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**Supplemental information**

**Unprecedented *endo*-oxidative cyclometallation  
and [4 + 3] cycloaddition  
of diene-vinylcyclopropanes**

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# Supplemental Experimental Procedures

## 1. General Information

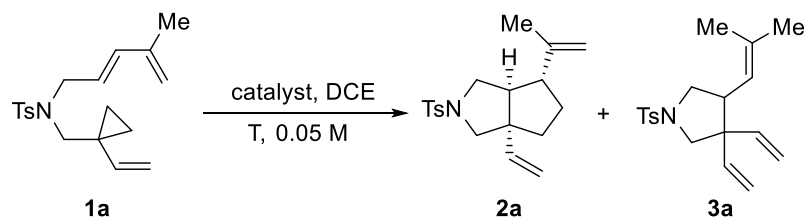
Air- and moisture-sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon. Reactions were stirred using Teflon coated magnetic stir bars. Elevated temperatures were maintained using thermostat-controlled silicone oil baths. Organic solutions were concentrated using a rotary evaporator with a desktop vacuum pump. Tetrahydrofuran (THF) and toluene were distilled from sodium and benzophenone prior to use. Dichloromethane (DCM) was distilled from  $\text{CaH}_2$  prior to use. *N,N*-dimethylformamide (DMF) and methanol were dried by molecular sieves prior to use. Synthetic reagents were purchased and used without further purification unless otherwise indicated. Super-dried DCE was purchased from J&K.  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  catalysts was purchased from Acros. Analytical TLC was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light and treatment with phosphomolybdic acid stain followed by gentle heating or iodine/silica-gel followed by water washing. Purification of products was accomplished by flash chromatography on silica gel, and the purified compounds showed a single spot by analytical TLC if not special instructions. The diastereomeric ratio was determined by  $^1\text{H}$  NMR of crude reaction mixtures. NMR spectra were recorded at Bruker AVANCE III 400 ( $^1\text{H}$  at 400 MHz,  $^{13}\text{C}$  at 101 MHz) and Bruker AVANCE III 500 ( $^1\text{H}$  at 500 MHz,  $^{13}\text{C}$  at 126 MHz) using  $\text{CDCl}_3$  ( $^1\text{H}$ , 7.26 ppm;  $^{13}\text{C}$ , 77.16 ppm) or  $\text{CD}_3\text{CN}$  ( $^1\text{H}$ , 1.96 ppm;  $^{13}\text{C}$ , 118.3 ppm,  $^{13}\text{CD}_3$ , 1.8 ppm) as internal standard. The following abbreviations were used to explain the multiplicities: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, ddd = doublet of doublet of doublets, dddd = doublet of doublet of doublet of doublets, m = multiplet, hept = heptet, coupling constant (Hz), and integration. HRMS were recorded on Bruker Apex IV FTMS mass spectrometer (ESI) or Micromass U.K. GCT GC-MS mass spectrometer (EI).

### Abbreviations:

$n\text{BuLi}$ = <i>n</i> -butyllithium;	$\text{BsNH}_2$ = 4-bromobenzenesulfonamide
DMF = <i>N,N</i> -dimethylformamide	$\text{NsNH}_2$ = 4-nitrobenzenesulfonamide
DIAD = diisopropyl azodiformate	PE = petroleum ether
THF = tetrahydrofuran	Bn = benzyl
$\text{ZrCp}_2\text{Cl}_2$ = Zirconocene dichloride	EA = ethyl acetate
Imida. = imidazole	DCM = dichloromethane
DCE = dichloroethane	PX = <i>p</i> -xylene
DME = 1,2-dimethoxyethane	PhMe = toluene
MP = melting point	COE = cyclooctadiene
COD = cyclooctene	

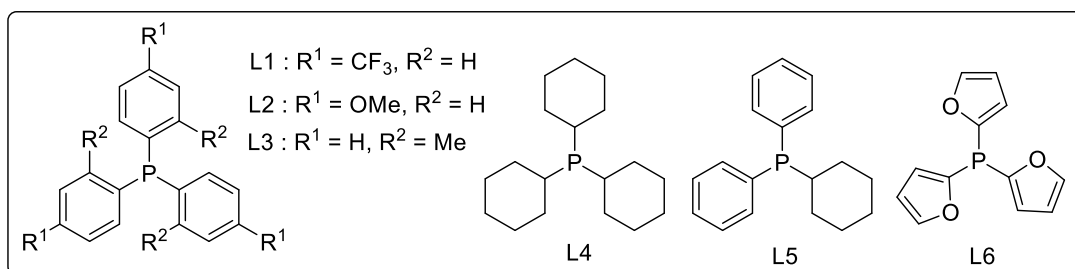
## 2. Screening Conditions of the [3+2] Cycloaddition

**Table S1.** Optimization of the Rh-catalyzed [3+2] cycloaddition.



entry <sup>a</sup>	catalyst	ligand	T/°C	yield <sup>b</sup>	2a : 3a <sup>c</sup>
1 <sup>d</sup>	[Rh(CO) <sub>2</sub> Cl] <sub>2</sub>	-	80	complex mixture	-
2 <sup>e</sup>	[Rh(CO) <sub>2</sub> ]SbF <sub>6</sub>	-	80	complex mixture	-
3 <sup>f</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	-	80	complex mixture	-
4 <sup>f,g</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	DPPP	80	no reaction	-
5 <sup>f,h</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	L1	80	83%	1 : 2.5
6 <sup>f,h</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	L2	80	no reaction	-
7 <sup>f,h</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	L3	80	complex mixture	-
8 <sup>f,h</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	L4	80	complex mixture	-
9 <sup>f,h</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	L5	80	63%	1 : 1.5
10 <sup>f,h</sup>	[Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ]SbF <sub>6</sub>	L6	80	63%	1 : 1.3
11 <sup>i</sup>	Rh(PPh <sub>3</sub> ) <sub>3</sub> SbF <sub>6</sub>	-	90	83%	5 : 1
12 <sup>i</sup>	Rh(PPh <sub>3</sub> ) <sub>3</sub> SbF <sub>6</sub>	-	60	83%	8 : 1
13 <sup>i</sup>	Rh(PPh <sub>3</sub> ) <sub>3</sub> SbF <sub>6</sub>	-	rt	84%	14 : 1
14 <sup>i,j</sup>	Rh(PPh <sub>3</sub> ) <sub>3</sub> SbF <sub>6</sub>	-	0	89%	18 : 1

<sup>a</sup>0.1 mmol substrate in 2 mL DCE. <sup>b</sup>Isolated yields. <sup>c</sup>Confirmed by <sup>1</sup>H NMR. <sup>d</sup>5 mol% [Rh(CO)<sub>2</sub>Cl]<sub>2</sub>. <sup>e</sup>5 mol% [Rh(CO)<sub>2</sub>]SbF<sub>6</sub>, 12 mol% AgSbF<sub>6</sub>. <sup>f</sup>5 mol% [Rh(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>]SbF<sub>6</sub>, 12 mol% AgSbF<sub>6</sub>. <sup>g</sup>6 mol% dppp. <sup>h</sup>5 mol% [Rh(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>]SbF<sub>6</sub> and 12 mol% ligand. <sup>i</sup>10 mol% Rh(PPh<sub>3</sub>)<sub>3</sub>Cl, 12 mol% AgSbF<sub>6</sub>. <sup>j</sup>Run 2 times.



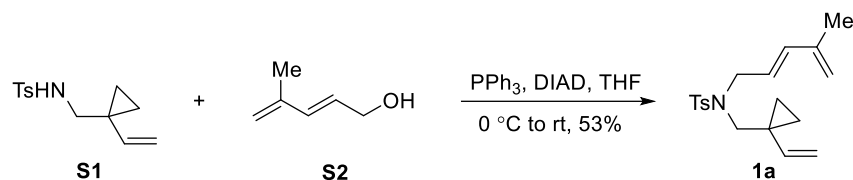
At first, we used **1a** to attempt [4+3] reaction and optimize the reaction conditions (Table S1). Under the catalysis of [Rh(CO)<sub>2</sub>Cl]<sub>2</sub>, [Rh(CO)<sub>2</sub>]SbF<sub>6</sub> and [Rh(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>]SbF<sub>6</sub> in DCE at 80 °C, we found all reactions gave complex mixtures (entries 1-3). Using bidentate phosphine ligand dppp did not help this reaction, catalysed by [Rh(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>]SbF<sub>6</sub> (entry 4). When monophosphine ligand L1 was used, a mixture of [3+2] cycloaddition product **2a** and β-hydride elimination product **3a** was generated (entry 5). With these results, we then planned to screen the reaction conditions to develop this as a [3+2] reaction to access highly functionalized 5/5 bicyclic products. We tested other monophosphine ligands with different substituents for this reaction. Unfortunately, the results were not satisfactory, because either complex mixture or low ratio of the target product with respect to the side product was observed (entries 6-10). We found that under the catalysis of [Rh(PPh<sub>3</sub>)<sub>3</sub>]SbF<sub>6</sub>, **2a**

became the major product (entry 11). Further investigation indicated that reaction temperature was important to the reaction outcomes. As the reaction temperature decreased, the ratio of **2a** and **3a** gradually increased (entries 12-14). When the reaction was carried out at 0 °C, we could get **2a** in 89% yield and high selectivity (entry 14).

### 3. Experimental Procedures and Characterization Data

#### 3.1 Syntheses of Substrates

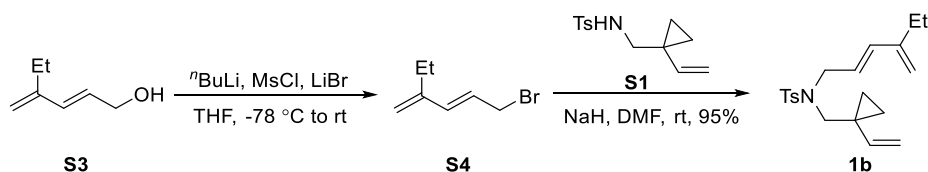
##### Substrate (1a)



To a solution of **S1**<sup>1</sup> (504.4 mg, 2.01 mmol) and  $\text{PPh}_3$  (1.05 g, 3.99 mmol) in THF (20 mL) was added **S2**<sup>2</sup> (228.1 mg, 2.33 mmol) under an argon atmosphere at  $0\text{ }^\circ\text{C}$ , and then DIAD (804.5 mg, 3.98 mmol) was added. The mixture was warmed up naturally and stirred for 10 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1) afforded the product **1a** (352.2 mg, 53%).

**1a**: white solid, MP =  $34\text{--}36\text{ }^\circ\text{C}$ . TLC  $R_f$  (PE/EA 5:1) = 0.66.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 (d,  $J = 8.2$  Hz, 2H), 7.28 (d,  $J = 8.2$  Hz, 2H), 6.12 (d,  $J = 15.8$  Hz, 1H), 5.90 (dd,  $J = 17.3, 10.7$  Hz, 1H), 5.28 (dt,  $J = 15.7, 6.5$  Hz, 1H), 4.99–4.85 (m, 4H), 3.97 (d,  $J = 6.5$  Hz, 2H), 3.23 (s, 2H), 2.41 (s, 3H), 1.65 (s, 3H), 0.74–0.65 (m, 2H), 0.65–0.56 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 141.2, 140.5, 137.8, 136.3, 129.6, 127.4, 124.2, 116.9, 112.4, 53.2, 49.1, 21.6, 20.1, 18.5, 13.3. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{26}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 332.1679, found 332.1686.

##### Substrate (1b)



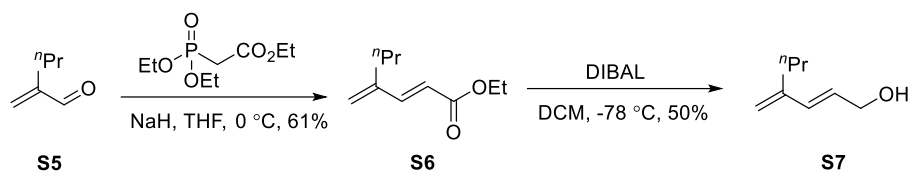
To a solution of **S3**<sup>3</sup> (174.3 mg, 1.55 mmol) in THF (4 mL) was added  $n\text{-BuLi}$  (1.1 mL, 1.6 M in hexane, 1.76 mmol) dropwise at  $-78\text{ }^\circ\text{C}$  under an argon atmosphere. After stirred for 15 min, MsCl (208.2 mg, 1.82 mmol) was added. The reaction mixture was stirred for 20 min at  $-78\text{ }^\circ\text{C}$ , and then LiBr (405.8 mg, 4.68 mmol) was added. The reaction mixture was warmed to room temperature and stirred for another 3 h.

To a solution of **S1** (251.7 mg, 1.0 mmol) in DMF (4 mL) was added NaH (56.5 mg, 60% weight in mineral oil, 1.41 mmol) at room temperature. After stirred for 5 min, the freshly prepared diene **S4** solution was transferred to the solution containing **S1**. The mixture was stirred for 14 h and then quenched with saturated aqueous ammonium chloride solution and water. This reaction mixture was then extracted with diethyl ether for three times. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 40:1, then 20:1) to give **1b** (327.5 mg, 95% yield).

**1b**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.37.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 (d,  $J = 8.2$  Hz, 2H), 7.27 (d,  $J = 8.2$  Hz, 2H), 6.06 (d,  $J = 16.0$  Hz, 1H), 5.90 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.28 (dt,  $J = 16.0, 6.4$  Hz, 1H), 4.99–4.86 (m, 4H), 3.97 (d,  $J = 6.0$  Hz, 2H), 3.23 (s, 2H), 2.41 (s, 3H), 1.99 (q,  $J = 7.6$  Hz, 2H), 0.97 (t,  $J = 7.6$  Hz, 3H), 0.72–0.65 (m, 2H), 0.65–0.57 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  146.8, 143.2, 140.5, 137.9,

135.8, 129.7, 127.4, 123.1, 114.8, 112.4, 53.1, 49.2, 24.7, 21.6, 21.0, 13.3, 12.6. HRMS (ESI): calcd for  $C_{20}H_{28}NO_2S^+$  ( $[M + H]^+$ ) 346.1835, found 346.1838.

#### Substrate (S7)

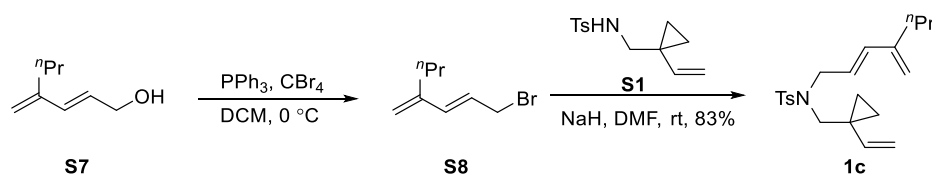


To a suspension of NaH (638.8 mg, 60% weight in mineral oil, 16.0 mmol) in THF (20 mL) was added ethyl 2-(diethoxyphosphoryl)acetate (3.4 mL, 17.3 mmol) dropwise at 0 °C under an argon atmosphere. A solution of **S5**<sup>4</sup> (1.31 g, in 10 mL THF, 13.3 mmol) was added dropwise at 0 °C. After stirred for 50 min at 0 °C, the reaction was quenched by saturated aqueous ammonium chloride solution and water. The reaction mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 100:1) to give **S6** (1.37 g, 61% yield) as a colorless oil.

To a solution of **S6** (1.34 g, 8.0 mmol) in DCM (27 mL) was added DIBAL (20.0 mL, 1.0 M in hexanes, 20.0 mmol) at -78 °C under an argon atmosphere. After stirred for 1 h at the same temperature, the reaction was quenched by saturated aqueous ammonium chloride solution and saturated potassium sodium tartrate tetrahydrate solution and then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 10:1) to give **S7** (502.3 mg, 50% yield) as a colorless oil.

**S7**: colorless oil. TLC  $R_f$  (PE/EA 5:1) = 0.33.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  6.26 (d,  $J = 16.0$  Hz, 1H), 5.86 (dt,  $J = 16.0, 6.0$  Hz, 1H), 5.01 (s, 1H), 4.97 (s, 1H), 4.21 (d,  $J = 6.0$  Hz, 2H), 2.18 (t,  $J = 7.2$  Hz, 2H), 1.51 (td,  $J = 7.2, 7.2$  Hz, 3H), 0.93 (t,  $J = 7.2$  Hz, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.5, 133.8, 127.7, 115.9, 63.9, 34.3, 21.4, 14.2. HRMS (ESI): calcd for  $\text{C}_8\text{H}_{15}\text{O}^+$  ( $[M + H]^+$ ) 127.1117, found 127.1119.

#### Substrate (1c)



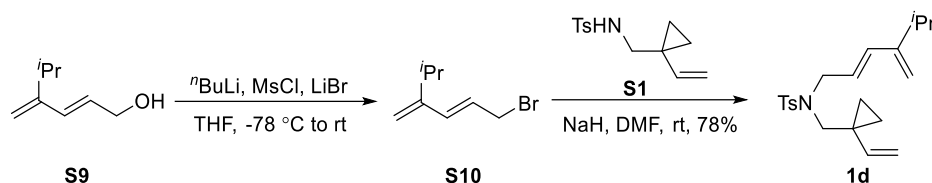
To a solution of **S7** (188.1 mg, 1.49 mmol) and  $\text{CBr}_4$  (595.6 mg, 1.80 mmol) in DCM (7 mL) at 0 °C under argon atmosphere was added  $\text{PPh}_3$  (438.2 mg in 2 mL DCM, 1.65 mmol). After stirred for 10 min, the solution was concentrated and filtered with silica gel, eluted with pentanes/ $\text{Et}_2\text{O}$  50:1 to give **S8**, which was immediately subjected to next step.

To a solution of **S1** (256.4 mg, 1.02 mmol) in DMF (6 mL) was added NaH (63.2 mg, 60% weight in mineral oil, 1.58 mmol) at room temperature. After stirred for 5 min, the freshly prepared diene **S8** was added. The mixture was stirred for 2 h and then quenched with saturated aqueous ammonium chloride solution and water. This reaction mixture was extracted with diethyl ether for three times. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 40:1) to give **1c** (303.3 mg, 83% yield).

**1c**: colorless oil. TLC  $R_f$  (PE/EA 5:1) = 0.65.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 (d,  $J = 8.2$  Hz, 2H), 7.27 (d,  $J = 8.2$  Hz, 2H), 6.03 (d,  $J = 16.0$  Hz, 1H), 5.91 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.25 (dt,  $J = 15.6, 6.8$  Hz, 1H),

4.96 (dd,  $J = 17.2, 0.8$  Hz, 1H), 4.93-4.87 (m, 3H), 3.98 (d,  $J = 6.8$  Hz, 2H), 3.24 (s, 2H), 2.41 (s, 3H), 1.94 (t,  $J = 7.8$  Hz, 2H), 1.34 (td,  $J = 7.8, 7.8$  Hz, 2H), 0.85 (t,  $J = 7.8$  Hz, 3H), 0.70 (dd,  $J = 7.2, 5.2$  Hz, 2H), 0.60 (dd,  $J = 7.2, 5.2$  Hz, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.2, 143.2, 140.5, 138.0, 135.9, 129.7, 127.4, 123.2, 115.9, 112.4, 53.1, 49.2, 34.2, 21.6, 21.3, 21.0, 14.1, 13.3. HRMS (ESI): calcd for  $\text{C}_{21}\text{H}_{30}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 360.1992, found 360.1998.

#### Substrate (1d)

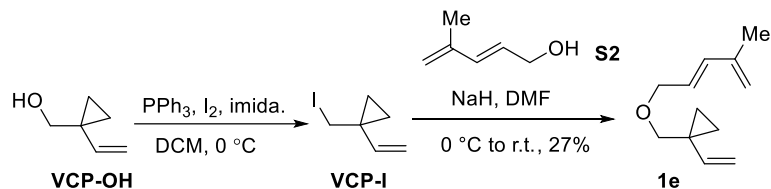


To a solution of **S9**<sup>5</sup> (125.6 mg, 1.0 mmol) in THF (3 mL) was added  $n\text{BuLi}$  (0.7 mL, 1.6 M in hexane, 1.12 mmol) dropwise at  $-78^\circ\text{C}$  under an argon atmosphere. After stirred for 15 min,  $\text{MsCl}$  (156.4 mg, 1.36 mmol) was added. The reaction mixture was stirred for 20 min at  $-78^\circ\text{C}$ , and then  $\text{LiBr}$  (261.8 mg, 3.02 mmol) was added. The reaction mixture was warmed to room temperature and stirred for another 2 h, generating **S10**, which was used immediately in the next step.

To a solution of **S1** (201.9 mg, 0.80 mmol) in DMF (3 mL) was added  $\text{NaH}$  (58.1 mg, 60% weight in mineral oil, 1.45 mmol) at room temperature. After stirred for 5 min, the freshly prepared diene **S10** solution was transferred to the solution containing **S1**. The mixture was stirred for 14 h, then quenched with saturated aqueous ammonium chloride solution and water and finally extracted with diethyl ether for three times. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 40:1, then 20:1) to give **1d** (226.1 mg, 78% yield).

**1d**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.42.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 (d,  $J = 8.2$  Hz, 2H), 7.27 (d,  $J = 8.2$  Hz, 2H), 6.01 (d,  $J = 15.6$  Hz, 1H), 5.91 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.31 (dt,  $J = 16.0, 6.4$  Hz, 1H), 4.96 (dd,  $J = 17.2, 1.0$  Hz, 1H), 4.92 (dd,  $J = 10.8, 1.0$  Hz, 1H), 4.91 (s, 1H), 4.87 (s, 1H), 3.98 (d,  $J = 6.4$  Hz, 2H), 3.24 (s, 2H), 2.41 (s, 3H), 2.29 (hept,  $J = 6.8$  Hz, 1H), 0.97 (d,  $J = 6.8$  Hz, 6H), 0.70 (dd,  $J = 6.8, 4.8$  Hz, 2H), 0.61 (dd,  $J = 6.8, 4.8$  Hz, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  151.8, 143.2, 140.5, 137.9, 135.6, 129.7, 127.4, 122.8, 112.7, 112.4, 53.1, 49.3, 29.3, 22.2, 21.6, 21.0, 13.3. HRMS (EI): calcd for  $\text{C}_{21}\text{H}_{30}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 360.1992, found 360.1992.

#### Substrate (1e)



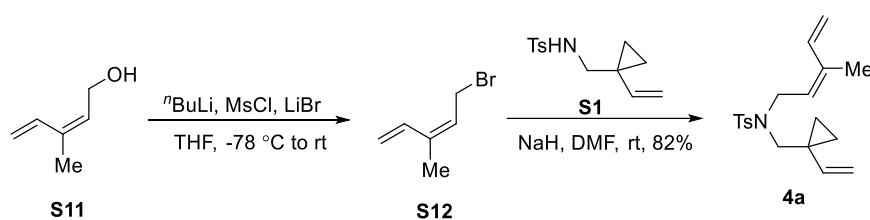
To a solution of **VCP-OH**<sup>6</sup> (391.7 mg, 4.00 mmol),  $\text{PPh}_3$  (1.258 g, 4.80 mmol) and imidazole (407.9 mg, 6.00 mmol) in DCM (8 mL) was added  $\text{I}_2$  (2.133 g, 8.40 mmol) at  $0^\circ\text{C}$ . The mixture was stirred for 20 min at the same temperature, then quenched by saturated sodium thiosulfate solution and water and finally was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by a flash short column chromatography (pentane/ $\text{Et}_2\text{O}$  50:1) to give intermediate **VCP-I**, which was concentrated and directly used in the next step.



To a solution of **S2** (588.0 mg, 6.00 mmol) in DMF (8 mL) was added NaH (241.1 mg, 60% weight in mineral oil, 6.03 mmol) at 0 °C. After stirred for 20 min under argon atmosphere, **VCP-I** was added. The mixture was warmed up naturally and stirred for 15 h, then quenched by saturated aqueous ammonium chloride solution and water, and finally extracted with diethyl ether. The combined organic layer was washed with water brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 300:1, 200:1) to give **1e** (195.4 mg, 27%).

**1e**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.93.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  6.32 (d,  $J$  = 15.6 Hz, 1H), 5.81 – 5.61 (m, 2H), 5.06 (dd,  $J$  = 17.4, 1.3 Hz, 1H), 5.00 – 4.93 (m, 3H), 4.06 (dd,  $J$  = 6.3, 1.4 Hz, 2H), 3.42 (s, 2H), 1.85 (s, 3H), 0.75 – 0.70 (m, 2H), 0.69 – 0.64 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  141.8, 141.6, 135.4, 126.4, 116.8, 111.5, 75.3, 71.5, 22.7, 18.7, 12.8. HRMS (EI): calcd for  $\text{C}_{12}\text{H}_{18}\text{O}$  ( $[\text{M}]^{+}$ ) 178.1352, found 178.1353.

#### Substrate (4a)

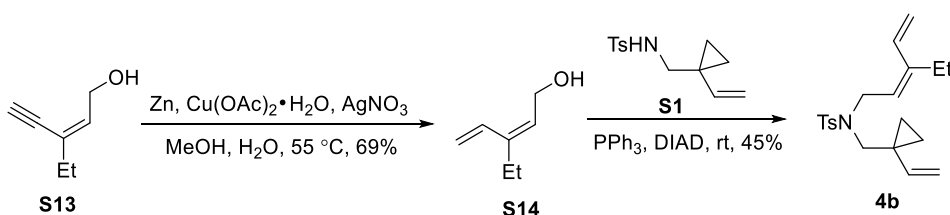


To a solution of **S11**<sup>7</sup> (306.3 mg, 3.12 mmol) in THF (10 mL) was added  $^n\text{BuLi}$  (2.1 mL, 1.6 M in hexane, 3.36 mmol) dropwise at -78 °C under an argon atmosphere. After stirred for 15 min, MsCl (467.5 mg, 4.08 mmol) was added. The reaction mixture was stirred for 20 min at -78 °C, and then LiBr (795.3 mg, 9.16 mmol) was added. The reaction mixture was allowed to warm to room temperature and stirred for 3 h, generating **S12**, which was used immediately in the next step.

To a solution of **S1** (752.2 mg, 2.99 mmol) in DMF (10 mL) was added NaH (183.2 mg, 60% weight in mineral oil, 4.58 mmol) at room temperature. After stirred for 5 min, the freshly prepared diene **S12** solution was transferred to the solution containing **S1**. The mixture was stirred for 19 h, then quenched by saturated aqueous ammonium chloride solution (20 mL) and water (10 mL), and finally extracted with diethyl ether (3 × 30 mL). The combined organic layer was washed with water (3 × 30 mL) and brine (30 mL), dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 50:1) to give **4a** (810.5 mg, 82% yield).

**4a**: white solid, Mp = 40–42 °C. TLC  $R_f$  (PE/EA 5:1) = 0.59.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.66 (d,  $J$  = 8.2 Hz, 2H), 7.27 (d,  $J$  = 8.2 Hz, 2H), 6.64 (dd,  $J$  = 17.2, 10.8 Hz, 1H), 5.89 (dd,  $J$  = 17.2, 10.6 Hz, 1H), 5.25 (d,  $J$  = 17.2 Hz, 1H), 5.17 (d,  $J$  = 10.8 Hz, 1H), 5.05 (t,  $J$  = 6.6 Hz, 1H), 4.97 (dd,  $J$  = 17.2, 1.2 Hz, 1H), 4.92 (dd,  $J$  = 10.6, 1.2 Hz, 1H), 4.10 (d,  $J$  = 6.6 Hz, 2H), 3.23 (s, 2H), 2.42 (s, 3H), 1.71 (d,  $J$  = 1.2 Hz, 3H), 0.68 (dd,  $J$  = 6.4, 4.5 Hz, 2H), 0.57 (dd,  $J$  = 6.4, 4.5 Hz, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 140.6, 137.6, 135.3, 132.8, 129.6, 127.5, 124.8, 115.7, 112.4, 53.2, 44.2, 21.6, 20.9, 19.8, 13.2. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{26}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 332.1679, found 332.1678.

#### Substrate (4b)

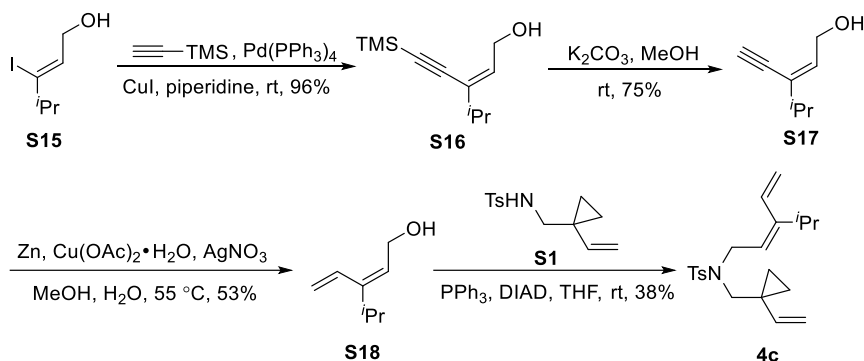


Zinc powder (5.26 g, 80.4 mmol) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated Zinc powder was washed with lots of water to neutral. To the above slurry of zinc in water (15 mL) was added Cu(OAc)<sub>2</sub> • H<sub>2</sub>O (802.8 mg, 4.02 mmol) at 0 °C. After stirred for 15 min, AgNO<sub>3</sub> (682.8 mg, 4.02 mmol) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 100 mL round bottom flask, and then **S13**<sup>8</sup> (443.0 mg, 4.02 mmol), water (15 mL), MeOH (20 mL) were added. The reaction mixture was stirred for 12 h at 55 °C and filtered through celite by washing with EA. The resulting mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 10:1, then 5:1) to give **S14** (312.3 mg, 69%) as a yellow oil.

To a solution of **S1** (377.2 mg, 1.50 mmol) and PPh<sub>3</sub> (786.8 mg, 3.00 mmol) in THF (15 mL) was added **S14** (222.6 mg, 1.98 mmol) under an argon atmosphere at 0 °C, and then DIAD (600.6 mg, 2.97 mmol) was added. The mixture was warmed up naturally and stirred for 12 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 100:1, then 50:1) afforded the product **4b** (234.3 mg, 45%).

**4b**: colorless oil, TLC R<sub>f</sub> (PE/EA 5:1) = 0.64. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 6.53 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.90 (dd, *J* = 17.4, 10.7 Hz, 1H), 5.26 (d, *J* = 17.5 Hz, 1H), 5.16 (d, *J* = 11.0 Hz, 1H), 4.99 (t, *J* = 6.4 Hz, 1H), 4.98 (dd, *J* = 17.4, 0.8 Hz, 1H), 4.93 (dd, *J* = 10.7, 0.8 Hz, 1H), 4.11 (d, *J* = 6.4 Hz, 2H), 3.24 (s, 2H), 2.41 (s, 3H), 2.10 (q, *J* = 7.3 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H), 0.72-0.63 (m, 2H), 0.63-0.51 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 143.2, 140.8, 140.6, 137.7, 132.1, 129.7, 127.4, 122.8, 115.3, 112.4, 53.3, 44.5, 25.7, 21.6, 20.9, 13.2, 12.8. HRMS (ESI): calcd for C<sub>20</sub>H<sub>28</sub>NO<sub>2</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 346.1835, found 346.1836.

#### Substrate (4c)



To a solution of **S15**<sup>9</sup> (1.26 g, 5.59 mmol), CuI (106.5 mg, 0.56 mmol) and Pd(PPh<sub>3</sub>)<sub>4</sub> (322.9 mg, 0.28 mmol) in piperidine (15 mL) was added ethynyltrimethylsilane (1.6 mL, 11.32 mmol) at room temperature under an argon atmosphere. After stirring for 8 h, the reaction mixture was filtered through celite by washing with Et<sub>2</sub>O, concentrated and purified by column chromatography (PE/EA 50:1, 20:1 and 15:1) to give **S16** (1.05 g, 96%) as a brown oil.

A solution of **S16** (1.05 g, 5.33 mmol) and K<sub>2</sub>CO<sub>3</sub> (36.9 mg, 0.27 mmol) in MeOH (7.8 mL) was stirred for 12 h at room temperature. It was quenched by saturated aqueous ammonium chloride solution and water, then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 20:1, 10:1) to give **S17** (493.7 mg, 75%).

**S17**: reddish brown oil, TLC  $R_f$  (PE/EA 5:1) = 0.3.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  5.96 (t,  $J$  = 6.4 Hz, 1H), 4.36 (dd,  $J$  = 6.4, 5.8 Hz, 2H), 3.19 (s, 1H), 2.41 (hept,  $J$  = 6.8 Hz, 1H), 1.53 (t,  $J$  = 5.8 Hz, 1H), 1.10 (d,  $J$  = 6.8 Hz, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  134.7, 131.4, 83.8, 80.1, 61.4, 35.1, 21.5. HRMS (EI): calcd for  $\text{C}_8\text{H}_{12}\text{O}^+$  ( $[\text{M}]^+$ ) 124.0883, found 124.0884.

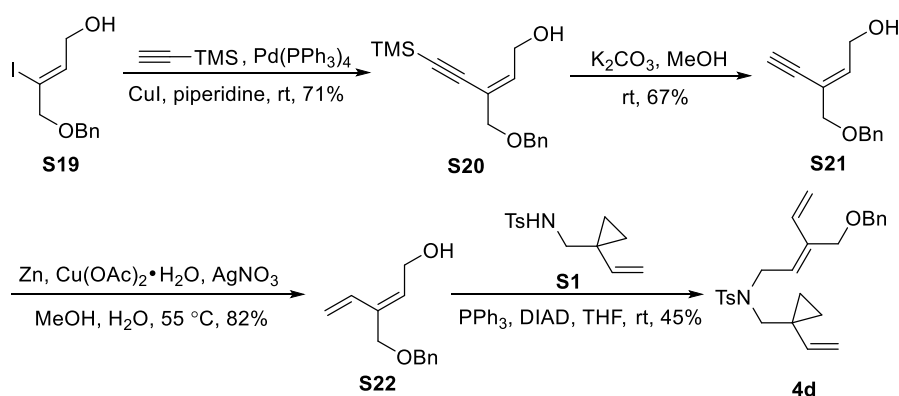
Zinc powder (4.89 g, 74.7 mmol) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated zinc powder was washed with lots of water to neutral. To the above slurry of zinc in water (10 mL) was added  $\text{Cu}(\text{OAc})_2\cdot\text{H}_2\text{O}$  (745.1 mg, 3.73 mmol) at 0 °C. After stirred for 15 min,  $\text{AgNO}_3$  (633.8 mg, 3.73 mmol) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 50 mL round bottom flask containing **S17** (462.7 mg, 3.73 mmol), water (10 mL), MeOH (13 mL) were added. The reaction mixture was stirred for 24 h at 55 °C. then filtered through celite by washing with EA and finally extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and the crude mixture was reprocessed under the same conditions to make this reaction complete.

Zinc powder (4.92 g, 75.2 mmol) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated zinc powder was washed with lots of water to neutral. To the above slurry of zinc in water (10 mL) was added  $\text{Cu}(\text{OAc})_2\cdot\text{H}_2\text{O}$  (744.7 mg, 3.73 mmol) at 0 °C. After stirred for 15 min,  $\text{AgNO}_3$  (634.3 mg, 3.73 mmol) was added. The reaction mixture was filtered, washed with water. The solid was transferred to a 100 mL round bottom flask containing above crude mixture, water (10 mL), MeOH (13 mL) were added. The reaction mixture was stirred for 20 h at 55 °C and filtered through celite by washing with EA. It was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated purified by column chromatography (PE/EA 15:1, 10:1) to give **S18** (249.6 mg, 53%) as a yellow oil.

To a solution of **S1** (363.5 mg, 1.45 mmol) and  $\text{PPh}_3$  (755.9 mg, 2.88 mmol) in THF (14 mL) was added **S18** (253.8 mg, 2.01 mmol) under an argon atmosphere at 0 °C, and then DIAD (586.4 mg, 2.90 mmol) was added. The mixture was warmed up naturally and stirred for 18 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 100:1, 50:1) afforded the product **4c** (196.0 mg, 38%).

**4c**: light yellow oil, TLC  $R_f$  (PE/EA 5:1) = 0.64.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 (d,  $J$  = 8.2 Hz, 2H), 7.27 (d,  $J$  = 8.2 Hz, 2H), 6.40 (dd,  $J$  = 17.5, 11.3 Hz, 1H), 5.88 (dd,  $J$  = 17.3, 10.7 Hz, 1H), 5.20 (d,  $J$  = 17.5 Hz, 1H), 5.19 (d,  $J$  = 10.0 Hz, 1H), 4.99 (d,  $J$  = 17.3 Hz, 1H), 4.96-4.90 (m, 2H), 4.11 (d,  $J$  = 6.4 Hz, 2H), 3.23 (s, 2H), 2.49 (hept,  $J$  = 6.8 Hz, 1H), 2.41 (s, 3H), 0.88 (d,  $J$  = 6.8 Hz, 6H), 0.69-0.61 (m, 2H), 0.61-0.51 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.7, 143.2, 140.6, 137.8, 132.3, 129.7, 127.4, 120.8, 115.8, 112.4, 53.2, 44.9, 30.0, 22.1, 21.6, 20.7, 13.2. HRMS (ESI): calcd for  $\text{C}_{21}\text{H}_{30}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 360.1992, found 360.1990.

#### **Substrate (4d)**



To a solution of **S19**<sup>10</sup> (1.64 g, 5.38 mmol), CuI (103.3 mg, 0.54 mmol) and Pd(PPh<sub>3</sub>)<sub>4</sub> (311.2 mg, 0.27 mmol) in piperidine (15 mL) was added ethynyltrimethylsilane (1.5 mL, 10.60 mmol) at room temperature under an argon atmosphere. After stirring for 5 h, the reaction mixture was filtered through celite by washing with Et<sub>2</sub>O, concentrated and purified by column chromatography (PE/EA 10:1 and 5:1) to give **S20** (1.04 g, 71%) as a brown oil.

A solution of **S20** (1.04 g, 3.78 mmol) and K<sub>2</sub>CO<sub>3</sub> (26.5 mg, 0.19 mmol) in MeOH (5.6 mL) was stirred for 12 h at room temperature. It was quenched by saturated aqueous ammonium chloride solution and water then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 10:1, 5:1) to give **S21** (513.0 mg, 67%).

