.51896	2.62251
H	-2.38387	-0.99114	3.41361
C	-0.32649	1.70202	3.48470
H	-0.06680	2.72743	3.20063
H	-0.90026	1.74043	4.41878
H	0.60502	1.15617	3.65807
C	-2.79024	1.85150	1.54016
C	-2.64506	3.20121	1.16201
C	-4.04942	1.24766	1.35962
C	-3.71168	3.91554	0.61619
H	-1.68421	3.69713	1.27095
C	-5.12235	1.96166	0.82386
H	-4.19699	0.20214	1.61334
C	-4.95330	3.29553	0.44673
H	-3.57423	4.95190	0.31931
H	-6.07928	1.46763	0.68572
H	-5.78437	3.85036	0.01899
C	-5.75573	-2.16608	-0.05171
F	-6.82385	-2.93647	0.19315
F	-4.95747	-2.17968	1.03543
F	-6.18696	-0.89267	-0.19407
S	-4.92266	-2.80474	-1.54500

**TS-2 (R=SCF3)**

Rh	3.36795	-1.82722	-0.60780
Rh	1.52902	-0.34641	0.20339
O	2.13943	-3.43382	-0.13072
O	0.46225	-2.07609	0.62087
O	4.10089	-1.82288	1.33945
O	2.40537	-0.48602	2.08588
O	2.73847	1.28076	-0.30268
O	4.43303	-0.07300	-1.01721
O	0.81842	-0.36800	-1.76218
O	2.50028	-1.72371	-2.49557
C	-0.00605	0.88181	0.86835
C	-1.33542	0.25345	0.78800
C	-1.92118	-0.14125	-0.43035

C	-1.99022	-0.09531	1.98823
C	-3.13277	-0.81590	-0.45352
H	-1.41440	0.08703	-1.35744
C	-3.17730	-0.82267	1.96857
H	-1.54306	0.17319	2.93941
C	-3.76125	-1.17481	0.74778
H	-3.58662	-1.08592	-1.40055
H	-3.65229	-1.11329	2.90016
C	0.15648	2.00762	1.80455
C	1.42641	2.37420	2.29916
C	-0.95437	2.81391	2.15565
C	1.57122	3.48011	3.13264
H	2.28928	1.78558	2.02761
C	-0.80206	3.92747	2.97472
H	-1.93211	2.57659	1.75151
C	0.46285	4.26063	3.47107
H	2.55526	3.74081	3.51172
H	-1.66575	4.53813	3.22328
H	0.58357	5.12945	4.11272
C	1.00293	-3.19723	0.35927
H	0.38222	-4.07394	0.59778
C	1.45502	-1.04143	-2.63620
H	1.02403	-1.00957	-3.64873
C	3.46491	-1.18200	2.21449
H	3.86970	-1.21683	3.23747
C	3.89397	1.03706	-0.78694
H	4.48786	1.93133	-1.03290
Si	-0.01148	2.94628	-1.49132
H	0.06007	1.72633	-0.53993
C	0.95284	4.30555	-0.62480
H	1.97912	3.96064	-0.46440
H	0.97716	5.21772	-1.23349
H	0.52962	4.55281	0.35365
C	0.74204	2.45558	-3.14184
H	0.17541	1.65250	-3.62150
H	0.77775	3.31430	-3.82335
H	1.76090	2.09134	-2.97994
C	-1.85132	3.28827	-1.59507
C	-2.66380	2.58582	-2.50568
C	-2.48088	4.17544	-0.70087
C	-4.04790	2.75808	-2.52308
H	-2.21208	1.89079	-3.21012
C	-3.86565	4.35125	-0.71363
H	-1.88386	4.73233	0.01669



C	-4.65156	3.64028	-1.62361
H	-4.65550	2.20464	-3.23418
H	-4.33160	5.04277	-0.01628
H	-5.73003	3.77375	-1.63298
C	-4.71034	-3.68320	0.17986
F	-3.78228	-4.19483	1.00395
F	-4.16269	-3.63928	-1.05091
F	-5.75755	-4.52373	0.14093
S	-5.32311	-2.05445	0.73452

### Dirhodium-C1

Conformations of each species were generated using Maestro with the OPLS3 force field. Conformational searches were conducted by restraining the position of the catalyst atoms and the Rh-C bond length. Geometry optimizations and frequency calculations were performed with Gaussian09 using ONIOM partitioning where carbon and hydrogen atoms in **C1** were modeled with UFF and all other atoms (including the carbene and silane) with B3LYP/6-31G(d)-LANL2DZ(Rh). All-DFT single point energy corrections were calculated at the M06/6-311++G(d,p)-SDD(Rh)/SMD(DCM) level of theory.

Structure	Electronic Energy	Zero Point Energy	Enthalpy	Free Energy
<b>TS-3</b>	-6835.565466	-6833.9538	-6833.8602	-6834.0875
<b>TS-4</b>	-6835.565181	-6833.9536	-6833.8602	-6834.0839
<b>TS-5</b>	-6835.558894	-6833.9472	-6833.8537	-6834.0785
<b>TS-6</b>	-6835.556087	-6833.9446	-6833.8512	-6834.0757
<b>TS-3'</b>	-6945.8393	-6944.2597	-6944.1659	-6944.392
<b>TS-4'</b>	-6945.8371	-6944.2577	-6944.1639	-6944.3904
<b>TS-5'</b>	-6945.8351	-6944.2556	-6944.1617	-6944.3881
<b>TS-6'</b>	-6945.8368	-6944.2574	-6944.1638	-6944.3881

### **TS-3**

Rh	-0.14295	0.01475	0.09776
Rh	-0.19853	0.31177	-2.52950
P	2.58202	0.86064	-1.18911
P	0.48631	-2.58190	-1.53673
P	-2.92088	-0.47371	-1.27909
P	-0.72711	2.91429	-0.97317
O	1.77818	0.82420	0.11482
O	1.83929	0.80597	-2.51391
O	3.47869	2.23140	-1.27657
O	3.65829	-0.37436	-1.03067
O	0.62554	-1.93335	-0.15377
O	0.30516	-1.70780	-2.76125
O	1.79293	-3.51014	-1.89474

O	-0.74006	-3.66806	-1.34265
O	-2.06592	-0.86347	-0.06416
O	-2.23989	-0.17511	-2.60001
O	-3.82078	0.78058	-0.70928
O	-3.99950	-1.66022	-1.64952
O	-0.86859	1.97319	0.23134
O	-0.77018	2.32470	-2.37234
O	-1.92938	4.03799	-0.94258
O	0.65684	3.75412	-0.70777
C	6.35336	1.24944	-1.16270
C	5.51796	1.89732	-0.10321
C	4.22729	2.44594	-0.19566
C	3.74004	3.16147	0.84577
C	4.48608	3.31271	2.03002
C	5.72476	2.67057	2.16742
H	6.28563	2.73954	3.08987
C	6.20959	1.93740	1.08540
C	7.45787	1.13688	1.03373
H	7.49668	0.40576	1.86936
H	8.34074	1.81078	1.06336
C	7.35499	0.41772	-0.32398
H	8.35128	0.31960	-0.80852
H	6.94811	-0.60520	-0.15548
C	5.65170	0.43243	-2.20139
C	4.49255	-0.47519	-2.06575
C	4.14862	-1.25708	-3.18010
H	3.29793	-1.91919	-3.13534
C	4.84331	-1.11791	-4.39257
C	5.86788	-0.17030	-4.53050
H	6.36219	-0.03891	-5.48445
C	6.23917	0.60479	-3.43099
C	7.27248	1.66811	-3.41378
H	7.08644	2.41648	-4.21404
H	8.28102	1.21637	-3.52986
C	7.10700	2.29872	-2.02174
H	8.09050	2.58957	-1.59128
H	6.49091	3.22102	-2.12311
C	0.63605	-6.34485	-1.80545
C	1.49810	-5.61426	-0.81646
C	2.11682	-4.35683	-0.92007
C	3.00351	-3.95568	0.09669
C	3.20508	-4.77009	1.22278
C	2.49900	-5.97292	1.35675
H	2.60475	-6.57489	2.24999

C	1.63416	-6.36277	0.33248
C	0.72308	-7.53420	0.34696
H	1.31116	-8.47198	0.25150
H	0.11050	-7.54993	1.27421
C	-0.16222	-7.30569	-0.89036
H	-1.10875	-6.81688	-0.56490
H	-0.42081	-8.26622	-1.38798
C	-0.25994	-5.55138	-2.71249
C	-0.97336	-4.37037	-2.44988
C	-1.82798	-3.86259	-3.44729
H	-2.38546	-2.95369	-3.27338
C	-1.91992	-4.49907	-4.69498
C	-1.13476	-5.62603	-4.96842
H	-1.16431	-6.09177	-5.94504
C	-0.29938	-6.12307	-3.96644
C	0.66204	-7.24310	-4.10417
H	1.30636	-7.10736	-4.99951
H	0.11253	-8.20708	-4.16239
C	1.49183	-7.15584	-2.81381
H	2.43498	-6.60729	-3.03744
H	1.76413	-8.16771	-2.44073
C	-6.61578	-0.34777	-0.64376
C	-6.00381	0.61946	-1.61155
C	-4.72945	1.20004	-1.58588
C	-4.39363	2.13884	-2.58022
H	-3.41794	2.60030	-2.58647
C	-5.30788	2.44946	-3.59945
C	-6.54891	1.80207	-3.65127
H	-7.23975	2.00287	-4.45997
C	-6.86688	0.87782	-2.65434
C	-8.08439	0.03567	-2.59676
H	-8.25677	-0.48213	-3.56498
H	-8.96284	0.66049	-2.32748
C	-7.76174	-0.97459	-1.48492
H	-8.66671	-1.21106	-0.88297
H	-7.41173	-1.91937	-1.95968
C	-5.74520	-1.40993	-0.03437
C	-4.66462	-2.12215	-0.59153
C	-4.20996	-3.28993	0.05247
H	-3.41359	-3.87041	-0.39487
C	-4.72619	-3.67625	1.23412
C	-5.74725	-2.83869	1.90414
H	-6.11722	-3.09099	2.88911
C	-6.20332	-1.71116	1.22750