**S21**: reddish brown oil, TLC R<sub>f</sub> (PE/EA 5:1) = 0.1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.41-7.27 (m, 5H), 6.26 (t, *J* = 6.4 Hz, 1H), 4.57 (s, 2H), 4.43 (d, *J* = 6.4 Hz, 2H), 4.05 (d, *J* = 1.1 Hz, 2H), 3.23 (s, 1H), 1.57 (brs, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 138.9, 138.0, 128.6, 127.93, 127.91, 121.4, 83.9, 79.4, 72.5, 72.1, 61.2. HRMS (ESI): calcd for C<sub>13</sub>H<sub>18</sub>NO<sub>2</sub><sup>+</sup> ([M + NH<sub>4</sub>]<sup>+</sup>) 220.1332, found 220.1325.

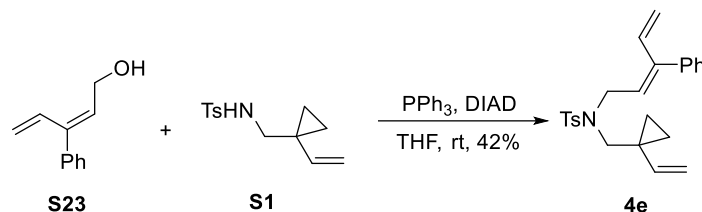
Zinc powder (2.62 g, 40.06 mmol) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated Zinc powder was washed with lots of water to neutral. To the above slurry of zinc in water (8 mL) was added Cu(OAc)<sub>2</sub> · H<sub>2</sub>O (399.5 mg, 2.00 mmol) at 0 °C. After stirred for 15 min, AgNO<sub>3</sub> (338.7 mg, 1.99 mmol) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 50 mL round bottom flask, and then **S21** (407.9 mg, 2.02 mmol), water (8 mL), MeOH (10 mL) were added. The reaction mixture was stirred for 15 h at 55 °C. After filtered through celite by washing with EA, the mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 5:1) to give **S22** (338.3 mg, 82%) as a yellow oil.

To a solution of **S1** (290.3 mg, 1.16 mmol) and PPh<sub>3</sub> (578.1 mg, 2.20 mmol) in THF (11 mL) was added **S22** (334.5 mg, 1.64 mmol) under an argon atmosphere at 0 °C, and then DIAD (448.3 mg, 2.22 mmol) was added. The mixture was warmed up naturally and stirred for 12 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 20:1, 15:1) afforded the product **4d** (229.4 mg, 45%).

**4d**: colorless oil, TLC R<sub>f</sub> (PE/EA 5:1) = 0.42. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.38-7.26 (m, 5H), 7.24 (d, *J* = 8.2 Hz, 2H), 6.52 (dd, *J* = 17.6, 11.2 Hz, 1H), 5.88 (dd, *J* = 17.3, 10.7 Hz, 1H), 5.44-5.33 (m, 2H), 5.24 (d, *J* = 11.2 Hz, 1H), 4.98 (dd, *J* = 17.3, 1.1 Hz, 1H), 4.93 (dd, *J* = 10.7, 1.1 Hz, 1H), 4.39 (s, 2H), 4.15 (d, *J* = 6.4 Hz, 2H), 4.04 (d, *J* = 0.9 Hz, 2H), 3.24 (s, 2H), 2.37 (s, 3H), 0.75-0.63 (m, 2H), 0.63-0.51 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 143.3, 140.4, 138.3, 137.5, 135.6, 130.5, 129.7, 128.5, 127.81,

127.76, 127.4, 126.9, 117.0, 112.6, 72.1, 71.3, 53.5, 44.4, 21.6, 20.9, 13.2. HRMS (ESI): calcd for  $C_{26}H_{35}N_2O_3S^+$  ( $[M + NH_4]^+$ ) 455.2363, found 455.2358.

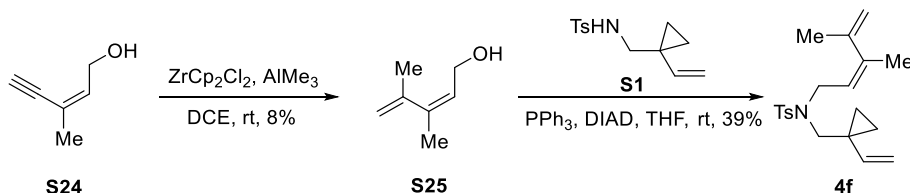
#### Substrate (4e)



To a solution of **S1** (360.4 mg, 1.43 mmol) and  $PPh_3$  (579.4 mg, 2.21 mmol) in THF (12 mL) was added **S23**<sup>11</sup> (177.1 mg, 1.11 mmol) under an argon atmosphere at 0 °C, and then DIAD (446.4 mg, 2.21 mmol) was added. The mixture was warmed up naturally and stirred for 32 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1, 20:1) afforded the product **4e** (183.2 mg, 42%).

**4e**: light yellow solid, MP = 65-67 °C. TLC  $R_f$  (PE/EA 5:1) = 0.55.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.69 (d,  $J$  = 8.2 Hz, 2H), 7.30-7.23 (m, 5H), 7.06 (apparent dd,  $J$  = 6.5, 2.9 Hz, 2H), 6.70 (dd,  $J$  = 17.3, 10.9 Hz, 1H), 5.91 (dd,  $J$  = 17.3, 10.7 Hz, 1H), 5.36 (d,  $J$  = 10.9 Hz, 1H), 5.23 (t,  $J$  = 6.5 Hz, 1H), 5.11 (d,  $J$  = 17.4 Hz, 1H), 5.02 (d,  $J$  = 17.3 Hz, 1H), 4.95 (d,  $J$  = 10.7 Hz, 1H), 4.26 (d,  $J$  = 6.5 Hz, 2H), 3.29 (s, 2H), 2.40 (s, 3H), 0.78-0.66 (m, 2H), 0.66-0.54 (m, 2H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  143.3, 142.0, 140.48, 140.45, 137.6, 132.4, 129.8, 128.5, 128.1, 127.5, 127.4, 126.0, 120.1, 112.6, 53.3, 44.9, 21.6, 20.8, 13.2. HRMS (ESI): calcd for  $C_{24}H_{31}N_2O_2S^+$  ( $[M + NH_4]^+$ ) 411.2101, found 411.2099.

#### Substrate (4f)



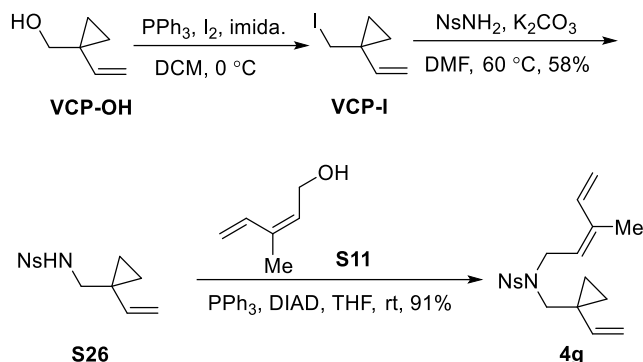
To a solution of  $ZrCp_2Cl_2$  (1.69 g, 5.79 mmol) in DCE (40 mL) was added  $AlMe_3$  (35 mL, 1 M in hexane, 35 mmol) at 0 °C under an argon atmosphere. The solution was stirred for 1 h at room temperature and then a solution of commercial available reagent **S24** (554.8 mg, 5.77 mmol) in DCE (10 mL) was added dropwise. The reaction mixture was stirred for 6 d at 25 °C. The reaction was quenched by 100 mL saturated potassium sodium tartrate tetrahydrate solution and stirred overnight. The reaction mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 10:1, 5:1) to give **S25** (51.2 mg, 8%) as a yellow oil.

To a solution of **S1** (99.5 mg, 0.40 mmol) and  $PPh_3$  (162.1 mg, 0.62 mmol) in THF (2 mL) was added **S25** (34.7 mg, 0.31 mmol) under an argon atmosphere at room temperature, and then DIAD (126.5 mg, 0.63 mmol) was added. The mixture was stirred for 4 d, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 100:1, 50:1) afforded product **4f** (53.5 mg, 39%).

**4f**: colorless oil. TLC  $R_f$  (PE/EA 5:1) = 0.60.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.68 (d,  $J$  = 8.2 Hz, 2H), 7.28 (d,  $J$  = 8.2 Hz, 2H), 5.88 (dd,  $J$  = 17.3, 10.7 Hz, 1H), 5.02-4.92 (m, 2H), 4.93 (d,  $J$  = 17.3 Hz, 1H), 4.90 (d,  $J$  = 10.7 Hz, 1H), 4.59 (s, 1H), 3.99 (d,  $J$  = 6.0 Hz, 2H), 3.20 (s, 2H), 2.42 (s, 3H), 1.80 (s, 3H), 1.70 (s, 3H), 0.70-0.61 (m, 2H), 0.60-0.51 (m, 2H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  143.7, 143.1, 141.3, 140.6, 137.8, 129.6,

127.5, 121.5, 114.6, 112.3, 53.3, 46.2, 22.8, 21.7, 21.6, 21.1, 13.0. HRMS (ESI): calcd for C<sub>20</sub>H<sub>28</sub>NO<sub>2</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 346.1835, found 346.1836.

#### Substrate (4g)



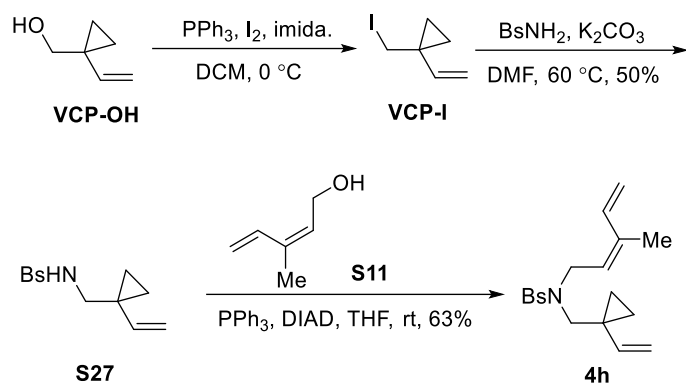
To a solution of **VCP-OH**<sup>6</sup> (391.3 mg, 3.99 mmol), PPh<sub>3</sub> (1.26 g, 4.82 mmol) and imidazole (409.6 mg, 6.01 mmol) in DCM (15 mL) was added I<sub>2</sub> (1.52 g, 6.00 mmol) at 0 °C. The mixture was stirred for 10 min at the same temperature. After quenched by saturated sodium thiosulfate solution (10 mL) and water (10 mL), the mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by a flash short column chromatography (pentane/Et<sub>2</sub>O 100:1) to give intermediate **VCP-I**, which was concentrated and directly used to the next step. To a solution of NsNH<sub>2</sub> (971.6 mg, 4.81 mmol) and K<sub>2</sub>CO<sub>3</sub> (885.1 mg, 6.40 mmol) in DMF (15 mL) was added **VCP-I** at 0 °C. The mixture was stirred for 4 h at 60 °C and cooled to room temperature, then quenched by saturated aqueous ammonium chloride solution and water then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 5:1). Recrystallization in PE/DCM to give **S26** (649.7 mg, 58%).

**S26**: light yellow solid, MP = 101-103 °C. TLC R<sub>f</sub> (PE/EA 5:1) = 0.21. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.37 (d, *J* = 8.8 Hz, 2H), 8.05 (d, *J* = 8.8 Hz, 2H), 5.45 (dd, *J* = 17.4, 10.7 Hz, 1H), 4.97 (d, *J* = 10.7 Hz, 1H), 4.87 (d, *J* = 17.4 Hz, 1H), 4.69 (t, *J* = 5.3 Hz, 1H), 3.07 (d, *J* = 5.3 Hz, 2H), 0.74-0.55 (m, 4H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 150.2, 146.1, 140.2, 128.4, 124.5, 113.2, 49.3, 22.6, 13.3. HRMS (ESI): calcd for C<sub>12</sub>H<sub>15</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 283.0747, found 283.0747.

To a solution of **S26** (282.7 mg, 1.00 mmol) and PPh<sub>3</sub> (524.3 mg, 2.00 mmol) in THF (10 mL) was added **S11** (153.4 mg, 1.56 mmol) under an argon atmosphere at 0 °C, and then DIAD (398.6 mg, 1.97 mmol) was added. The mixture was warmed up naturally and stirred for 12 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 100:1, 50:1 then 20:1) afforded the product **4g** (328.9 mg, 91%).

**4g**: white solid, MP = 103-104 °C. TLC R<sub>f</sub> (PE/EA 5:1) = 0.55. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.31 (d, *J* = 8.8 Hz, 2H), 7.95 (d, *J* = 8.8 Hz, 2H), 6.66 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.88 (dd, *J* = 17.3, 10.6 Hz, 1H), 5.30 (d, *J* = 17.2 Hz, 1H), 5.23 (d, *J* = 10.8 Hz, 1H), 5.02-4.88 (m, 3H), 4.18 (d, *J* = 6.8 Hz, 2H), 3.30 (s, 2H), 1.70 (s, 3H), 0.76-0.66 (m, 2H), 0.66-0.53 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 150.0, 146.7, 139.9, 136.5, 132.4, 128.6, 124.2, 123.2, 116.7, 113.1, 53.4, 44.1, 21.0, 19.8, 13.1. HRMS (ESI): calcd for C<sub>18</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 363.1373, found 363.1373.

#### Substrate (4h)



To a solution of **VCP-OH**<sup>6</sup> (400.3 mg, 4.08 mmol), PPh<sub>3</sub> (1.26 g, 4.80 mmol) and imidazole (409.6 mg, 6.01 mmol) in DCM (15 mL) was added I<sub>2</sub> (1.52 g, 5.99 mmol) at 0 °C. The mixture was stirred for 10 min at the same temperature and then quenched by 10 mL saturated sodium thiosulfate solution and water (10 mL). It was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by a flash short column chromatography (pentane/Et<sub>2</sub>O 100:1) to give intermediate **VCP-I**. It was concentrated and directly used to the next step.

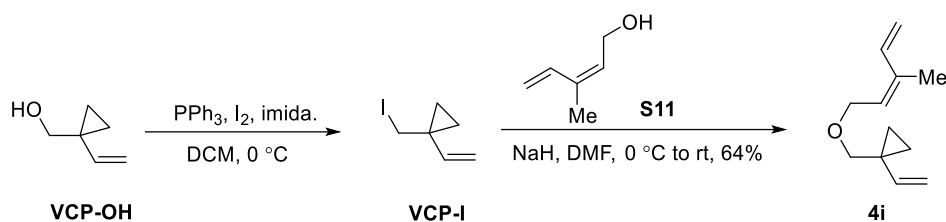
To a suspension of BsNH<sub>2</sub> (1.13 g, 4.79 mmol) and K<sub>2</sub>CO<sub>3</sub> (889.0 mg, 6.43 mmol) in DMF (15 mL) was added **VCP-I** at 0 °C. The mixture was stirred for 4 h at 60 °C and cooled to room temperature, then quenched by saturated aqueous ammonium chloride solution and water then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 20:1, 10:1). Recrystallization in PE/DCM afforded **S27** (644.3 mg, 50%).

**S27**: white solid, MP = 89-90 °C. TLC R<sub>f</sub> (PE/EA 5:1) = 0.42. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.72 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 8.8 Hz, 2H), 5.44 (dd, *J* = 17.4, 10.7 Hz, 1H), 4.96 (d, *J* = 10.7 Hz, 1H), 4.86 (d, *J* = 17.4 Hz, 1H), 4.61 (brs, 1H), 2.99 (d, *J* = 5.6 Hz, 2H), 0.71-0.50 (m, 4H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 140.5, 139.1, 132.5, 128.8, 127.7, 113.0, 49.0, 22.5, 13.3. HRMS (ESI): calcd for C<sub>12</sub>H<sub>15</sub>BrNO<sub>2</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 316.0001, found 316.0004.

To a solution of **S27** (315.4 mg, 1.00 mmol) and PPh<sub>3</sub> (525.2 mg, 2.00 mmol) in THF (10 mL) was added **S11** (125.9 mg, 1.28 mmol) under an argon atmosphere at 0 °C, and then DIAD (485.8 mg, 2.40 mmol) was added. The mixture was warmed up naturally and stirred for 11 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 400:1, 100:1) afforded the product **4h** (249.9 mg, 63%).

**4h**: light yellow solid, MP = 44-45 °C. TLC R<sub>f</sub> (PE/EA 5:1) = 0.73. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.64 (d, *J* = 9.0 Hz, 2H), 7.61 (d, *J* = 9.0 Hz, 2H), 6.65 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.88 (dd, *J* = 17.3, 10.6 Hz, 1H), 5.28 (d, *J* = 17.3 Hz, 1H), 5.20 (d, *J* = 10.8 Hz, 1H), 5.02 (t, *J* = 6.7 Hz, 1H), 4.97 (d, *J* = 17.2 Hz, 1H), 4.93 (dd, *J* = 10.6 Hz, 1H), 4.12 (d, *J* = 6.7 Hz, 2H), 3.24 (s, 2H), 1.72 (d, *J* = 1.2 Hz, 3H), 0.73-0.64 (m, 2H), 0.64-0.54 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 140.3, 139.8, 135.9, 132.6, 132.2, 130.0, 127.3, 124.0, 116.2, 112.8, 53.2, 44.1, 20.9, 19.8, 13.1. HRMS (ESI): calcd for C<sub>18</sub>H<sub>23</sub>BrNO<sub>2</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 396.0627, found 396.0625.

#### Substrate (4i)

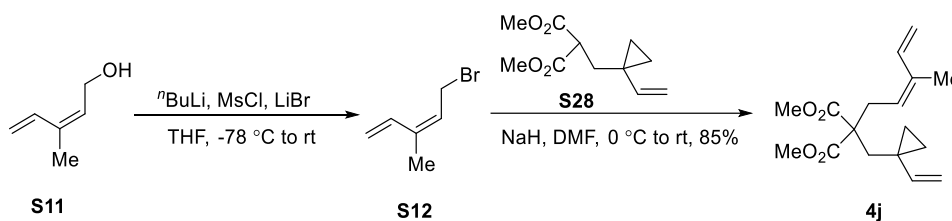


To a solution of **VCP-OH**<sup>6</sup> (198.8 mg, 2.03 mmol), PPh<sub>3</sub> (630.5 mg, 2.40 mmol) and imidazole (203.8 mg, 2.99 mmol) in DCM (8 mL) was added I<sub>2</sub> (766.0 mg, 3.02 mmol) at 0 °C. The mixture was stirred for 10 min at the same temperature. After quenched by saturated sodium thiosulfate solution and water, the mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by a flash short column chromatography (pentane/Et<sub>2</sub>O 100:1) to give intermediate **VCP-I**. It was concentrated and directly used to the next step.

To a solution of **S11** (295.5 mg, 3.01 mmol) in DMF (8 mL) was added NaH (120.1 mg, 60% weight in mineral oil, 3.00 mmol) at 0 °C. After stirred for 10 min under argon atmosphere, **VCP-I** was added. The mixture was warmed up naturally and stirred for 15 h. After quenched by saturated aqueous ammonium chloride solution and water then extracted with diethyl ether, the combined organic layer was washed with water brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 200:1, 100:1) to give **4i** (230.2 mg, 64%).

**4i**: yellow oil. TLC R<sub>f</sub> (PE/EA 50:1) = 0.30. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 6.72 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.66 (ddd, *J* = 17.4, 10.7, 1.7 Hz, 1H), 5.54 (t, *J* = 6.7 Hz, 1H), 5.27 (d, *J* = 17.3 Hz, 1H), 5.15 (d, *J* = 10.8 Hz, 1H), 5.06 (d, *J* = 17.4 Hz, 1H), 4.96 (d, *J* = 10.7 Hz, 1H), 4.14 (d, *J* = 6.7 Hz, 2H), 3.41 (d, *J* = 1.6 Hz, 2H), 1.86 (s, 3H), 0.76-0.59 (m, 4H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 141.9, 136.0, 133.4, 126.9, 115.3, 111.5, 75.3, 66.2, 22.7, 19.8, 12.8. HRMS (ESI): calcd for C<sub>12</sub>H<sub>22</sub>NO<sup>+</sup> ([M + NH<sub>4</sub>]<sup>+</sup>) 196.1696, found 196.1695.

#### Substrate (**4j**)



To a solution of **S11** (257.8 mg, 2.63 mmol) in THF (8 mL) was added <sup>n</sup>BuLi (1.8 mL, 1.6 M in hexane, 2.88 mmol) dropwise at -78 °C under an argon atmosphere. After stirred for 15 min, MsCl (349.6 mg, 3.05 mmol) was added. The reaction mixture was stirred for 20 min at -78 °C, and then LiBr (1.02 g, 11.75 mmol) was added. The reaction mixture was allowed to warm to room temperature and stirred for 3 h.

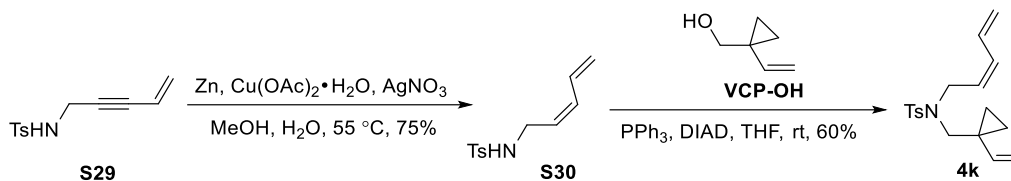
To a solution of **S28**<sup>1</sup> (422.3 mg, 1.99 mmol) in DMF (8 mL) was added NaH (123.0 mg, 60% weight in mineral oil, 3.08 mmol) at 0 °C. After stirred for 10 min, the freshly prepared diene bromide **S12** solution was transferred to the solution containing **S28**. The mixture was stirred for 24 h at room temperature and then quenched by saturated aqueous ammonium chloride solution and water. This reaction mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 100:1, 50:1) to give **4j** (494.1 mg, 85% yield).

**4j**: purplish oil. TLC R<sub>f</sub> (PE/EA 20:1) = 0.39. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 6.75 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.92 (dd, *J* = 17.2, 10.0, 1.7 Hz, 1H), 5.23 (d, *J* = 16.9 Hz, 1H), 5.19 (t, *J* = 7.6 Hz, 1H), 5.12 (d, *J* = 10.8 Hz, 1H), 4.90-4.74 (m, 2H), 3.66 (s, 6H), 2.91 (d, *J* = 7.6 Hz, 2H), 2.12 (s, 2H), 1.81 (s, 3H), 0.68-0.57 (m, 2H),



0.56-0.44 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{CN}$ ):  $\delta$  161.8, 132.2, 125.9, 124.0, 115.1, 104.8, 102.2, 48.5, 42.0, 30.7, 21.6, 10.7, 10.4, 4.0. HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{25}\text{O}_4^+$  ( $[\text{M} + \text{H}]^+$ ) 293.1747, found 293.1742.

#### Substrate (4k)

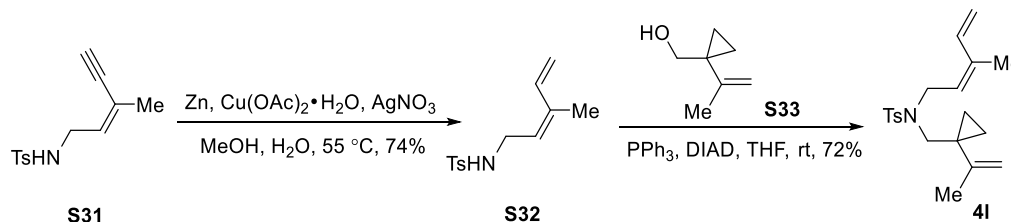


Zinc powder (2.72 g, 41.60 mmol) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated Zinc powder was washed with lots of water to neutral. To the above slurry of zinc in water (10 mL) was added  $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$  (412.3 mg, 2.07 mmol) at 0 °C. After stirred for 15 min,  $\text{AgNO}_3$  (354.9 mg, 2.09 mmol) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 50 mL round bottom flask, and then **S29**<sup>12</sup> (486.7 mg, 2.07 mmol), water (6 mL), MeOH (10 mL) were added. The reaction mixture was stirred for 17 h at 55 °C and filtered through celite by washing with EA. The reaction mixture was then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 5:1) to give **S30** (368.3 mg, 75%) as a white solid.

To a solution of **S30** (110.9 mg, 0.47 mmol) and  $\text{PPh}_3$  (246.4 mg, 0.94 mmol) in THF (5 mL) was added **VCP-OH** (61.8 mg, 0.63 mmol) under an argon atmosphere at 0 °C, and then DIAD (186.3 mg, 0.92 mmol) was added. The mixture was warmed up naturally and stirred for 8 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1, 30:1) afforded product **4k** (88.2 mg, 60%).

**4k**: light yellow solid, MP = 50-51 °C. TLC  $R_f$  (PE/EA 5:1) = 0.58.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 (d,  $J$  = 8.2 Hz, 2H), 7.28 (d,  $J$  = 8.2 Hz, 2H), 6.53 (ddd,  $J$  = 16.7, 10.7, 10.7 Hz, 1H), 5.99 (dd,  $J$  = 11.2, 11.2 Hz, 1H), 5.89 (d,  $J$  = 17.3, 10.7 Hz, 1H), 5.23 (d,  $J$  = 17.2 Hz, 1H), 5.20 (d,  $J$  = 10.4 Hz, 1H), 5.11 (dt,  $J$  = 10.8, 6.5 Hz, 1H), 4.99 (dd,  $J$  = 17.3, 1.0 Hz, 1H), 4.93 (dd,  $J$  = 10.7, 1.0 Hz, 1H), 4.12 (dd,  $J$  = 6.5, 1.5 Hz, 2H), 3.23 (s, 2H), 2.42 (s, 3H), 0.75-0.64 (m, 2H), 0.63-0.54 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.3, 140.5, 137.6, 131.9, 131.2, 129.7, 127.4, 126.4, 119.7, 112.5, 53.2, 44.4, 21.7, 20.8, 13.2. HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{24}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 318.1522, found 318.1523.

#### Substrate (4l)



Zinc powder (3.52 g, 53.88 mmol) was added to a round bottomed flask and treated with 3 M HCl. The liquid was decanted and freshly activated Zinc powder was washed with lots of water to neutral. To a slurry of zinc in water (10 mL) was added  $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$  (534.9 mg, 2.68 mmol) at 0 °C. After stirred for 15 min,  $\text{AgNO}_3$  (461.5 mg, 2.72 mmol) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 50 mL round bottomed flask, and then **S31**<sup>13</sup> (670.4 mg, 2.69 mmol), water (10 mL), MeOH (13 mL) were added. The reaction mixture was stirred for 24 h at 55 °C

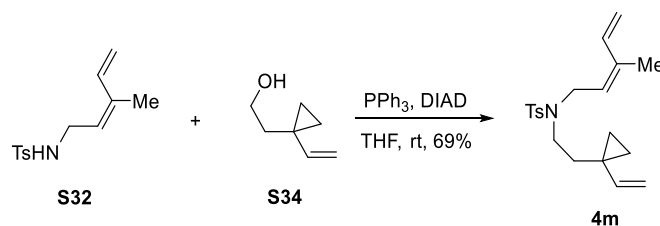
and filtered through celite by washing with EA. The reaction mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 10:1, 5:1) to give **S32** (498.4 mg, 74%).

**S32**: white solid, MP = 66-67 °C. TLC  $R_f$  (PE/EA 5:1) = 0.24.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.75 (d,  $J = 8.2$  Hz, 2H), 7.31 (d,  $J = 8.2$  Hz, 2H), 6.51 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.27 (d,  $J = 17.2$  Hz, 1H), 5.25 (t,  $J = 6.9$  Hz, 1H), 5.15 (d,  $J = 10.8$  Hz, 1H), 4.29 (brs, 1H), 3.71 (dd,  $J = 6.9, 6.9$  Hz, 2H), 2.44 (s, 3H), 1.76 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.6, 137.1, 137.0, 132.3, 129.9, 127.4, 123.8, 116.6, 40.2, 21.7, 19.8. HRMS (ESI): calcd for  $\text{C}_{13}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+$  ( $[\text{M} + \text{NH}_4]^+$ ) 269.1318, found 269.1317.

To a solution of **S32** (225.9 mg, 0.90 mmol) and  $\text{PPh}_3$  (472.5 mg, 1.80 mmol) in THF (9 mL) was added **S33**<sup>14</sup> (123.9 mg, 1.10 mmol) under an argon atmosphere at room temperature, and then DIAD (361.2 mg, 1.79 mmol) was added. The mixture was stirred for 34 h and then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1, 30:1 then 20:1) afforded product **4i** (224.2 mg, 72%).

**4i**: white solid, MP = 75-76 °C. TLC  $R_f$  (PE/EA 5:1) = 0.60.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.65 (d,  $J = 8.2$  Hz, 2H), 7.25 (d,  $J = 8.2$  Hz, 2H), 6.64 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.25 (d,  $J = 17.2$  Hz, 1H), 5.17 (d,  $J = 10.8$  Hz, 1H), 5.01 (t,  $J = 6.6$  Hz, 1H), 4.82 (s, 1H), 4.78 (s, 1H), 4.10 (d,  $J = 6.5$  Hz, 2H), 3.21 (s, 2H), 2.41 (s, 3H), 1.80 (s, 3H), 1.68 (s, 3H), 0.68-0.56 (m, 2H), 0.54-0.38 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  146.0, 143.1, 137.7, 135.3, 132.8, 129.5, 127.6, 124.8, 115.6, 113.0, 52.2, 43.9, 25.4, 21.6, 20.7, 19.8, 11.3. HRMS (ESI): calcd for  $\text{C}_{20}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1835, found 346.1834.

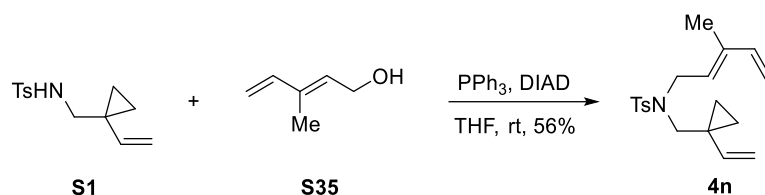
#### Substrate (4m)



To a solution of **S32** (201.7 mg, 0.80 mmol) and  $\text{PPh}_3$  (420.0 mg, 1.60 mmol) in THF (8 mL) was added **S34**<sup>15</sup> (115.5 mg, 1.03 mmol) under an argon atmosphere at room temperature, and then DIAD (320.9 mg, 1.59 mmol) was added. The mixture was stirred for 17 h and then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1, 30:1 then 20:1) afforded product **4m** (191.5 mg, 69%).

**4m**: light yellow solid, MP = 38-39 °C. TLC  $R_f$  (PE/EA 5:1) = 0.64.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 (d,  $J = 8.2$  Hz, 2H), 7.29 (d,  $J = 8.2$  Hz, 2H), 6.65 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.39 (dd,  $J = 17.4, 10.6$  Hz, 1H), 5.30 (d,  $J = 17.2$  Hz, 1H), 5.23 (t,  $J = 7.2$  Hz, 1H), 5.18 (d,  $J = 10.8$  Hz, 1H), 4.91 (d,  $J = 17.2$  Hz, 1H), 4.88 (d,  $J = 10.6$  Hz, 1H), 3.94 (d,  $J = 7.2$  Hz, 2H), 3.20-3.05 (m, 2H), 2.43 (s, 3H), 1.79 (s, 3H), 1.70-1.60 (m, 2H), 0.60-0.44 (m, 4H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 143.0, 137.2, 136.6, 132.4, 129.8, 127.3, 124.7, 116.3, 111.3, 45.7, 45.0, 35.3, 21.7, 20.6, 20.0, 14.3. HRMS (ESI): calcd for  $\text{C}_{20}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1835, found 346.1834.

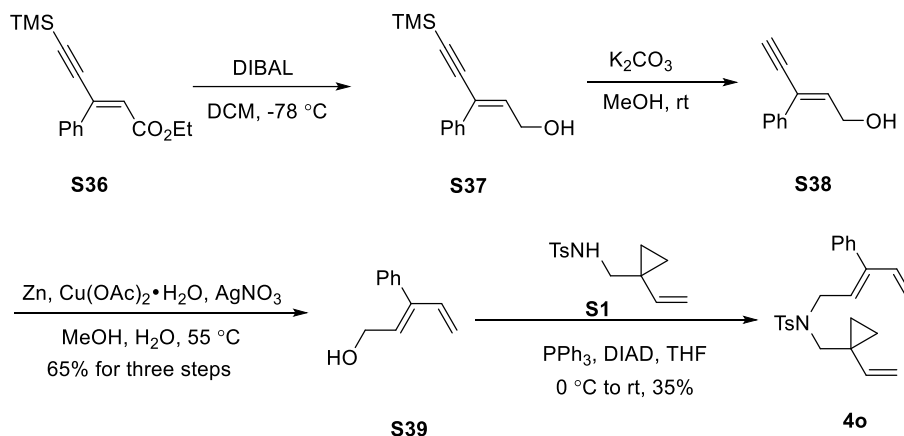
#### Substrate (4n)



To a solution of **S1** (175.5 mg, 0.70 mmol) and  $\text{PPh}_3$  (367.4 mg, 1.40 mmol) in THF (7 mL) was added **S35**<sup>16</sup> (91.8 mg, 0.94 mmol) under an argon atmosphere at room temperature, and then DIAD (283.1 mg, 1.40 mmol) was added. The mixture was stirred for 15 h and then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1, 20:1) afforded product **4n** (130.4 mg, 56%).

**4n**: colorless oil. TLC  $R_f$  (PE/EA 5:1) = 0.66.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.67 (d,  $J = 8.2$  Hz, 2H), 7.27 (d,  $J = 8.2$  Hz, 2H), 6.15 (dd,  $J = 17.2, 10.7$  Hz, 1H), 5.88 (dd,  $J = 17.2, 10.7$  Hz, 1H), 5.13 (t,  $J = 6.6$  Hz, 1H), 5.12 (d,  $J = 17.2$  Hz, 1H), 4.99 (d,  $J = 17.2$  Hz, 1H), 4.98 (d,  $J = 10.7$  Hz, 1H), 4.93 (d,  $J = 10.7$  Hz, 1H), 4.08 (d,  $J = 6.6$  Hz, 2H), 3.22 (s, 2H), 2.42 (s, 3H), 1.72 (s, 3H), 0.75-0.63 (m, 2H), 0.63-0.50 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 140.53, 140.50, 137.6, 136.4, 129.7, 127.4, 126.9, 112.6, 112.5, 53.3, 45.2, 21.6, 20.9, 13.2, 12.0. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{26}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 332.1679, found 332.1677.

#### Substrate (**4o**)



To a solution of **S36**<sup>17</sup> (721.9 mg, 2.65 mmol) in DCM (13.2 mL) was added DIBAL (16.6 mL, 1.0 M in hexanes, 6.3 mmol) at  $-78$  °C under an argon atmosphere. After stirred for 2 h at the same temperature, the reaction was quenched by saturated aqueous ammonium chloride solution and saturated potassium sodium tartrate tetrahydrate solution. The reaction mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated to give intermediate **S37** and directly used to the next step.

The suspension of **S37** and  $\text{K}_2\text{CO}_3$  (732.5 mg, 5.3 mmol) in MeOH (12.0 mL) was stirred for 3.5 h at room temperature. It was quenched by saturated aqueous ammonium chloride solution and water then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated to give intermediate **S38** and directly used to the next step.

Zinc powder (3.47 g, 20.1 mmol) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated Zinc powder was washed with lots of water to neutral. To a saturated aqueous  $\text{Cu(OAc)}_2 \cdot \text{H}_2\text{O}$  (527.4 mg, 2.64 mmol) was added the above slurry of zinc at 0 °C. After stirred for 15 min,  $\text{AgNO}_3$  (447.8 mg, 2.64 mmol) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 100 mL round bottom flask, and then **S38** obtained in the last step and water (20.0 mL) and MeOH (16.0 mL) were added under an argon atmosphere. The reaction

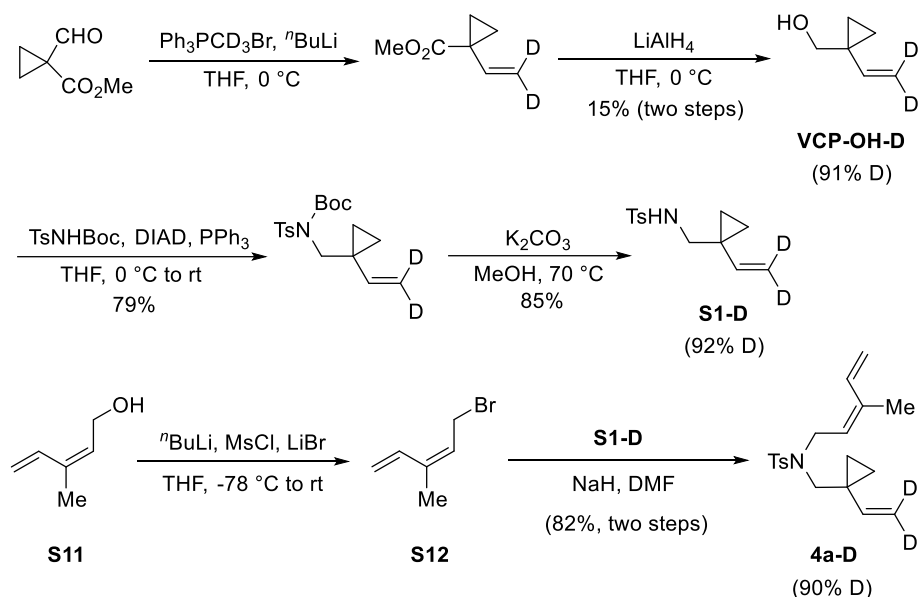
mixture was stirred for 11 h at 55 °C and filtered through celite by washing with EA. The resulting reaction mixture was then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 5:1) to give **S39** (275.9mg, 65%) as a yellow oil.

**S39**: yellow oil. TLC  $R_f$  (PE/EA 5:1) = 0.2.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35 (m, 3H), 7.16 – 7.10 (m, 2H), 6.58 (dd,  $J = 17.3, 10.5$  Hz, 1H), 5.89 (t,  $J = 6.9$  Hz, 1H), 5.14 (d,  $J = 10.5$  Hz, 1H), 4.83 (d,  $J = 17.3$  Hz, 1H), 4.05 (d,  $J = 6.9$  Hz, 2H), 1.37 (s, 1H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.5, 140.0, 136.7, 131.0, 129.4, 128.3, 127.5, 117.3, 60.3. HRMS (ESI): calcd for  $\text{C}_{11}\text{H}_{13}\text{O}^+$  ( $[\text{M} + \text{H}]^+$ ) 161.0961, found 161.0963.

To a solution of **S1** (175.3 mg, 0.64 mmol) and  $\text{PPh}_3$  (220.0 mg, 0.84 mmol) in THF (6 mL) was added **S39** (111.9 mg, 0.7 mmol) under an argon atmosphere at 0 °C, and then DIAD (0.17 mL, 0.84 mmol) was added. The mixture was warmed up naturally and stirred for 16 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1) afforded product **4o** (96.0 mg, 35%).

**4o**: colorless oil. TLC  $R_f$  (PE/EA 5:1) = 0.8.  $^1\text{H NMR}$  (400 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  7.59 (d,  $J = 8.3$  Hz, 2H), 7.42-7.33 (m, 3H), 7.29 (d,  $J = 8.0$  Hz, 2H), 7.14-7.09 (m, 2H), 6.41 (dd,  $J = 17.3, 10.6$  Hz, 1H), 5.76 (dd,  $J = 17.3, 10.7$  Hz, 1H), 5.47 (t,  $J = 6.3$  Hz, 1H), 5.06 (d,  $J = 10.5$  Hz, 1H), 4.93-4.71 (m, 3H), 3.78 (d,  $J = 6.3$  Hz, 2H), 3.14 (s, 2H), 2.41 (s, 3H), 0.57-0.53 (m, 2H), 0.46-0.42 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 143.1, 140.3, 139.6, 137.2, 136.2, 129.6, 129.5, 128.3, 128.2, 127.6, 127.3, 116.4, 112.3, 53.8, 46.3, 21.5, 21.0, 12.9. HRMS (ESI): calcd for  $\text{C}_{24}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 394.1835, found 394.1833.

#### Substrate (4a-D)



All the labelling ratios below were determined by  $^1\text{H NMR}$ .

To a solution of (bromo-1,2-methyl)triphenyl-1,7-phosphane- $d_3$ <sup>18</sup> (11.51 g, 31.95 mmol) in THF (30 mL) was added  $t\text{BuLi}$  (13.31 mL, 2.4 M in hexane, 31.95 mmol) at 0 °C under a nitrogen atmosphere. After stirred for 1 h, this mixture was added to a solution of methyl 1-formylcyclopropane-1-carboxylate<sup>19</sup> (3.72 g, 29.04 mmol) in THF (30 mL). The reaction mixture was then stirred for 0.5 h. After quenched by saturated aqueous ammonium chloride solution, the mixture was extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated to give a residue. *n*-Pentane was then added to the residue and stirred until white precipitation generated and this mixture was

filtered, washed by *n*-pentane and diethyl ether (*n*-pentane:diethyl ether = 20:1). The residue was concentrated to give crude methyl 1-(vinyl-2,2-*d*<sub>2</sub>)cyclopropane-1-carboxylate and directly used to the next step.

To a suspension of LiAlH<sub>4</sub> (1.38 g, 36.3 mmol) in THF (20 mL) was added a solution of the above crude product in THF (25 mL) dropwise at 0 °C under a nitrogen atmosphere. After stirred for 3 h at the same temperature, the reaction was quenched by saturated aqueous ammonium chloride solution and saturated potassium sodium tartrate tetrahydrate solution. The mixture was then extracted with diethyl ether. The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (*n*-pentane:diethyl ether 10:1, 5:1) to give **VCP-OH-D** (435.3 mg, 15% for 2 steps) as a yellow oil.

**VCP-OH-D**: yellow oil. TLC R<sub>f</sub> (PE/EA 5:1) = 0.23. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 5.67-5.56 (m, 1H), 3.56 (s, 2H), 1.89 (s, 1H), 0.71-0.66 (m, 2H), 0.66-0.61 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 141.1, 67.9, 25.1, 12.3. HRMS (EI): calcd for C<sub>6</sub>H<sub>8</sub>D<sub>2</sub>O<sup>+</sup> ([M]<sup>+</sup>) 100.0852, found 100.0850.

To a solution of *tert*-butyl tosylcarbamate (1.27 g, 4.67 mmol), triphenylphosphine (2.04 g, 7.78 mmol) and **VCP-OH-D** (389.8 mg, 3.89 mmol) in THF (15 mL) was added DIAD (1.54 mL, 7.78 mmol) dropwise at 0 °C under a nitrogen atmosphere. The mixture was warmed up naturally and stirred for 24 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1, 20:1) afforded the product *tert*-butyl tosyl((1-(vinyl-2,2-*d*<sub>2</sub>)cyclopropyl)methyl)carbamate (1.0919 g, 79%) as a white solid.

To a solution of *tert*-butyl tosyl((1-(vinyl-2,2-*d*<sub>2</sub>)cyclopropyl)methyl)carbamate (1.0919 g, 3.09 mmol) in methanol (15 mL) was added potassium carbonate (1.28 g, 9.27 mmol). The mixture was stirred to reflux at 70 °C for 16 h. After filtered, the residue was purified by column chromatography (PE/EA 10:1, with 2 drop of triethylamine in every 100 mL eluent) to give **S1-D** (666.3 mg, 85%) as a white solid.

**S1-D**: white solid. MP = 57-60 °C. TLC R<sub>f</sub> (PE/EA 5:1) = 0.27. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.42 (s, 1H), 4.46 (s, 1H), 2.97 (d, *J* = 5.6 Hz, 2H), 2.43 (s, 3H), 0.62 (m, 2H), 0.61 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 143.4, 140.4, 136.9, 129.8, 127.2, 48.8, 22.3, 21.6, 13.1. HRMS (ESI): calcd for C<sub>13</sub>H<sub>16</sub>D<sub>2</sub>NO<sub>2</sub>S<sup>+</sup> ([M + H]<sup>+</sup>) 254.1178, found 254.1185.

To a solution of **S11**<sup>7</sup> (301.3 mg, 3.07 mmol) in THF (15 mL) was added <sup>n</sup>BuLi (1.41 mL, 2.4 M in hexane, 3.38 mmol) dropwise at -78 °C under a nitrogen atmosphere. After stirred for 15 min, MsCl (0.26 mL, 3.38 mmol) was added. The reaction mixture was stirred for 20 min at -78 °C, and then LiBr (799.9 mg, 9.21 mmol) was added. The reaction mixture was allowed to warm to room temperature and stirred for 3 h, generating **S12**, which was used immediately in the next step.

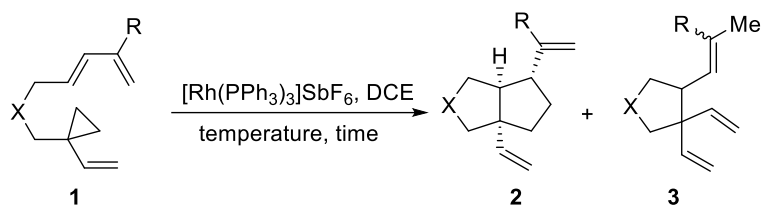
To a solution of **S1-D** (598.3 mg, 2.36 mmol) in DMF (12 mL) was added NaH (188.8 mg, 60% weight in mineral oil, 4.72 mmol) at room temperature under a nitrogen atmosphere. After stirred for 5 min, the freshly prepared diene **S12** solution was transferred to the solution containing **S1-D**. The mixture was stirred for 20 h. After quenched by saturated aqueous ammonium chloride solution and water, the mixture was extracted with diethyl ether (4 × 10 mL). The combined organic layer was washed with water and brine, dried over anhydrous sodium sulphate, filtered, concentrated and purified by column chromatography (PE/EA 50:1) to give **4a-D** (641.6 mg, 82% yield for 2 steps) as a white solid.

**4a-D**: white solid. MP = 32-33 °C. TLC R<sub>f</sub> (PE/EA 5:1) = 0.58. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.66 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 6.64 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.88 (s, 1H), 5.25 (d, *J* = 17.2 Hz, 1H), 5.16 (d, *J* = 10.8 Hz, 1H), 5.05 (t, *J* = 6.6 Hz, 1H), 4.10 (d, *J* = 6.7 Hz, 2H), 3.23 (s, 2H), 2.41 (s, 3H), 1.76-1.67 (m, 3H), 0.70-0.65 (m, 2H), 0.60-0.55 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 143.1, 140.3, 137.5,

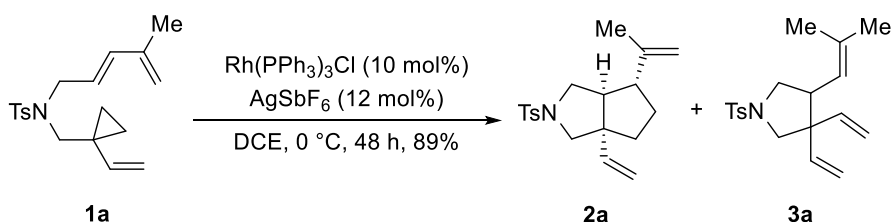
135.2, 132.7, 129.5, 127.3, 124.6, 115.6, 53.1, 44.1, 21.5, 20.7, 19.6, 13.1. HRMS (ESI): calcd for  $C_{19}H_{24}D_2NO_2S^+$  ( $[M + H]^+$ ) 334.1804, found 334.1798.

### 3.2 [3+2] Cycloadditions

The NMR spectrum of **3a**<sup>20</sup> (cycloisomerization product of **1a**) was previously reported. The other cycloisomerization products were proposed by checking the NMR of the reactions, by analogy to the characteristic NMR data of **3a**. The present reaction has limited use because several of them gave inseparable mixtures (see below) and here we only report either the major [3+2] products if they can be isolated or the mixture of inseparable **2** and **3**.



#### Product (2a)

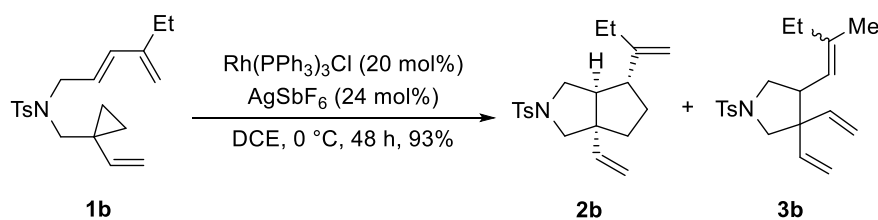


To a solution of  $Rh(PPh_3)_3Cl$  (9.4 mg, 0.01 mmol) and  $AgSbF_6$  (4.2 mg, 0.012 mmol) was added anhydrous DCE (1.0 mL). The mixture was stirred at room temperature for 10 min. Then the solution of **1a** (33.1 mg, 0.1 mmol) in DCE (1 mL) was added at 0 °C. The reaction mixture was stirred for 48 h at 0 °C then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1, 20:1) afforded **2a** + **3a** (28.7 mg, 87%). The ratio (**2a**:**3a**) was 18:1, determined by  $^1H$  NMR. Here we just report the  $^1H$  NMR and  $^{13}C$  NMR of major product.

Run 2:  $Rh(PPh_3)_3Cl$  (9.3 mg, 0.01 mmol),  $AgSbF_6$  (4.1 mg, 0.012 mmol), **1a** (33.2 mg, 0.1 mmol), **2a** + **3a** (29.9 mg, 90%). So the average yield of two runs was 89%.

**2a**: white solid. MP = 48-51 °C. TLC  $R_f$  (PE/EA 10:1) = 0.31.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.68 (d,  $J$  = 8.1 Hz, 2H), 7.33 (d,  $J$  = 8.1 Hz, 2H), 5.77 (dd,  $J$  = 17.4, 10.4 Hz, 1H), 4.91 (d,  $J$  = 17.4 Hz, 1H), 4.90 (d,  $J$  = 10.4 Hz, 1H), 4.69 (s, 1H), 4.65 (s, 1H), 3.23 (d,  $J$  = 9.2 Hz, 1H), 3.22 (d,  $J$  = 9.6 Hz, 1H), 2.87 (dd,  $J$  = 9.6, 7.1 Hz, 1H), 2.75 (d,  $J$  = 9.5 Hz, 1H), 2.44 (s, 3H), 2.31-2.21 (m, 1H), 2.12 (dd,  $J$  = 8.4, 7.2 Hz, 1H), 1.98-1.89 (m, 1H), 1.84-1.69 (m, 2H), 1.66 (s, 3H), 1.58-1.43 (m, 1H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  146.2, 143.7, 143.2, 132.2, 129.7, 128.1, 111.8, 110.5, 58.5, 55.8, 54.6, 53.2, 52.6, 37.0, 31.1, 21.7, 20.4. HRMS (ESI): calcd for  $C_{19}H_{26}NO_2S^+$  ( $[M + H]^+$ ) 332.1679, found 332.1677.

#### Product (2b)

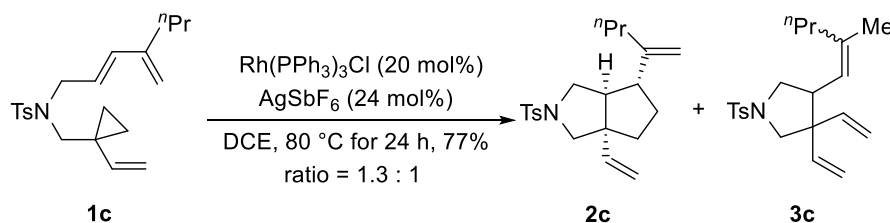


To a solution of  $\text{Rh(PPh}_3)_3\text{Cl}$  (18.5 mg, 0.02 mmol) and  $\text{AgSbF}_6$  (8.3 mg, 0.024 mmol) was added anhydrous DCE (1.0 mL). The mixture was stirred at room temperature for 10 min. Then the solution of **1b** (34.6 mg, 0.1 mmol) in DCE (1 mL) was added at 0 °C. The reaction mixture was stirred for 48 h at 0 °C then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1, 20:1) afforded **2b** (31.5 mg, 91%). The ratio (**2b**:**3b**) was 16:1, determined by  $^1\text{H NMR}$ . Here we just report the  $^1\text{H NMR}$  and  $^{13}\text{C NMR}$  of major product.

Run 2:  $\text{Rh(PPh}_3)_3\text{Cl}$  (18.4 mg, 0.02 mmol),  $\text{AgSbF}_6$  (8.2 mg, 0.024 mmol), **1b** (34.6 mg, 0.1 mmol), **2b** + **3b** (32.8 mg, 95%). So the average yield of two runs was 93%.

**2b**: white solid. MP = 44-45°C. TLC  $R_f$  (PE/EA 10:1) = 0.32.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 (d,  $J$  = 8.0 Hz, 2H), 7.33 (d,  $J$  = 8.0 Hz, 2H), 5.78 (dd,  $J$  = 17.2, 10.9 Hz, 1H), 4.92 (d,  $J$  = 17.2 Hz, 1H), 4.92 (d,  $J$  = 10.9 Hz, 1H), 4.71 (d,  $J$  = 1.2 Hz, 1H), 4.69 (d,  $J$  = 1.2 Hz, 1H), 3.23 (d,  $J$  = 9.6 Hz, 1H), 3.22 (dd,  $J$  = 9.6, 1.2 Hz, 1H), 2.89 (dd,  $J$  = 9.6, 6.8 Hz, 1H), 2.77 (d,  $J$  = 9.6 Hz, 1H), 2.44 (s, 3H), 2.34-2.23 (m, 1H), 2.19-2.11 (m, 1H), 2.00-1.89 (m, 3H), 1.87-1.79 (m, 1H), 1.78-1.68 (m, 1H), 1.57-1.43 (m, 1H), 1.01 (t,  $J$  = 7.2 Hz, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.2, 143.7, 143.3, 132.2, 129.7, 128.1, 111.7, 107.7, 58.5, 55.7, 53.9, 53.3, 53.0, 37.0, 31.7, 27.0, 21.7, 12.6. HRMS (ESI): calcd for  $\text{C}_{20}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1835, found 346.1839.

#### Products (**2c** and **3c**)

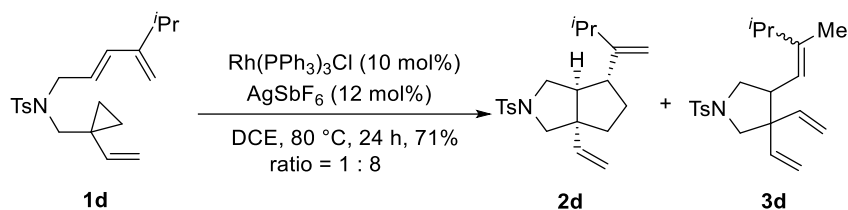


To a solution of  $\text{Rh(PPh}_3)_3\text{Cl}$  (18.5 mg, 0.02 mmol) and  $\text{AgSbF}_6$  (8.3 mg, 0.024 mmol) was added anhydrous DCE (1.0 mL). The mixture was stirred at room temperature for 10 min. Then the solution of **1c** (36.0 mg, 0.1 mmol) in DCE (1 mL) was added at 80 °C. The reaction mixture was stirred for 24 h at 80 °C. It was concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1) afforded the inseparable mixture of **2c** and **3c** (28.2 mg, 78%). The ratio (**2c**:**3c**) was 1.3:1, determined by  $^1\text{H NMR}$ .

Run 2:  $\text{Rh(PPh}_3)_3\text{Cl}$  (18.5 mg, 0.02 mmol),  $\text{AgSbF}_6$  (8.2 mg, 0.024 mmol), **1c** (35.9 mg, 0.1 mmol), **2c** + **3c** (27.0 mg, 75%). So the average yield of two runs was 77%.

**2c** + **3c**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.75.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.73 (d,  $J$  = 8.4 Hz, 2H), 7.68 (d,  $J$  = 8.0 Hz, 2H), 7.33 (d,  $J$  = 7.6 Hz, 4H), 5.76 (dd,  $J$  = 17.6, 10.8 Hz, 1H), 5.72-5.59 (m, 2H), 5.10-5.03 (m, 2H), 4.99-4.86 (m, 4H), 4.71 (d,  $J$  = 10.0 Hz, 1H), 3.46 (d,  $J$  = 10.0 Hz, 2H), 3.28 (d,  $J$  = 10.0 Hz, 1H), 3.23-3.16 (m, 2H), 3.01 (t,  $J$  = 9.2 Hz, 1H), 2.84 (dd,  $J$  = 9.6, 6.8 Hz, 1H), 2.81-2.72 (m, 2H), 2.44 (s, 6H), 2.20-2.10 (m, 1H), 2.10-2.00 (m, 1H), 2.00-1.84 (m, 5H), 1.74-1.64 (m, 2H), 1.64-1.55 (m, 2H), 1.51 (s, 3H), 1.48 (s, 3H), 1.32 (q,  $J$  = 7.2 Hz, 2H), 0.92 (t,  $J$  = 7.6 Hz, 3H), 0.80 (t,  $J$  = 7.2 Hz, 3H).

#### Products (**2d** and **3d**)

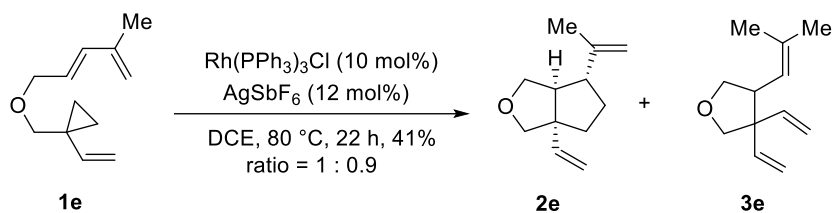


To a solution of  $\text{Rh(PPh}_3)_3\text{Cl}$  (9.2 mg, 0.01 mmol) and  $\text{AgSbF}_6$  (4.2 mg, 0.012 mmol) was added anhydrous DCE (1.0 mL). The mixture was stirred at room temperature for 10 min. Then the solution of **1d** (36.0 mg, 0.1 mmol) in DCE (1 mL) was added at 80 °C. The reaction mixture was stirred for 24 h at 80 °C. The reaction solution was concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1) afforded the inseparable mixture of **2d** and **3d** (26.4 mg, 73%). The ratio (**2d**:**3d**) was 1:8 determined by  $^1\text{H NMR}$ . Here we just report the  $^1\text{H NMR}$  of major product.

Run 2:  $\text{Rh(PPh}_3)_3\text{Cl}$  (9.2 mg, 0.01 mmol),  $\text{AgSbF}_6$  (4.2 mg, 0.012 mmol), **1d** (35.9 mg, 0.1 mmol), **2d** + **3d** (24.3 mg, 68%). So the average yield of two runs was 71%.

**3d**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.58.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.74 (d,  $J = 8.2$  Hz, 2H), 7.33 (d,  $J = 8.2$  Hz, 2H), 5.68 (dd,  $J = 17.6, 10.8$  Hz, 1H), 5.63 (dd,  $J = 17.6, 10.8$  Hz, 1H), 5.06 (d,  $J = 10.8$  Hz, 1H), 5.05 (d,  $J = 10.8$  Hz, 1H), 4.94 (d,  $J = 17.6$  Hz, 1H), 4.91 (d,  $J = 17.6$  Hz, 1H), 4.73 (d,  $J = 9.6$  Hz, 1H), 3.52-3.42 (m, 2H), 3.29 (d,  $J = 9.8$  Hz, 1H), 3.00 (dd,  $J = 9.8, 8.8$  Hz, 1H), 2.74 (dd,  $J = 16.8, 8.8$  Hz, 1H), 2.44 (s, 3H), 2.13 (hept,  $J = 6.8$  Hz, 1H), 1.49 (s, 3H), 0.90 (d,  $J = 6.8$  Hz, 6H).

#### Products (2e and 3e)



To a solution of  $\text{Rh(PPh}_3)_3\text{Cl}$  (18.7 mg, 0.02 mmol) and  $\text{AgSbF}_6$  (8.3 mg, 0.024 mmol) was added anhydrous DCE (2.0 mL). The mixture was stirred at room temperature for 10 min. Then the solution of **1e** (35.6 mg, 0.2 mmol) in DCE (2 mL) was added. The reaction mixture was stirred for 22 h at 80 °C. The reaction solution was concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 200:1) afforded the inseparable mixture of **2e** and **3e** (14.1 mg, 40%). The ratio (**2e**:**3e**) was 1:0.9 determined by  $^1\text{H NMR}$ .

Run 2:  $\text{Rh(PPh}_3)_3\text{Cl}$  (18.8 mg, 0.02 mmol),  $\text{AgSbF}_6$  (8.4 mg, 0.024 mmol), **1e** (35.5 mg, 0.2 mmol), **2e** + **3e** (14.6 mg, 41%). So the average yield of two runs was 41%.

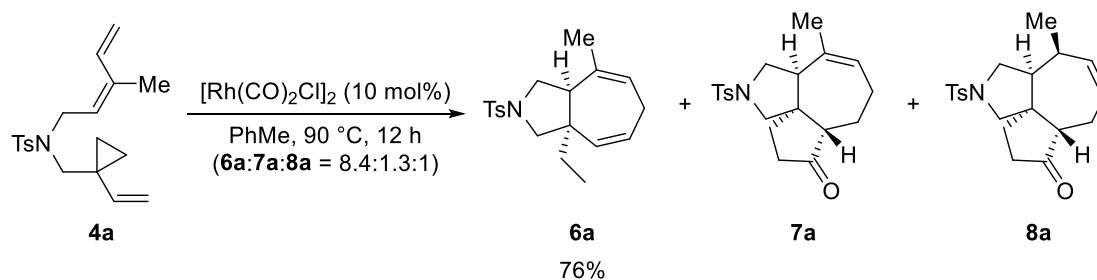
**2e** + **3e**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.26.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  5.99-5.89 (m, 1.6H), 5.85 (dd,  $J = 17.5, 10.8$  Hz, 1H), 5.23 (d,  $J = 10.8$  Hz, 1H), 5.15 (d,  $J = 10.8$  Hz, 1H), 5.11 (d,  $J = 4.0$  Hz, 0.9H), 5.07 (d,  $J = 5.6$  Hz, 0.9H), 5.02 (d,  $J = 10.4$  Hz, 0.9H), 5.00 (d,  $J = 17.0$  Hz, 1H), 4.97 (d,  $J = 11.2$  Hz, 0.9H), 4.72 (s, 0.7H), 4.71 (s, 0.7H), 3.98 (d,  $J = 7.9$  Hz, 0.9H), 3.95 (d,  $J = 8.2$  Hz, 1H), 3.78 (d,  $J = 8.5$  Hz, 1H), 3.74-3.69 (m, 1.9H), 3.52 (dd,  $J = 8.7, 8.7$  Hz, 1H), 3.47 (d,  $J = 8.8$  Hz, 0.7H), 3.08 (dd,  $J = 17.2, 9.5$  Hz, 1H), 2.37-2.21 (m, 1.7H), 2.08-2.01 (m, 1H), 1.84-1.77 (m, 1H), 1.72 (s, 5.5H), 1.66 (s, 3H), 1.64-1.58 (m, 3H).



### 3.3 [4+3] Cycloadditions

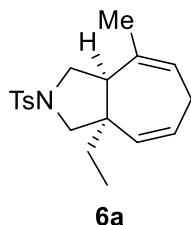
#### General procedure:

A solution of substrate (0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous toluene (2 mL, 0.05 M) was stirred at 90 °C for 12 h under an argon atmosphere. Then the reaction mixture was cooled to room temperature. It was concentrated in vacuo. Purification of the residue through column chromatography on silica gel afforded the corresponding products.



We point out here that, the present [4+3] reaction could have side reactions such as CO (from the used catalyst) insertion, which decreased the reaction yields of the target reaction slightly. For example, reaction of **4a** gave products **6a**, **7a**, and **8a** with a ratio of 8.4:1.3:1 (**6a:7a:8a**). These side products became the major products when carrying out the reactions under the CO atmosphere. These results (together with their characterization data) will be reported in the future. Therefore, we did not separate these possible polar byproducts from the reaction system in for all [4+3] reactions carried out in this investigation.

#### Product (6a):



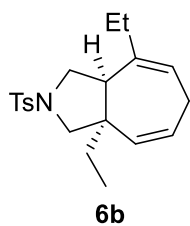
Eluted with PE/EA 40:1, 20:1

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4a** (33.1 mg, 0.1 mmol), **6a** (25.2 mg, 76%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4a** (33.3 mg, 0.1 mmol), **6a** (25.0 mg, 75%). So the average yield of two runs was 76%.

**6a**: white solid, MP = 74-77 °C. TLC  $R_f$  (PE/EA 10:1) = 0.33.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.71 (d,  $J$  = 7.8 Hz, 2H), 7.30 (d,  $J$  = 7.8 Hz, 2H), 5.39 (dd,  $J$  = 5.0, 5.0 Hz, 1H), 5.31 (ddd,  $J$  = 12.0, 5.2, 5.2 Hz, 1H), 4.99 (d,  $J$  = 12.0 Hz, 1H), 3.63 (dd,  $J$  = 8.0, 8.0 Hz, 1H), 3.33 (d,  $J$  = 9.6 Hz, 1H), 3.24 (dd,  $J$  = 11.4, 9.4 Hz, 1H), 2.94 (d,  $J$  = 9.6 Hz, 1H), 2.77-2.60 (m, 2H), 2.43 (s, 3H), 2.21 (dd,  $J$  = 11.4, 8.0 Hz, 1H), 1.68 (d,  $J$  = 1.6 Hz, 3H), 1.67 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 1.33 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 0.83 (dd,  $J$  = 7.5, 7.5 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.3, 135.0, 133.2, 131.9, 129.7, 128.5, 127.6, 123.9, 61.3, 52.9, 51.3, 49.5, 30.5, 29.4, 27.8, 21.7, 10.0. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{26}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 332.1679, found 332.1672.

#### Product (6b):



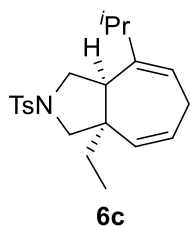
Eluted with PE/EA 50:1, 40:1

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4b** (34.7 mg, 0.1 mmol), **6b** (26.7 mg, 77%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4b** (34.8 mg, 0.1 mmol), **6b** (28.3 mg, 81%). So the average yield of two runs was 79%.

**6b**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.28.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.71 (d,  $J$  = 8.3 Hz, 2H), 7.30 (d,  $J$  = 8.3 Hz, 2H), 5.39 (dd,  $J$  = 4.8, 4.8 Hz, 1H), 5.25 (ddd,  $J$  = 12.1, 4.8, 4.8 Hz, 1H), 4.98 (dq,  $J$  = 12.1, 1.8 Hz, 1H), 3.57 (dd,  $J$  = 9.0, 7.8 Hz, 1H), 3.32 (d,  $J$  = 9.9 Hz, 1H), 3.29 (dd,  $J$  = 11.6, 9.0 Hz, 1H), 2.96 (d,  $J$  = 9.9 Hz, 1H), 2.79-2.61 (m, 2H), 2.44 (s, 3H), 2.20 (dd,  $J$  = 11.6, 7.8 Hz, 1H), 1.93 (q,  $J$  = 7.4 Hz, 2H), 1.60 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 1.33 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 0.93 (t,  $J$  = 7.4 Hz, 3H), 0.83 (dd,  $J$  = 7.6, 7.6 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.3, 137.7, 134.9, 132.7, 129.6, 127.9, 127.6, 123.2, 61.3, 51.8, 51.6, 49.4, 34.1, 31.0, 29.6, 21.7, 13.3, 10.0. HRMS (ESI): calcd for  $\text{C}_{20}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1835, found 346.1833.

**Product (6c):**



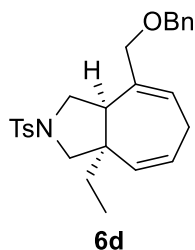
Eluted with PE/EA 50:1, 20:1, concentrated then purified further by preparative TLC (PE/EA 50:1)

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4c** (36.1 mg, 0.1 mmol), **6c** (14.5 mg, 40%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (4.0 mg, 0.01 mmol), **4c** (36.2 mg, 0.1 mmol), **6c** (15.6 mg, 43%). So the average yield of two runs was 42%.

**6c**: colorless oil. TLC  $R_f$  (PE/EA 10:1) = 0.37.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.71 (d,  $J$  = 8.1 Hz, 2H), 7.30 (d,  $J$  = 8.1 Hz, 2H), 5.42 (dd,  $J$  = 6.0, 4.0 Hz, 1H), 5.19 (ddd,  $J$  = 12.0, 4.2, 4.2 Hz, 1H), 4.98 (d,  $J$  = 12.0 Hz, 1H), 3.51 (dd,  $J$  = 8.4, 8.4 Hz, 1H), 3.32 (d,  $J$  = 9.6 Hz, 1H), 3.29 (d,  $J$  = 9.6 Hz, 1H), 2.94 (d,  $J$  = 9.6 Hz, 1H), 2.82-2.60 (m, 2H), 2.43 (s, 3H), 2.23-2.07 (m, 2H), 1.60 (dq,  $J$  = 15.2, 7.6 Hz, 1H), 1.33 (dq,  $J$  = 15.2, 7.6 Hz, 1H), 0.91 (d,  $J$  = 6.8 Hz, 6H), 0.83 (dd,  $J$  = 7.5, 7.5 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.3, 141.8, 134.9, 132.2, 129.6, 127.6, 127.4, 122.8, 61.3, 51.9, 50.1, 49.3, 38.3, 31.6, 29.8, 22.0, 21.9, 21.7, 10.1. HRMS (ESI): calcd for  $\text{C}_{21}\text{H}_{30}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 360.1992, found 360.1990.

**Product (6d):**



Eluted with PE/EA 15:1, 10:1

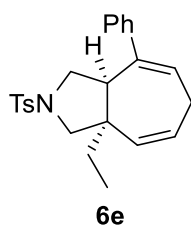
Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4d** (43.6 mg, 0.1 mmol), **6d** (30.5 mg, 70%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4d** (43.6 mg, 0.1 mmol), **6d** (30.7 mg, 70%). So the average yield of two runs was 70%.

**6d**: colorless oil. TLC  $R_f$  (PE/EA 5:1) = 0.30.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 (d,  $J$  = 8.2 Hz, 2H), 7.39-7.21 (m, 7H), 5.70 (dd,  $J$  = 4.6, 4.6 Hz, 1H), 5.34 (ddd,  $J$  = 12.0, 4.6, 4.6 Hz, 1H), 5.13 (dq,  $J$  = 12.0, 1.6 Hz, 1H), 4.41 (s, 2H), 3.79 (s, 2H), 3.62 (dd,  $J$  = 8.8, 8.0 Hz, 1H), 3.37 (d,  $J$  = 9.5 Hz, 1H), 3.31 (dd,  $J$  = 11.7, 9.0 Hz, 1H), 2.91 (d,  $J$  = 9.5 Hz, 1H), 2.87-2.74 (m, 2H), 2.47-2.34 (m, 1H), 2.41 (s, 3H), 1.62 (dq,  $J$  = 14.2, 7.6 Hz, 1H), 1.32 (dq,  $J$  = 14.2, 7.6 Hz, 1H), 0.83 (dd,  $J$  = 7.6, 7.6 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{CN}$ ):  $\delta$  144.7, 139.7, 135.2, 134.2, 134.1, 130.6, 129.3, 128.9, 128.5, 128.43, 128.41, 128.3, 77.7, 72.2, 61.8, 52.7, 50.2, 49.7, 31.2, 30.2, 21.5, 10.0. HRMS (ESI): calcd for  $\text{C}_{26}\text{H}_{32}\text{NO}_3\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 438.2097, found 438.2096.

We proposed the dq (5.13 ppm) split in the  $^1\text{H}$  NMR comes from the couplings of the adjacent alkenyl CH and the bridgehead methyl group.

**Product (6e):**



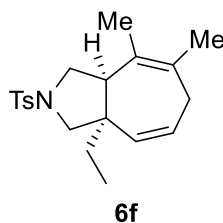
Eluted with PE/EA 50:1, 20:1.

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.8 mg, 0.01 mmol), **4e** (39.3 mg, 0.1 mmol), **6e** (22.5 mg, 57%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4e** (39.3 mg, 0.1 mmol), **6e** (23.3 mg, 59%). So the average yield of two runs was 58%.

**6e**: white solid, MP = 132-134 °C. TLC  $R_f$  (PE/EA 5:1) = 0.39.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.72 (d,  $J$  = 8.2 Hz, 2H), 7.31 (d,  $J$  = 8.2 Hz, 2H), 7.29-7.19 (m, 3H), 7.18-7.11 (m, 2H), 5.82 (dd,  $J$  = 5.0, 5.0 Hz, 1H), 5.35 (ddd,  $J$  = 12.0, 4.8, 4.8 Hz, 1H), 5.10 (dq,  $J$  = 12.0, 1.6 Hz, 1H), 3.68 (dd,  $J$  = 9.2, 7.8 Hz, 1H), 3.46 (dd,  $J$  = 11.6, 9.2 Hz, 1H), 3.38 (d,  $J$  = 9.8 Hz, 1H), 3.00 (d,  $J$  = 9.8 Hz, 1H), 2.96-2.85 (m, 2H), 2.76 (dd,  $J$  = 11.6, 7.8 Hz, 1H), 2.44 (s, 3H), 1.66 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 1.41 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 0.84 (dd,  $J$  = 7.5, 7.5 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.4, 143.4, 137.5, 134.8, 133.2, 129.7, 128.9, 128.4, 127.6, 127.3, 127.0, 126.3, 61.4, 52.1, 51.8, 49.7, 31.1, 30.0, 21.7, 10.1. HRMS (ESI): calcd for  $\text{C}_{24}\text{H}_{28}\text{NO}_3\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 394.1835, found 394.1832.

**Product (6f):**



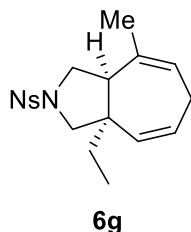
Eluted with PE/EA 50:1, 20:1.

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4f** (34.5 mg, 0.1 mmol), **6f** (20.4 mg, 59%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (4.0 mg, 0.01 mmol), **4f** (34.5 mg, 0.1 mmol), **6f** (21.1 mg, 61%). So the average yield of two runs was 60%.

**6f**: white solid, MP = 75-78 °C. TLC  $R_f$  (PE/EA 5:1) = 0.52.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.70 (d,  $J$  = 8.2 Hz, 2H), 7.29 (d,  $J$  = 8.2 Hz, 2H), 5.24 (ddd,  $J$  = 12.0, 5.5, 4.3 Hz, 1H), 4.96 (dq,  $J$  = 12.0, 1.6 Hz, 1H), 3.53 (dd,  $J$  = 8.8, 8.0 Hz, 1H), 3.30 (d,  $J$  = 8.8 Hz, 1H), 3.27 (d,  $J$  = 9.6 Hz, 1H), 2.94 (d,  $J$  = 9.6 Hz, 1H), 2.76 (d,  $J$  = 21.6 Hz, 1H), 2.58 (dd,  $J$  = 21.6, 5.4 Hz, 1H), 2.43 (s, 3H), 2.23 (dd,  $J$  = 11.2, 8.0 Hz, 1H), 1.65 (s, 3H), 1.60 (s, 3H), 1.61-1.53 (m, 1H), 1.32 (dq,  $J$  = 14.9, 7.5 Hz, 1H), 0.81 (dd,  $J$  = 7.5, 7.5 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 134.9, 132.2, 130.1, 129.6, 127.7, 127.6, 124.0, 60.8, 54.3, 50.4, 49.2, 36.3, 30.7, 23.7, 22.9, 21.7, 9.9. HRMS (ESI): calcd for  $\text{C}_{20}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1835, found 346.1835.

**Product (6g):**



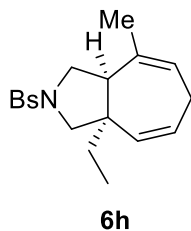
Eluted with PE/EA 50:1, 20:1

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (4.0 mg, 0.01 mmol), **4g** (36.1 mg, 0.1 mmol), **6g** (25.4 mg, 70%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4g** (36.1 mg, 0.1 mmol), **6g** (24.6 mg, 68%). So the average yield of two runs was 69%.

**6g**: white solid, MP = 110-113 °C. TLC  $R_f$  (PE/EA 5:1) = 0.52.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.36 (d,  $J$  = 8.8 Hz, 2H), 8.01 (d,  $J$  = 8.8 Hz, 2H), 5.42 (dd,  $J$  = 4.7, 4.7 Hz, 1H), 5.28 (ddd,  $J$  = 12.0, 4.8, 4.8 Hz, 1H), 4.93 (dq,  $J$  = 12.0, 1.7 Hz, 1H), 3.68 (dd,  $J$  = 8.7, 7.9 Hz, 1H), 3.35 (d,  $J$  = 9.8 Hz, 1H), 3.24 (dd,  $J$  = 11.6, 8.7 Hz, 1H), 3.02 (d,  $J$  = 9.8 Hz, 1H), 2.76-2.58 (m, 2H), 2.32 (dd,  $J$  = 11.6, 7.9 Hz, 1H), 1.70 (d,  $J$  = 1.6 Hz, 3H), 1.68 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 1.36 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 0.85 (dd,  $J$  = 7.5, 7.5 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  150.1, 144.0, 132.6, 131.5, 129.0, 128.5, 124.3, 124.2, 61.5, 52.9, 51.3, 49.6, 30.4, 29.5, 27.8, 9.9. HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{23}\text{N}_2\text{O}_4\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 363.1373, found 363.1375.