C	-7.19938	-0.72306	1.71341
H	-6.88756	-0.29256	2.68942
H	-8.19784	-1.20293	1.79913
C	-7.19498	0.35059	0.60996
H	-6.52350	1.18233	0.92259
H	-8.21250	0.76768	0.44326
C	-0.41286	6.64004	-0.32619
C	-1.22375	5.75106	0.56703
C	-2.03453	4.65064	0.23737
C	-2.85926	4.11653	1.24223
C	-2.78425	4.62757	2.54956
C	-1.86000	5.63855	2.85830
H	-1.76137	5.99079	3.87729
C	-1.10303	6.16094	1.87975
C	-0.05371	7.20047	2.04207
H	-0.52325	8.17695	2.28896
H	0.67771	6.91060	2.82720
C	0.61748	7.24507	0.65801
H	1.53205	6.60998	0.68550
H	0.92265	8.27967	0.38695
C	0.23266	6.01522	-1.52147
C	0.87873	4.68946	-1.63209
C	1.50135	4.37076	-2.85438
H	1.96971	3.40804	-2.99082
C	1.46572	5.23417	-3.88922
C	0.77846	6.45570	-3.78906
H	0.72159	7.11851	-4.64299
C	0.15747	6.80044	-2.58406
C	-0.65014	8.02121	-2.34106
H	-1.43497	8.14088	-3.11892
H	0.01154	8.91362	-2.31433
C	-1.27716	7.75580	-0.96556
H	-1.31799	8.68389	-0.35390
H	-2.32042	7.39560	-1.11486
H	-4.35616	-4.56798	1.72296
H	-3.41116	4.21720	3.32913
H	4.08197	3.88808	2.85267
H	3.87288	-4.44726	2.01043
H	-2.56810	-4.09395	-5.46112
H	-5.03887	3.16345	-4.36698
H	1.93671	4.96537	-4.82616
H	4.55001	-1.71418	-5.24683
C	-0.10251	-0.08278	2.23649
C	1.28565	-0.09156	2.75809

C	-1.16198	0.53567	3.05327
C	2.15569	-1.16819	2.48675
C	1.81493	1.02624	3.44062
C	-2.42442	0.84774	2.48716
C	-1.02378	0.73895	4.44639
C	3.46537	-1.17357	2.93716
H	1.78873	-1.99284	1.88984
C	3.12100	1.02357	3.91854
H	1.20036	1.90597	3.59163
C	-3.46347	1.33624	3.25733
H	-2.58505	0.68693	1.43334
C	-2.05248	1.25610	5.22816
H	-0.09736	0.46736	4.93898
C	3.92900	-0.08455	3.67615
H	4.13260	-2.00091	2.73293
H	3.51792	1.86213	4.47748
C	-3.28708	1.56260	4.63265
H	-4.42618	1.56656	2.81162
H	-1.89045	1.40547	6.28964
H	-3.34913	-3.22106	3.92105
C	-2.76446	-2.33429	3.64582
Si	-1.03315	-2.85198	3.13039
H	-2.76906	-1.64542	4.49441
H	-3.26434	-1.82702	2.81684
C	0.07978	-3.15681	4.61390
C	-1.02257	-4.28520	1.91957
H	-0.45707	-1.56618	2.36201
C	1.20711	-3.99517	4.51416
C	-0.17499	-2.55790	5.86408
H	-1.32304	-3.96338	0.92051
H	-0.02409	-4.71954	1.83481
H	-1.70225	-5.07425	2.26582
C	2.04504	-4.22485	5.60484
H	1.43406	-4.48244	3.57133
C	0.65967	-2.78314	6.95964
H	-1.03829	-1.91023	5.98881
H	2.90834	-4.87612	5.49776
C	1.77381	-3.61504	6.83141
H	0.44031	-2.31134	7.91403
H	2.42608	-3.78866	7.68307
H	-3.51970	3.28835	1.02022
H	2.75737	3.60836	0.78635
H	3.50239	-2.99704	0.03383
O	-4.35673	2.06751	5.29201

C	-4.23327	2.35768	6.67888
H	-5.19612	2.77107	6.98246
H	-4.02684	1.45113	7.26159
H	-3.44410	3.09721	6.86292
N	5.29173	-0.11153	4.21112
O	6.01046	-1.06461	3.90420
O	5.64063	0.81578	4.94473

**TS-4**

Rh	0.11885	-0.00436	0.08427
Rh	0.28878	0.44131	-2.51873
P	2.22035	2.14847	-0.81699
P	2.15183	-1.82098	-1.47418
P	-1.88843	-1.58746	-1.65841
P	-1.76801	2.25364	-1.00985
O	1.31904	1.67121	0.32279
O	1.77557	1.92097	-2.24924
O	2.48419	3.76041	-0.66831
O	3.67962	1.44742	-0.49135
O	1.79363	-1.27406	-0.08486
O	1.75898	-1.04191	-2.71150
O	3.77687	-2.01527	-1.62637
O	1.53699	-3.34971	-1.44302
O	-1.16399	-1.62014	-0.30254
O	-1.14164	-1.05901	-2.87177
O	-3.28031	-0.77174	-1.38530
O	-2.36409	-3.11240	-2.06607
O	-1.53486	1.28790	0.15778
O	-1.14998	1.94089	-2.36452
O	-3.36821	2.40935	-1.34358
O	-1.28286	3.71779	-0.43587
C	5.40468	4.01124	0.10771
C	4.17591	4.12990	0.95626
C	2.82347	4.11079	0.57276
C	1.86924	4.34126	1.50782
C	2.21335	4.53958	2.85870
C	3.55392	4.46198	3.26055
H	3.82563	4.55742	4.30341
C	4.52213	4.22640	2.28489
C	5.97012	3.98773	2.50434
H	6.13338	3.20546	3.27627
H	6.46913	4.93580	2.79830
C	6.45805	3.50752	1.12533
H	7.48454	3.87553	0.90674

H	6.48120	2.39398	1.12452
C	5.32714	3.14827	-1.11451
C	4.64648	1.85001	-1.31514
C	4.87492	1.17605	-2.52514
H	4.38240	0.23547	-2.72317
C	5.67280	1.75571	-3.52473
C	6.22697	3.03279	-3.35367
H	6.80238	3.48653	-4.15034
C	6.02456	3.71542	-2.15307
C	6.51052	5.07726	-1.82439
H	6.20111	5.80826	-2.60220
H	7.61653	5.06753	-1.71777
C	5.82921	5.38241	-0.48057
H	6.50415	5.95541	0.19268
H	4.92879	6.00804	-0.67606
C	4.03244	-5.07188	-1.67718
C	4.31191	-4.08840	-0.57778
C	4.32264	-2.68383	-0.61286
C	4.82209	-1.98610	0.50222
C	5.22568	-2.68465	1.65141
C	5.09068	-4.07831	1.71202
H	5.34750	-4.61633	2.61526
C	4.61822	-4.75717	0.58739
C	4.37389	-6.21679	0.47405
H	5.34216	-6.76168	0.46942
H	3.72821	-6.58177	1.30091
C	3.65994	-6.34789	-0.88214
H	2.56078	-6.37399	-0.70378
H	3.94920	-7.28631	-1.40442
C	2.99973	-4.72721	-2.70989
C	1.79340	-4.02590	-2.56056
C	0.92688	-3.92970	-3.66574
H	-0.01390	-3.40566	-3.57412
C	1.29998	-4.46847	-4.90755
C	2.55152	-5.07918	-5.06154
H	2.86526	-5.45258	-6.02780
C	3.39070	-5.18234	-3.95046
C	4.77291	-5.71911	-3.94046
H	5.38892	-5.24833	-4.73671
H	4.75011	-6.82278	-4.06699
C	5.29103	-5.33226	-2.54575
H	5.88803	-4.39658	-2.63765
H	5.95353	-6.12224	-2.12831
C	-5.41634	-2.87129	-1.52709

C	-5.06908	-1.81452	-2.52875
C	-4.10659	-0.80270	-2.43009
C	-3.95392	0.08961	-3.51080
H	-3.21188	0.87193	-3.47504
C	-4.73636	-0.05568	-4.66734
C	-5.64686	-1.11444	-4.77135
H	-6.21600	-1.26209	-5.68011
C	-5.78068	-1.99301	-3.69513
C	-6.59632	-3.22953	-3.67099
H	-6.41156	-3.84702	-4.57648
H	-7.67349	-2.96929	-3.59007
C	-6.10431	-3.95105	-2.40696
H	-6.94155	-4.46840	-1.88871
H	-5.36239	-4.72429	-2.71055
C	-4.30734	-3.46437	-0.70524
C	-2.96940	-3.74498	-1.05846
C	-2.20957	-4.58891	-0.22519
H	-1.20005	-4.85284	-0.51447
C	-2.70502	-5.04039	0.94235
C	-4.04025	-4.59964	1.40148
H	-4.42092	-4.88968	2.37203
C	-4.79081	-3.81001	0.53625
C	-6.14737	-3.25992	0.78597
H	-6.17136	-2.66588	1.72450
H	-6.88810	-4.08690	0.82984
C	-6.39345	-2.36319	-0.43987
H	-6.14549	-1.31230	-0.16897
H	-7.45738	-2.39682	-0.76223
C	-3.94081	5.34286	-0.68360
C	-4.26108	4.09818	0.08406
C	-4.10559	2.75434	-0.29002
C	-4.72491	1.77341	0.50251
C	-5.40774	2.15359	1.66889
C	-5.41034	3.49711	2.07858
H	-5.88353	3.77996	3.01026
C	-4.83160	4.42384	1.29759
C	-4.73180	5.87875	1.58280
H	-5.74110	6.34225	1.54428
H	-4.25754	6.06006	2.57143
C	-3.84099	6.40182	0.44117
H	-2.79139	6.46505	0.80787
H	-4.15525	7.41680	0.11231
C	-2.73618	5.32516	-1.57036
C	-1.41783	4.69617	-1.33178