**Product (6h):**

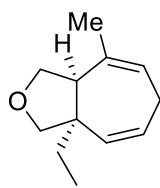


Eluted with PE/EA 50:1, 20:1

Run 1:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol), **4h** (39.6 mg, 0.1 mmol), **6h** (28.5 mg, 72%).

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (4.0 mg, 0.01 mmol), **4h** (39.7 mg, 0.1 mmol), **6h** (27.3 mg, 69%). So the average yield of two runs was 71%.

**6h**: white solid, MP = 94-96 °C. TLC  $R_f$  (PE/EA 10:1) = 0.39.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.70 (d,  $J$  = 8.8 Hz, 2H), 7.65 (d,  $J$  = 8.8 Hz, 2H), 5.41 (dd,  $J$  = 4.7, 4.7 Hz, 1H), 5.33 (ddd,  $J$  = 12.0, 4.8, 4.8 Hz, 1H), 4.97 (dq,  $J$  = 12.0, 1.7 Hz, 1H), 3.63 (dd,  $J$  = 8.7, 7.8 Hz, 1H), 3.32 (d,  $J$  = 9.8 Hz, 1H), 3.22 (dd,  $J$  = 11.6, 8.7 Hz, 1H), 2.97 (d,  $J$  = 9.8 Hz, 1H), 2.80-2.60 (m, 2H), 2.27 (dd,  $J$  = 11.6, 7.8 Hz, 1H), 1.70 (d,  $J$  = 1.5 Hz, 3H), 1.68 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 1.35 (dq,  $J$  = 15.0, 7.5 Hz, 1H), 0.85 (dd,  $J$  = 7.5, 7.5 Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  137.0, 132.9, 132.3, 131.7, 129.0, 128.8, 127.5, 124.1, 61.4, 52.9, 51.3, 49.6, 30.5, 29.4, 27.8, 10.0. HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{23}\text{BrNO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 396.0627, found 396.0636.

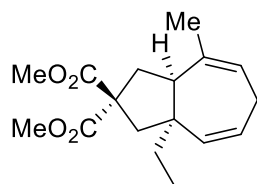
**Product (6i):****6i**

Eluted with PE/EA 200:1

Run 1: [Rh(CO)<sub>2</sub>Cl]<sub>2</sub> (4.0 mg, 0.01 mmol), **4i** (17.7 mg, 0.1 mmol), **6i** (8.9 mg, 50%).

Run 2: [Rh(CO)<sub>2</sub>Cl]<sub>2</sub> (4.0 mg, 0.01 mmol), **4i** (17.8 mg, 0.1 mmol), **6i** (8.7 mg, 49%). So the average yield of two runs was 50%.

**6i**: light yellow oil. TLC R<sub>f</sub> (PE/EA 30:1) = 0.30. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.70 (ddd, *J* = 12.0, 4.8, 4.8 Hz, 1H), 5.50-5.38 (m, 2H), 4.11 (dd, *J* = 7.6, 7.6 Hz, 1H), 3.80 (dd, *J* = 11.2, 7.2 Hz, 1H), 3.78 (d, *J* = 7.9 Hz, 1H), 3.49 (d, *J* = 7.9 Hz, 1H), 2.84-2.71 (m, 2H), 2.50 (dd, *J* = 10.0, 9.2 Hz, 1H), 1.76 (d, *J* = 1.6 Hz, 3H), 1.75 (dq, *J* = 15.0, 7.5 Hz, 1H), 1.45 (dq, *J* = 15.0, 7.5 Hz, 1H), 0.92 (dd, *J* = 7.5, 7.5 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 134.5, 132.5, 128.8, 123.3, 81.6, 71.8, 53.8, 50.1, 30.2, 29.1, 28.1, 10.4. HRMS (EI): calcd for C<sub>12</sub>H<sub>18</sub>O<sup>+</sup> ([M]<sup>+</sup>) 178.1352, found 178.1354.

**Product (6j):****6j**

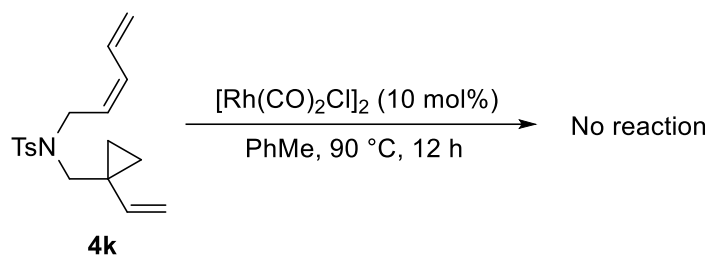
Eluted with PE/EA 100:1, 50:1

Run 1: [Rh(CO)<sub>2</sub>Cl]<sub>2</sub> (3.8 mg, 0.01 mmol), **4j** (29.0 mg, 0.1 mmol), **6j** (18.6 mg, 64%) with trace of inseparable impurity.

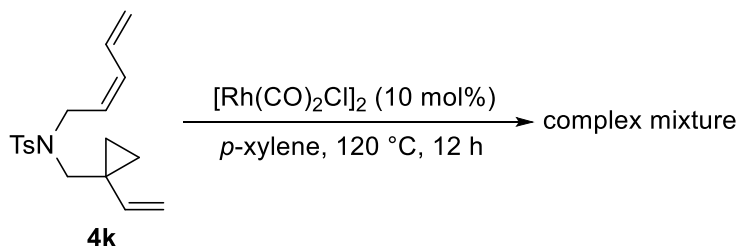
Run 2: [Rh(CO)<sub>2</sub>Cl]<sub>2</sub> (3.9 mg, 0.01 mmol), **4j** (29.1 mg, 0.1 mmol), **6j** (17.6 mg, 60%) with trace of inseparable impurity. So the average yield of two runs was 62%.

**6j**: colorless oil. TLC R<sub>f</sub> (PE/EA 10:1) = 0.54. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.47 (ddd, *J* = 12.0, 4.8, 4.8 Hz, 1H), 5.37 (dd, *J* = 4.8, 4.8 Hz, 1H), 5.28 (dq, *J* = 12.0, 1.7 Hz, 1H), 3.714 (s, 3H), 3.707 (s, 3H), 2.84-2.71 (m, 2H), 2.55 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.53 (d, *J* = 13.6 Hz, 1H), 2.40 (dd, *J* = 13.2, 12.8 Hz, 1H), 2.19 (dd, *J* = 12.8, 7.2 Hz, 1H), 1.87 (d, *J* = 13.6 Hz, 1H), 1.75 (d, *J* = 1.6 Hz, 3H), 1.71 (dq, *J* = 15.0, 7.5 Hz, 1H), 1.40 (dq, *J* = 15.0, 7.5 Hz, 1H), 0.90 (dd, *J* = 7.5, 7.5 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 173.9, 172.9, 135.5, 135.0, 127.3, 122.5, 57.1, 54.1, 53.0, 52.8, 50.6, 48.0, 38.6, 33.1, 29.6, 27.9, 10.1. HRMS (ESI): calcd for C<sub>17</sub>H<sub>25</sub>O<sub>4</sub><sup>+</sup> ([M + H]<sup>+</sup>) 293.1747, found 293.1745.

**Reaction of 4k:**

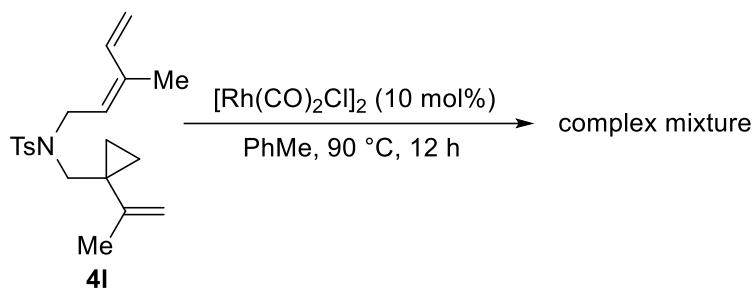


A solution of **4k** (31.6 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous toluene (2 mL, 0.05 M) was stirred at 90 °C for 12 h under an argon atmosphere. There's no reaction occurred as indicated by the TLC. Then the reaction mixture was cooled to room temperature. It was concentrated in vacuo. Purification of the residue through column chromatography (PE/EA 50:1) on silica gel recovered the substrate **4k** (22.0 mg, 70%).



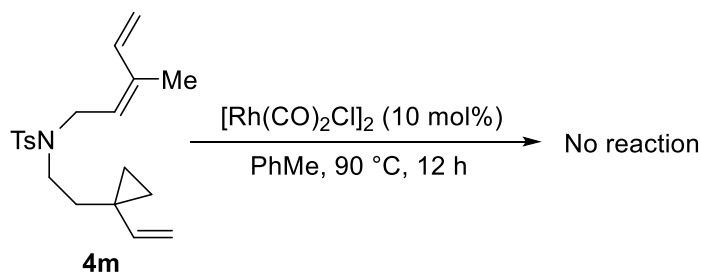
A solution of **4k** (31.6 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous *p*-xylene (2 mL, 0.05 M) was stirred at 120 °C for 12 h under an argon atmosphere. The reaction gave complex mixture as indicated by TLC.

**Reaction 4l:**



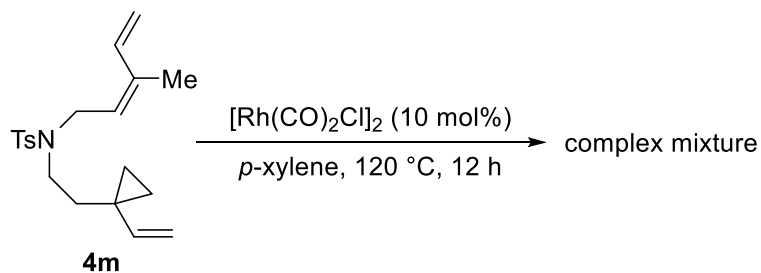
A solution of **4l** (34.6 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous toluene (2 mL, 0.05 M) was stirred at 90 °C for 12 h under an argon atmosphere. Then the reaction mixture was cooled to room temperature. It was concentrated in vacuo. Purification of the residue through column chromatography (PE/EA 20:1) on silica gel gives a colorless oil (32.1 mg), which is complex mixture as indicated by  $^1\text{H}$  NMR.

**Reaction 4m:**



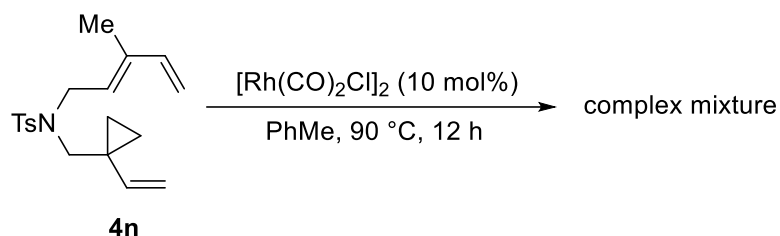
A solution of **4m** (34.6 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous toluene (2 mL, 0.05 M) was stirred at 90 °C for 12 h under an argon atmosphere. There's no reaction occurred as

indicated by the TLC. Then the reaction mixture was cooled to room temperature. It was concentrated in vacuo. Purification of the residue through column chromatography (PE/EA 40:1, 20:1) on silica gel recovered the substrate **4m** (28.6 mg, 83%).



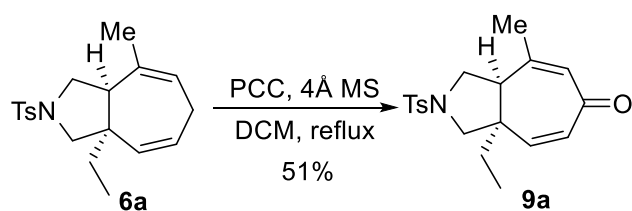
A solution of **4m** (34.6 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous *p*-xylene (2 mL, 0.05 M) was stirred at 120 °C for 12 h under an argon atmosphere. The reaction gave complex mixture as indicated by TLC.

#### Reaction 4n:



A solution of **4n** (33.2 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (3.9 mg, 0.01 mmol, 10 mol%) in anhydrous toluene (2 mL, 0.05 M) was stirred at 90 °C for 12 h under an argon atmosphere. Then the reaction mixture was cooled to room temperature. It was concentrated in vacuo. Purification of the residue through column chromatography (PE/EA 25:1) on silica gel gave a colorless oil (20.0 mg), which was complex mixture as indicated by  $^1\text{H}$  NMR.

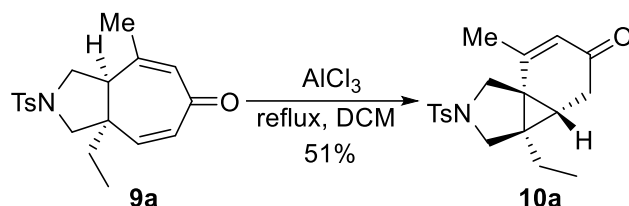
### 3.4 Transformations of the Cycloadduct **6a**



**6a** (16.6 mmol, 0.05 mmol), PCC (32.3 mg, 0.15 mmol), 4 Å MS (32.3 mg) and DCM (1 mL) were added in a reaction flask with an air condenser. The reaction mixture was heated to reflux for 17 h in a 50 °C oil bath. The reaction mixture was filtered through silica gel and washed with EA. Then the crude product was concentrated and purified by preparative TLC to afford **9a** as a white solid. Run 1: **9a** (9.1 mg, 53%); Run 2: **9a** (8.4 mg, 49%). The average yield of two runs was 51%.

**9a**: white solid. MP = 145.1-147.0 °C. TLC  $R_f$  (PE/EA 1:1) = 0.36.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J$  = 8.3 Hz, 2H), 7.34 (d,  $J$  = 8.0 Hz, 2H), 6.04 (apparent t,  $J$  = 1.7 Hz, 1H), 5.80 (dd,  $J$  = 12.5, 1.7 Hz, 1H), 5.74 (dd,  $J$  = 12.5, 1.7 Hz, 1H), 3.80 (dd,  $J$  = 9.2, 7.7 Hz, 1H), 3.59 (d,  $J$  = 10.1 Hz, 1H), 3.25 (dd,  $J$  = 11.8, 9.2 Hz, 1H), 3.15 (d,  $J$  = 10.1 Hz, 1H), 2.52-2.47 (m, 1H), 2.46 (s, 3H), 1.97 (d,  $J$  = 1.4 Hz, 3H), 1.72 (dq,  $J$  = 13.8,

7.6 Hz, 1H), 1.45 (dq,  $J = 15.1, 7.6$  Hz, 1H), 0.88 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  189.4, 149.6, 146.0, 144.1, 134.3, 132.6, 131.0, 130.0, 127.5, 61.4, 53.2, 52.3, 51.0, 30.6, 28.3, 21.7, 9.7. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{24}\text{NO}_3\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1471, found 346.1478.

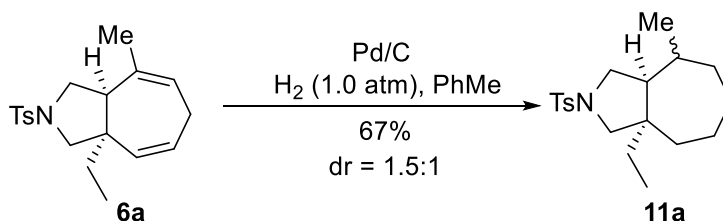


**9a** (10.0 mg, 0.029 mmol) and  $\text{AlCl}_3$  (3.9 mg, 0.029 mmol) were dissolved in super-dry DCM (1 mL) under argon atmosphere and the resulting mixture was heated to reflux for 24 h. After that, another portion of  $\text{AlCl}_3$  (7.8 mg, 0.058 mmol) was added, and the resulting mixture was heated to reflux for another 24 h (attention: DCM was added for several times during the reaction to avoid the system to be totally evaporated). After cooled to r.t., the mixture was purified by preparative TLC (PE/EA = 3:1) to give product **10a** (5.0 mg, 0.014 mmol, 50%) as a yellow oil.

Run 2: **9a** (10.0 mg, 0.029 mmol) was converted to the title compound **10a** (5.2 mg, 0.015 mmol, 52%) using the same procedure as above.

The average yield of two runs was 51%.

**10a**: colourless oil, TLC  $R_f$  (PE/EA 1:1) = 0.30.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.2$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 5.87 (d,  $J = 1.5$  Hz, 1H), 3.66 (d,  $J = 9.3$  Hz, 1H), 3.64 (d,  $J = 9.5$  Hz, 1H), 3.47 (d,  $J = 9.3$  Hz, 1H), 3.09 (d,  $J = 9.4$  Hz, 1H), 2.64 (dd,  $J = 19.9, 8.5$  Hz, 1H), 2.52 (d,  $J = 19.9$  Hz, 1H), 2.46 (s, 3H), 1.96 (d,  $J = 1.3$  Hz, 3H), 1.65 (d,  $J = 8.4$  Hz, 1H), 1.31-1.23 (m, 1H), 1.23-1.13 (m, 1H), 0.82 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ):  $\delta$  195.6, 156.4, 144.0, 133.9, 130.0, 127.6, 125.9, 53.0, 51.0, 40.9, 33.0, 31.8, 23.5, 23.2, 21.7, 17.1, 11.1. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{24}\text{NO}_3\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 346.1471, found 346.1470.



To a solution of **6a** (16.6 mg, 0.05 mmol) in PhMe (1 mL) was added Pd/C (53.2 mg, 0.05 mmol, 10 mol % on dry basis) and bubbled with  $\text{H}_2$  (1 atm) for 10 min. The reaction mixture was stirred under  $\text{H}_2$  atmosphere (1 atm) for 2.5 h. The mixture was purified by preparative TLC (PE/EA = 10:1) to give product **11a** (10.8 mg, 0.032 mmol, 64%) as a colorless oil.

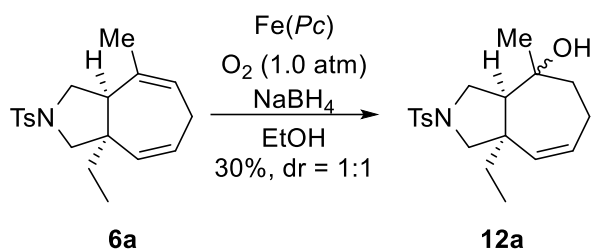
Run 2: **6a** (16.6 mg, 0.05 mmol) was converted to the title compound **11a** (11.6 mg, 0.035 mmol, 69%) using the same procedure as above.

The average yield of two runs was 67%.

**11a**: colourless oil, TLC  $R_f$  (PE/EA 4:1) = 0.58. The ratio of diastereomers (1.5:1) is determined by the  $^1\text{H}$  NMR.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.8$  Hz, 2H), 7.67 (d,  $J = 7.8$  Hz, 3H), 7.33 (d,  $J = 7.8$  Hz, 5H), 3.61 (t,  $J = 8.6$  Hz, 1.5H), 3.31 (d,  $J = 9.4$  Hz, 1.5H), 3.26 (t,  $J = 9.1$  Hz, 1H), 3.13 (t,  $J = 9.4$  Hz, 1H), 3.01 (d,  $J = 9.5$  Hz, 1H), 2.93 (d,  $J = 9.4$  Hz, 1H), 2.45 (s, 7.5H), 2.24 (t,  $J = 9.5$  Hz, 1.5H), 2.11 (d,  $J = 9.4$  Hz, 1.5H), 1.91-1.84 (m, 1.5 H), 1.77-1.70 (m, 3H), 1.62-1.54 (m, 7H), 1.52-1.45 (m, 4.5H), 1.44-1.37 (m,



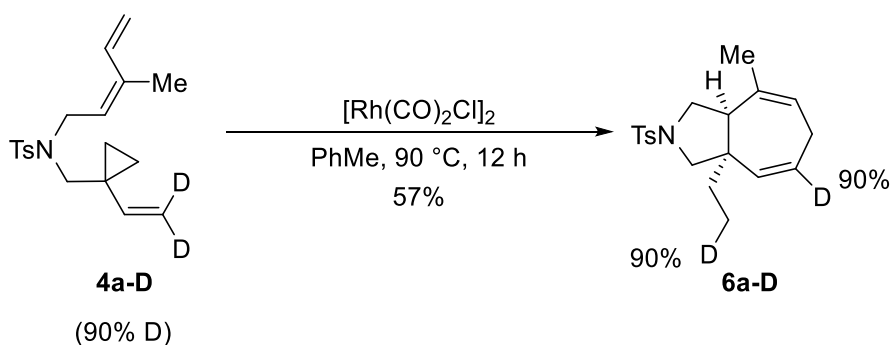
3.5H), 1.37-1.26 (m, 6.5H), 1.25-1.19 (m, 4.5H), 0.87 (d,  $J = 7.1$  Hz, 3H), 0.85-0.78 (m, 11H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.6, 143.4, 133.1, 131.7, 129.64, 129.62, 128.3, 127.9, 59.9, 59.4, 56.8, 55.0, 53.0, 48.7, 47.0, 46.8, 37.6, 37.2, 33.8, 33.5, 33.4, 32.8, 30.71, 30.67, 28.7, 23.9, 23.8, 23.6, 22.3, 21.7, 9.2, 9.1. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{30}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 336.1992, found 336.1982.



To a solution of **6a** (16.6 mmol, 0.05 mmol),  $\text{Fe(Pc)}$  (1.4 mg, 5 mol%) in EtOH (0.6 mL) was added  $\text{NaBH}_4$  (5.8 mg, 0.15 mmol) and then charged with  $\text{O}_2$  (1.0 atm). The reaction mixture was stirred at room temperature for 16 h. The reaction was quenched by 1 N HCl and extracted with DCM. The organic phase was washed with brine and dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 4:1 petroleum ether/EtOAc) afforded **12a** as a colorless oil. Run 1: **12a** (4.9 mg, 28%); Run 2: **12a** (5.6 mg, 32%). The average yield of two runs was 30%.

**12a**: colourless oil, TLC **12a-1**  $R_f$  (PE/EA 2:1) = 0.37, **12a-2**  $R_f$  (PE/EA 2:1) = 0.36, The ratio of diastereomers (1:1) is determined by the  $^1\text{H}$  NMR.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.0$  Hz, 2H), 7.70 (d,  $J = 8.0$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 4H), 5.72-5.60 (m, 2H), 5.24 (d,  $J = 11.6$  Hz, 1H), 5.13 (dd,  $J = 11.6, 2.4$  Hz, 1H), 3.54 (dd,  $J = 9.6, 8.4$  Hz, 1H), 3.41-3.20 (m, 4H), 3.10 (d,  $J = 9.0$  Hz, 1H), 3.04 (d,  $J = 9.1$  Hz, 1H), 2.95 (d,  $J = 9.2$  Hz, 1H), 2.44 (s, 3H), 2.43 (s, 3H), 2.41-2.32 (m, 1H), 2.20-2.10 (m, 2H), 2.10-2.00 (m, 2H), 1.95-1.86 (m, 2H), 1.80-1.71 (m, 2H), 1.70-1.61 (m, 2H), 1.60-1.53 (m, 1H), 1.47-1.39 (m, 2H), 1.33 (m, 2H), 1.21 (s, 3H), 1.08 (s, 3H), 0.87 (t,  $J = 7.5$  Hz, 3H), 0.83 (t,  $J = 7.5$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.49, 143.47, 134.8, 134.4, 134.1, 133.4, 131.8, 130.6, 129.8, 129.7, 127.9, 127.6, 73.9, 73.4, 61.7, 61.2, 56.4, 55.8, 50.1, 49.7, 49.6, 48.7, 37.6, 36.6, 33.5, 31.6, 31.4, 30.6, 29.8, 24.1, 22.5, 21.7, 10.2, 9.8. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{28}\text{NO}_3\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 350.1784, found 350.1801.

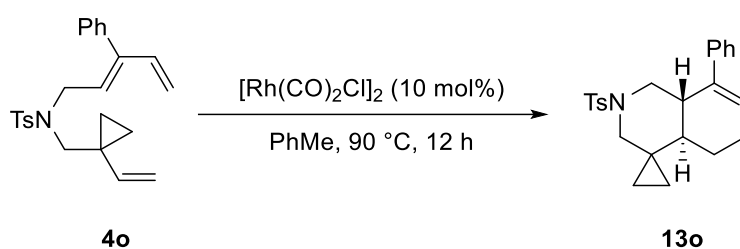
### 3.5 Deuterium Labeling Experiment



A solution of **4a-D** (468.6 mg, 1.40 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (54.4 mg, 0.14 mmol, 10 mol%) in anhydrous toluene (28 mL) was stirred at 90  $^\circ\text{C}$  for 12 h under an argon atmosphere. Then the reaction mixture was cooled to room temperature. It was concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 50:1, 20:1) afforded **6a-D** (267.8 mg, 57%) as a white solid.

**6a-D**: white solid. MP = 92.6-95.2 °C. TLC  $R_f$  (PE/EA 10:1) = 0.27.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J$  = 8.1 Hz, 2H), 7.28 (d,  $J$  = 8.0 Hz, 2H), 5.37 (dd,  $J$  = 4.1, 4.1 Hz, 1H), 4.96 (s, 1H), 3.60 (dd,  $J$  = 8.3, 8.3 Hz, 1H), 3.31 (d,  $J$  = 9.7 Hz, 1H), 3.22 (dd,  $J$  = 11.7, 9.0 Hz, 1H), 2.92 (d,  $J$  = 9.7 Hz, 1H), 2.71-2.59 (m, 2H), 2.40 (s, 3H), 2.18 (dd,  $J$  = 11.3, 8.0 Hz, 1H), 1.70-1.65 (m, 3H), 1.65-1.58 (m, 1H), 1.37-1.19 (m, 1H), 0.79 (t,  $J$  = 7.3 Hz, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.2, 134.8, 133.0, 131.8, 129.6, 127.4, 123.8, 61.2, 52.8, 51.2, 49.4, 30.3, 29.2, 27.7, 21.6. HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{24}\text{D}_2\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 334.1804, found 334.1800.

### 3.6 [4+2] Cycloaddition

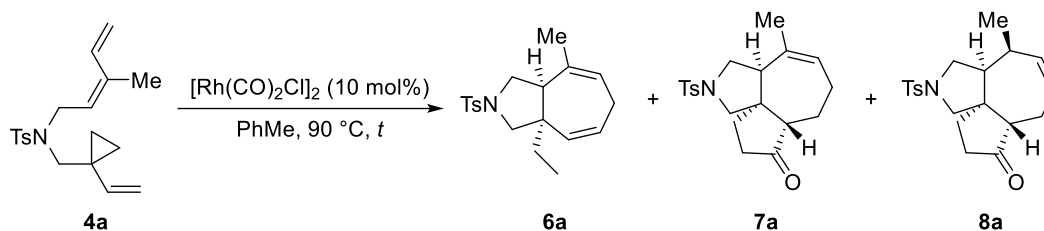


A solution of **4o** (39.4 mg, 0.10 mmol) and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (4.1 mg, 0.01 mmol, 10 mol%) in anhydrous PhMe (2 mL, 0.05 M) was stirred at 90 °C for 12 h under an argon atmosphere. Then the reaction mixture was cooled to room temperature and then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA 40:1) afforded the **13o** (18.6 mg, 47%). The configuration of **13o** was determined by 2D NMR (see the attached spectrum)

Run 2:  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (4.0 mg, 0.01 mmol), **4o** (39.5 mg, 0.1 mmol), **13o** (17.3 mg, 44%). So the average yield of two runs was 46%.

**13o**: white solid, MP = 145-147 °C. TLC  $R_f$  (PE/EA 5:1) = 0.63.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.50 (d,  $J$  = 8.0 Hz, 2H), 7.33-7.30 (m, 2H), 7.26-7.21 (m, 3H), 7.21-7.15 (m, 2H), 5.82-5.78 (m, 1H), 3.88 (ddd,  $J$  = 11.7, 3.6, 1.7 Hz, 1H), 2.99 (dd,  $J$  = 11.7, 1.8 Hz, 1H), 2.81 (dd,  $J$  = 11.8, 1.9 Hz, 2H), 2.39 (s, 3H), 2.29-2.19 (m, 1H), 2.16-2.02 (m, 1H), 1.88 (dd,  $J$  = 11.6, 11.6 Hz, 1H), 1.69-1.59 (m, 1H), 1.38 (dd,  $J$  = 12.3, 5.5 Hz, 1H), 0.98 (dddd,  $J$  = 12.0, 12.0, 12.0, 5.4 Hz, 1H), 0.77-0.68 (m, 1H), 0.62-0.52 (m, 2H), 0.33-0.22 (m, 1H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.3, 141.0, 138.8, 134.1, 129.6, 128.5, 128.5, 127.7, 126.9, 126.6, 56.3, 50.8, 41.6, 41.2, 25.9, 21.8, 21.6, 21.1, 7.5, 6.9. HRMS (ESI): calcd for  $\text{C}_{24}\text{H}_{28}\text{NO}_2\text{S}^+$  ( $[\text{M} + \text{H}]^+$ ) 394.1835, found 394.1834.

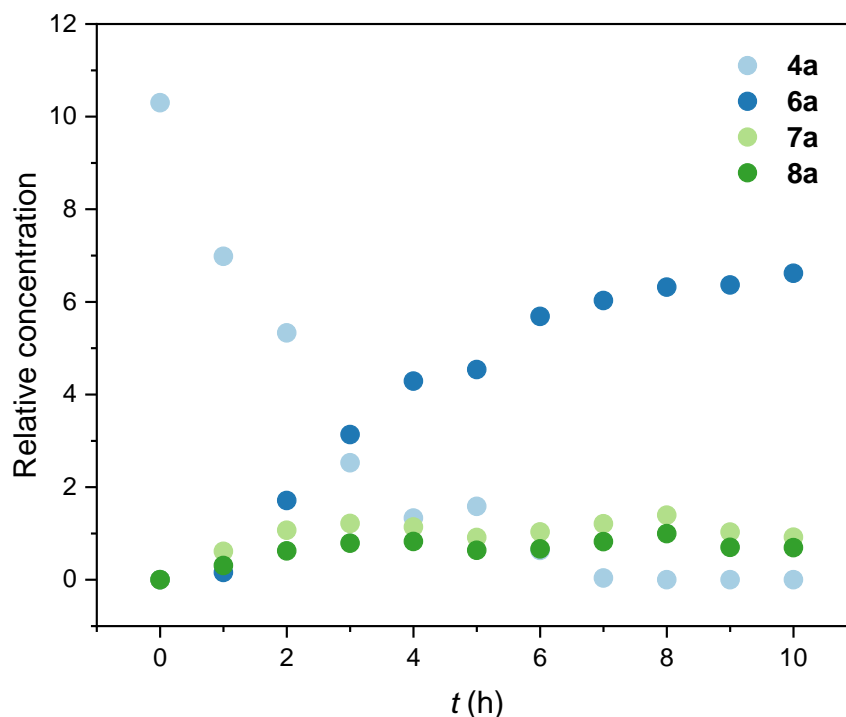
## 4. Visual Kinetic Analysis



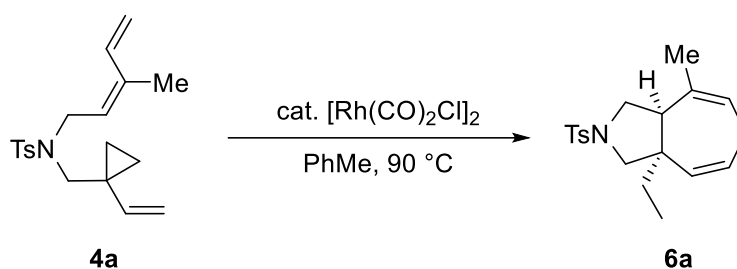
**Concentration Profile Measurements.** To a 10 mL volumetric flask was added 1,3,5-trimethoxybenzene (8.2 mg, 98% purity, internal standard) and  $\text{CDCl}_3$  to prepare a 4.78 mmol/L concentration solution. To a NMR tube was added **4a** (8.3 mg, 25.0  $\mu\text{mol}$ ),  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (1.0 mg, 2.5  $\mu\text{mol}$ ) and PhMe (0.5 mL). Ten such tubes were heated at 90 °C in an oil bath. Taking out one NMR tube every hour and pouring the solution into a sharp bottom bottle. Rinsing NMR tube with DCM and it was concentrated in vacuo. After removing the solvent, 0.5 mL of internal standard solution were added to measure  $^1\text{H}$  NMR. The horizontal axis is the reaction time and the vertical axis is the relative concentration of the substrate and products to the internal standard.

**Table S2.** Kinetic data for [4+3] cycloaddition of substrate **4a**

t / h	<b>4a</b>	<b>6a</b>	<b>7a</b>	<b>8a</b>
0	10.3	0	0	0
1	6.983	0.157	0.6129	0.308
2	5.33	1.71	1.07	0.625
3	2.526	3.134	1.216	0.789
4	1.333	4.289	1.14	0.826
5	1.584	4.54	0.913	0.638
6	0.633	5.686	1.033	0.667
7	0.038	6.03	1.208	0.822
8	0	6.318	1.395	0.997
9	0	6.364	1.028	0.699
10	0	6.617	0.921	0.693



**Figure S1.** Concentration profile of substrate **4a** and products.



**Visual Kinetic Measurements.** A solution of substrate **4a**, 1,3,5-trimethoxybenzene (internal standard), and  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  in toluene was split into a reaction tube. The reaction mixture was stirred at 90 °C for an indicated time under argon atmosphere. After cooling, the solvent was removed through a rotary evaporator, and  $\text{CDCl}_3$  was added. Nuclear magnetic resonance (NMR) spectra were measured on Bruker AVANCE III 400 ( $^1\text{H}$  at 400 MHz).

We must point out here that, because the reaction at the beginning produced **6a**, **7a** and **8a** (Figure S1), measuring the kinetics cannot give the orders of substrate, catalyst at the early stage. Therefore, we measured the kinetic data after 60 or 70 minutes, assuming that comparable results from these can be obtained.

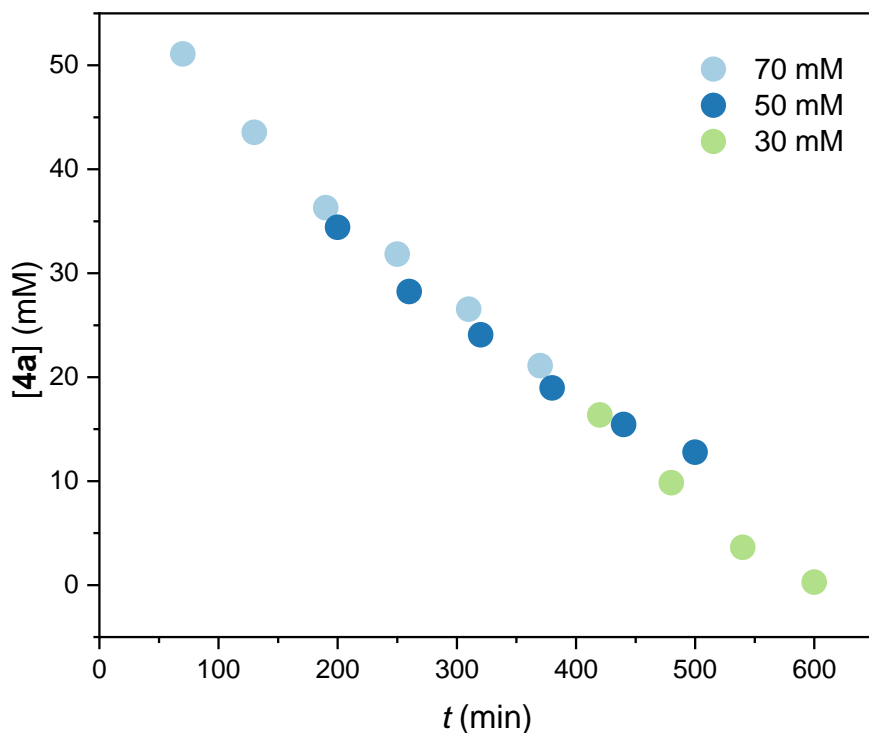
**Table S3.** Visual kinetic data for [4+3] cycloaddition of substrate **4a**

$[\mathbf{4a}]_0$ / mM	$[\text{Cat}]_T$ / mM <sup>a</sup>	$t$ / min	$[\mathbf{4a}]$ / mM	$[\mathbf{6a}]$ / mM
50	5	60	34.42	2.41
50	5	120	28.23	7.9
50	5	180	24.07	13.48
50	5	240	18.96	16.68
50	5	300	15.45	20.39

50	5	360	12.78	22.88
50	3.75	60	38.15	1.14
50	3.75	120	32.11	5.14
50	3.75	180	26.94	9.7
50	3.75	240	21.64	13.64
50	3.75	300	17.2	17.72
50	3.75	360	13.29	21.39
50	6.25	60	30.75	3.08
50	6.25	120	24.24	9.21
50	6.25	180	19.06	14.48
50	6.25	240	14.07	19.13
50	6.25	300	9.47	23.76
50	6.25	360	5.37	27.08
70	5	70	51.09	1.53
70	5	130	43.56	5.23
70	5	190	36.3	10.89
70	5	250	31.83	17.19
70	5	310	26.53	22.02
70	5	370	21.11	27.66
30	5	70	16.37	0.49
30	5	130	9.85	4.73
30	5	190	3.62	10.06
30	5	250	0.29	14.55

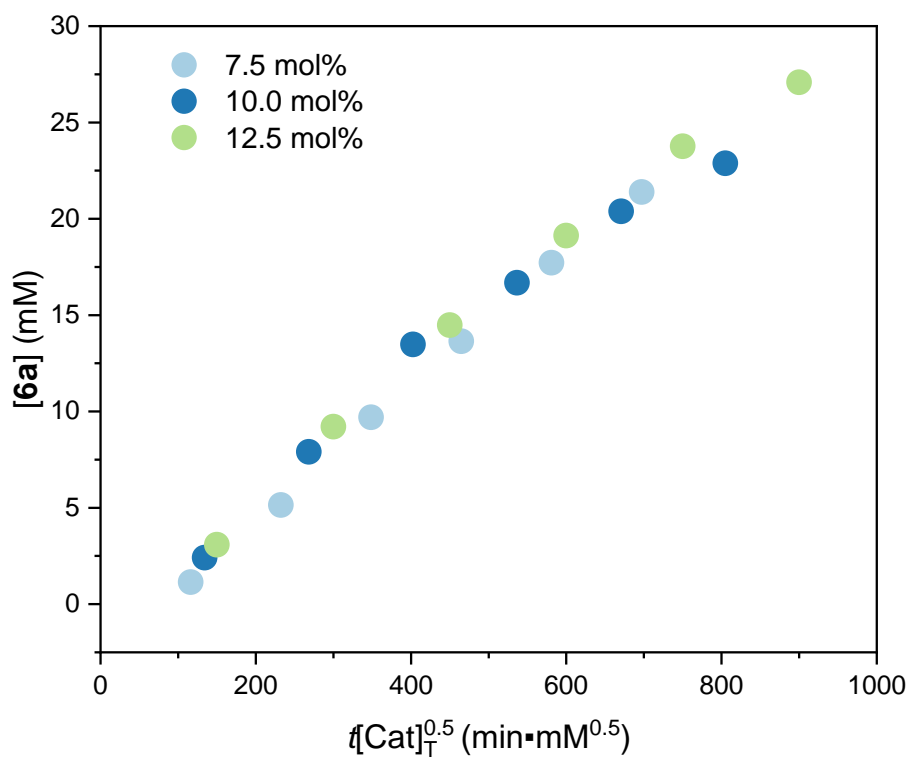
<sup>a</sup>[Cat]<sub>T</sub> is the total concentration of catalyst added.

**Time adjustment.** To identify catalyst deactivation or product inhibition, we shifted the concentration profiles of substrate **4a** on the time scale (Figure S2).<sup>21</sup> The overlay of the concentration profiles indicates the absence of catalyst deactivation and product inhibition.



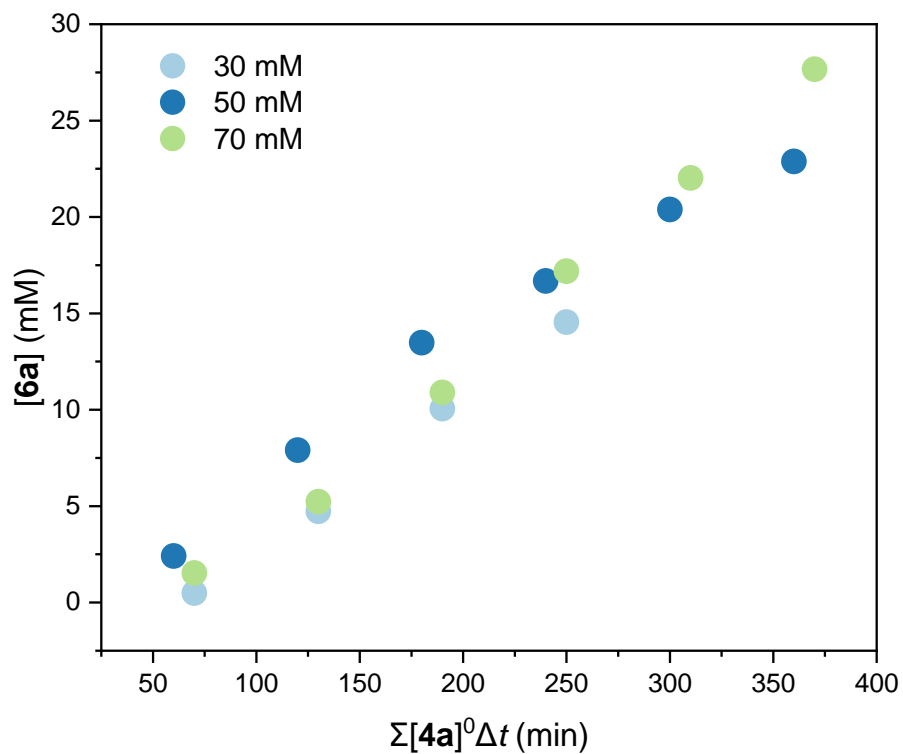
**Figure S2.** Concentration profiles of **4a** after time adjustment (+140 min for  $[\mathbf{4a}]_0 = 50$  mM; +350 min for  $[\mathbf{4a}]_0 = 30$  mM). Reaction conditions: **4a** (30, 50, 70 mM),  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (5.0 mM), toluene, 90 °C.

**Order in catalyst.** To determine the order in catalyst ( $n$ ), we performed normalized time scale analysis<sup>22</sup> via plotting the concentration of **6a** against  $t[\text{Cat}]_T^n$  ( $[\text{Cat}]_T$  is the total concentration of catalyst added).  $n$  was adjusted until the concentration profiles overlaid. As shown in Figure S3,  $n$  equals 0.5.



**Figure S3.** Normalized time scale analysis to determine the order in catalyst. Reaction conditions: **4a** (50 mM),  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (7.5, 10.0, 12.5 mol %), toluene, 90 °C.

**Order in substrate.** To determine the order in substrate ( $a$ ), we performed variable time normalization analysis<sup>23</sup> via plotting the concentration of cycloadduct **6a** against  $\Sigma[4\mathbf{a}]^a\Delta t$ .  $a$  was adjusted until the concentration profiles overlaid and became straight lines. As shown in Figure S4,  $a$  equals 0.



**Figure S4.** Variable time normalization analysis to determine the order in substrate **4a**. Reaction conditions: **4a** (30, 50, 70 mM),  $[\text{Rh}(\text{CO})_2\text{Cl}]_2$  (5.0 mM), toluene, 90 °C.

## 5. Computational Details

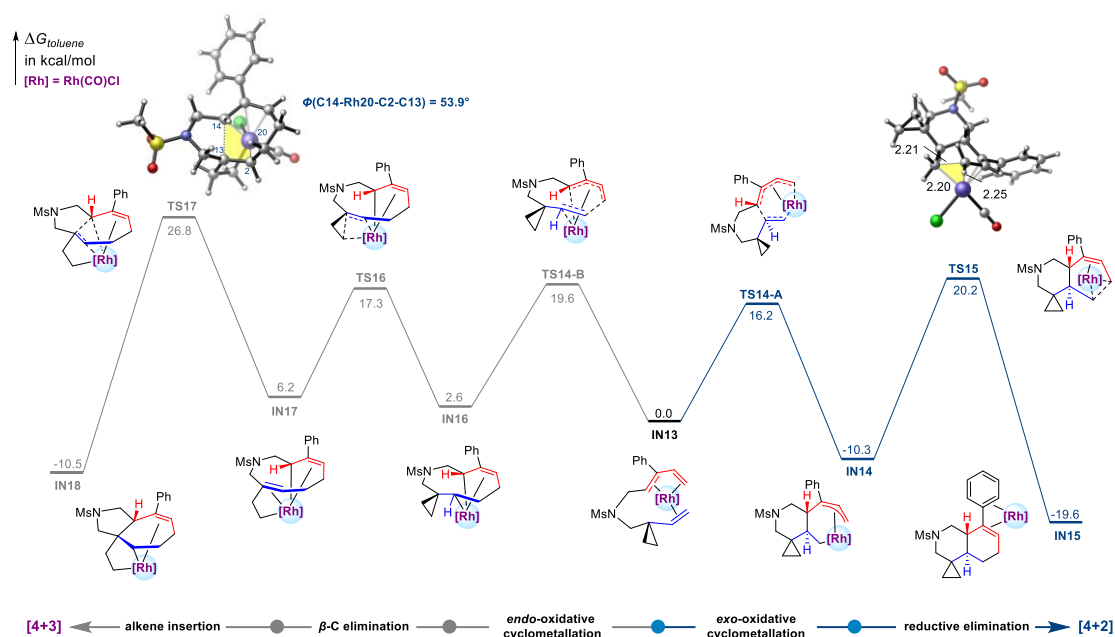
### 5.1 Computational Methods

DFT calculations were performed with Gaussian 09.<sup>24</sup> Geometry optimizations of the stationary points were carried out at the BMK/6-31G(d)/LANL2DZ<sup>25-27</sup> level without any constraints in the gas phase. In structure optimizations, the keyword “5D” was used to specify that five d-type orbitals were used for all elements. Solution phase single point energies in toluene (solvent for formal [4+3] cycloaddition) or DCE (solvent for [3+2] cycloaddition) solution based on the gas phase structures were obtained at the same level using the SMD solvation model<sup>28</sup>. Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. IRC<sup>29</sup> calculations were carried out to confirm that the transition state structures connect corresponding reactants and products. On the basis of the optimized structures, single-point energies were computed at the BMK/def2-TZVPP<sup>30-31</sup> level unless otherwise specified. For some key transition states, DLPNO-CCSD(T)/def2-TZVPP<sup>32</sup> single point energy calculations were performed to improve accuracy using ORCA 4.2.1.<sup>33-34</sup> The auxiliary basis set def2-TZVPP/C,<sup>35</sup> “TightPNO” and “TightSCF” settings were applied during the single point energy calculations. IBO analysis<sup>31</sup> was done by using ORCA at PBE0/def2-SVP<sup>30</sup> level along the IRC computed at the BMK/6-31G(d)/LANL2DZ level. All the discussed energy differences were based on Gibbs energies at 298 K. Reference states for solutes in toluene or DCE solution are the hypothetical states at 1 mol/L, respectively. 3D molecular structures were prepared by CYLview.<sup>37</sup>



## 5.2 Mechanism of [4+2] Cycloaddition of *E*-diene-VCPs

To understand why [4+2] but not [4+3] cycloaddition could occur, DFT calculations were applied using a model substrate with a NMs tether (**Figure S5**).



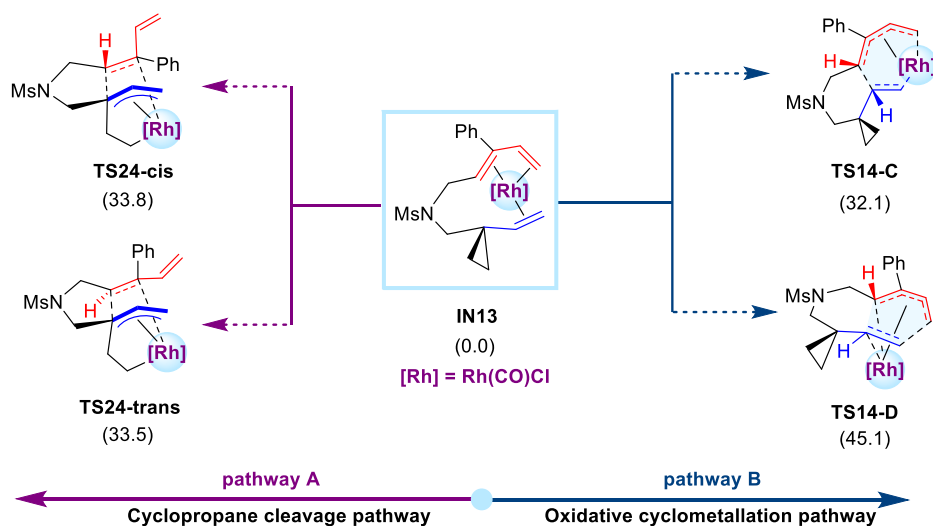
**Figure S5.** Gibbs energy profile of the Rh catalyzed [4+2] cycloaddition of *E*-diene-VCP. Computed at the SMD(toluene)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level. Color scheme: H, white; C, gray; O, red; S, yellow; N, blue; Cl, green; Rh, violet. Bond lengths are reported in Å.

In the [4+2] pathway leading to the experimentally observed *trans* product, substrate/Rh catalyst complex **IN13** gives **IN14** via *exo*-oxidative cyclometallation (*exo*-OCM) transition state **TS14-A** (with an activation free energy of 16.2 kcal/mol), followed by reductive elimination process via **TS15** to give [4+2] product/catalyst complex. The reductive elimination step is the most difficult process for this [4+2] reaction pathway and has an activation free energy of 30.5 kcal/mol (from **IN14** to **TS15**). In contrast, in the [4+3] product formation pathway (pathway B), the *endo*-oxidative cyclometallation (*endo*-OCM) via **TS14-B** is more difficult than the *exo*-OCM. Although the  $\beta$ -C elimination step is relatively easier, there's another very difficult transition state to overcome, which is alkene insertion transition state **TS17**. This transition state is higher in energy than **TS15** by 6.6 kcal/mol. Therefore, according to the Curtin-Hammett principle, the reaction will give [4+2] product. The major reason for this is that, the [4+3] pathway generates *trans* intermediate **IN18**, which is highly strained. In contrast, when *Z*-diene-VCP is used as substrate, the alkene insertion prefers to give a *cis* product (see Figure 3 in the main text).

Here we analyze why **TS17** is disfavored. **TS17** is highly strained with a significant geometry change to push alkene into the insertion transition state. It is proposed that alkene/alkyne insertion into the M–C bond usually prefers to have a planar structure.<sup>38</sup> The dihedral angle  $\Phi(\text{C14-Rh20-C2-C13})$  of **TS17**, however, is up to  $53.9^\circ$  (indicating the transition state structure is far from planar), which is much higher than  $\Phi(\text{C1-Rh28-C6-C2})$  of **TS7** ( $38.7^\circ$ ). With the above analysis, we can conclude that *E*-diene-VCPs could not undergo [4+3] cycloadditions due to the disfavored *endo*-OCM and alkene insertion.

### 5.3 Other Disfavored Pathways of IN13

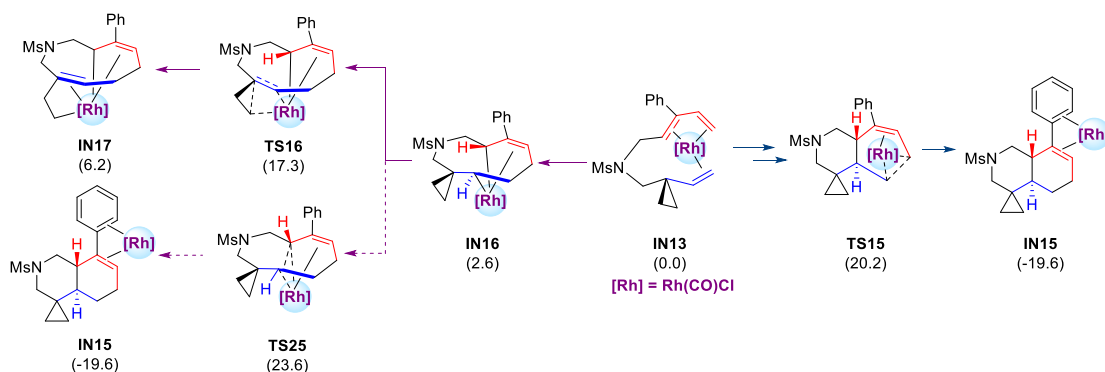
Except for the *trans exo*-OCM (via **TS14-A**) and *trans endo*-OCM (via **TS14-B**) for the [4+2] reaction shown in Figure S1, **IN13** has some other transformation pathways, which were also considered here (**Figure S6**). *Cis exo*-OCM (via **TS14-C**) and *cis endo*-OCM (via **TS14-D**) have an activation free energy of 32.1 kcal/mol and 45.1 kcal/mol, respectively, which are much higher than *trans exo*-OCM and *trans endo*-OCM. Besides, the alkene insertions (via **TS24-cis** or **TS24-trans**) in the cyclopropane oxidative addition pathway (pathway A) are also disfavored due to high activation free energy (33.5 kcal/mol for *trans* alkene insertion and 33.8 kcal/mol for *cis* alkene insertion).



**Figure S6.** Other disfavored pathways of **IN13**. Gibbs energies given in the brackets are reported in kcal/mol. Computed at SMD(toluene)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ.

### 5.4 Reductive Elimination of IN16

The direct reductive elimination process of **IN16** (via **TS25**) was also considered, which needs an activation free energy of 21.0 kcal/mol (**Figure S7**, from **IN16** to **TS21**). It's 6.3 kcal/mol disfavored over  $\beta$ -C elimination via **TS16**. Besides, **TS25** is 3.4 kcal/mol higher than **TS15** in terms of Gibbs free energy, suggesting that this process can be excluded according to Curtin-Hammett principle.

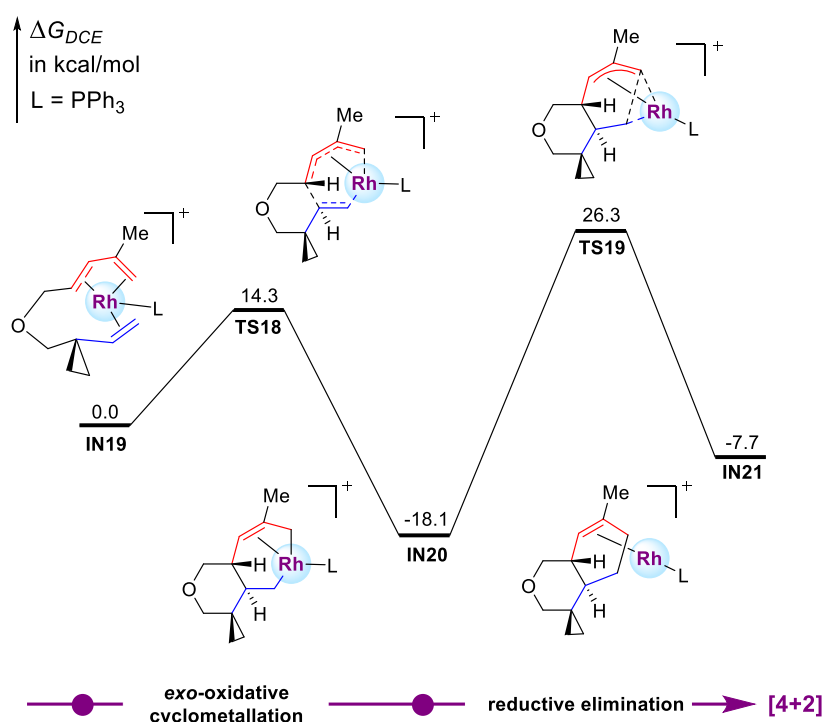


**Figure S7.** Reductive elimination of **IN16**. Gibbs energies given in the brackets are reported in kcal/mol. Computed at SMD(toluene)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ.

## 5.5 Mechanism of [3+2] Cycloaddition and Cycloisomerization for *E*-diene-VCPs under Cationic Rh Conditions

DFT calculations were also applied to understand the mechanism of the [3+2] cycloaddition (major reaction) and cycloisomerization (side reaction) of *E*-diene-VCPs catalyzed by cationic Rh species. The oxygen tethered **1e** was the model substrate for computation to understand the mechanism and answer why [4+2] reaction did not take place as a competing reaction (**Figure S8** and **S9**).

As for the possible [4+2] cycloaddition pathway (**Figure S8**), the first step in this pathway is *exo*-oxidative cyclometallation (from **IN19** to **IN20** via **TS18**) is easy with an activation free energy of 14.3 kcal/mol. But the second step, reductive elimination via **TS19** is very difficult with an activation free energy of 44.4 kcal/mol. Thus, this pathway can be safely ruled out.

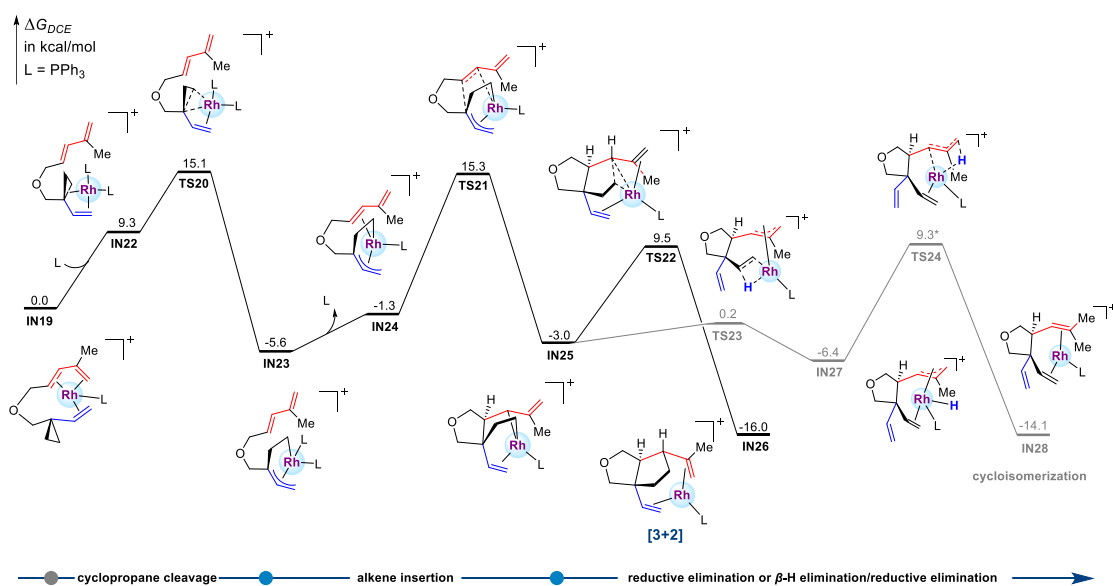


**Figure S8.** Gibbs energy profile of the [4+2] cycloaddition pathway under cationic Rh conditions.

The [3+2] cycloaddition and cycloisomerization reactions have the cyclopropane cleavage and alkene insertion steps in common (**Figure S9**), which is similar to our previous report.<sup>39</sup> These two steps start with the formation of complex **IN22** between vinylcyclopropane and alkene after **IN19** is coordinated by another  $PPh_3$  ligand. Oxidative addition of **IN22** occurs via **TS20**, giving rise to the cyclopropane cleaved product **IN23**, which then dissociates a  $PPh_3$  ligand to form **IN24**. Subsequently, **IN24** undergoes alkene insertion via **TS21** to form **IN25**, with an activation free energy of 16.6 kcal/mol (from **IN24** to **TS21**).

In the [3+2] cycloaddition process, a reductive elimination with an activation free energy of 12.5 kcal/mol (via **TS22**) converts **IN25** to **IN26**, which, via ligand exchange reaction, affords the final experimentally observed [3+2] cycloaddition product.

While in the cycloisomerization process, **IN25** undergoes  $\beta$ -H elimination via **TS23** to give the Rh-H complex **IN27**, which then affords **IN28** via the reductive elimination transition state **TS24**. This two-step process is energetically comparable with [3+2] cycloaddition because the Gibbs energy of **TS24** is only 0.2 kcal/mol more favored over **TS22**. Therefore, DFT calculations suggest that  $\beta$ -H elimination product can also be generated, which is consistent with experimental observation in Scheme 2 (the main text).



**Figure S9.** Gibbs energy profile of the cationic Rh catalyzed [3+2] cycloaddition and cycloisomerization of *E*-diene-VCP **1e**. Computed at the SMD(DCE)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level. \*The reported energy of **TS24** is the relative energy with respect to **TS22** computed by the SMD(DCE)/PBE0-D3(BJ)//def2-TZVPP//BMK/6-31G(d)/LANL2DZ level which was proven to be a better functional for calculating the energy gap as supported by the benchmark study (*vide infra*).

## 5.6 Benchmark Study for TS22 and TS24

To obtain a more accurate computational selectivity for Rh catalyzed [3+2] and cycloisomerization, we carried out the benchmark study using the DLPNO-CCSD(T) method as the reference (**Table S4**). In the benchmark study, the ligand PPh<sub>3</sub> was modeled by PMe<sub>3</sub> to reduce the computational cost. According to the DLPNO-CCSD(T) computational results, **TS24'** is -1.9 kcal/mol lower than **TS22'** in terms of Gibbs free energy. Among all the tested functionals in **Table S3**, PBE0-D3(BJ)<sup>40-42</sup> shows the best performance, which gives the closest energy difference compared to DLPNO-CCSD(T) among the tested functionals. M06-D3,<sup>42-43</sup> ωB97X-D,<sup>44</sup> M11,<sup>45</sup> and B3LYP-D3(BJ),<sup>42,46-47</sup> underestimate the energy difference while there is large overestimation for BMK. Therefore, we applied PBE0-D3(BJ) to calculate the Gibbs free energy difference of **TS22** and **TS24**, which is used for discussion in the above calculations of [3+2] reaction. **TS24** is calculated to be 0.2 kcal/mol favored over **TS22** using PBE0-D3(BJ) method.

**Table S4.** Benchmark Study for the Key Transition States<sup>a</sup>

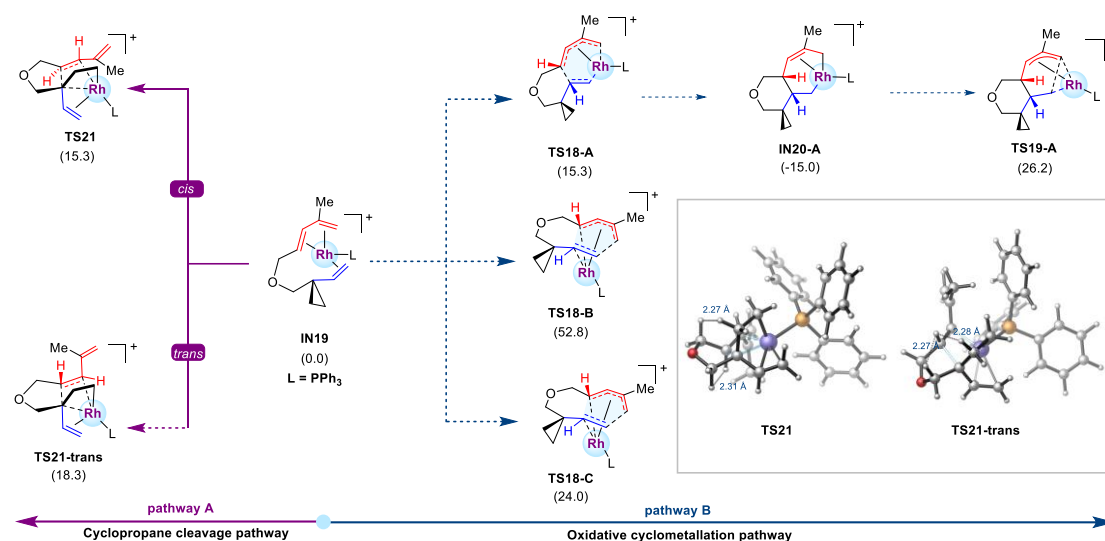
	TS22	TS24		TS22'		TS24'	
Method	DLPNO-CCSD(T)	BMK	M06-D3	ωB97X-D	PBE0-D3(BJ)	M11	B3LYP-D3(BJ)
TS22'	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS24'	-1.9	5.5	-4.2	-4.0	-0.5	-3.8	-4.4

<b>TS22</b>	-	0.0	0.0	0.0	0.0	0.0	0.0
<b>TS24</b>	-	5.7	-3.8	-3.3	-0.2	-3.0	-4.7

<sup>a</sup>The computational level is SMD(DCE)/Method/def2-TZVPP//BMK/6-31G(d)//LANL2DZ and the Gibbs energy differences are shown in kcal/mol.

## 5.7 Other Disfavored Pathways of IN19

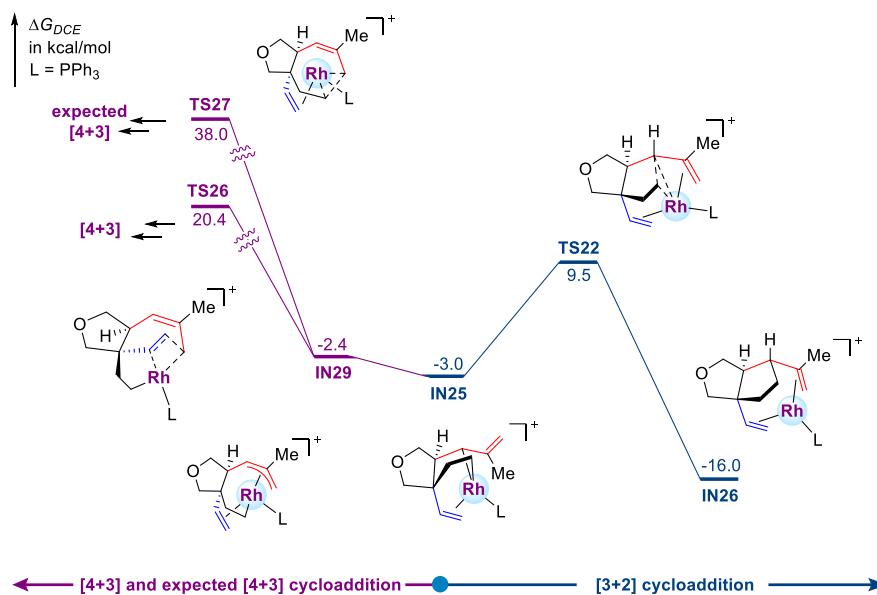
As mentioned above, *cis*-[3+2] cycloaddition pathway via **TS21** is the most favored process. In comparison, *trans*-[4+2] cycloaddition pathway via **TS18** and **TS19** is disfavored. In addition to these two pathways, **IN19** has some other transformation pathways (**Figure S10**). In consistent with experimental observations that no *trans*-[3+2] cycloadduct was detected, *trans*-[3+2] cycloaddition pathway via **TS21-trans** was found to be 3.0 kcal/mol more difficult compared to *cis*-[3+2] cycloaddition pathway via **TS21**. Similar to *trans*-[4+2] cycloaddition pathway, *cis*-[4+2] cycloaddition pathway via **TS18-A** and **TS19-A** is also disfavored since it requires more activation free energy of 10.9 kcal/mol than **TS21** does. Besides, DFT calculations showed that *cis* *endo*-OCM transition state **TS18-B** and *trans* *endo*-OCM transition state **TS18-C** are disfavored over the *cis*-alkene insertion transition state **TS21** by 37.5 and 8.7 kcal/mol, respectively. Thus *endo*-OCMs of **IN19** would not take place either.



**Figure S10.** Gibbs energy profile of different transformation pathways of **IN19**. Computed at SMD(DCE)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ. Color scheme: H, white; C, gray; O, red; P, orange; Rh, violet. Bond lengths are reported in Å.

## 5.8 Competing [4+3] and Expected [4+3] Pathway of IN25

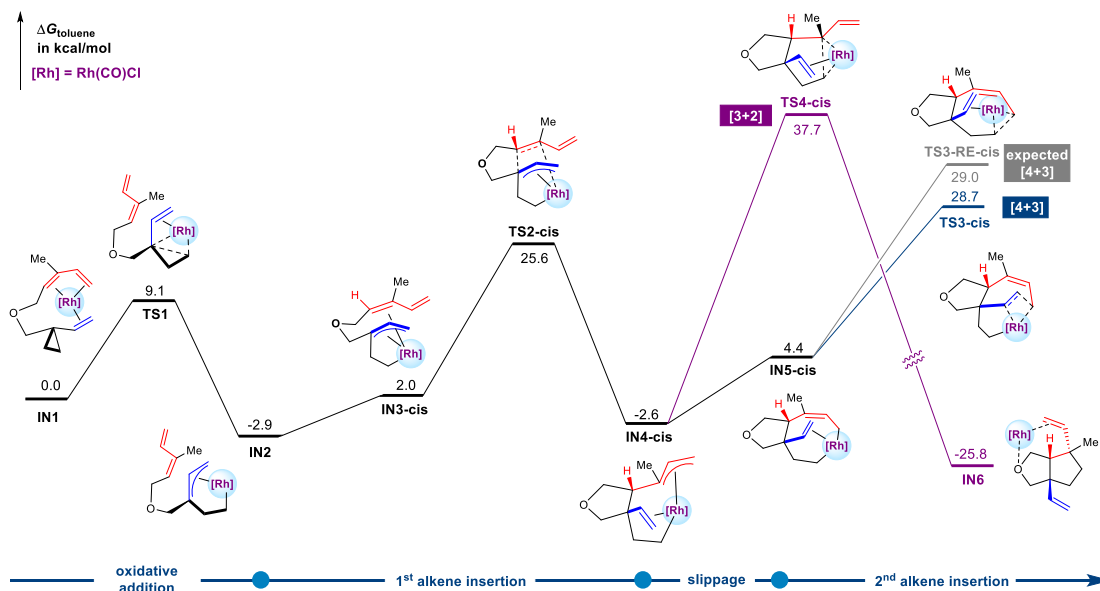
The competing [4+3] and expected [4+3] pathways of **IN25** was also examined (**Figure S11**). DFT calculations suggest that **TS26** and **TS27** are disfavored over **TS22** by 10.9 and 28.5 kcal/mol, respectively, which indicates neither [4+3] cycloaddition nor expected [4+3] cycloaddition may occur.



**Figure S11.** Gibbs energy profile of different transformation pathways of **IN25**. Computed at SMD(DCE)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ.

## 5.9 Discussion on *cis*-Cycloaddition in Pathway A

After oxidative addition step, the formed **IN2** has two reaction pathways to continue the reaction: the *cis* and *trans*-cycloaddition pathway. The *trans* pathway has been discussed detailly in the main text. The *cis*-cycloaddition pathway is shown in **Figure S12**. It was found that, similar to the *trans* pathway, alkene insertion via **TS2-cis** (25.6 kcal/mol) is much higher than *endo*-OCM via **TS5** (in pathway B, 17.4 kcal/mol) in terms of Gibbs energy, which indicates *cis*-cycloaddition in pathway A is also highly disfavored.



**Figure S12.** Gibbs energy profile of the *cis*-cycloaddition in pathway A. Computed at SMD(toluene)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ.

## 5.10 Different Oxidative Cyclometallation (OCM) Transition States for 5/6 and 6/6 Systems

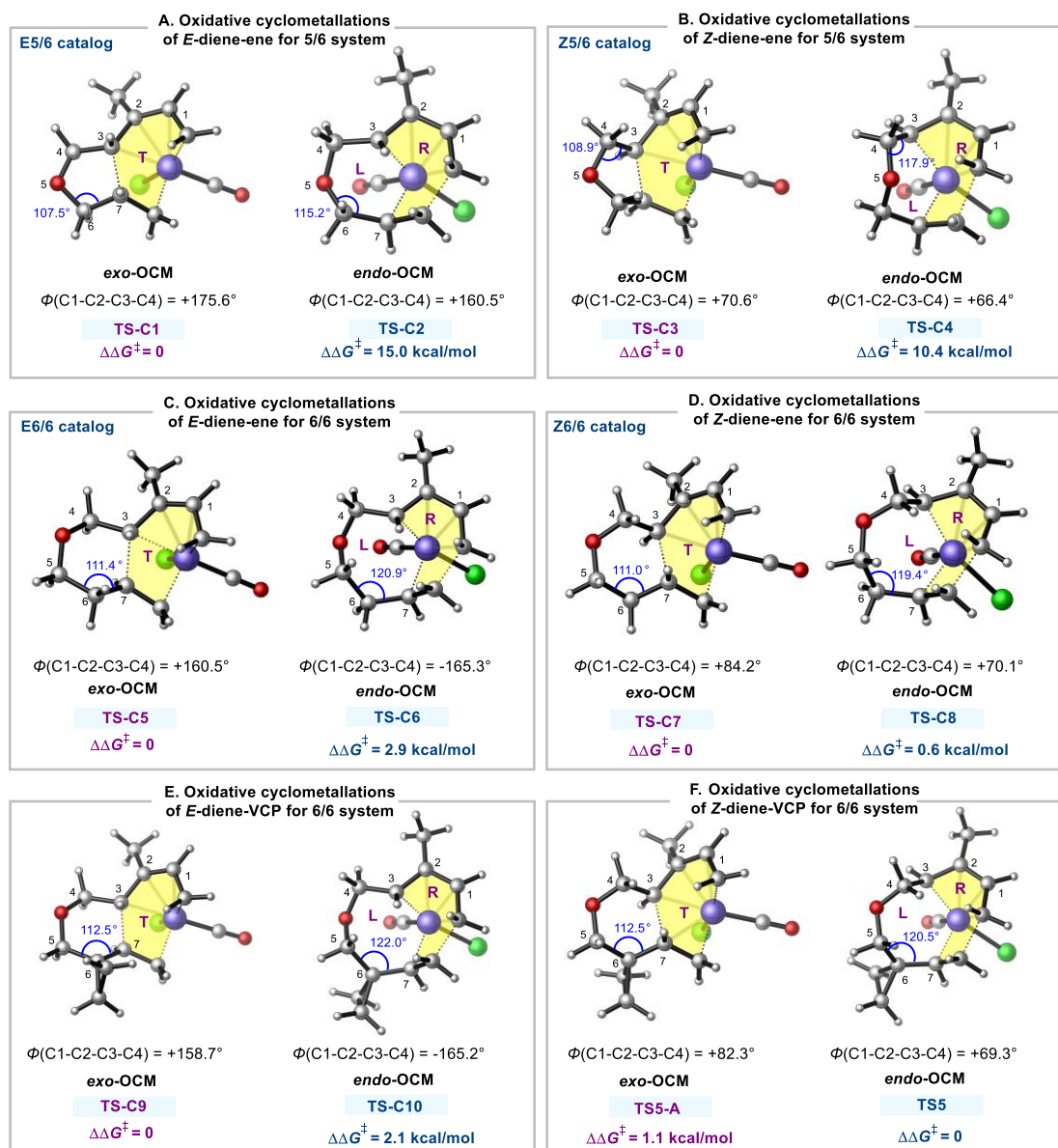
The comparison of different OCMs has been briefly described in the main text, and here we give more structural comparison.

As for the E5/6 catalog (**Figure S13A**), the bond angle  $\Phi(\text{O5-C6-C7})$  of the *exo*-OCM transition state **TS-C1** is  $107.5^\circ$  (close to the angle for normal  $\text{sp}^3$  hybridization), which means there's almost no ring distortion. While it was found  $\Phi(\text{O5-C6-C7})$  has become  $115.2^\circ$  for the *endo*-OCM transition state **TS-C2**, which implies **TS-C2** has larger L (left) ring distortion. Besides, the dihedral angle  $\Phi(\text{C1-C2-C3-C4})$  of **TS-C2** is  $+160.5^\circ$ , which suggests **TS-C2** has larger R (right) ring distortion compared to **TS-C1** ( $+175.6^\circ$ ). The above reasons make *endo*-OCM much less favored. The energy difference between the two types of OCMs for Z5/6 catalog is 10.4 kcal/mol, which is relatively smaller than E5/6 catalog because *endo*-OCM via **TS-C4** suffers from smaller R ring distortion (**Figure S13B**).