C	-0.39827	4.95491	-2.26638
H	0.57562	4.50878	-2.13975
C	-0.64398	5.69623	-3.36522
C	-1.92885	6.20319	-3.62294
H	-2.12142	6.75859	-4.53188
C	-2.95573	5.97970	-2.69985
C	-4.36681	6.41460	-2.84762
H	-4.78671	6.08074	-3.82102
H	-4.43457	7.51967	-2.75183
C	-5.06991	5.71389	-1.67725
H	-5.85390	6.36298	-1.22867
H	-5.56257	4.79110	-2.05974
H	-2.11669	-5.69982	1.56233
H	-5.90585	1.40527	2.26775
H	1.43796	4.70482	3.59529
H	5.59637	-2.14045	2.51037
H	0.63586	-4.37679	-5.75709
H	-4.60759	0.62874	-5.49572
H	0.14795	5.86632	-4.08343
H	5.82314	1.22998	-4.45873
C	0.07945	-0.25220	2.21739
C	1.18104	0.32758	3.01533
C	-1.30575	-0.17995	2.73778
C	2.48731	0.41816	2.46747
C	1.02933	0.74391	4.35592
C	-2.19810	-1.26709	2.63805
C	-1.80169	1.02900	3.28000
C	3.54977	0.91897	3.19599
H	2.66104	0.06978	1.46102
C	2.08761	1.26142	5.09903
H	0.06181	0.66631	4.83874
C	-3.47354	-1.20860	3.17859
H	-1.87585	-2.17144	2.13944
C	-3.07641	1.10006	3.82692
H	-1.17758	1.91489	3.26991
C	3.36264	1.35203	4.51957
H	4.54017	0.98954	2.75741
H	1.91367	1.57755	6.12123
C	-3.88736	-0.03481	3.80708
H	-4.13961	-2.06093	3.14700
H	-3.44570	2.01359	4.27690
H	1.88183	-5.11936	2.08405
C	1.16340	-4.37626	1.71616
Si	0.88865	-3.07783	3.04159

H	0.24266	-4.90177	1.45409
H	1.54947	-3.92876	0.79875
C	-0.39599	-3.59113	4.31017
C	2.47835	-2.57831	3.90912
H	0.36423	-1.70107	2.30510
C	-0.73721	-2.75192	5.39027
C	-1.01840	-4.85124	4.24059
H	3.13680	-1.99279	3.26711
H	2.28595	-1.98781	4.80937
H	3.00527	-3.49378	4.20934
C	-1.67551	-3.14495	6.34307
H	-0.26854	-1.77591	5.48843
C	-1.95563	-5.25192	5.19438
H	-0.75441	-5.54151	3.44524
H	-1.92918	-2.47739	7.16214
C	-2.29244	-4.39490	6.24284
H	-2.42111	-6.23095	5.11783
H	-3.02826	-4.69977	6.98198
H	-4.66604	0.72886	0.23208
H	0.82375	4.33286	1.22723
H	4.86279	-0.90462	0.49233
N	-5.19554	0.00460	4.46060
O	-5.51096	1.03868	5.05450
O	-5.90661	-0.99985	4.38685
O	4.46385	1.82848	5.14904
C	4.33757	2.30928	6.48119
H	3.62052	3.13739	6.54143
H	4.02960	1.51080	7.16791
H	5.32911	2.66679	6.76266

**TS-5**

Rh	-0.08704	-0.00003	0.07542
Rh	0.09650	0.24826	-2.55745
P	2.75820	0.75548	-1.01158
P	0.66365	-2.63782	-1.40650
P	-2.73594	-0.48181	-1.53479
P	-0.47957	2.89426	-1.11790
O	1.85751	0.74240	0.22659
O	2.12420	0.73113	-2.39269
O	3.71131	2.09086	-1.01523
O	3.78531	-0.51443	-0.79274
O	0.66758	-1.96046	-0.02951
O	0.58140	-1.79358	-2.66146
O	2.01018	-3.55462	-1.62299

O	-0.56165	-3.73465	-1.29244
O	-1.99728	-0.86294	-0.24357
O	-1.93958	-0.20431	-2.79319
O	-3.66574	0.79094	-1.05692
O	-3.78867	-1.66168	-1.98659
O	-0.76554	1.98211	0.08370
O	-0.43401	2.28103	-2.50688
O	-1.62834	4.07030	-1.20429
O	0.91504	3.67109	-0.73879
C	6.53724	1.01550	-0.74895
C	5.66172	1.67106	0.27321
C	4.39152	2.25335	0.11857
C	3.84756	2.93454	1.15546
C	4.51623	3.02148	2.39168
C	5.73451	2.35347	2.58031
H	6.23870	2.37477	3.53663
C	6.27543	1.65334	1.50403
C	7.50184	0.81880	1.50806
H	7.46657	0.06509	2.32402
H	8.39917	1.46570	1.61200
C	7.46551	0.13833	0.12780
H	8.48736	0.02703	-0.29699
H	7.02583	-0.87829	0.24391
C	5.87000	0.23444	-1.83675
C	4.67512	-0.63536	-1.77918
C	4.36730	-1.38658	-2.92545
H	3.49178	-2.01668	-2.94212
C	5.13348	-1.25378	-4.09480
C	6.19526	-0.34012	-4.16003
H	6.74549	-0.21096	-5.08318
C	6.52986	0.40572	-3.02916
C	7.59218	1.43648	-2.93824
H	7.47403	2.20086	-3.73626
H	8.59164	0.95543	-3.00466
C	7.36759	2.05340	-1.54818
H	8.33333	2.30884	-1.05903
H	6.78484	2.99472	-1.66958
C	0.88932	-6.40193	-1.52753
C	1.65460	-5.62291	-0.49684
C	2.26482	-4.36137	-0.59545
C	3.05861	-3.91055	0.47606
C	3.17321	-4.67908	1.64540
C	2.46865	-5.88460	1.76679
H	2.50218	-6.44935	2.68946

C	1.69923	-6.32537	0.68795
C	0.80041	-7.50624	0.66998
H	1.40262	-8.43988	0.66291
H	0.11003	-7.49323	1.54086
C	0.02346	-7.33650	-0.64749
H	-0.95199	-6.84712	-0.42458
H	-0.18223	-8.31856	-1.12738
C	0.06985	-5.65592	-2.54193
C	-0.68041	-4.47829	-2.38998
C	-1.44906	-4.02107	-3.47729
H	-2.03409	-3.11648	-3.38586
C	-1.41918	-4.70377	-4.70341
C	-0.59786	-5.82721	-4.86242
H	-0.53390	-6.32937	-5.81911
C	0.15020	-6.27403	-3.77149
C	1.13110	-7.38553	-3.77893
H	1.85284	-7.27440	-4.61672
H	0.59865	-8.35816	-3.85006
C	1.83930	-7.24033	-2.42302
H	2.79460	-6.69004	-2.58147
H	2.08492	-8.23431	-1.98837
C	-6.46858	-0.30807	-1.23701
C	-5.75946	0.64392	-2.15212
C	-4.48815	1.21453	-2.01252
C	-4.05557	2.14782	-2.97359
H	-3.08023	2.60319	-2.88958
C	-4.86962	2.46007	-4.07415
C	-6.10513	1.82040	-4.23817
H	-6.71720	2.02261	-5.10766
C	-6.52075	0.90319	-3.27097
C	-7.74624	0.07193	-3.32021
H	-7.83332	-0.45204	-4.29648
H	-8.63999	0.70630	-3.13757
C	-7.53707	-0.93230	-2.17606
H	-8.49583	-1.15669	-1.65869
H	-7.15277	-1.88362	-2.60944
C	-5.66977	-1.37192	-0.53894
C	-4.55250	-2.10328	-0.98836
C	-4.17362	-3.26968	-0.29474
H	-3.34558	-3.86313	-0.66041
C	-4.80264	-3.63905	0.83644
C	-5.87049	-2.78275	1.40211
H	-6.33414	-3.02190	2.35002
C	-6.24632	-1.65532	0.67765

C	-7.27156	-0.65175	1.06025
H	-7.04493	-0.21295	2.05594
H	-8.27887	-1.12065	1.06000
C	-7.15561	0.40879	-0.04973
H	-6.50968	1.23946	0.31452
H	-8.14973	0.83149	-0.31450
C	-0.06230	6.59660	-0.41584
C	-0.99482	5.73893	0.38431
C	-1.82519	4.68592	-0.03755
C	-2.76669	4.18387	0.87706
C	-2.78475	4.66961	2.19592
C	-1.84280	5.62717	2.60601
H	-1.81896	5.95819	3.63652
C	-0.97492	6.12443	1.70962
C	0.10690	7.10533	1.98519
H	-0.33286	8.10152	2.20680
H	0.74804	6.76664	2.82761
C	0.90308	7.13401	0.66830
H	1.77817	6.45204	0.76666
H	1.28341	8.15497	0.44475
C	0.65591	5.95490	-1.55978
C	1.24934	4.60224	-1.63264
C	1.96445	4.26824	-2.79860
H	2.40323	3.28793	-2.90506
C	2.05935	5.14303	-3.82009
C	1.42188	6.39408	-3.76311
H	1.47240	7.06836	-4.60846
C	0.71265	6.75472	-2.61260
C	-0.05250	8.01154	-2.42220
H	-0.75985	8.17831	-3.26317
H	0.64709	8.86955	-2.32547
C	-0.80890	7.76379	-1.10994
H	-0.85469	8.68585	-0.48958
H	-1.85258	7.46132	-1.35420
H	-4.49059	-4.53059	1.36467
H	-3.49734	4.27677	2.90848
H	4.06916	3.57011	3.21028
H	3.76768	-4.31548	2.47351
H	-2.00149	-4.33812	-5.53912
H	-4.52607	3.16925	-4.81595
H	2.60036	4.86320	-4.71504
H	4.86781	-1.82594	-4.97422
C	-0.27752	-0.01068	2.21397
C	1.00856	0.09462	2.92272

C	-1.48800	0.59113	2.87812
C	2.03478	-0.85140	2.67922
C	1.31780	1.16189	3.78962
C	-2.62087	0.95183	2.12233
C	-1.58564	0.69189	4.28643
C	3.24679	-0.79261	3.33758
H	1.85012	-1.63835	1.95761
C	2.54258	1.24074	4.45093
H	0.60332	1.96385	3.93656
C	-3.78981	1.39807	2.73217
H	-2.59727	0.87048	1.04981
C	-2.73763	1.16046	4.90968
H	-0.75816	0.36893	4.90652
C	3.50267	0.24081	4.25724
H	4.01878	-1.53538	3.16277
H	2.73390	2.08133	5.10802
C	-3.83082	1.50830	4.11827
H	-4.65954	1.66073	2.14295
H	-2.80741	1.24223	5.98756
H	-3.64328	-3.23535	3.55503
C	-3.06431	-2.31625	3.40095
Si	-1.26285	-2.75080	3.09298
H	-3.21100	-1.67196	4.27076
H	-3.46926	-1.78948	2.53256
C	-0.29951	-3.00751	4.68414
C	-1.05206	-4.17830	1.89989
H	-0.62538	-1.44086	2.36999
C	0.92903	-3.69634	4.67244
C	-0.77455	-2.54438	5.92736
H	-1.40617	-3.91920	0.90096
H	0.00123	-4.44668	1.80456
H	-1.59866	-5.05708	2.26571
C	1.65353	-3.91356	5.84340
H	1.32402	-4.07388	3.73512
C	-0.05498	-2.75985	7.10357
H	-1.72281	-2.01709	5.98435
H	2.59834	-4.44917	5.80457
C	1.16241	-3.44289	7.06304
H	-0.44591	-2.39859	8.05120
H	1.72362	-3.61140	7.97839
H	-3.44421	3.39410	0.58003
H	2.87729	3.40173	1.04905
H	3.55145	-2.94894	0.41942
N	-5.06248	1.98551	4.76639

O	-6.01991	2.25740	4.04308
O	-5.06074	2.08294	5.99394
O	4.70466	0.19078	4.89025
C	4.94669	1.10463	5.95097
H	4.20191	0.99134	6.74910
H	5.93727	0.85826	6.33678
H	4.94361	2.14576	5.60500

**TS-6**

Rh	0.05318	-0.03205	0.10444
Rh	0.11685	0.43177	-2.50883
P	2.16605	2.08078	-0.89549
P	1.96465	-1.89070	-1.54920
P	-2.06871	-1.54597	-1.57895
P	-1.81480	2.28689	-0.90090
O	1.34213	1.58244	0.29317
O	1.62315	1.89538	-2.29933
O	2.44730	3.68505	-0.72008
O	3.63973	1.35971	-0.69441
O	1.67515	-1.35274	-0.13944
O	1.54918	-1.08410	-2.76084
O	3.57668	-2.12953	-1.76361
O	1.30825	-3.40100	-1.50734
O	-1.29714	-1.60384	-0.25060
O	-1.35208	-1.03695	-2.81763
O	-3.42598	-0.69135	-1.25044
O	-2.60121	-3.05465	-1.97664
O	-1.54570	1.31706	0.25468
O	-1.27898	1.96175	-2.28677
O	-3.42663	2.48110	-1.15041
O	-1.26387	3.73874	-0.35337
C	5.42507	3.94181	-0.31206
C	4.31909	4.02840	0.69330
C	2.93047	3.99176	0.48410
C	2.09812	4.16146	1.54092
C	2.60799	4.31622	2.84448
C	3.99096	4.26358	3.06896
H	4.39207	4.32727	4.07205
C	4.83157	4.09612	1.96870
C	6.30304	3.91066	1.99068
H	6.59818	3.12558	2.71756
H	6.80090	4.87348	2.23459
C	6.62230	3.47032	0.55155
H	7.59628	3.88310	0.20815

H	6.69104	2.35887	0.52869
C	5.20479	3.06435	-1.50563
C	4.53677	1.74645	-1.60267
C	4.66155	1.04618	-2.81296
H	4.17679	0.08919	-2.93756
C	5.33025	1.62220	-3.90558
C	5.85507	2.92079	-3.82652
H	6.32669	3.37005	-4.69101
C	5.76346	3.62737	-2.62643
C	6.24847	5.00712	-2.37687
H	5.82582	5.71734	-3.11979
H	7.35905	5.02793	-2.40662
C	5.72892	5.31550	-0.96252
H	6.46335	5.91808	-0.38411
H	4.79120	5.90960	-1.05192
C	3.74689	-5.19176	-1.81422
C	4.09093	-4.21399	-0.72807
C	4.14129	-2.81048	-0.76884
C	4.69069	-2.12394	0.32952
C	5.10335	-2.82979	1.47083
C	4.93087	-4.21900	1.54014
H	5.19536	-4.76119	2.43865
C	4.41002	-4.88775	0.43075
C	4.11738	-6.33951	0.33062
H	5.06781	-6.91409	0.29862
H	3.48651	-6.68221	1.17812
C	3.35838	-6.45245	-1.00268
H	2.26492	-6.44264	-0.79079
H	3.60144	-7.40143	-1.52941
C	2.69502	-4.81681	-2.81705
C	1.51494	-4.07949	-2.63360
C	0.62093	-3.95530	-3.71374
H	-0.30064	-3.40293	-3.59508
C	0.94176	-4.50462	-4.96550
C	2.16853	-5.15451	-5.15462
H	2.44252	-5.53765	-6.12912
C	3.03560	-5.28412	-4.06793
C	4.39950	-5.86508	-4.09723
H	5.00695	-5.41476	-4.91169
H	4.33755	-6.96750	-4.22152
C	4.97023	-5.49464	-2.71879
H	5.59524	-4.57954	-2.82970
H	5.61804	-6.30588	-2.31946
C	-5.62368	-2.73195	-1.33339



C	-5.28100	-1.67701	-2.33860
C	-4.28995	-0.69078	-2.26475
C	-4.15461	0.20980	-3.34085
H	-3.39412	0.97448	-3.32344
C	-4.98048	0.09578	-4.47039
C	-5.91960	-0.93957	-4.55259
H	-6.52408	-1.06350	-5.44188
C	-6.03744	-1.82566	-3.48074
C	-6.88461	-3.04027	-3.43852
H	-6.74692	-3.65449	-4.35454
H	-7.95111	-2.75228	-3.31928
C	-6.36984	-3.78543	-2.19749
H	-7.20283	-4.28453	-1.65507
H	-5.65967	-4.57553	-2.53194
C	-4.50525	-3.36135	-0.55246
C	-3.18841	-3.67603	-0.95198
C	-2.42464	-4.54663	-0.15075
H	-1.43373	-4.83695	-0.47672
C	-2.89242	-4.99230	1.03024
C	-4.19922	-4.51879	1.53686
H	-4.55560	-4.80659	2.51722
C	-4.95683	-3.70340	0.70193
C	-6.29037	-3.12094	0.99853
H	-6.27114	-2.53610	1.94282
H	-7.05069	-3.92903	1.05715
C	-6.55011	-2.20603	-0.21097
H	-6.26283	-1.16510	0.06035
H	-7.62442	-2.20621	-0.49885
C	-3.89785	5.42327	-0.46986
C	-4.20605	4.18827	0.31805
C	-4.09677	2.84084	-0.05810
C	-4.68480	1.87304	0.77370
C	-5.29382	2.26974	1.97503
C	-5.25243	3.61552	2.37616
H	-5.66900	3.91182	3.33027
C	-4.70223	4.52873	1.55962
C	-4.55861	5.98227	1.83278
H	-5.55905	6.46593	1.84493
H	-4.02968	6.15745	2.79443
C	-3.71834	6.48340	0.64399
H	-2.64999	6.52664	0.95524
H	-4.02879	7.50358	0.32783
C	-2.73940	5.37648	-1.41576
C	-1.42312	4.72162	-1.24058