As for E6/6 catalog, *endo*-OCM via **TS-C6** is still more disfavored over *exo*-OCM by 2.9 kcal/mol (**Figure S13C**) due to L ring distortion. But for the Z6/6 catalog, the *endo*-OCM (via **TS-C8**) and *exo*-OCM (via **TS-C7**) has almost the same Gibbs energy, which can be attributed to the trade off between L ring distortion and R ring distortion. As shown in **Figure S13D**,  $\Phi(\text{C5-C6-C7})$  of **TS-C7** and **TS-C8** is  $111.0^\circ$  and  $119.4^\circ$ , respectively, indicating **TS-C8** suffers larger L ring distortion. The dihedral angle  $\Phi(\text{C1-C2-C3-C4})$  should be  $0^\circ$  for common diene structure, however it has been distorted to  $+84.2^\circ$  and  $+70.1^\circ$  for **TS-C7** and **TS-C8**, respectively, which suggests the R ring distortion for **TS-C8** is much smaller.

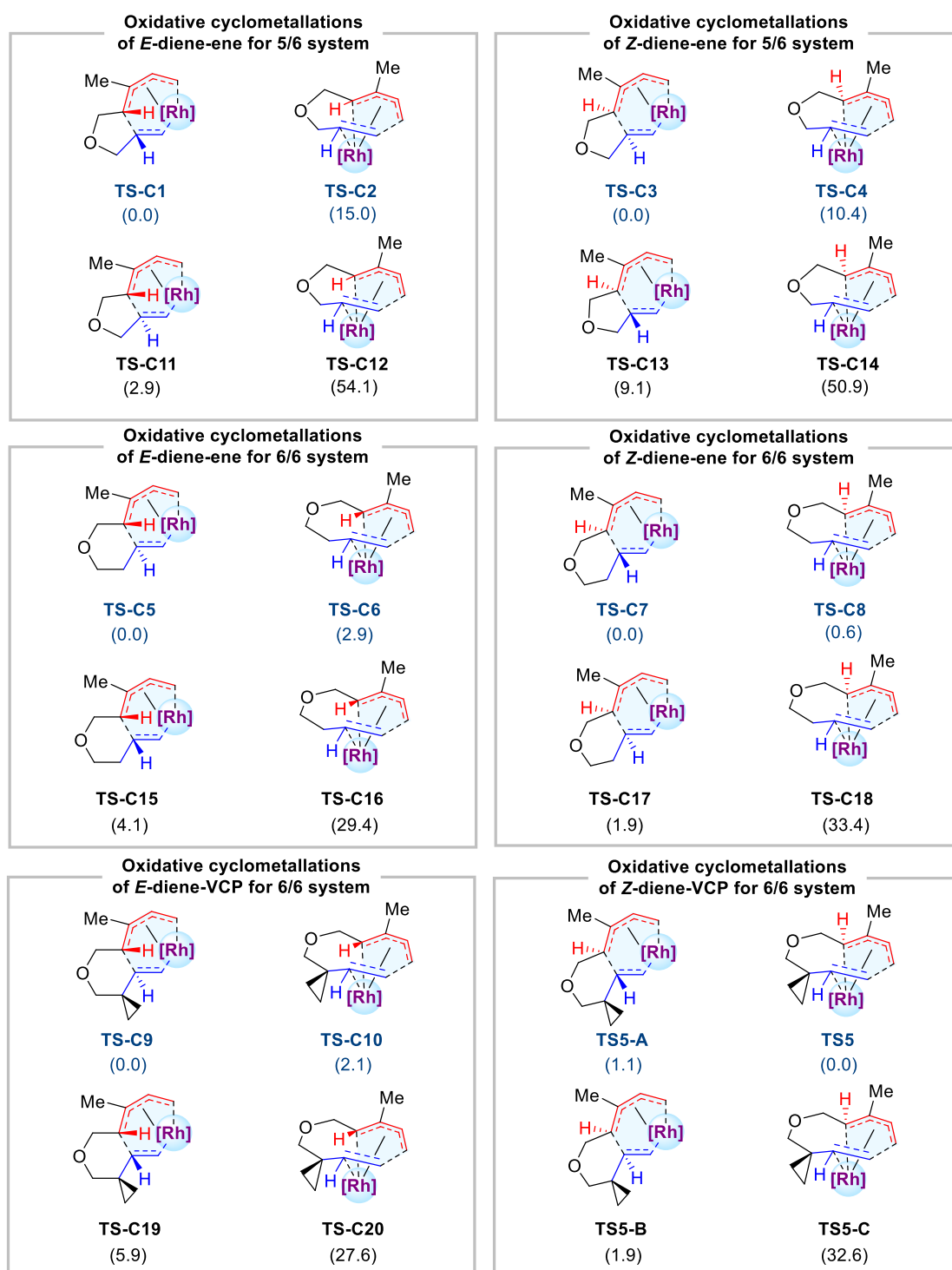
It's similar when cyclopropane was introduced to the tether, as shown in **Figure S13E** and **S13F**. And it should be noted that *endo*-OCM for Z-diene-VCP becomes more favored than *exo*-OCM.

Except for the most favored *exo* and *endo*-OCM transition states mentioned in the main text, the other disfavored transition states are listed in **Figure S14**.



**Figure S13.** *Exo* and *endo*-ene/diene oxidative cyclometallations. Computed at SMD(toluene)/DLPNO-CCSD(T)/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level. Color scheme: H, white; C, gray; O, red; Cl, green; Rh, violet.



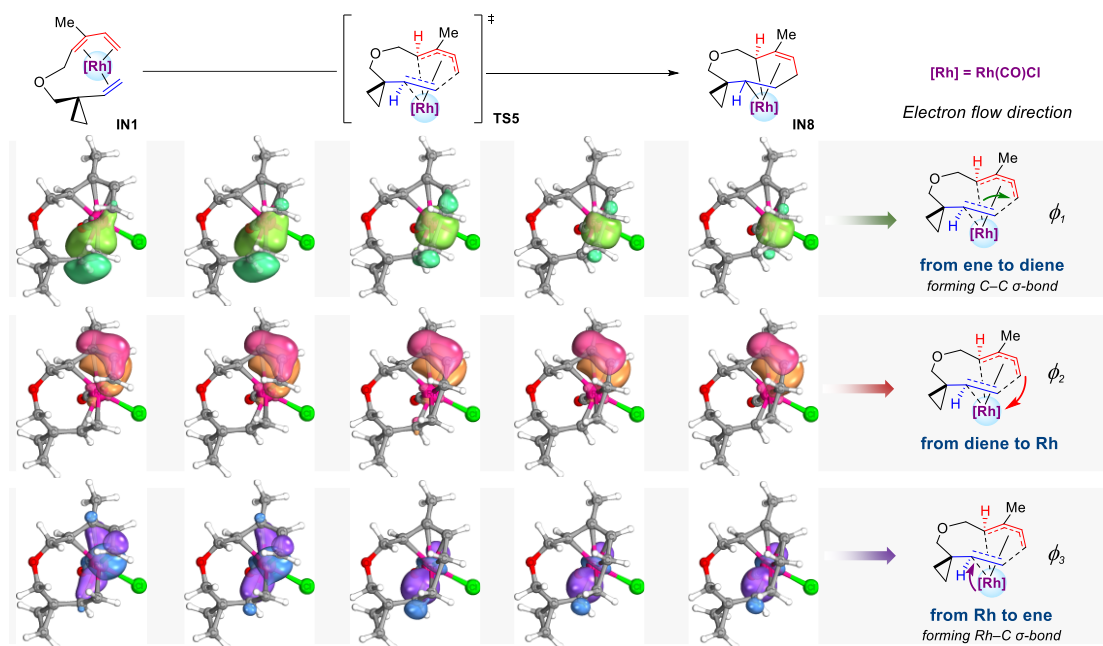


**Figure S14.** Summary of different oxidative cyclometallation transition states of 5/6 and 6/6 systems. Gibbs energies given in the brackets are reported in kcal/mol. [Rh] = Rh(CO)Cl. Computed at SMD(toluene)/DLPNO-CCSD(T)/def2-TZVPP//BMK/LANL2DZ/6-31G(d) level.

## 5.11 Intrinsic Bonding Orbital (IBO) Analysis of TS5

To have a better understanding of the unexpected *endo*-OCM process, we carried out intrinsic bonding orbitals (IBOs) analysis<sup>36,48</sup> (**Figure S15**). Three IBOs were found to undergo significant displacement along the intrinsic reaction coordinate (IRC) through **IN1** → **TS5** → **IN8**. Among these IBOs,  $\phi_I$ , which corresponds to

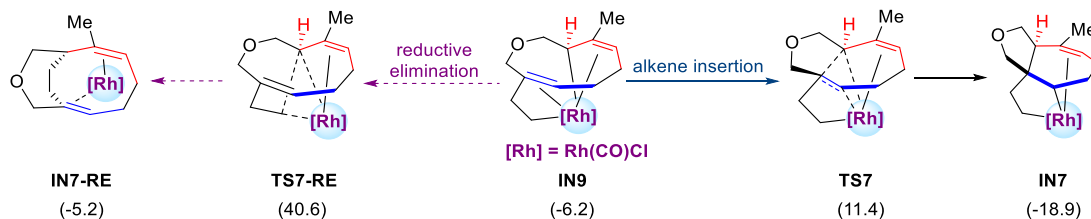
the localized  $\pi(\text{C}-\text{C})$  bond of the ene fragment, encapsulates its density to construct the newly formed  $\sigma(\text{C}-\text{C})$  bond of **IN8**. Similarly,  $\phi_2$  and  $\phi_3$  track the transformations that the diene part gives its density to Rh center and Rh gives its density to the ene part forming a  $\sigma(\text{Rh}-\text{C})$  bond, respectively. This result undoubtedly provides a clear picture of how electron flows in the *endo*-OCM.



**Figure S15.** IBO analysis of **TS5**. Computed at PBE0/def2-SVP level.

## 5.12 Discussion on Different Reaction Pathways of **IN9**

For **IN9**, it has two reaction pathways, as shown in **Figure S16**. One is alkene insertion via **TS7**, which has an activation free energy of 17.6 kcal/mol. While reductive elimination of **IN9** via **TS7-RE** is disfavored by 29.2 kcal/mol, which can be safely ruled out.



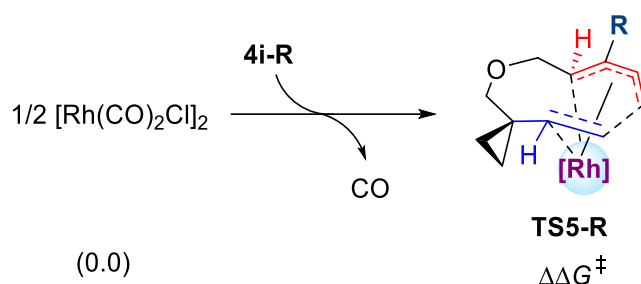
**Figure S16.** Comparison of different pathways of **IN9**. Gibbs energies given in the brackets are reported in kcal/mol. Computed at SMD(toluene)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ.

## 5.13 Substitution Effects of the Diene Moiety

It was observed that substrate **4k** with no methyl group on the diene group did not react under the standard conditions. To know the difference between substrates with different substitutions on the diene group, we calculated the Gibbs energy differences of OCM transition states for different substrates. As is shown in **Table S5**, the activation free energy ( $\Delta\Delta G^\ddagger$ ) increases as the substitution group becomes more electron deficient. **TS5-H** is 2.4 kcal/mol higher than **TS5**, indicating that **4i-H** is difficult to undergo [4+3] reaction, which is in consistent with the experimental observation. It's proposed that methyl group can increase the orbital

coefficient of the diene group so as to lower the energy barrier via hyperconjugation. Indeed, as the substitution group becomes more electron donating, the energy barrier for the *endo*-OCM become lower. For example, **TS5-N** is 5.1 kcal/mol lower compared to **TS5**. This explains why substitution is necessary.

**Table S5.** Diene substitution effects on the OCM step.<sup>a</sup>



entry	R	Substrate (4i-R)	Transition State (TS5-R)	ΔΔG <sup>‡</sup> (kcal/mol)
1	CN	4i-CN	TS5-CN	38.5
2	F	4i-F	TS5-F	35.5
3	H	4i-H	TS5-H	34.1
4	Me	4i	TS5	31.7
5	OMe	4i-O	TS5-O	30.9
6	NMe <sub>2</sub>	4i-N	TS5-N	26.6

<sup>a</sup>Computed at SMD(toluene)/BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ.

## 5.14 Computed Energies for the Stationary Points

**Table S6.** Thermal Corrections to Gibbs Energies (TCGs) and Single Point Energies (SPEs) (PART1)

Stationary Point	TCG <sup>a,b</sup> /a.u.	SPE(L) <sup>a</sup> /a.u.	SPE(sol) <sup>c</sup> /a.u.	SPE(H1) <sup>d</sup> /a.u.	SPE(H2) <sup>e</sup> /a.u.
4i	0.231033	-542.832863	-542.844922	-543.047951	
6i	0.244201	-542.902236	-542.913025	-543.10691	
CO	-0.013873	-113.260871	-113.256415	-113.309262	
[Rh(CO) <sub>2</sub> Cl] <sub>2</sub>	-0.008513	-1591.32025	-1591.32213	-1593.843897	
IN1	0.244721	-1225.219104	-1225.237808	-1226.642205	
TS1	0.233536	-1225.190383	-1225.209886	-1226.615725	
IN2	0.237383	-1225.21149	-1225.23208	-1226.637658	
IN3	0.246698	-1225.227651	-1225.242894	-1226.649692	
IN3-cis	0.246262	-1225.22165	-1225.237102	-1226.643751	
TS2	0.246017	-1225.182833	-1225.198299	-1226.604141	-1225.621964
TS2-cis	0.24625	-1225.184312	-1225.199968	-1226.606004	-1225.624202
IN4	0.24625	-1225.228178	-1225.246352	-1226.645294	
IN4-cis	0.249192	-1225.234924	-1225.250757	-1226.653694	
IN5	0.247088	-1225.21776	-1225.237818	-1226.633722	
IN5-cis	0.249521	-1225.224079	-1225.243137	-1226.639642	
TS3	0.246359	-1225.184733	-1225.204963	-1226.600738	
TS3-cis	0.248024	-1225.182066	-1225.202637	-1226.597904	
TS4	0.247473	-1225.185409	-1225.204594	-1226.605516	

<b>TS4-cis</b>	0.246339	-1225.167788	-1225.184225	-1226.585955	
<b>TS3-RE</b>	0.245524	-1225.176915	-1225.195278	-1226.592103	
<b>TS3-RE-cis</b>	0.245005	-1225.18073	-1225.198454	-1226.597291	
<b>IN6</b>	0.248861	-1225.252303	-1225.269942	-1226.667904	
<b>IN6-cis</b>	0.24868	-1225.269149	-1225.287129	-1226.685297	
<b>TS5</b>	0.246077	-1225.191088	-1225.210932	-1226.614686	-1225.626277
<b>TS5-C</b>	0.245507	-1225.131967	-1225.152279	-1226.553966	-1225.573294
<b>TS5-B</b>	0.246126	-1225.191231	-1225.207875	-1226.614282	-1225.626491
<b>TS5-A</b>	0.246167	-1225.193801	-1225.209817	-1226.618312	-1225.628414
<b>IN8</b>	0.24855	-1225.23011	-1225.251334	-1226.646414	
<b>TS6</b>	0.246422	-1225.213944	-1225.232911	-1226.628241	
<b>TS6-RE</b>	0.246253	-1225.184655	-1225.203932	-1226.6028	
<b>IN9</b>	0.248617	-1225.240777	-1225.259037	-1226.656496	
<b>TS7</b>	0.247837	-1225.212516	-1225.229842	-1226.628537	
<b>TS7-RE</b>	0.249778	-1225.166859	-1225.18437	-1226.583797	
<b>IN7</b>	0.250436	-1225.265966	-1225.284885	-1226.677872	
<b>IN7-RE</b>	0.25167	-1225.247919	-1225.266875	-1226.656975	
<b>IN10</b>	0.246173	-1225.241692	-1225.26478	-1226.657097	
<b>TS8</b>	0.242741	-1225.218978	-1225.23947	-1226.637313	
<b>IN11</b>	0.244569	-1225.23237	-1225.250845	-1226.652864	
<b>TS9</b>	0.243653	-1225.22032	-1225.238198	-1226.641463	
<b>IN12</b>	0.245217	-1225.288019	-1225.305687	-1226.7025	
<b>IN13</b>	0.33864	-1984.63932	-1984.667697	-1986.274601	
<b>TS14-A</b>	0.338694	-1984.612305	-1984.639606	-1986.249869	
<b>TS14-B</b>	0.341605	-1984.609787	-1984.640139	-1986.244361	
<b>TS14-C</b>	0.341565	-1984.593806	-1984.620047	-1986.228546	
<b>TS14-D</b>	0.341028	-1984.568925	-1984.599026	-1986.203428	
<b>IN14</b>	0.341214	-1984.658852	-1984.689906	-1986.29086	
<b>IN16</b>	0.343018	-1984.64383	-1984.675282	-1986.27181	
<b>TS15</b>	0.338773	-1984.608304	-1984.638887	-1986.240312	
<b>TS16</b>	0.343482	-1984.62441	-1984.654159	-1986.250521	
<b>TS25</b>	0.341036	-1984.609674	-1984.637375	-1986.240035	
<b>IN15</b>	0.343707	-1984.683924	-1984.71139	-1986.311788	
<b>IN17</b>	0.34512	-1984.640225	-1984.669323	-1986.270489	
<b>TS17</b>	0.342337	-1984.604913	-1984.632772	-1986.236082	
<b>IN18</b>	0.344067	-1984.674632	-1984.703157	-1986.296593	
<b>TS24-trans</b>	0.341599	-1984.593459	-1984.618895	-1986.226632	
<b>TS24-cis</b>	0.340622	-1984.591149	-1984.616432	-1986.226223	
<b>4i-H</b>	0.203319	-503.545975	-503.55764	-503.747433	
<b>TS5-H</b>	0.22005	-1185.902164	-1185.92143	-1187.312189	
<b>4i-CN</b>	0.197931	-595.740458	-595.7536	-595.974543	
<b>TS5-CN</b>	0.215374	-1278.090446	-1278.111126	-1279.533122	
<b>4i-F</b>	0.1942	-602.754052	-602.765057	-602.998323	
<b>TS5-F</b>	0.210822	-1285.107589	-1285.126093	-1286.560909	

<b>4i-O</b>	0.236511	-618.013589	-618.024982	-618.259057	
<b>TS5-O</b>	0.251315	-1300.372549	-1300.391962	-1301.82659	
<b>4i-N</b>	0.273764	-637.420711	-637.433788	-637.670463	
<b>TS5-N</b>	0.291394	-1319.789564	-1319.811428	-1321.246841	
<b>TS-C1</b>	0.187943	-1108.594604	-1108.608662	-1109.975092	-1109.155152
<b>TS-C2</b>	0.186556	-1108.565427	-1108.583772	-1109.945158	-1109.125639
<b>TS-C3</b>	0.185182	-1108.594479	-1108.609096	-1109.975959	-1109.15596
<b>TS-C4</b>	0.186088	-1108.577257	-1108.593368	-1109.956646	-1109.138828
<b>TS-C5</b>	0.214832	-1147.867042	-1147.882312	-1149.262592	-1148.387683
<b>TS-C6</b>	0.212674	-1147.857953	-1147.877047	-1149.252027	-1148.377011
<b>TS-C7</b>	0.214885	-1147.862028	-1147.877078	-1149.257861	-1148.382313
<b>TS-C8</b>	0.2145	-1147.858621	-1147.876278	-1149.253252	-1148.378422
<b>TS-C9</b>	0.246936	-1225.197345	-1225.214246	-1226.621847	-1225.63267
<b>TS-C10</b>	0.245756	-1225.189857	-1225.210709	-1226.613084	-1225.624118
<b>TS-C11</b>	0.186016	-1108.58506	-1108.599672	-1109.967543	-1109.148073
<b>TS-C12</b>	0.18507	-1108.491915	-1108.509824	-1109.871585	-1109.062211
<b>TS-C13</b>	0.185542	-1108.579472	-1108.593798	-1109.96201	-1109.142068
<b>TS-C14</b>	0.184868	-1108.50423	-1108.521589	-1109.883471	-1109.071813
<b>TS-C15</b>	0.215647	-1147.861281	-1147.876706	-1149.255939	-1148.381761
<b>TS-C16</b>	0.214193	-1147.814608	-1147.833716	-1149.206676	-1148.336407
<b>TS-C17</b>	0.21579	-1147.859334	-1147.874621	-1149.25337	-1148.380001
<b>TS-C18</b>	0.212408	-1147.797902	-1147.816564	-1149.190783	-1148.323011
<b>TS-C19</b>	0.247717	-1225.190165	-1225.206242	-1226.613588	-1225.624805
<b>TS-C20</b>	0.245388	-1225.146682	-1225.167553	-1226.567207	-1225.583241

<sup>a</sup>Computed at BMK/6-31G(d)/LANL2DZ level.

<sup>b</sup>Computed at 1 atm and 298 K.

<sup>c</sup>Computed at SMD(toluene)/BMK/6-31G(d)/LANL2DZ//BMK/6-31G(d)/LANL2DZ level.

<sup>d</sup>Computed at BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level.

<sup>e</sup>Computed at DLPNO-CCSD(T)/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level.

**Table S7.** Thermal Corrections to Gibbs Energies (TCGs) and Single Point Energies (SPEs) (PART2)

<b>Stationary Point</b>	<b>TCG<sup>a,b</sup> / a.u.</b>	<b>SPE(L)<sup>a</sup> / a.u.</b>	<b>SPE(sol)<sup>c</sup> / a.u.</b>	<b>SPE(H1)<sup>d</sup> / a.u.</b>	<b>SPE(H2)<sup>e</sup> / a.u.</b>
<b>PPh<sub>3</sub></b>	0.230512	-1035.679748	-1035.701919	-1035.969817	
<b>IN19</b>	0.496838	-1687.358377	-1687.441371	-1688.980397	
<b>IN22</b>	0.748713	-2723.05183	-2723.148516	-2724.962247	
<b>TS20</b>	0.749877	-2723.044794	-2723.140417	-2724.955199	
<b>IN23</b>	0.751401	-2723.072853	-2723.173843	-2724.984409	
<b>IN24</b>	0.501823	-1687.357224	-1687.449071	-1688.978609	
<b>TS21</b>	0.500439	-1687.329147	-1687.422553	-1688.949172	
<b>TS21-trans</b>	0.500214	-1687.322384	-1687.416943	-1688.943059	
<b>IN25</b>	0.499006	-1687.355082	-1687.457241	-1688.968216	
<b>IN29</b>	0.499928	-1687.354461	-1687.456936	-1688.967767	
<b>TS26</b>	0.499143	-1687.311646	-1687.418165	-1688.926743	
<b>TS27</b>	0.498257	-1687.303537	-1687.388668	-1688.919157	
<b>TS22</b>	0.501114	-1687.346651	-1687.433792	-1688.965391	

<b>IN26</b>	0.504229	-1687.392109	-1687.480863	-1689.007479	
<b>TS23</b>	0.490402	-1687.336641	-1687.428729	-1688.964475	
<b>IN27</b>	0.491465	-1687.35107	-1687.44164	-1688.977632	
<b>TS24</b>	0.492583	-1687.323082	-1687.406629	-1688.951368	
<b>IN28</b>	0.49373	-1687.370073	-1687.466304	-1688.986453	
<b>TS18-A</b>	0.497675	-1687.327877	-1687.418351	-1688.94937	
<b>TS18</b>	0.494659	-1687.322768	-1687.415784	-1688.945424	
<b>TS18-B</b>	0.500979	-1687.277488	-1687.362942	-1688.897978	
<b>TS18-C</b>	0.49847	-1687.315104	-1687.405515	-1688.936297	
<b>IN20-A</b>	0.499096	-1687.376	-1687.474297	-1688.991186	
<b>IN20</b>	0.497782	-1687.368619	-1687.476492	-1688.985283	
<b>TS19-A</b>	0.499636	-1687.312606	-1687.410527	-1688.926504	
<b>TS19</b>	0.497216	-1687.310929	-1687.404525	-1688.928274	
<b>IN21</b>	0.502584	-1687.371201	-1687.467342	-1688.985284	
<b>TS22'</b>	0.352611	-1112.543751	-1112.625049	-1113.959973	-1112.96069
<b>TS24'</b>	0.342024	-1112.522323	-1112.598139	-1113.947539	-1112.958664

<sup>a</sup>Computed at BMK/6-31G(d)/LANL2DZ level.

<sup>b</sup>Computed at 1 atm and 298 K.

<sup>c</sup>Computed at SMD(DCE)/BMK/6-31G(d)/LANL2DZ//BMK/6-31G(d)/LANL2DZ level.

<sup>d</sup>Computed at BMK/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level.

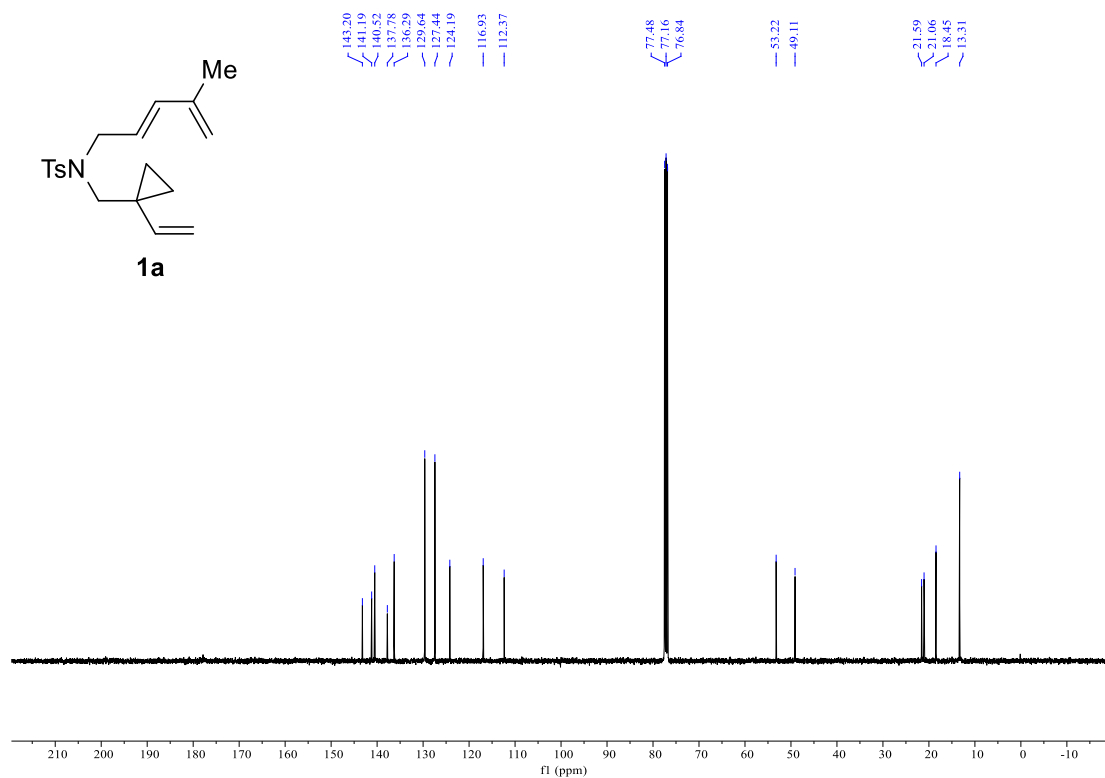
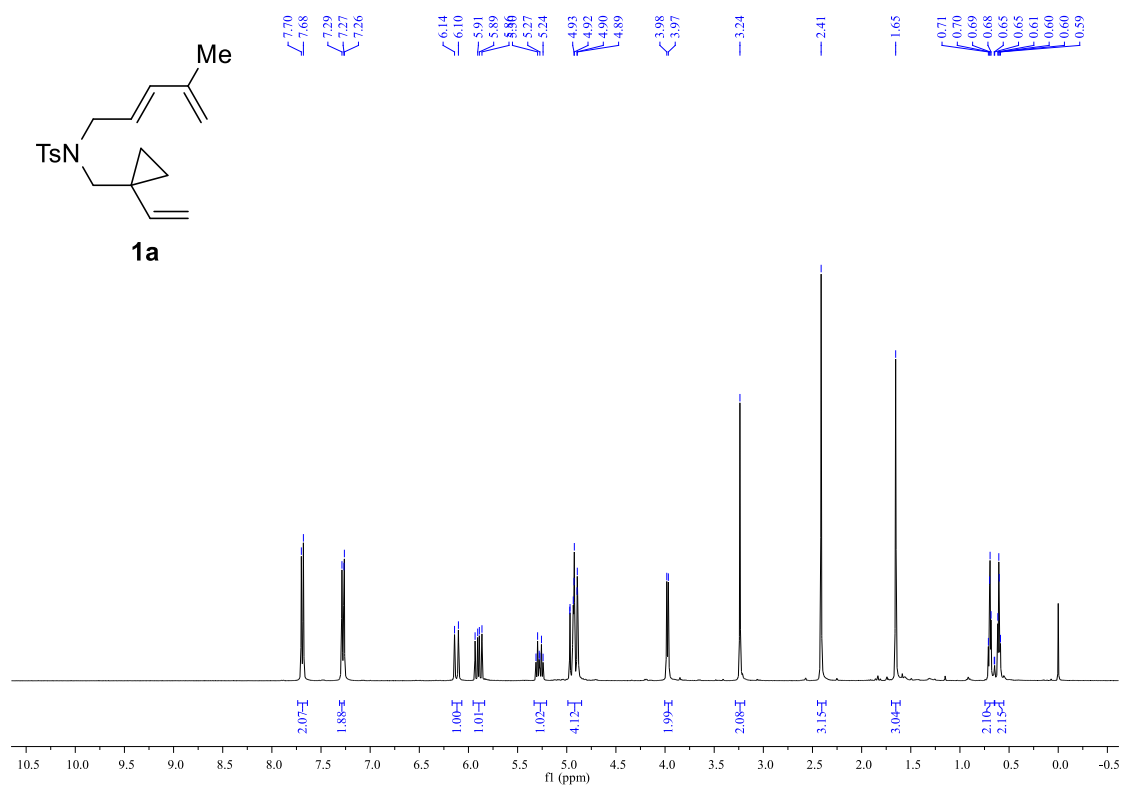
<sup>e</sup>Computed at DLPNO-CCSD(T)/def2-TZVPP//BMK/6-31G(d)/LANL2DZ level.

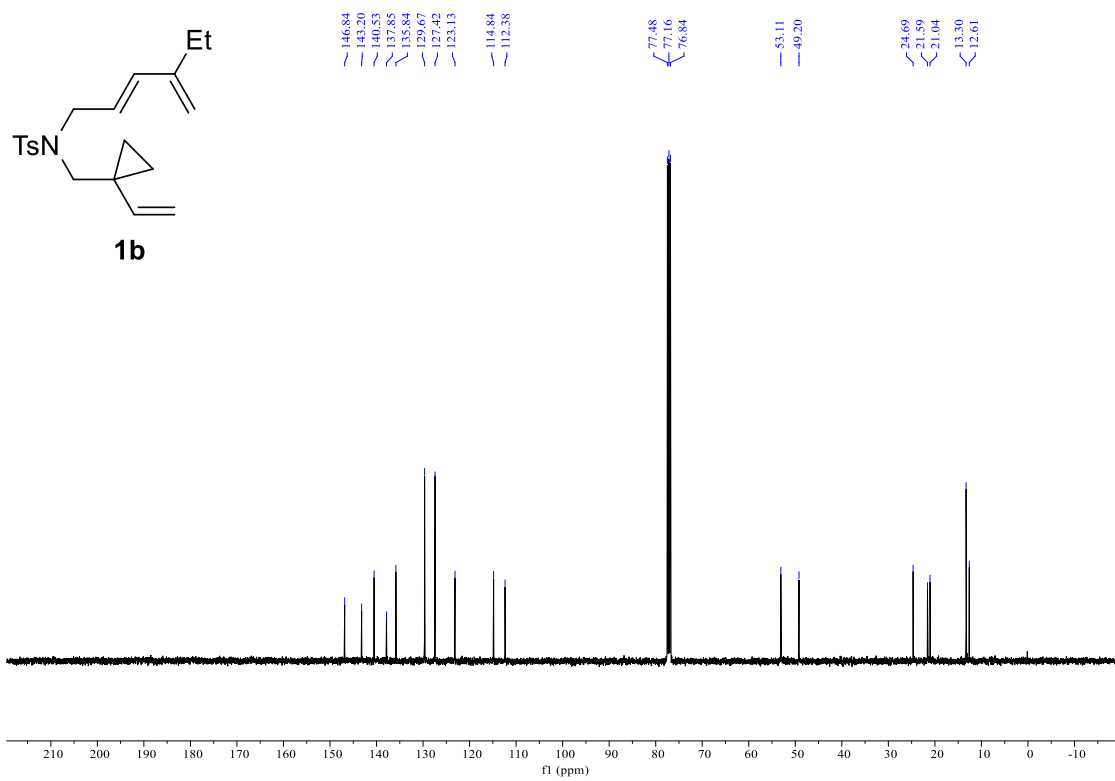
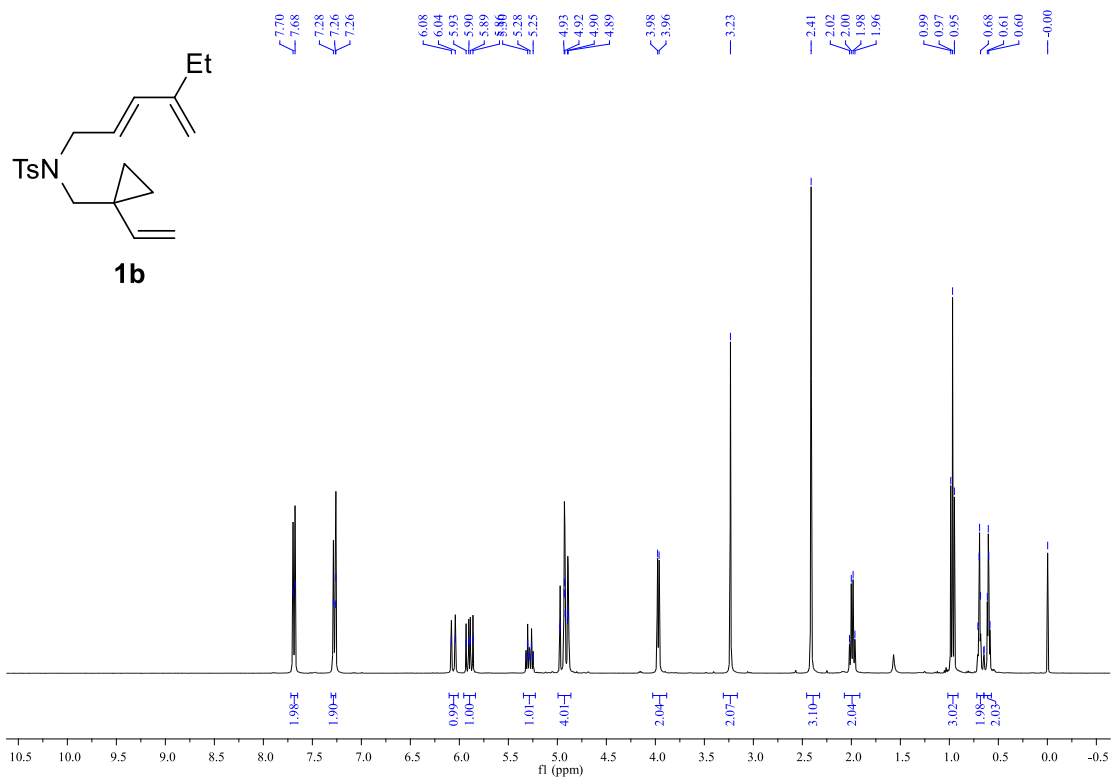
**Table S8.** Single Point Energies (SPEs) of **TS22**, **TS24**, **TS22'** and **TS24'** Calculated by Different Methods<sup>a</sup>

<b>Method</b>	<b>M06-D3</b>	<b><math>\omega</math>B97X-D</b>	<b>PBE0-D3(BJ)</b>	<b>M11</b>	<b>B3LYP-D3(BJ)</b>
<b>TS22'</b>	-1114.53244	-1114.874066	-1114.160935	-1114.486181	-1115.201832
<b>TS24'</b>	-1114.534032	-1114.875275	-1114.156601	-1114.487172	-1115.204587
<b>TS22</b>	-1689.497581	-1690.075025	-1688.922673	-1689.55624	-1690.681666
<b>TS24</b>	-1689.498647	-1690.075413	-1688.918055	-1689.556132	-1690.684214

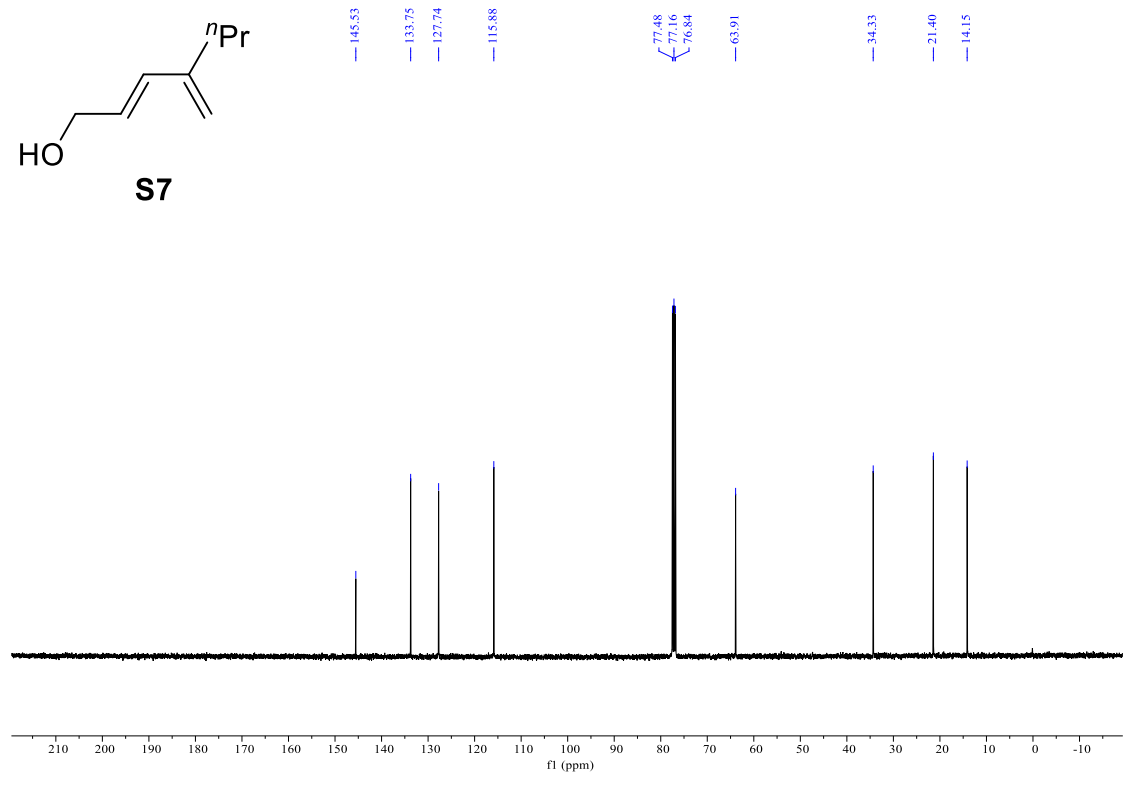
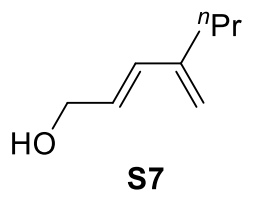
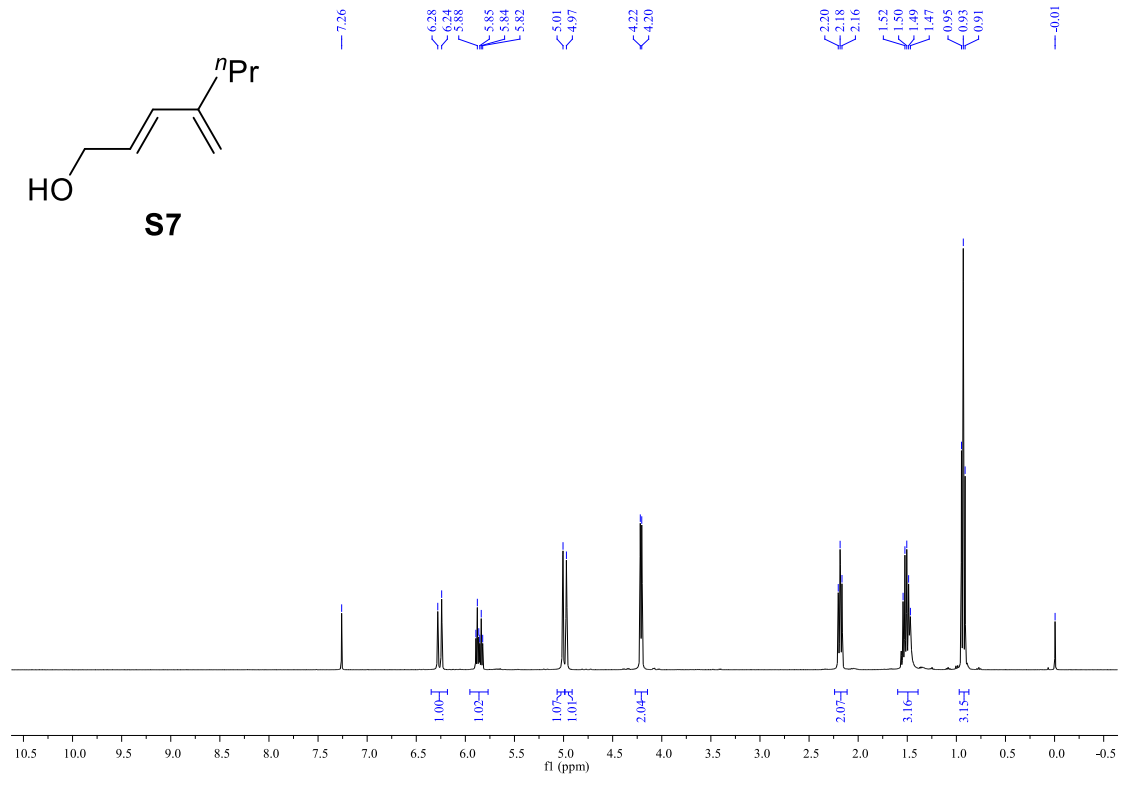
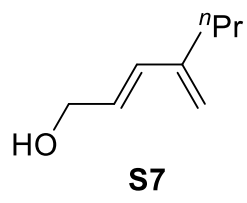
<sup>a</sup>The computational level is Method/def2-TZVPP//BMK/6-31G(d)/LANL2DZ and the unit is a.u.