C	-0.44476	4.96194	-2.22295
H	0.52586	4.49814	-2.14293
C	-0.72920	5.70739	-3.30961
C	-2.01528	6.23814	-3.50599
H	-2.24074	6.79723	-4.40507
C	-3.00046	6.03493	-2.53414
C	-4.40755	6.49980	-2.61300
H	-4.88214	6.17362	-3.56360
H	-4.44676	7.60623	-2.51694
C	-5.06666	5.81625	-1.40737
H	-5.81361	6.48262	-0.92239
H	-5.59683	4.90338	-1.76246
H	-2.30160	-5.67229	1.62527
H	-5.77029	1.53234	2.60452
H	1.92968	4.43018	3.67997
H	5.51188	-2.29345	2.31747
H	0.25690	-4.39204	-5.79584
H	-4.86448	0.78597	-5.29588
H	0.03039	5.86257	-4.06518
H	5.39700	1.07629	-4.83770
C	0.06752	-0.24857	2.22718
C	1.25966	0.26246	2.98960
C	-1.27038	-0.11473	2.83717
C	2.53064	0.28106	2.37175
C	1.19415	0.65365	4.34605
C	-2.24973	-1.12168	2.67451
C	-1.66251	1.04593	3.53492
C	3.66817	0.69820	3.05419
H	2.62730	-0.05598	1.35178
C	2.31953	1.08873	5.03914
H	0.25403	0.60431	4.88042
C	-3.48300	-1.04065	3.29393
H	-2.01613	-1.98623	2.06578
C	-2.91167	1.14910	4.14706
H	-0.99506	1.89936	3.57789
C	3.54682	1.10157	4.38192
H	4.63723	0.71087	2.57033
H	2.26417	1.39196	6.07740
C	-3.81011	0.07761	4.07773
H	-4.20472	-1.84620	3.21265
H	-3.16743	2.06215	4.67286
H	1.71873	-5.18285	2.03648
C	1.03080	-4.40086	1.69208
Si	0.81402	-3.12283	3.04775

H	0.08662	-4.87747	1.42004
H	1.43104	-3.94528	0.78495
C	-0.49090	-3.60821	4.30679
C	2.43037	-2.72745	3.92426
H	0.33219	-1.72323	2.34653
C	-0.83449	-2.75835	5.37697
C	-1.11926	-4.86572	4.24375
H	3.13474	-2.19696	3.28212
H	2.27412	-2.12089	4.82097
H	2.89216	-3.67394	4.23492
C	-1.77950	-3.13910	6.32803
H	-0.36343	-1.78316	5.46864
C	-2.06320	-5.25441	5.19580
H	-0.85423	-5.56325	3.45483
H	-2.03331	-2.46336	7.14035
C	-2.40095	-4.38721	6.23562
H	-2.53211	-6.23233	5.12534
H	-3.14000	-4.68394	6.97510
H	-4.65849	0.82618	0.50510
H	1.02533	4.13744	1.39414
H	4.76126	-1.04401	0.31400
O	-5.01440	0.03003	4.71086
C	-5.34659	1.07676	5.61034
H	-5.44363	2.04216	5.09818
H	-6.31042	0.80400	6.04359
H	-4.59917	1.16978	6.40914
N	4.74653	1.51837	5.12416
O	4.58713	1.98146	6.25363
O	5.83695	1.37152	4.57384

**TS-3'**

Rh	-0.01177	-0.01845	0.04102
Rh	0.25913	0.31092	-2.56924
P	2.57305	1.51971	-0.83669
P	1.50622	-2.33098	-1.42282
P	-2.33502	-1.14918	-1.73464
P	-1.13623	2.66332	-1.16057
O	1.61718	1.24912	0.33096
O	2.07647	1.30664	-2.25738
O	3.09429	3.07434	-0.80359
O	3.89237	0.59584	-0.50010
O	1.26206	-1.68956	-0.05010
O	1.27683	-1.51560	-2.67925
O	3.05301	-2.86131	-1.56451

O	0.60213	-3.70824	-1.38052
O	-1.59538	-1.34906	-0.40225
O	-1.55583	-0.67663	-2.94531
O	-3.57236	-0.14615	-1.32060
O	-3.04416	-2.54801	-2.22887
O	-1.22337	1.68551	0.02098
O	-0.81750	2.11234	-2.53915
O	-2.56920	3.45438	-1.32438
O	-0.05845	3.80699	-0.69468
C	6.07406	2.84634	-0.23469
C	4.94949	3.23230	0.67491
C	3.59154	3.44176	0.37697
C	2.78571	3.97902	1.32368
C	3.27788	4.27336	2.60933
C	4.60161	3.95660	2.94499
H	4.97539	4.12661	3.94624
C	5.41712	3.40593	1.95727
C	6.81902	2.94393	2.10936
H	6.91015	2.21768	2.94532
H	7.48857	3.81515	2.27412
C	7.11244	2.26724	0.75775
H	8.16335	2.43928	0.43678
H	6.95822	1.16980	0.86794
C	5.76893	1.91017	-1.36106
C	4.86881	0.73810	-1.39679
C	4.89994	-0.06734	-2.54665
H	4.24444	-0.92037	-2.62851
C	5.70986	0.27915	-3.64024
C	6.47365	1.45520	-3.62625
H	7.05497	1.73629	-4.49498
C	6.47085	2.26250	-2.48791
C	7.18747	3.54986	-2.32148
H	6.94108	4.25174	-3.14717
H	8.28298	3.36918	-2.27782
C	6.66059	4.07615	-0.97671
H	7.46276	4.59006	-0.40262
H	5.85514	4.81819	-1.17947
C	2.70411	-5.90381	-1.59731
C	3.18513	-4.99174	-0.50593
C	3.44794	-3.61190	-0.53872
C	4.04196	-3.01157	0.58732
C	4.29962	-3.76952	1.74104
C	3.93682	-5.12211	1.78976
H	4.08020	-5.69662	2.69583

C	3.35864	-5.70444	0.66059
C	2.80925	-7.07944	0.56203
H	3.63821	-7.81919	0.56428
H	2.10033	-7.28453	1.39311
C	2.07817	-7.06883	-0.79161
H	0.99822	-6.86455	-0.61077
H	2.16425	-8.05044	-1.30748
C	1.76256	-5.36242	-2.63447
C	0.72360	-4.42758	-2.49453
C	-0.09321	-4.15445	-3.60838
H	-0.89883	-3.43860	-3.52774
C	0.16655	-4.76490	-4.84547
C	1.26222	-5.62569	-4.98811
H	1.49686	-6.06071	-5.95104
C	2.05563	-5.89557	-3.87157
C	3.29662	-6.70667	-3.85432
H	3.99774	-6.37950	-4.65214
H	3.04595	-7.78260	-3.97330
C	3.88198	-6.42551	-2.46159
H	4.65992	-5.63442	-2.55883
H	4.36656	-7.33246	-2.03744
C	-6.00521	-1.90375	-1.58833
C	-5.51891	-0.81169	-2.49209
C	-4.43028	0.05201	-2.31795
C	-4.19729	1.04998	-3.28346
H	-3.36458	1.72815	-3.17631
C	-5.01941	1.14443	-4.41762
C	-6.05784	0.22454	-4.61128
H	-6.66646	0.26350	-5.50551
C	-6.27689	-0.75559	-3.64148
C	-7.26117	-1.86013	-3.71898
H	-7.18222	-2.39675	-4.68907
H	-8.28830	-1.46078	-3.57728
C	-6.85703	-2.77482	-2.55246
H	-7.75131	-3.22051	-2.06377
H	-6.23947	-3.60842	-2.95775
C	-4.99333	-2.73709	-0.85477
C	-3.71581	-3.17160	-1.26116
C	-3.08580	-4.20751	-0.54362
H	-2.12644	-4.58072	-0.87816
C	-3.64015	-4.71464	0.57335
C	-4.90363	-4.14564	1.09591
H	-5.32422	-4.48715	2.03248
C	-5.52185	-3.14895	0.34678

C	-6.77334	-2.42575	0.68679
H	-6.69354	-1.94181	1.68419
H	-7.63465	-3.12714	0.66074
C	-6.88448	-1.37258	-0.43085
H	-6.47321	-0.40782	-0.05659
H	-7.94264	-1.20697	-0.73067
C	-1.85581	6.32268	-0.47698
C	-2.54623	5.22732	0.27791
C	-3.00346	3.97766	-0.17675
C	-3.80547	3.21536	0.69030
C	-4.04580	3.67095	1.99799
C	-3.45555	4.86294	2.44778
H	-3.59244	5.18293	3.47296
C	-2.72051	5.59690	1.59655
C	-1.99340	6.85131	1.92190
H	-2.71889	7.67372	2.10136
H	-1.33477	6.71325	2.80657
C	-1.16039	7.11660	0.65549
H	-0.13160	6.72164	0.81742
H	-1.08306	8.20495	0.43986
C	-0.90883	5.92236	-1.56274
C	0.05458	4.80063	-1.57656
C	0.90651	4.68940	-2.69219
H	1.61307	3.87581	-2.75718
C	0.80900	5.55672	-3.71976
C	-0.16506	6.56966	-3.72177
H	-0.25901	7.23104	-4.57351
C	-1.01990	6.70634	-2.62297
C	-2.12911	7.68423	-2.50127
H	-2.79812	7.63976	-3.38771
H	-1.71800	8.70881	-2.37417
C	-2.86411	7.22199	-1.23558
H	-3.21778	8.08830	-0.63430
H	-3.75538	6.62770	-1.54028
H	-3.13597	-5.49985	1.12146
H	-4.65232	3.08397	2.67362
H	2.61958	4.70095	3.35423
H	4.73919	-3.29813	2.61019
H	-0.45661	-4.53806	-5.70066
H	-4.82804	1.90708	-5.16124
H	1.46224	5.44666	-4.57596
H	5.70485	-0.34290	-4.52588
C	-0.27745	-0.12408	2.13636
C	0.94650	0.21825	2.89157