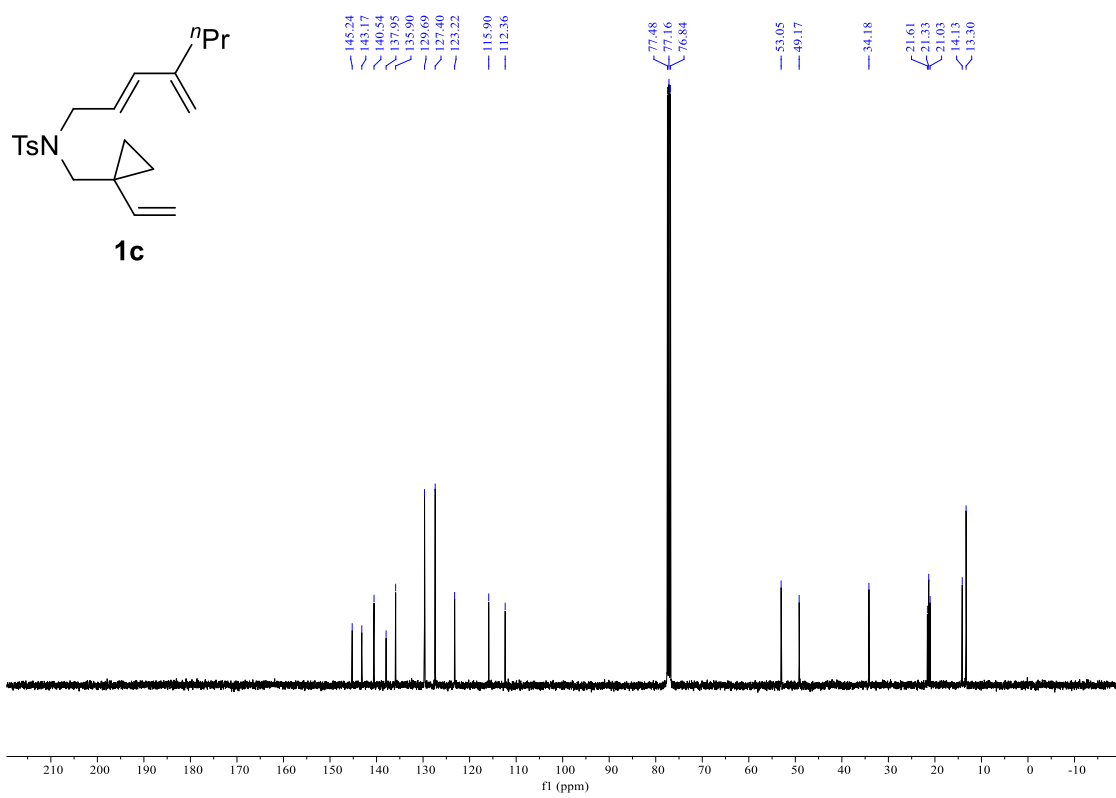
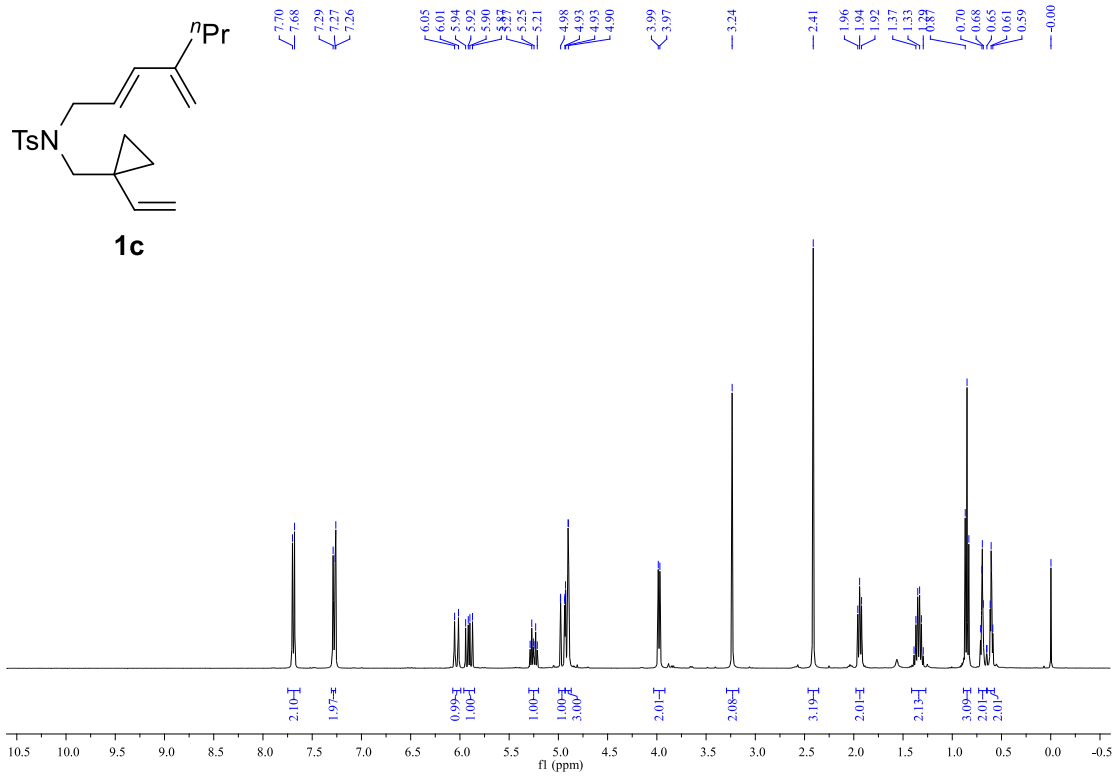
## 6. Data S1 (<sup>1</sup>H and <sup>13</sup>C NMR)

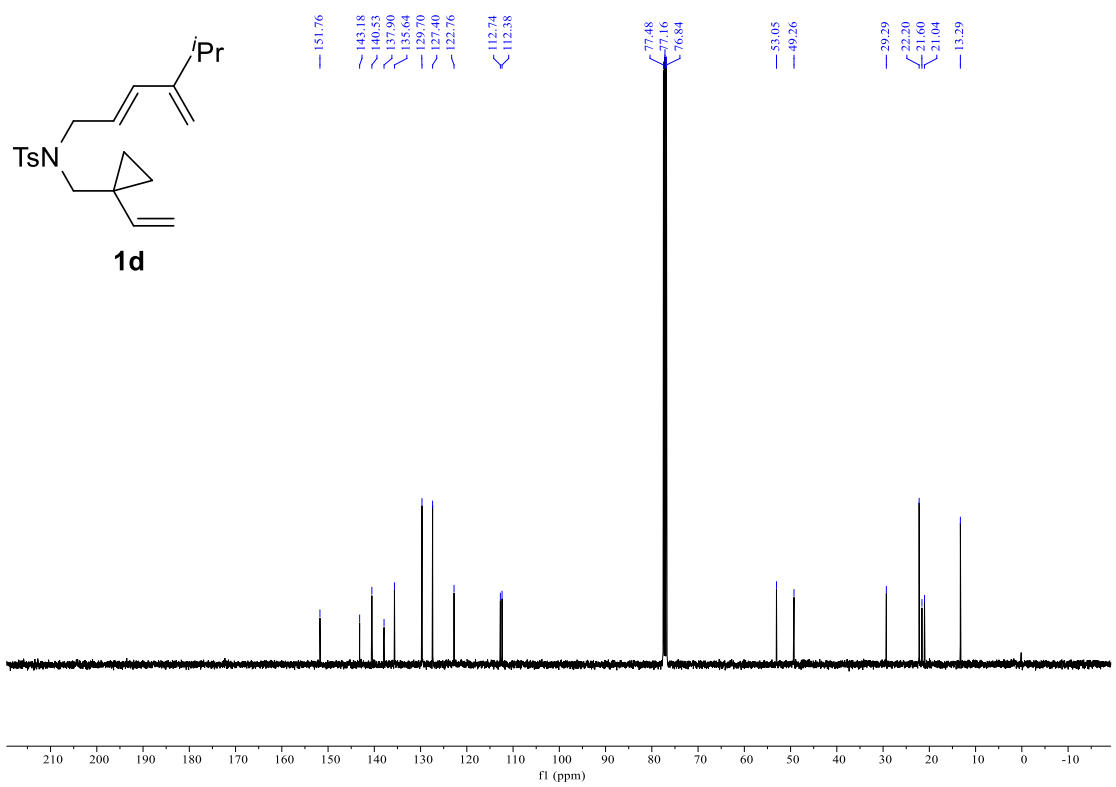
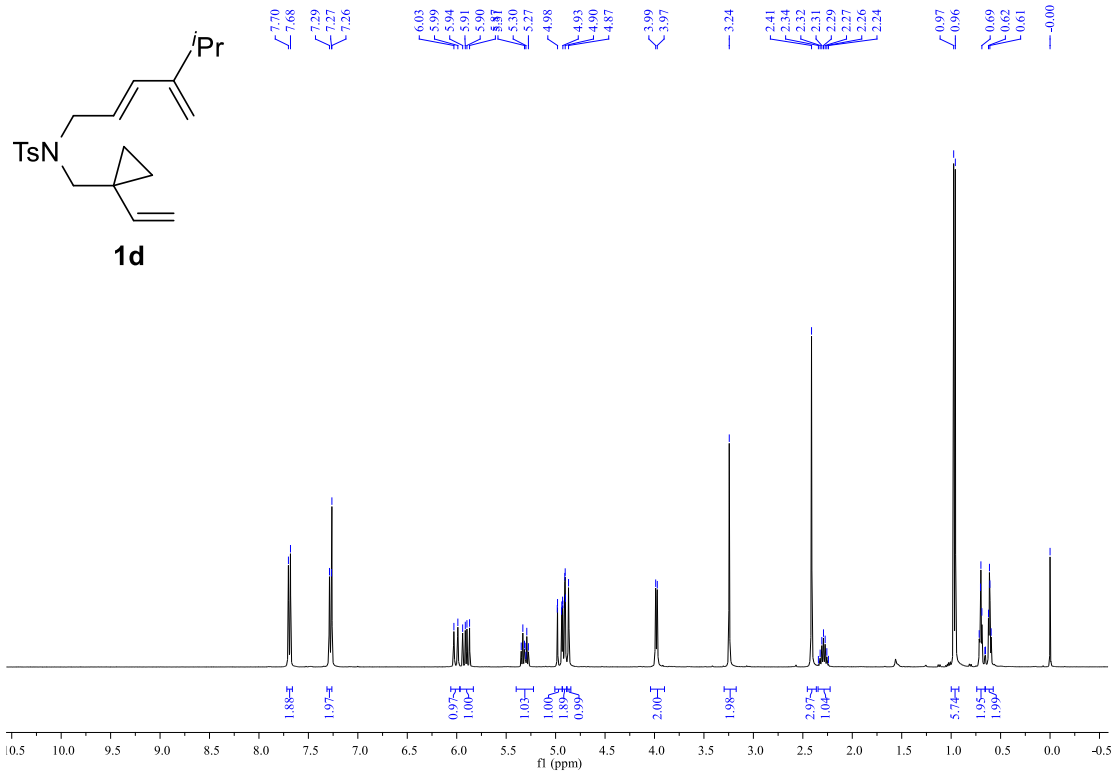


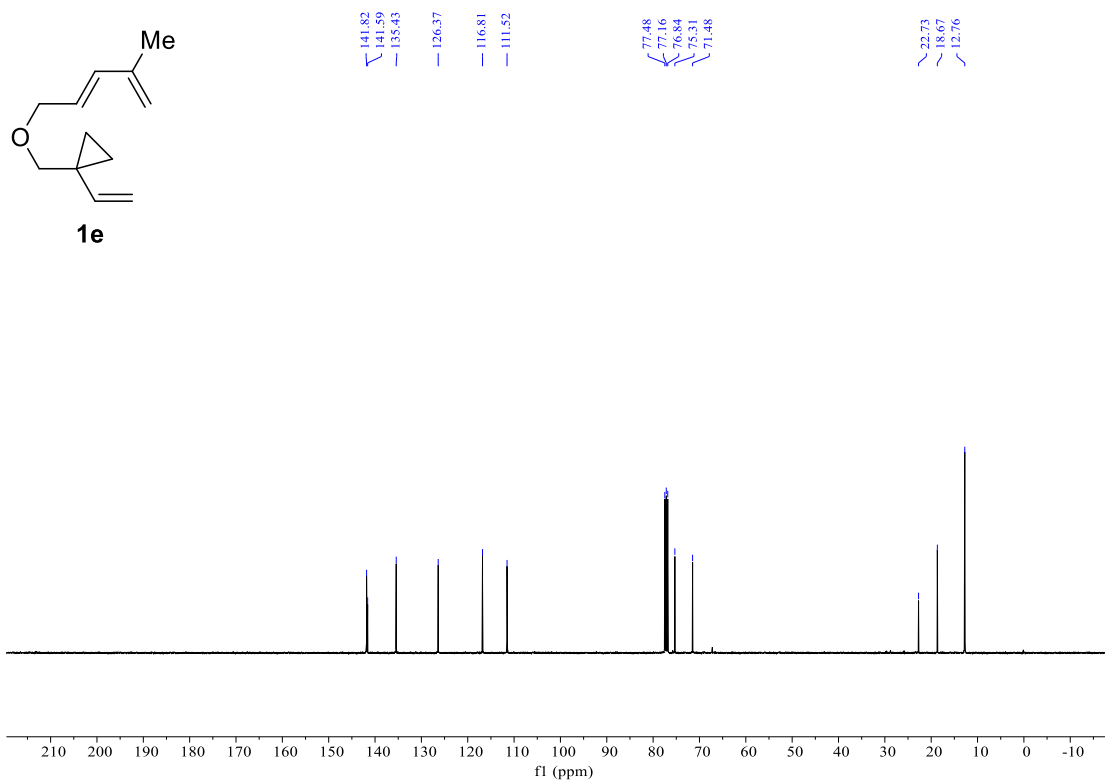
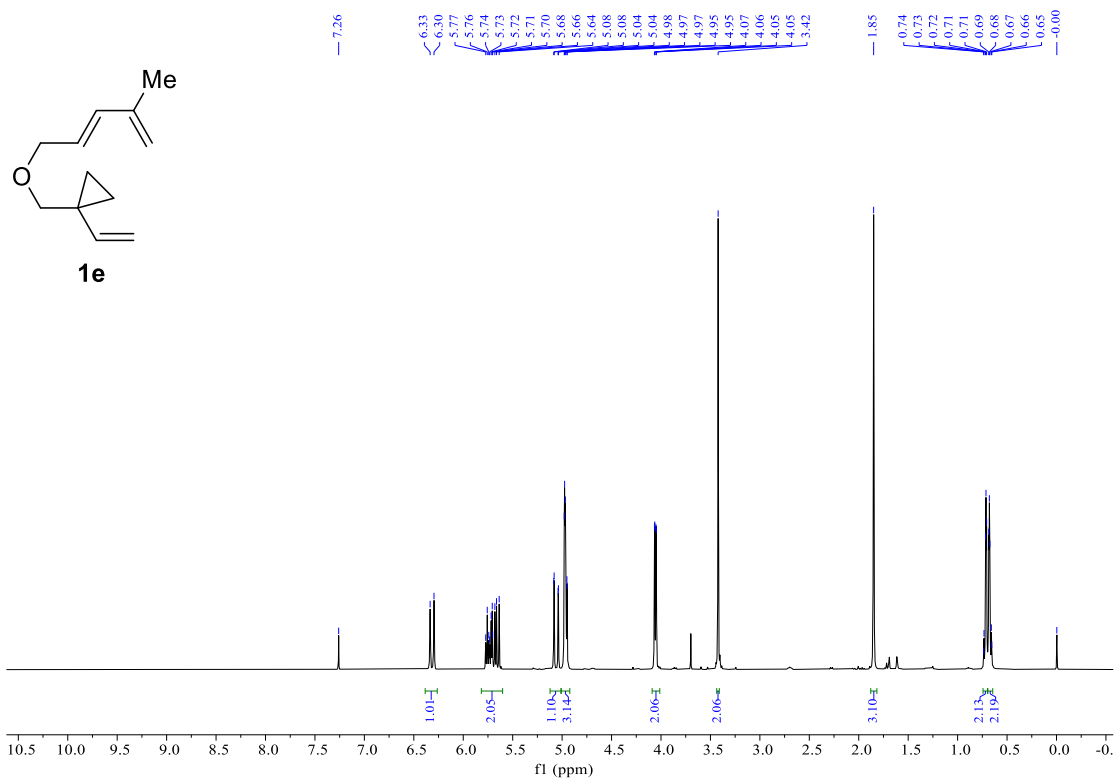


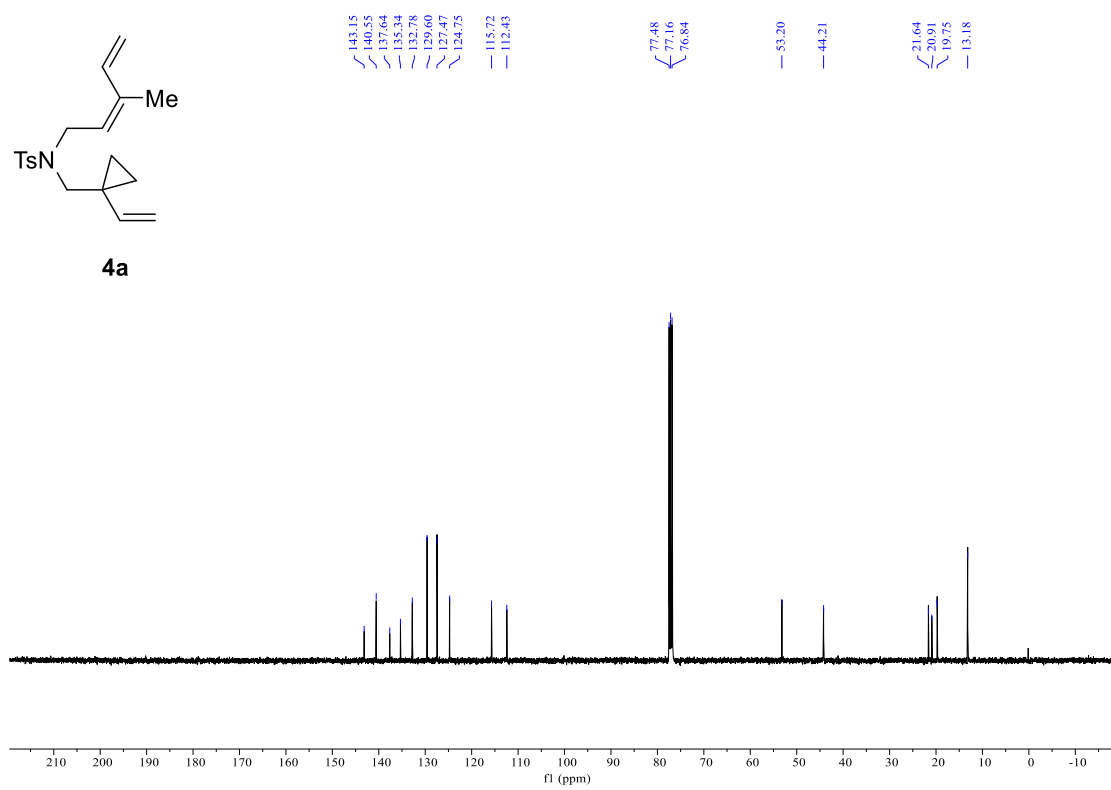
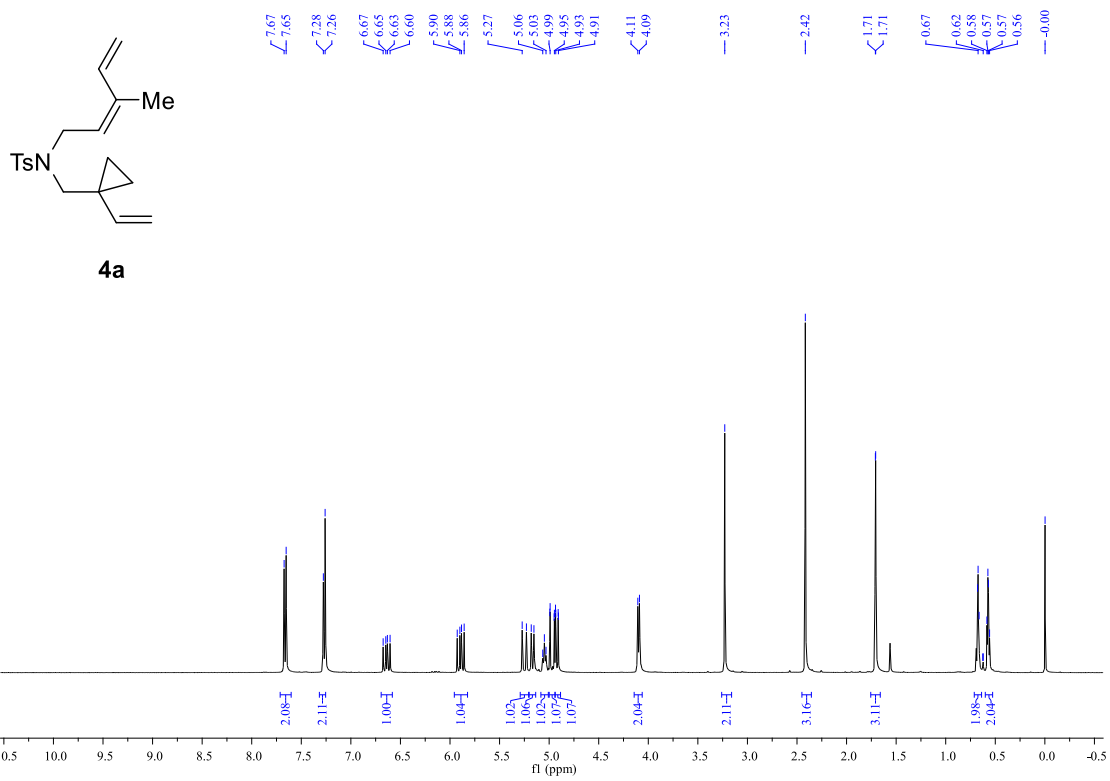


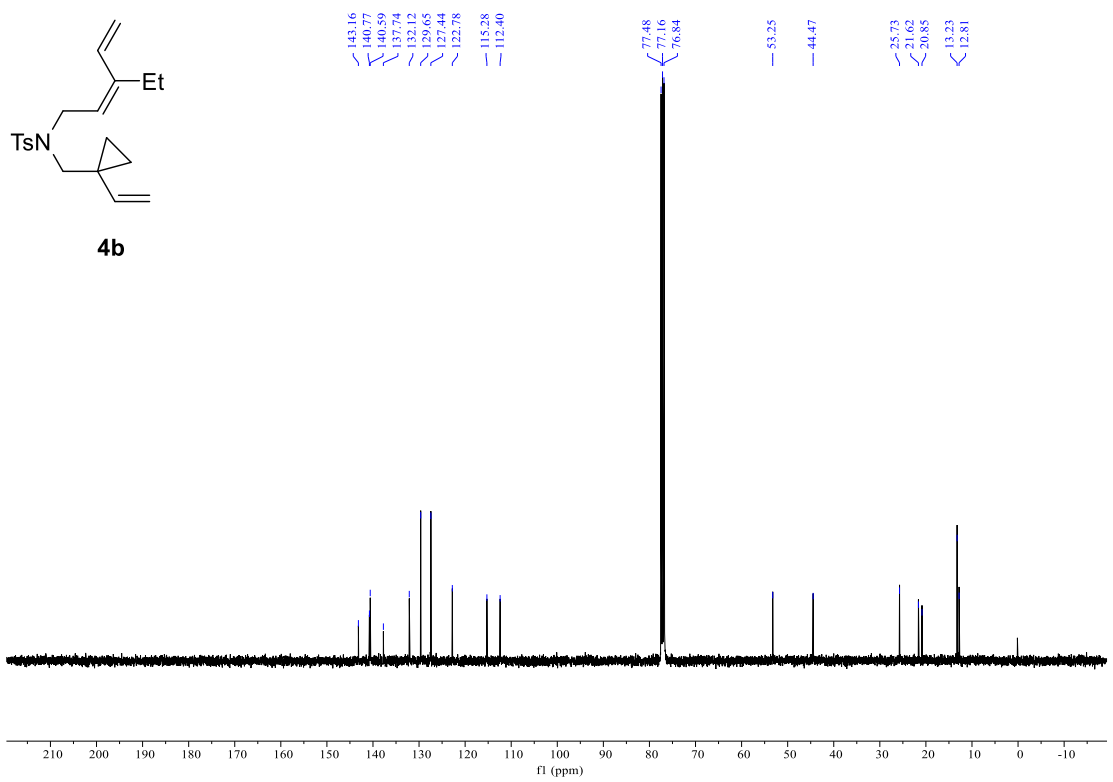
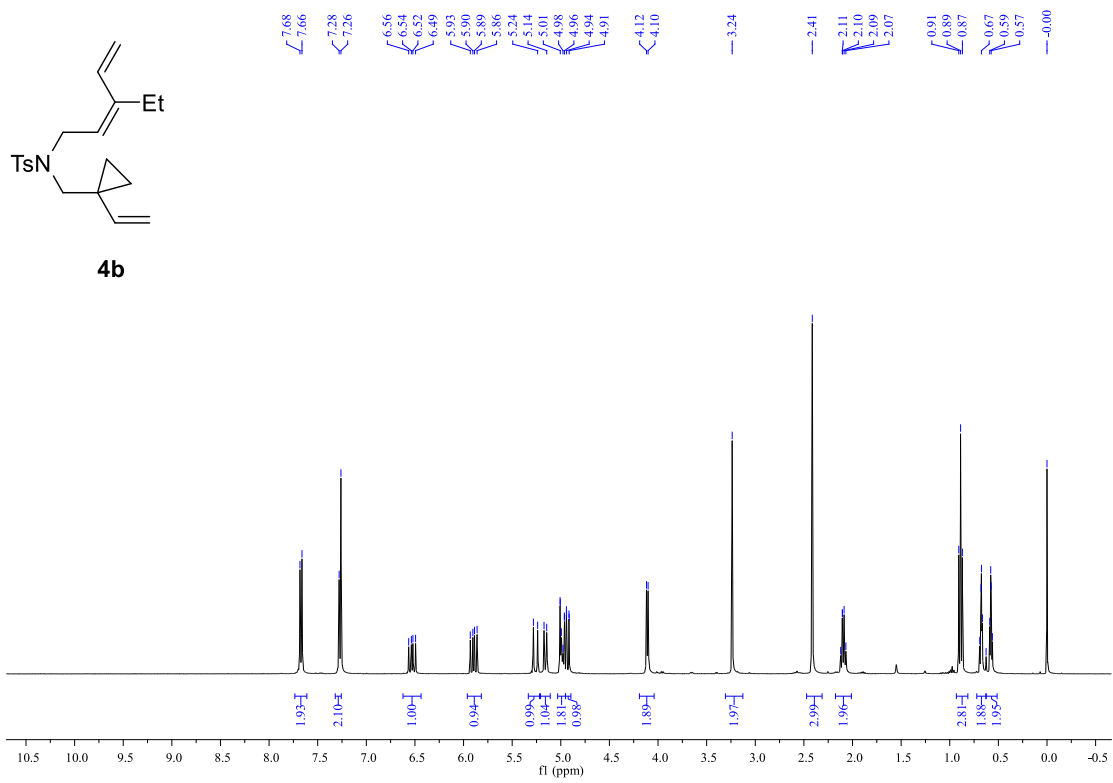


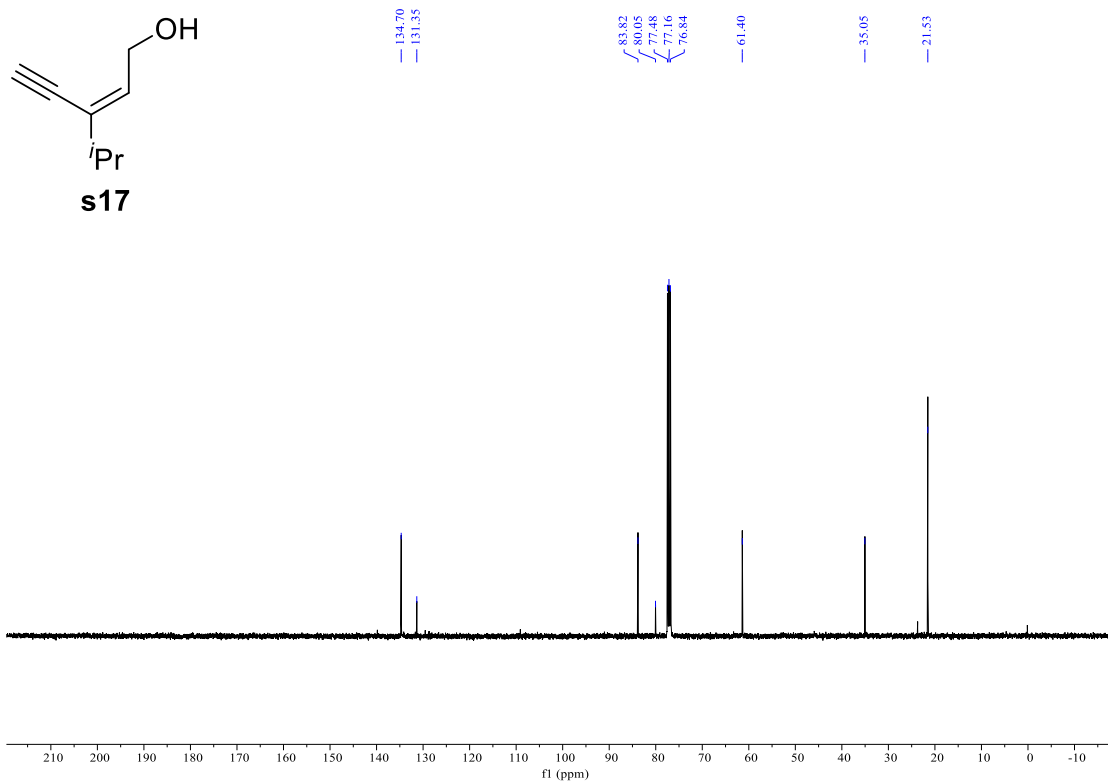
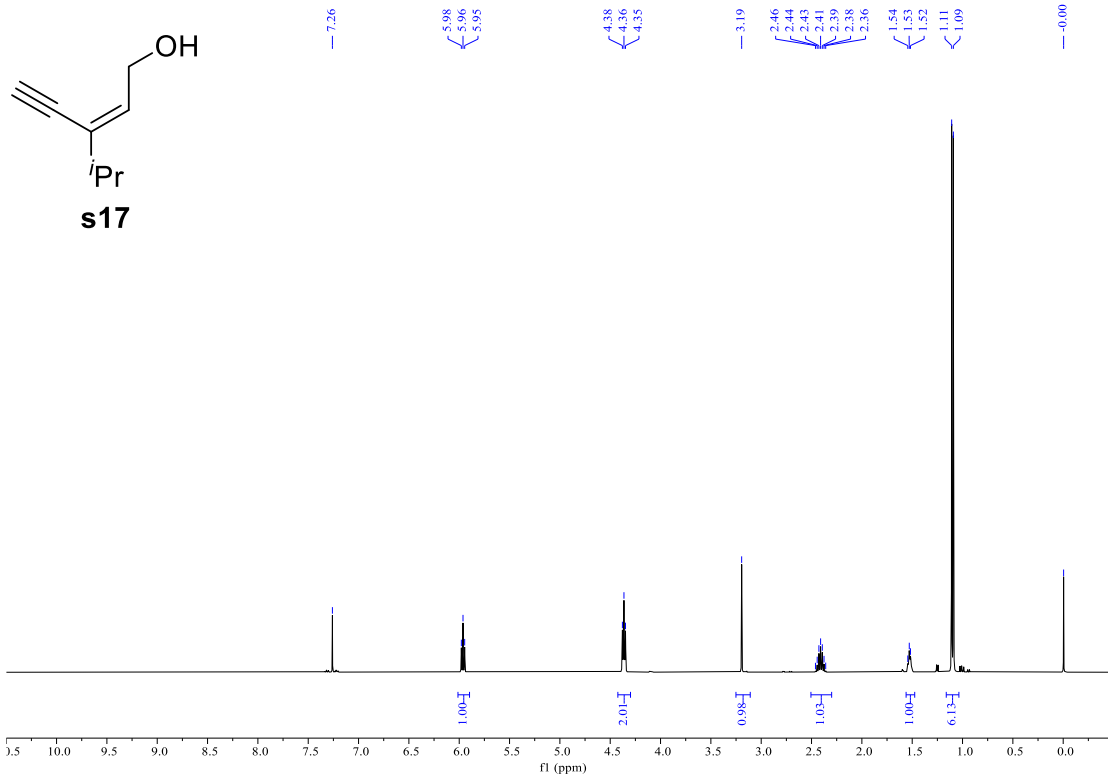