C	-1.59682	0.13243	2.77201
C	2.11242	-0.56479	2.76105
C	1.02552	1.39430	3.66842
C	-2.77411	0.13237	1.99403
C	-1.74200	0.27547	4.17278
C	3.27812	-0.24062	3.43327
H	2.08666	-1.42550	2.10557
C	2.19336	1.72802	4.34569
H	0.17346	2.06194	3.72760
C	-4.02744	0.26330	2.58274
H	-2.70653	0.01376	0.92598
C	-2.99318	0.42893	4.76116
H	-0.86782	0.24015	4.81199
C	3.32481	0.90345	4.25028
H	4.16160	-0.86139	3.33039
H	2.23258	2.62586	4.95416
C	-4.14264	0.41788	3.96511
H	-4.91552	0.25655	1.95952
H	-3.07985	0.54776	5.83625
H	-2.76724	-4.15350	3.45881
C	-2.41071	-3.12580	3.31732
Si	-0.55868	-3.13194	2.98773
H	-2.68417	-2.54895	4.20461
H	-2.94306	-2.68641	2.46951
C	0.43588	-3.18711	4.58267
C	-0.03387	-4.46169	1.77211
H	-0.26111	-1.73316	2.30293
C	1.72238	-3.75829	4.60934
C	-0.06746	-2.66575	5.79141
H	-0.35438	-4.21477	0.75836
H	1.05327	-4.56345	1.74219
H	-0.45674	-5.43220	2.06033
C	2.47816	-3.80329	5.78041
H	2.13731	-4.18511	3.70265
C	0.68309	-2.70629	6.96705
H	-1.06181	-2.22867	5.82150
H	3.46764	-4.25269	5.77040
C	1.95982	-3.27255	6.96324
H	0.27112	-2.30004	7.88712
H	2.54558	-3.30323	7.87796
H	-4.19905	2.26005	0.36805
H	1.74300	4.16615	1.10836
H	4.26687	-1.95285	0.58237
C	-5.50617	0.49566	4.59976

F	-5.99731	-0.74003	4.85337
F	-5.47832	1.15949	5.77526
F	-6.39806	1.11666	3.79937
C	4.51950	1.22255	4.97291
N	5.49142	1.47819	5.55988

**TS-4'**

Rh	-0.01585	-0.02240	0.06489
Rh	-0.10705	0.47340	-2.53354
P	2.16631	1.94855	-1.05833
P	1.64910	-1.97676	-1.73344
P	-2.35549	-1.36258	-1.47039
P	-1.78048	2.44167	-0.78131
O	1.39560	1.49200	0.18295
O	1.50866	1.82401	-2.41928
O	2.57400	3.52523	-0.88876
O	3.59449	1.12149	-0.97877
O	1.49440	-1.43795	-0.30245
O	1.19769	-1.13080	-2.90560
O	3.22326	-2.30747	-2.06477
O	0.90609	-3.44503	-1.66003
O	-1.49048	-1.49168	-0.20558
O	-1.69893	-0.87630	-2.75087
O	-3.62504	-0.43171	-1.02318
O	-3.00682	-2.82676	-1.85044
O	-1.50175	1.43426	0.34160
O	-1.37665	2.08944	-2.20465
O	-3.38481	2.76330	-0.90744
O	-1.07061	3.83340	-0.26638
C	5.58671	3.56031	-0.70932
C	4.56918	3.70887	0.37864
C	3.16974	3.77857	0.27660
C	2.43548	3.99792	1.39496
C	3.05375	4.10211	2.65590
C	4.44209	3.94531	2.77271
H	4.92363	3.97676	3.74071
C	5.18103	3.72404	1.61094
C	6.63247	3.43196	1.51869
H	6.92264	2.61538	2.21245
H	7.21693	4.35197	1.73408
C	6.80930	2.99245	0.05489
H	7.78130	3.34106	-0.35818
H	6.79670	1.87943	0.01544
C	5.21445	2.71984	-1.89157



C	4.44363	1.45701	-1.95160
C	4.41700	0.77454	-3.17849
H	3.85146	-0.13972	-3.27814
C	5.03794	1.32072	-4.31371
C	5.66434	2.57455	-4.25953
H	6.09676	3.00528	-5.15346
C	5.72227	3.26199	-3.04646
C	6.32311	4.59935	-2.81999
H	5.89659	5.35020	-3.51949
H	7.42669	4.54190	-2.93620
C	5.93742	4.91981	-1.36625
H	6.75543	5.45945	-0.84021
H	5.04069	5.58018	-1.37579
C	3.20009	-5.36993	-2.20322
C	3.68342	-4.44757	-1.12184
C	3.81231	-3.04863	-1.12915
C	4.48346	-2.42809	-0.05954
C	4.94498	-3.19172	1.02452
C	4.69882	-4.57074	1.06993
H	5.00251	-5.15494	1.92884
C	4.05335	-5.17411	-0.01098
C	3.67210	-6.60382	-0.12678
H	4.58312	-7.22792	-0.24954
H	3.09046	-6.93779	0.75862
C	2.80678	-6.63349	-1.39824
H	1.73534	-6.57261	-1.10003
H	2.95519	-7.57680	-1.96854
C	2.09423	-4.90805	-3.10692
C	0.97751	-4.11093	-2.81052
C	0.00719	-3.90929	-3.81026
H	-0.86770	-3.30881	-3.60451
C	0.19348	-4.44167	-5.09608
C	1.36226	-5.15173	-5.40048
H	1.53460	-5.52187	-6.40289
C	2.30568	-5.35815	-4.39216
C	3.62870	-6.00956	-4.54751
H	4.19232	-5.56892	-5.39799
H	3.49628	-7.10314	-4.69286
C	4.32838	-5.70922	-3.21208
H	4.99057	-4.82465	-3.35130
H	4.96164	-6.56404	-2.88733
C	-5.94546	-2.33572	-0.96872
C	-5.61631	-1.28071	-1.97879
C	-4.56385	-0.35717	-1.96557

C	-4.45675	0.55748	-3.03282
H	-3.65054	1.27350	-3.06221
C	-5.37351	0.51945	-4.09529
C	-6.37880	-0.45484	-4.12138
H	-7.05760	-0.52127	-4.96184
C	-6.46737	-1.35675	-3.05996
C	-7.38338	-2.51773	-2.97283
H	-7.35635	-3.11808	-3.90781
H	-8.41713	-2.16777	-2.76435
C	-6.82156	-3.32125	-1.79023
H	-7.63959	-3.78085	-1.19291
H	-6.19076	-4.14554	-2.19419
C	-4.81283	-3.05195	-0.28997
C	-3.55229	-3.43576	-0.79584
C	-2.78730	-4.37352	-0.07547
H	-1.84283	-4.71358	-0.48146
C	-3.19426	-4.82457	1.12584
C	-4.42828	-4.28810	1.74042
H	-4.72862	-4.58178	2.73767
C	-5.19084	-3.40150	0.98645
C	-6.45688	-2.74326	1.39858
H	-6.32728	-2.18636	2.35114
H	-7.26211	-3.50231	1.49832
C	-6.74678	-1.78112	0.23318
H	-6.37070	-0.76857	0.50367
H	-7.83749	-1.70444	0.02953
C	-3.55109	5.73095	-0.16473
C	-3.90336	4.51226	0.63009
C	-3.94543	3.16710	0.23069
C	-4.57325	2.24499	1.08467
C	-5.06376	2.67516	2.32846
C	-4.86528	4.00177	2.74499
H	-5.18969	4.31650	3.72870
C	-4.28393	4.87438	1.90608
C	-3.99232	6.30455	2.18540
H	-4.94230	6.87404	2.27603
H	-3.38259	6.41493	3.10804
C	-3.19840	6.75154	0.94437
H	-2.11076	6.69549	1.17686
H	-3.43955	7.80026	0.66306
C	-2.47689	5.60461	-1.19768
C	-1.21245	4.83849	-1.13157
C	-0.29658	5.00927	-2.18638
H	0.63322	4.46304	-2.18824

C	-0.59869	5.79395	-3.24017
C	-1.84501	6.43637	-3.32947
H	-2.09029	7.02746	-4.20253
C	-2.76583	6.30161	-2.28543
C	-4.12976	6.88488	-2.24956
H	-4.70186	6.61681	-3.16394
H	-4.06678	7.98878	-2.13828
C	-4.75045	6.23792	-1.00419
H	-5.39855	6.95610	-0.45520
H	-5.38237	5.37957	-1.32736
H	-2.60489	-5.55570	1.65830
H	-5.56820	1.97632	2.97914
H	2.45210	4.26035	3.54140
H	5.44965	-2.70601	1.84964
H	-0.54869	-4.26881	-5.86450
H	-5.27944	1.21991	-4.91488
H	0.11045	5.89559	-4.05181
H	4.98724	0.79066	-5.25594
C	0.11036	-0.30340	2.15772
C	1.33734	0.11872	2.89022
C	-1.20063	-0.15770	2.83075
C	2.58887	0.11160	2.23602
C	1.32326	0.46477	4.26186
C	-2.17497	-1.17376	2.78843
C	-1.54187	1.05235	3.47679
C	3.76004	0.45028	2.90977
H	2.64139	-0.18613	1.19996
C	2.48901	0.80816	4.93530
H	0.39130	0.45488	4.81347
C	-3.37298	-1.05246	3.47507
H	-1.97502	-2.07334	2.22249
C	-2.74491	1.18565	4.15857
H	-0.85839	1.89296	3.43802
C	3.71461	0.79472	4.26133
H	4.70744	0.43857	2.38157
H	2.45227	1.07162	5.98789
C	-3.65596	0.11665	4.20001
H	-4.08455	-1.87032	3.47933
H	-2.97835	2.11278	4.67263
H	1.46023	-5.38126	1.80198
C	0.80534	-4.55096	1.51045
Si	0.77471	-3.27409	2.88438
H	-0.18524	-4.96138	1.30187
H	1.17147	-4.11581	0.57894

C	-0.43465	-3.70757	4.25499
C	2.48002	-2.96118	3.61189
H	0.31167	-1.86218	2.24791
C	-0.60186	-2.86897	5.37560
C	-1.17632	-4.90282	4.21852
H	3.13426	-2.42906	2.92028
H	2.43226	-2.37961	4.53711
H	2.93907	-3.93051	3.84613
C	-1.48800	-3.19754	6.40018
H	-0.03518	-1.94427	5.45107
C	-2.06250	-5.23943	5.24344
H	-1.04685	-5.59445	3.39144
H	-1.60585	-2.53124	7.25043
C	-2.22636	-4.38203	6.33227
H	-2.62225	-6.16950	5.19128
H	-2.92087	-4.63696	7.12815
H	-4.66607	1.20590	0.79988
H	1.35590	4.05594	1.33064
H	4.61433	-1.35366	-0.05103
C	4.97047	1.07741	5.04249
F	4.84807	2.19527	5.79213
F	5.24545	0.06465	5.89793
F	6.04757	1.23209	4.24769
C	-4.85540	0.20776	4.97718
N	-5.82730	0.27592	5.61392

**TS-5'**

Rh	-0.20388	0.06083	0.09410
Rh	-0.29593	0.50186	-2.51130
P	2.59458	0.36663	-1.29895
P	-0.20981	-2.51843	-1.66653
P	-3.07766	0.25665	-1.16141
P	-0.15503	3.07080	-0.83851
O	1.85415	0.37925	0.04206
O	1.79765	0.54131	-2.58067
O	3.72182	1.55397	-1.34606
O	3.43372	-1.05104	-1.28751
O	0.10212	-1.98432	-0.26093
O	-0.24577	-1.56362	-2.84312
O	0.86891	-3.67044	-2.11703
O	-1.62565	-3.33673	-1.46408
O	-2.27758	-0.36438	-0.00637
O	-2.39635	0.48333	-2.49529
O	-3.67233	1.63543	-0.48585

O	-4.38746	-0.66109	-1.54097
O	-0.45615	2.12475	0.33517
O	-0.41457	2.58068	-2.25283
O	-1.04542	4.44520	-0.68150
O	1.40295	3.53111	-0.62350
C	6.36242	0.11609	-1.62129
C	5.76385	0.78172	-0.42288
C	4.57287	1.51837	-0.32245
C	4.28641	2.15610	0.83769
C	5.14264	2.04763	1.95033
C	6.27955	1.22951	1.88589
H	6.92004	1.10060	2.74822
C	6.55636	0.58064	0.68331
C	7.65699	-0.37748	0.41637
H	7.67146	-1.19148	1.17195
H	8.62974	0.15923	0.40358
C	7.30979	-0.92832	-0.97836
H	8.22628	-1.11359	-1.58061
H	6.77562	-1.89763	-0.85437
C	5.42340	-0.49647	-2.61269
C	4.16118	-1.23718	-2.39068
C	3.60859	-1.91210	-3.49063
H	2.68277	-2.45580	-3.38221
C	4.19145	-1.80171	-4.76384
C	5.31560	-0.98936	-4.97368
H	5.72595	-0.87512	-5.96873
C	5.90095	-0.33369	-3.88980
C	7.08102	0.56441	-3.93506
H	6.92619	1.38774	-4.66520
H	7.99029	-0.01962	-4.19362
C	7.16554	1.10936	-2.49943
H	8.22219	1.22439	-2.17174
H	6.68547	2.11397	-2.47315
C	-0.83695	-6.21436	-2.07560
C	0.19137	-5.71629	-1.10132
C	1.05120	-4.60862	-1.19054
C	2.04070	-4.44178	-0.20347
C	2.11332	-5.32773	0.88361
C	1.17922	-6.36466	1.00987
H	1.19265	-7.01308	1.87640
C	0.21411	-6.52534	0.01388
C	-0.91688	-7.48630	0.02934
H	-0.53774	-8.51930	-0.12415
H	-1.48504	-7.41646	0.98201

C	-1.78145	-7.02992	-1.15880
H	-2.59460	-6.37245	-0.77508
H	-2.24998	-7.89562	-1.67661
C	-1.58285	-5.21848	-2.91691
C	-2.03283	-3.93017	-2.58427
C	-2.80125	-3.21903	-3.52566
H	-3.15711	-2.22474	-3.29565
C	-3.06357	-3.77089	-4.78939
C	-2.53332	-5.02051	-5.13436
H	-2.69133	-5.42960	-6.12389
C	-1.78165	-5.71747	-4.18656
C	-1.07521	-7.00282	-4.40248
H	-0.44781	-6.96365	-5.31898
H	-1.81212	-7.83167	-4.47011
C	-0.20142	-7.14033	-3.14602
H	0.82616	-6.78720	-3.39073
H	-0.13015	-8.20112	-2.81904
C	-6.64074	1.11432	-0.37550
C	-5.86281	1.98911	-1.31118
C	-4.49564	2.29188	-1.29861
C	-3.99611	3.20632	-2.24527
H	-2.94645	3.45807	-2.25754
C	-4.84974	3.76388	-3.21053
C	-6.19860	3.38851	-3.25640
H	-6.85165	3.77948	-4.02591
C	-6.67775	2.48595	-2.30502
C	-8.04220	1.91101	-2.25092
H	-8.34120	1.50087	-3.23964
H	-8.76495	2.68554	-1.91578
C	-7.91051	0.78900	-1.20929
H	-8.83072	0.70651	-0.58990
H	-7.77427	-0.17633	-1.74789
C	-5.99802	-0.13842	0.14871
C	-5.10812	-1.02979	-0.48278
C	-4.90421	-2.30563	0.07909
H	-4.26257	-3.01542	-0.42674
C	-5.46806	-2.64464	1.25350
C	-6.27019	-1.65064	2.00295
H	-6.66833	-1.87904	2.98280
C	-6.48502	-0.41179	1.40620
C	-7.24078	0.73207	1.97630
H	-6.82519	1.03002	2.96308
H	-8.31582	0.46700	2.06908
C	-7.03414	1.84372	0.93156

H	-6.19669	2.49756	1.26552
H	-7.94468	2.47272	0.82039
C	1.09833	6.54545	0.01127
C	0.12628	5.81627	0.88882
C	-0.95172	4.98512	0.53480
C	-1.84517	4.59967	1.54883
C	-1.58791	4.96653	2.88101
C	-0.42334	5.68270	3.20141
H	-0.19555	5.91406	4.23424
C	0.40126	6.07513	2.21669
C	1.68766	6.79966	2.38572
H	1.49456	7.83906	2.72813
H	2.35264	6.27081	3.10237
C	2.28951	6.78799	0.96938
H	3.01130	5.94281	0.89646
H	2.83754	7.73105	0.75209
C	1.51118	5.88168	-1.26318
C	1.79690	4.45138	-1.50429
C	2.25154	4.08659	-2.78642
H	2.45357	3.05185	-3.01802
C	2.38216	5.01233	-3.75778
C	2.03502	6.35469	-3.52942
H	2.10446	7.07768	-4.33205
C	1.58428	6.74446	-2.26388
C	1.12518	8.10368	-1.88597
H	0.35954	8.47808	-2.59939
H	1.99195	8.79790	-1.84455
C	0.51888	7.89173	-0.49206
H	0.74670	8.74668	0.18194
H	-0.58783	7.81968	-0.59423
H	-5.29094	-3.62398	1.67857
H	-2.26535	4.66286	3.66737
H	4.90186	2.56588	2.86918
H	2.86324	-5.18206	1.64995
H	-3.64281	-3.21191	-5.51269
H	-4.45688	4.45714	-3.94280
H	2.71975	4.71121	-4.74130
H	3.73574	-2.30860	-5.60449
C	-0.11342	-0.11471	2.19977
C	1.23965	-0.42430	2.70922
C	-1.03563	0.64250	3.09186
C	1.89042	-1.61876	2.33552
C	1.96247	0.50295	3.48728
C	-2.17925	1.28094	2.56698

C	-0.86762	0.65687	4.49797
C	3.16543	-1.91315	2.78883
H	1.37499	-2.30258	1.67351
C	3.24782	0.20967	3.94062
H	1.52619	1.46638	3.72590
C	-3.10186	1.90780	3.39600
H	-2.35323	1.27338	1.50430
C	-1.77150	1.30138	5.33310
H	-0.03197	0.13224	4.94535
C	3.84384	-1.00680	3.61331
H	3.64487	-2.84274	2.49952
H	3.78230	0.92678	4.55398
C	-2.90096	1.93410	4.78477
H	-3.97896	2.38185	2.96735
H	-1.61993	1.30643	6.40784
H	-3.97485	-2.64340	3.87136
C	-3.21667	-1.88362	3.64506
Si	-1.63657	-2.71205	3.05097
H	-3.07132	-1.27454	4.54082
H	-3.60477	-1.22483	2.86334
C	-0.58642	-3.33661	4.47952
C	-1.95049	-4.04424	1.76758
H	-0.81160	-1.55498	2.34380
C	0.40296	-4.31687	4.26936
C	-0.75729	-2.85767	5.79364
H	-2.20031	-3.61176	0.79687
H	-1.06477	-4.66816	1.62838
H	-2.76992	-4.69599	2.09603
C	1.18798	-4.79766	5.31639
H	0.56025	-4.71672	3.27266
C	0.02411	-3.33541	6.84684
H	-1.51619	-2.10906	6.00418
H	1.94340	-5.55497	5.12455
C	1.00034	-4.30514	6.60961
H	-0.13144	-2.95438	7.85280
H	1.61010	-4.67698	7.42859
H	-2.70297	3.98394	1.31158
H	3.38131	2.74197	0.92733
H	2.72358	-3.60342	-0.25639
C	5.18654	-1.39114	4.16767
F	5.82012	-0.35314	4.75398
F	6.00300	-1.87817	3.20562
F	5.07206	-2.36508	5.10266
C	-3.84739	2.58980	5.63874



N	-4.61705	3.12202	6.32993
<b>TS-6'</b>			
Rh	0.18256	0.01034	0.05651
Rh	0.57603	0.49465	-2.51560
P	2.39582	2.12882	-0.62155
P	2.29658	-1.82976	-1.35765
P	-1.70475	-1.49286	-1.89134
P	-1.54404	2.33282	-1.14695
O	1.39570	1.64824	0.43317
O	2.05874	1.93970	-2.08713
O	2.67986	3.72897	-0.41207
O	3.80753	1.38257	-0.20047
O	1.83351	-1.29256	0.00541
O	2.02768	-1.01977	-2.60836
O	3.92295	-2.06279	-1.36735
O	1.64793	-3.34274	-1.40292
O	-1.08571	-1.56781	-0.48513
O	-0.85726	-0.95535	-3.03191
O	-3.09745	-0.65362	-1.70309
O	-2.17625	-2.99921	-2.36290
O	-1.44331	1.33070	0.01027
O	-0.84451	2.01837	-2.46068
O	-3.10790	2.57080	-1.58570
O	-1.03242	3.75433	-0.49789
C	5.54368	3.89292	0.56681
C	4.26311	4.01571	1.33409
C	2.94026	4.03966	0.85850
C	1.92865	4.26172	1.73338
C	2.18231	4.40704	3.11062
C	3.48998	4.28622	3.60044
H	3.69041	4.34038	4.66245
C	4.51891	4.06370	2.68559
C	5.94461	3.79417	2.99524
H	6.04347	2.98609	3.75080
H	6.43615	4.72436	3.35222
C	6.51929	3.34736	1.63918
H	7.56245	3.70770	1.50179
H	6.53052	2.23404	1.60832
C	5.53124	3.05518	-0.67445
C	4.84367	1.77304	-0.94241
C	5.14465	1.11364	-2.14466
H	4.65038	0.18599	-2.39276
C	6.01963	1.69435	-3.07704

C	6.58116	2.95915	-2.84755
H	7.21778	3.41480	-3.59501
C	6.30754	3.62657	-1.65258
C	6.79345	4.97348	-1.26633
H	6.54844	5.72381	-2.04866
H	7.88962	4.94205	-1.08714
C	6.02984	5.26659	0.03557
H	6.66837	5.81390	0.76347
H	5.15533	5.91243	-0.20631
C	4.11888	-5.11974	-1.43762
C	4.31781	-4.15791	-0.30216
C	4.35720	-2.75357	-0.31526
C	4.74362	-2.07961	0.85805
C	5.00312	-2.79912	2.03527
C	4.84445	-4.19130	2.05884
H	4.99087	-4.74526	2.97695
C	4.49007	-4.84754	0.87850
C	4.23096	-6.30021	0.71940
H	5.18516	-6.86381	0.79894
H	3.50249	-6.66458	1.47452
C	3.64807	-6.39829	-0.70054
H	2.53661	-6.40442	-0.62792
H	3.96775	-7.33561	-1.20678
C	3.19046	-4.73716	-2.55333
C	1.98998	-4.01106	-2.50234
C	1.22968	-3.87968	-3.67975
H	0.29630	-3.33457	-3.66526
C	1.70214	-4.40984	-4.89105
C	2.94922	-5.04655	-4.94106
H	3.34110	-5.41362	-5.88085
C	3.68223	-5.18377	-3.76070
C	5.04645	-5.75146	-3.63488
H	5.74158	-5.28356	-4.36493
H	5.01199	-6.85247	-3.78043
C	5.44485	-5.39589	-2.19327
H	6.06721	-4.47258	-2.21616
H	6.05014	-6.20621	-1.73043
C	-5.25140	-2.71581	-2.05342
C	-4.80978	-1.64467	-3.00162
C	-3.84576	-0.64807	-2.80543
C	-3.60476	0.27054	-3.84697
H	-2.86079	1.04372	-3.73411
C	-4.29893	0.16348	-5.06258
C	-5.20916	-0.88175	-5.26245

H	-5.71024	-0.99916	-6.21466
C	-5.43318	-1.78513	-4.22234
C	-6.26600	-3.00861	-4.28955
H	-6.01997	-3.60934	-5.19172
H	-7.34232	-2.73275	-4.28684
C	-5.88484	-3.76503	-3.00766
H	-6.76755	-4.27901	-2.56740
H	-5.13315	-4.54390	-3.27000
C	-4.22024	-3.34409	-1.15986
C	-2.86314	-3.63819	-1.41352
C	-2.17767	-4.49778	-0.53295
H	-1.15129	-4.76879	-0.74639
C	-2.76520	-4.95418	0.58897
C	-4.12803	-4.50489	0.94820
H	-4.58454	-4.79944	1.88409
C	-4.80202	-3.69881	0.03616
C	-6.16706	-3.13407	0.18798
H	-6.25954	-2.55701	1.13265
H	-6.91926	-3.95119	0.15667
C	-6.30302	-2.21179	-1.03587
H	-6.06132	-1.17007	-0.72604
H	-7.33887	-2.22210	-1.44069
C	-3.60676	5.49182	-0.80447
C	-4.02213	4.22251	-0.12729
C	-3.90353	2.89504	-0.56826
C	-4.60554	1.90146	0.13459
C	-5.33244	2.24771	1.28436
C	-5.30011	3.56567	1.76918
H	-5.80860	3.81783	2.69107
C	-4.64224	4.50676	1.07231
C	-4.49264	5.93720	1.44618
H	-5.47658	6.44991	1.38325
H	-4.06427	6.04023	2.46653
C	-3.51910	6.47991	0.38372
H	-2.48870	6.47139	0.80607
H	-3.76888	7.52568	0.09909
C	-2.35978	5.46670	-1.63095
C	-1.08326	4.76816	-1.36198
C	-0.00895	5.02013	-2.23503
H	0.93715	4.52351	-2.08476
C	-0.16730	5.82364	-3.30588
C	-1.41346	6.40459	-3.59602
H	-1.53602	7.01225	-4.48341
C	-2.49339	6.18595	-2.73422

C	-3.87407	6.69472	-2.92563
H	-4.25940	6.43154	-3.93437
H	-3.89627	7.79547	-2.77460
C	-4.66611	5.96997	-1.82913
H	-5.44008	6.63310	-1.38367
H	-5.18241	5.09423	-2.28416
H	-2.23111	-5.62303	1.24686
H	-5.89106	1.49014	1.81380
H	1.36105	4.56442	3.79754
H	5.28366	-2.27216	2.93803
H	1.11993	-4.29130	-5.79556
H	-4.10175	0.86737	-5.86062
H	0.66535	5.98971	-3.97748
H	6.22553	1.18044	-4.00700
C	-0.05874	-0.23615	2.14700
C	1.01773	0.24906	3.06444
C	-1.47024	-0.11517	2.58154
C	2.35598	0.29076	2.61266
C	0.77795	0.61253	4.40925
C	-2.40243	-1.13763	2.31819
C	-1.94591	1.05597	3.21135
C	3.39060	0.70908	3.43942
H	2.58339	-0.02633	1.60747
C	1.80402	1.03785	5.24515
H	-0.22370	0.55357	4.81627
C	-3.69740	-1.07324	2.81243
H	-2.08966	-1.99914	1.74286
C	-3.24758	1.12601	3.70041
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H	4.40676	0.74206	3.05983
H	1.59452	1.31474	6.27334
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H	-4.37958	-1.90039	2.65130
H	-3.58610	2.02192	4.21044
H	1.66717	-5.17124	2.17432
C	1.02266	-4.40020	1.73479
Si	0.55956	-3.15043	3.05442
H	0.14927	-4.89486	1.30522
H	1.55145	-3.91838	0.91094
C	-0.92066	-3.68799	4.07844
C	2.01497	-2.73495	4.17141
H	0.16970	-1.75951	2.30754
C	-1.53073	-2.82923	5.01421

C	-1.43896	-4.99099	3.95351
H	2.80753	-2.19968	3.64534
H	1.71538	-2.13107	5.03259
H	2.43046	-3.67827	4.54992
C	-2.63041	-3.23991	5.76638
H	-1.15642	-1.81773	5.14822
C	-2.53014	-5.41352	4.71481
H	-0.97933	-5.69387	3.26389
H	-3.10533	-2.54679	6.45509
C	-3.13510	-4.53384	5.61382
H	-2.90986	-6.42540	4.60086
H	-3.99503	-4.85447	6.19573
H	-4.57463	0.87113	-0.18988
H	0.90500	4.28479	1.38211
H	4.80466	-0.99931	0.86784
C	-5.44106	0.01266	4.24831
F	-5.90734	1.25119	4.51882
F	-5.35383	-0.63906	5.43738
F	-6.38346	-0.63196	3.52545
C	4.18766	1.50449	5.63010
N	5.05224	1.84024	6.33243

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