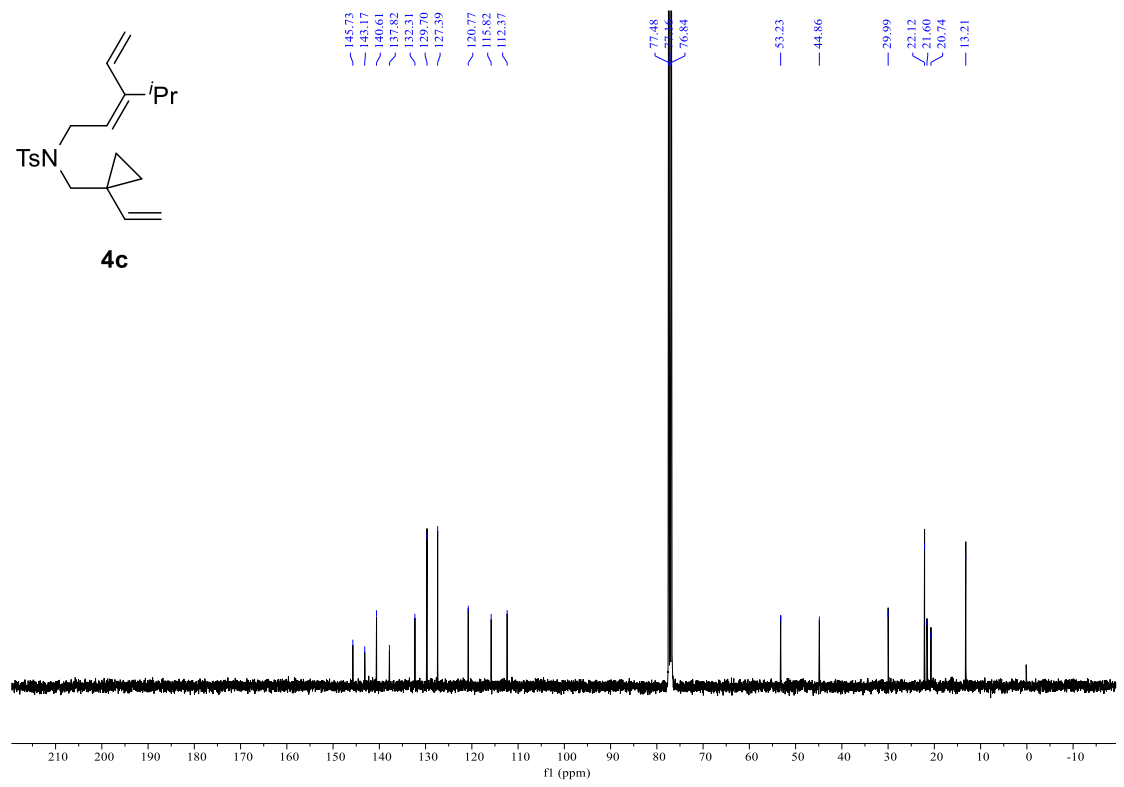
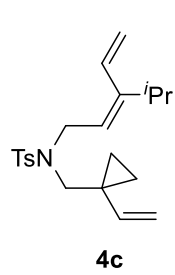
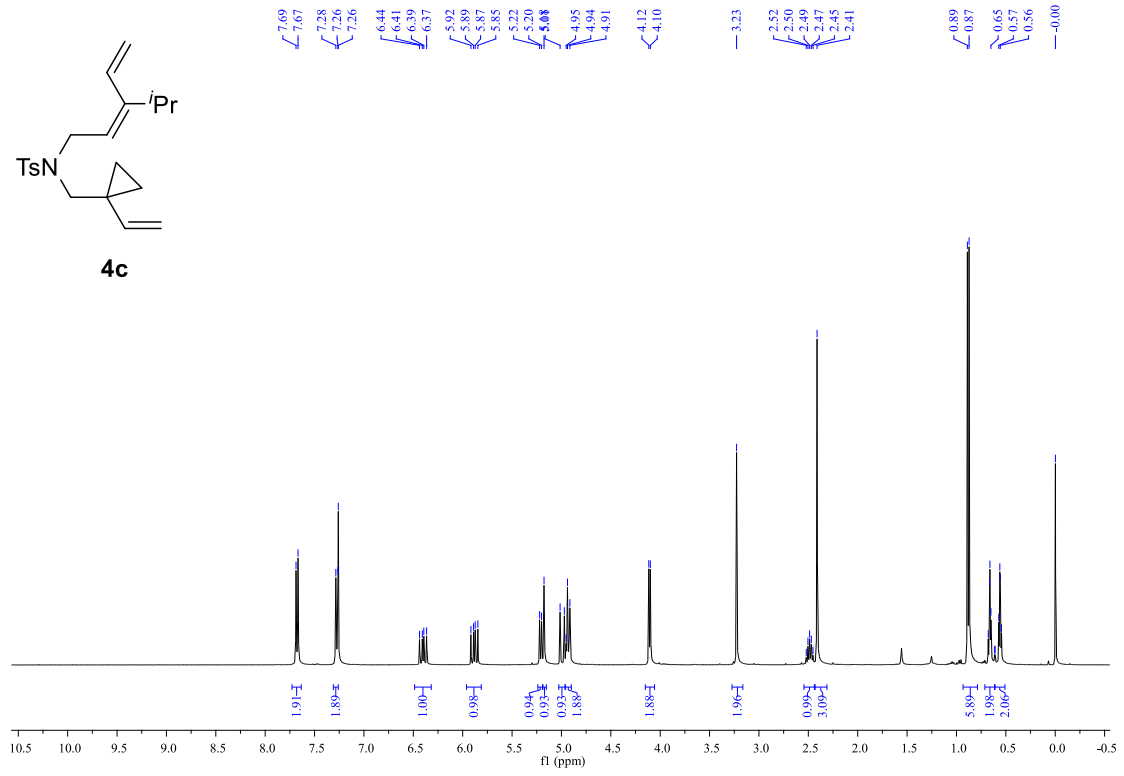
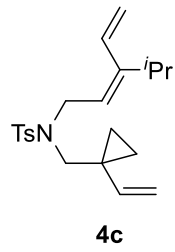




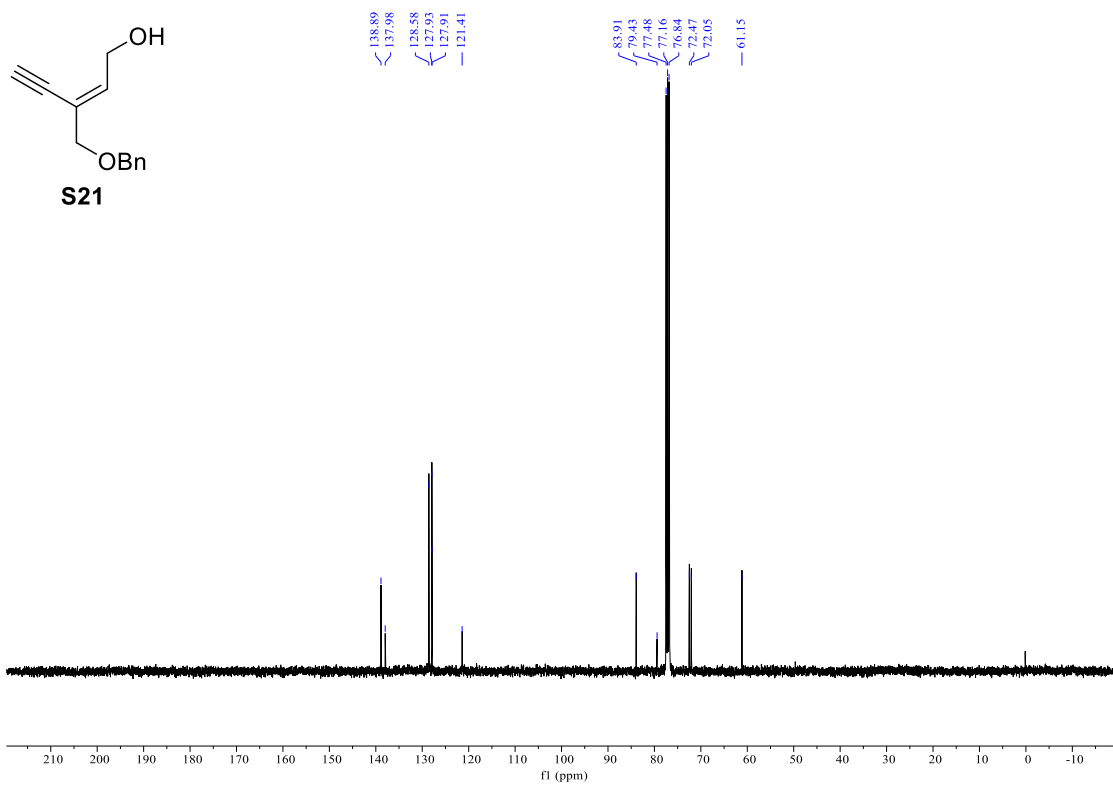
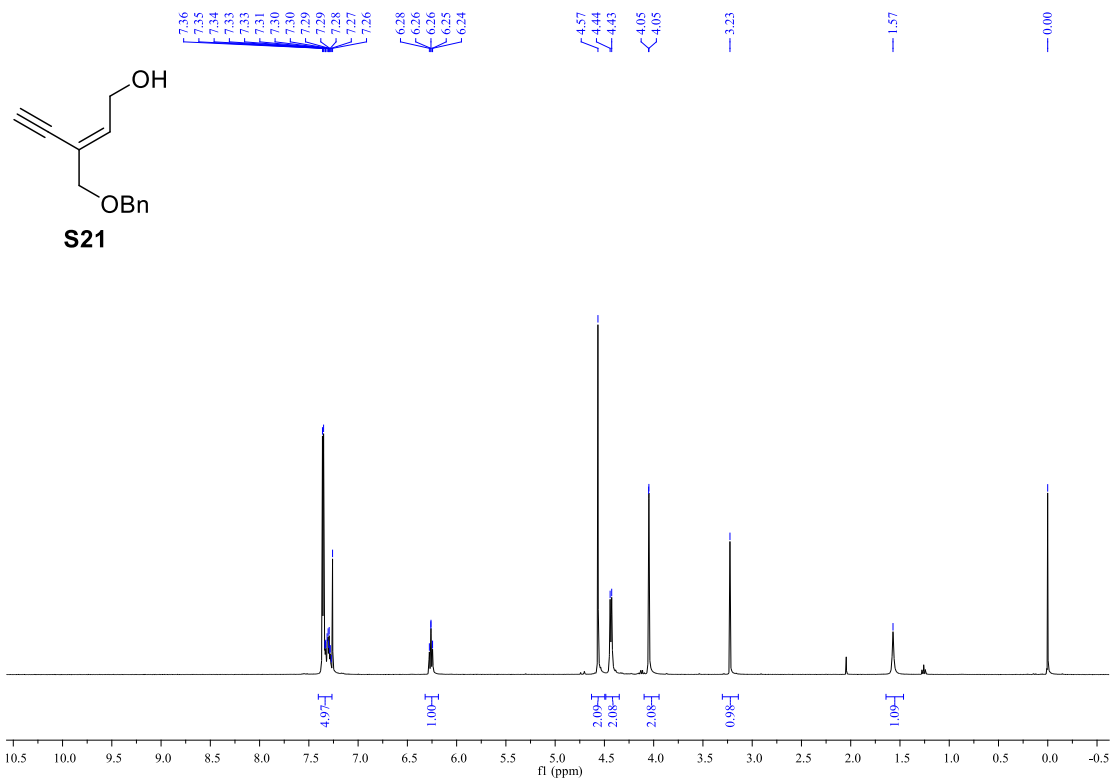


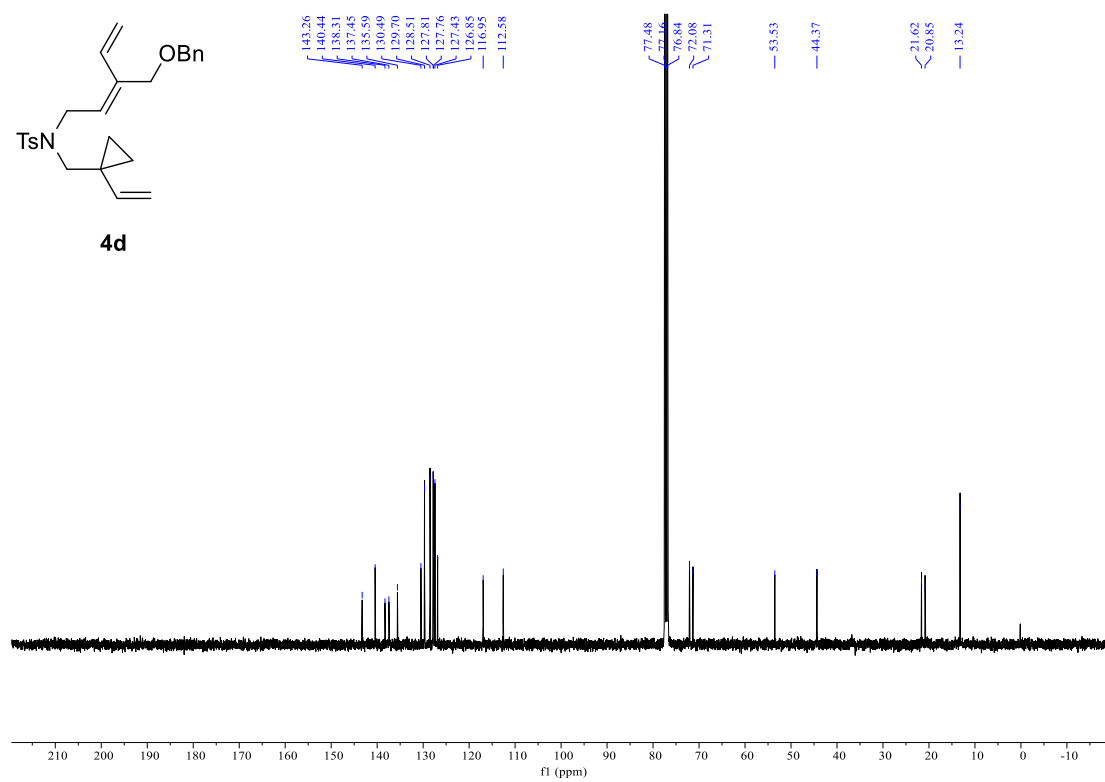
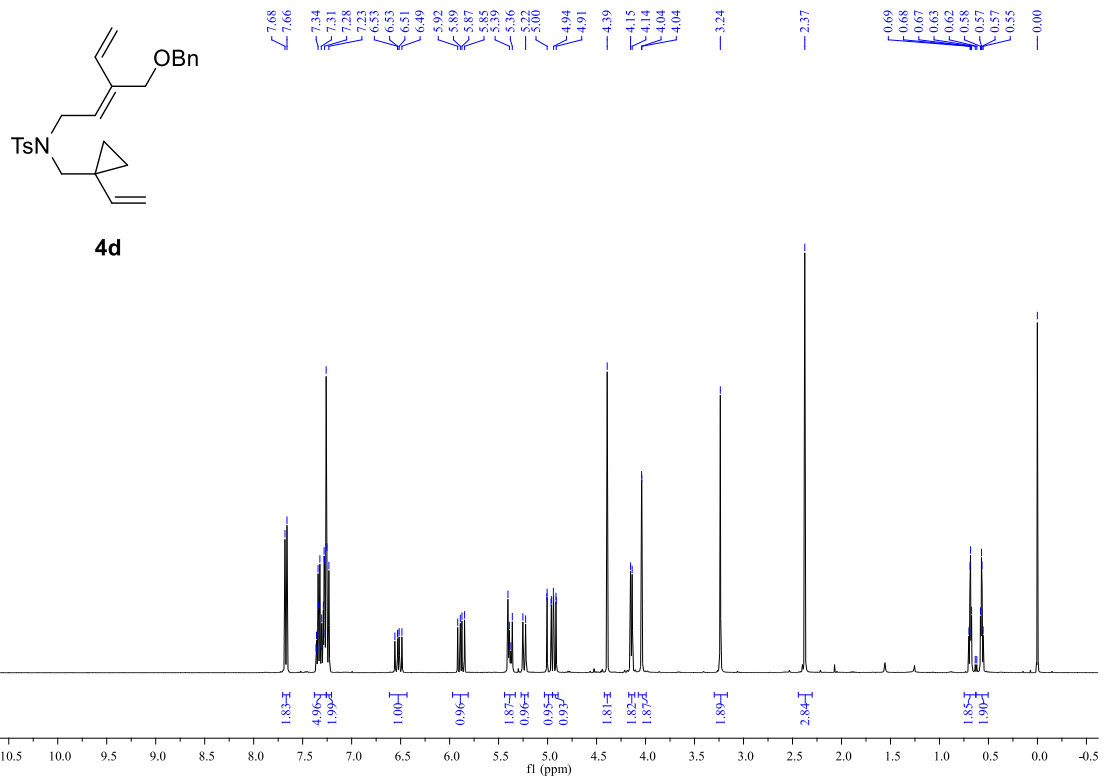


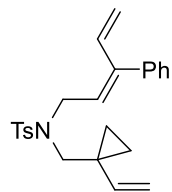




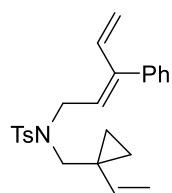
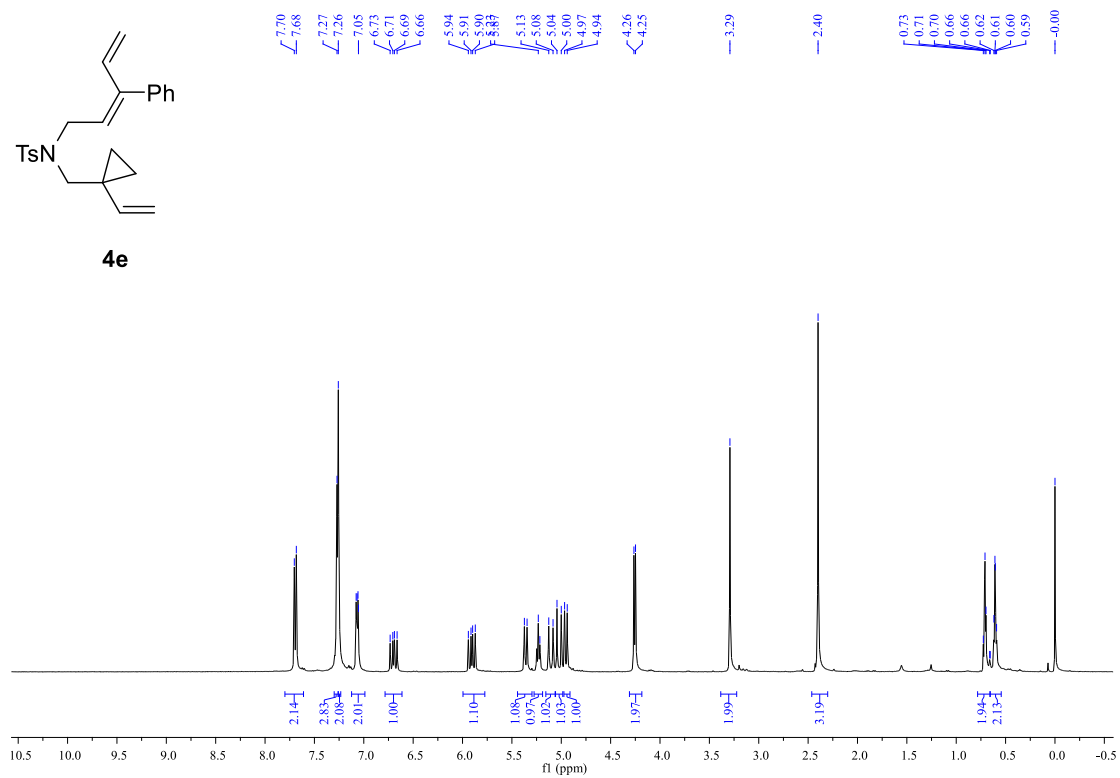




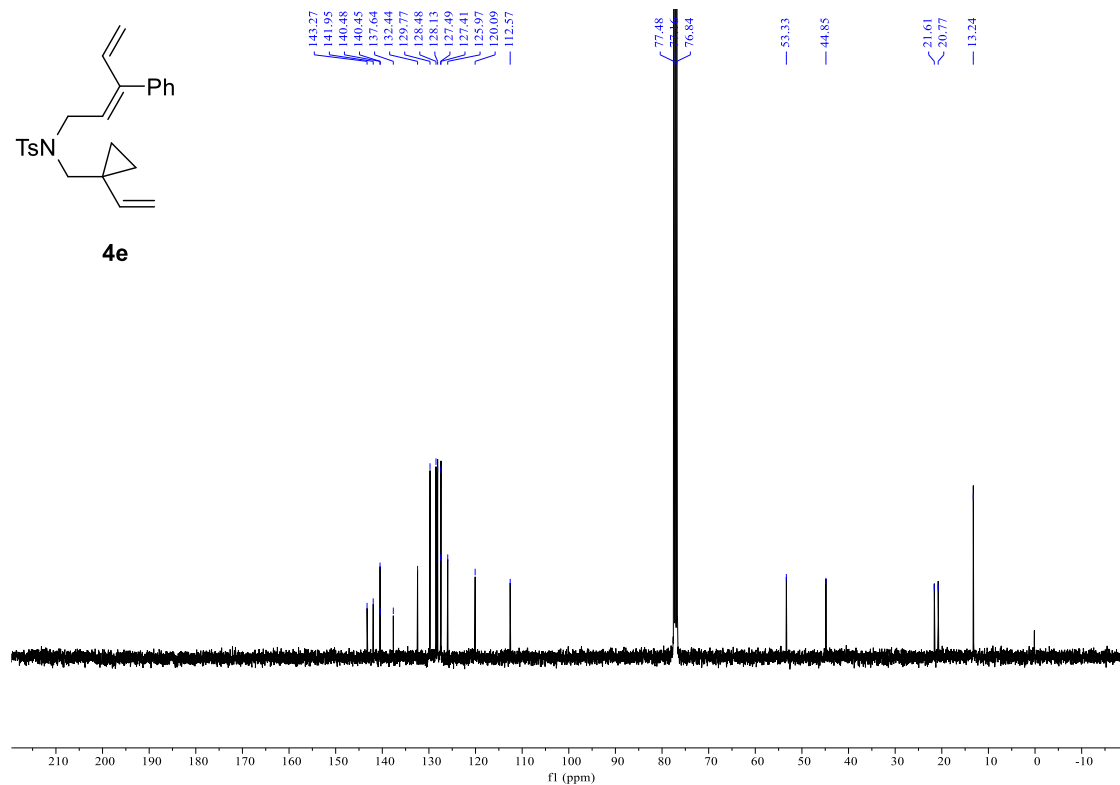


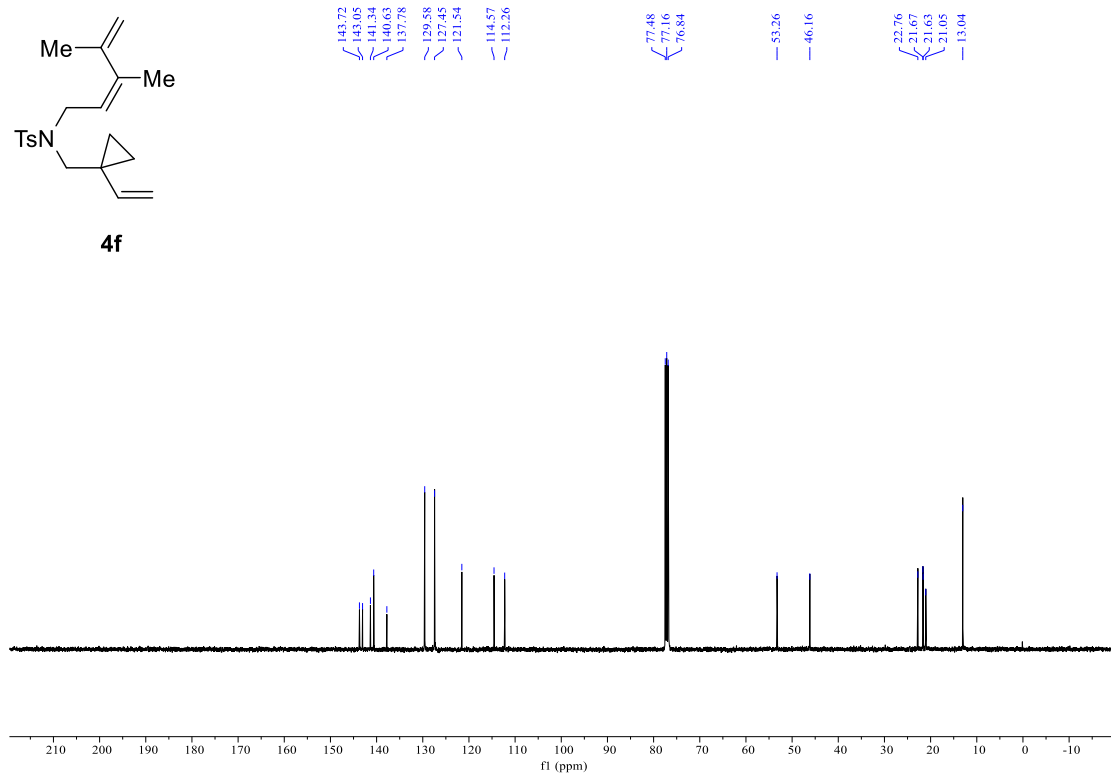
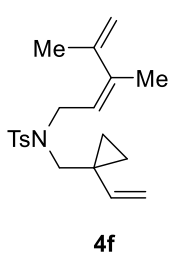
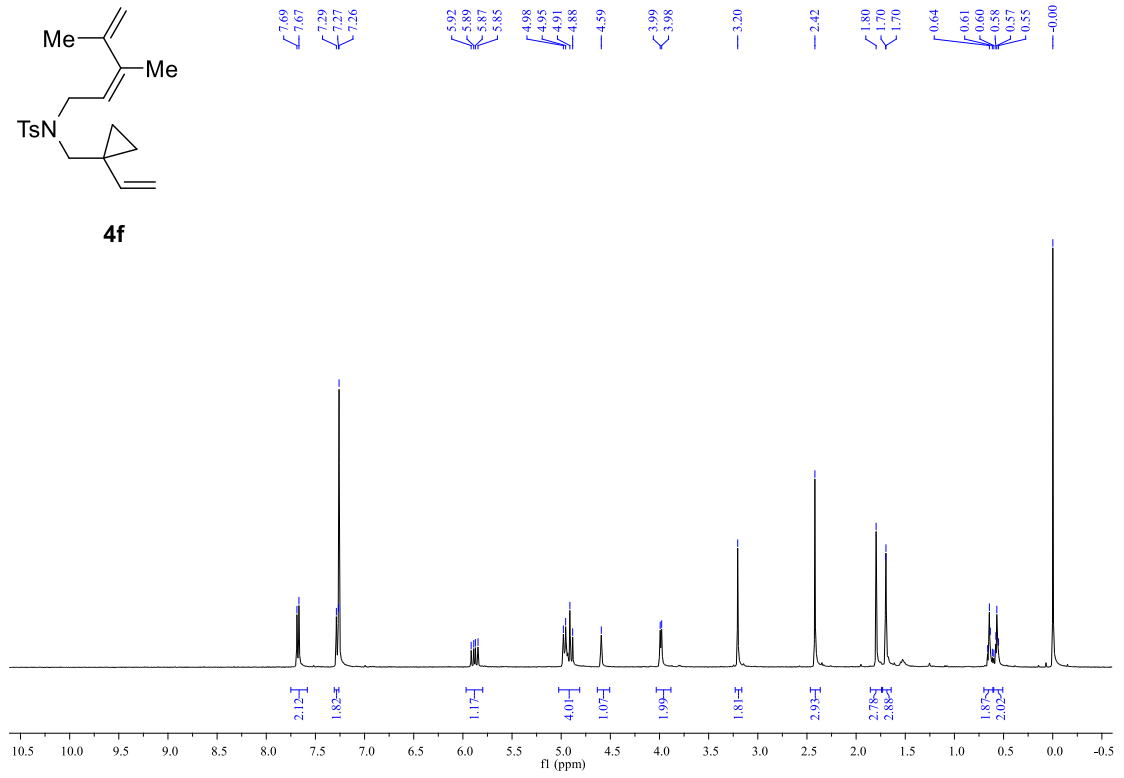
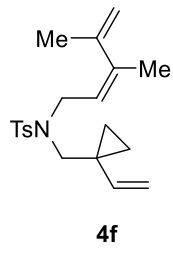


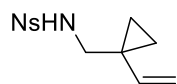
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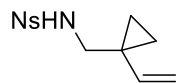
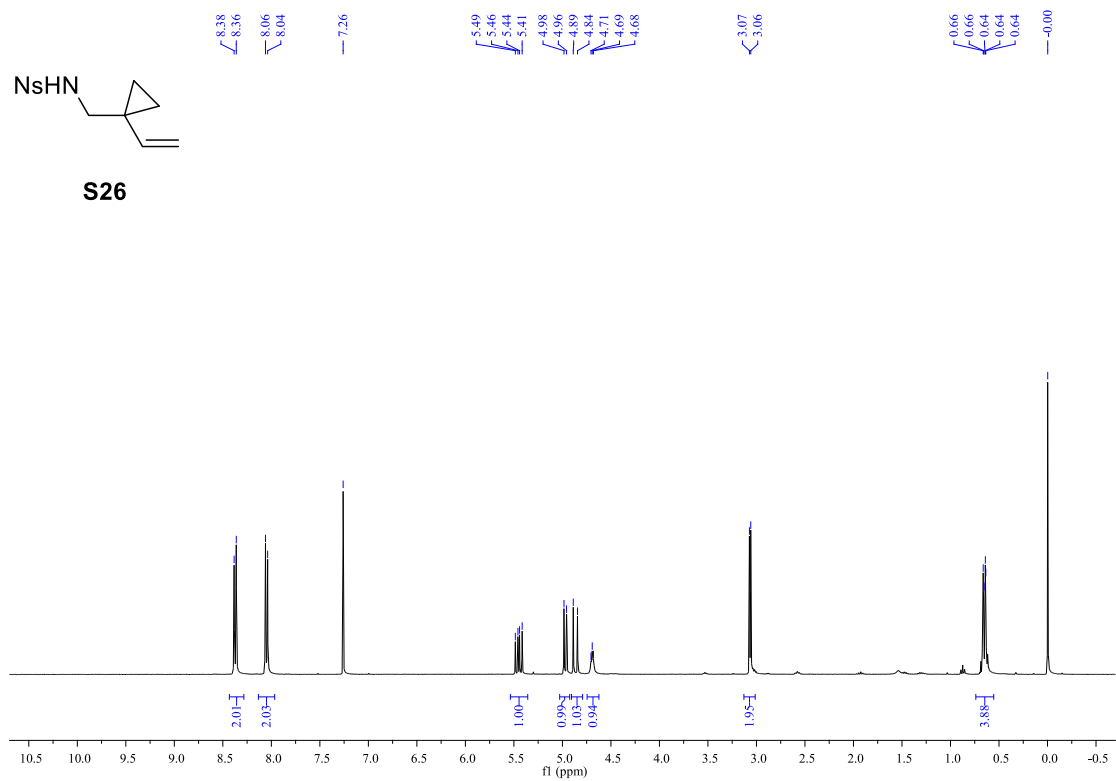
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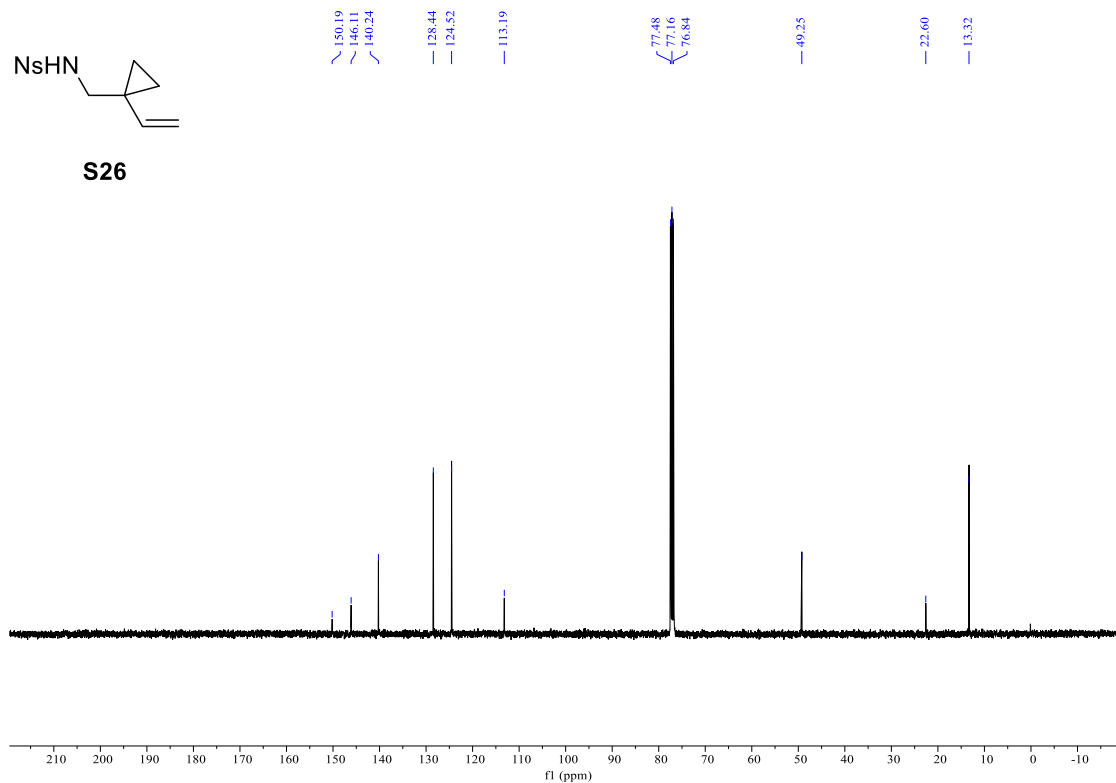


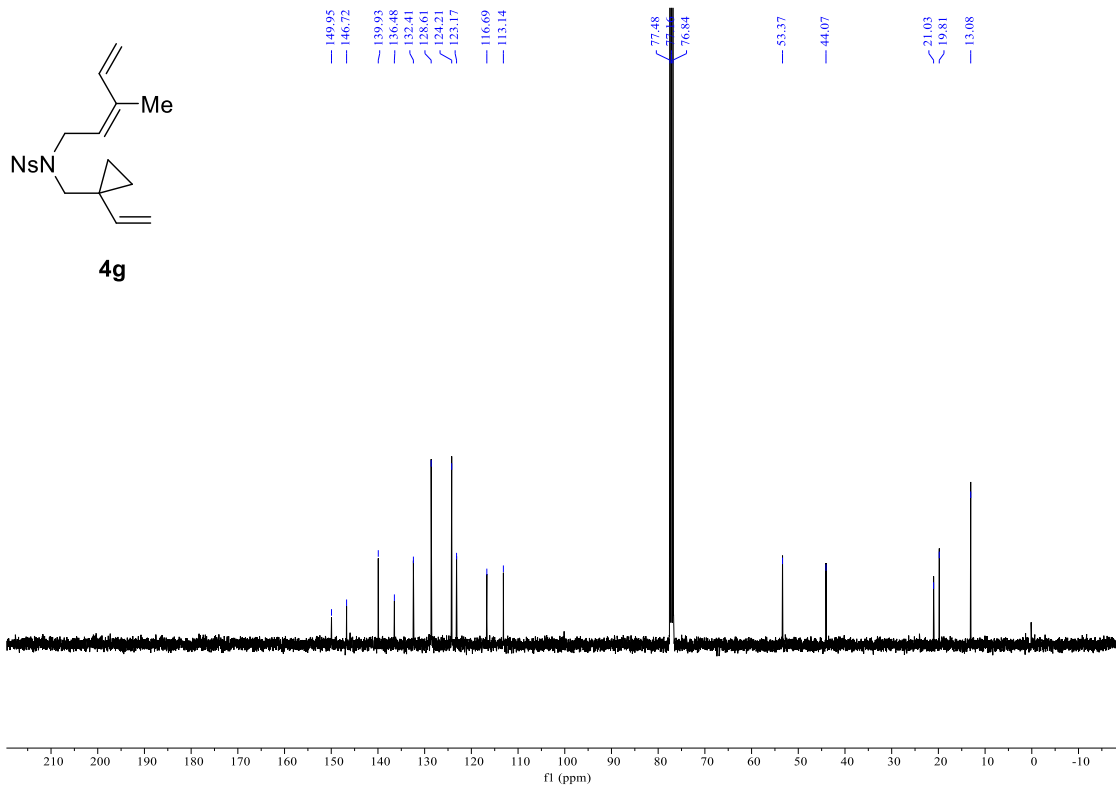
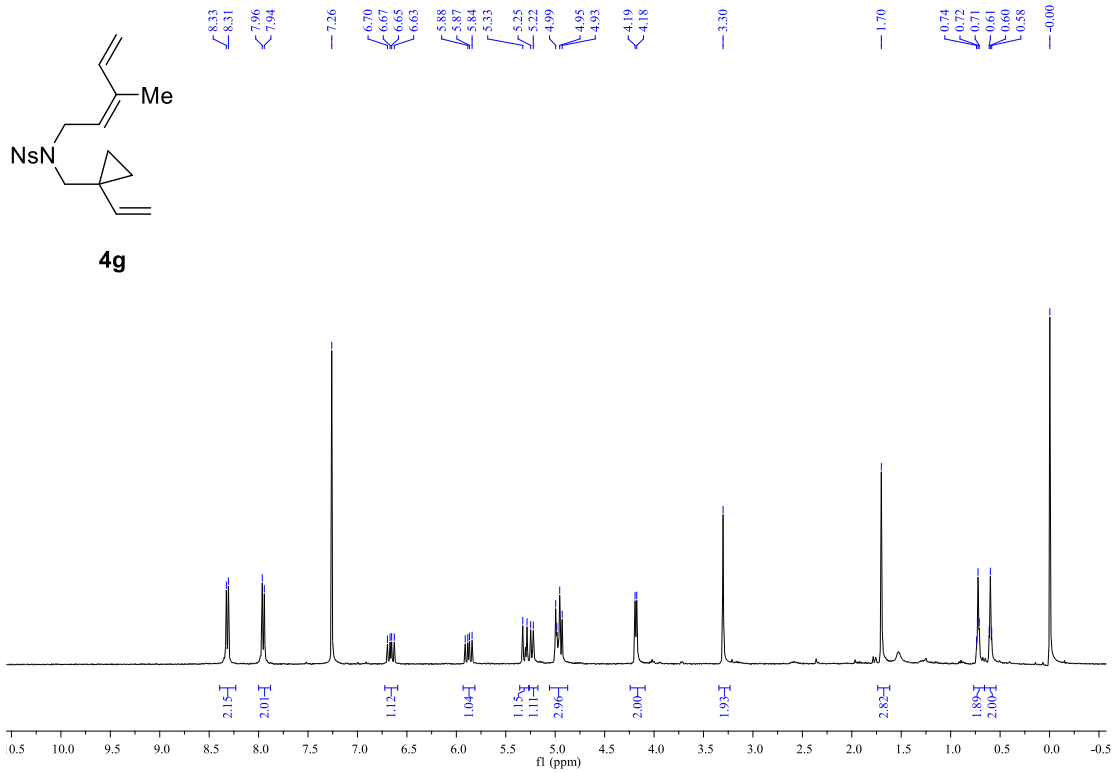


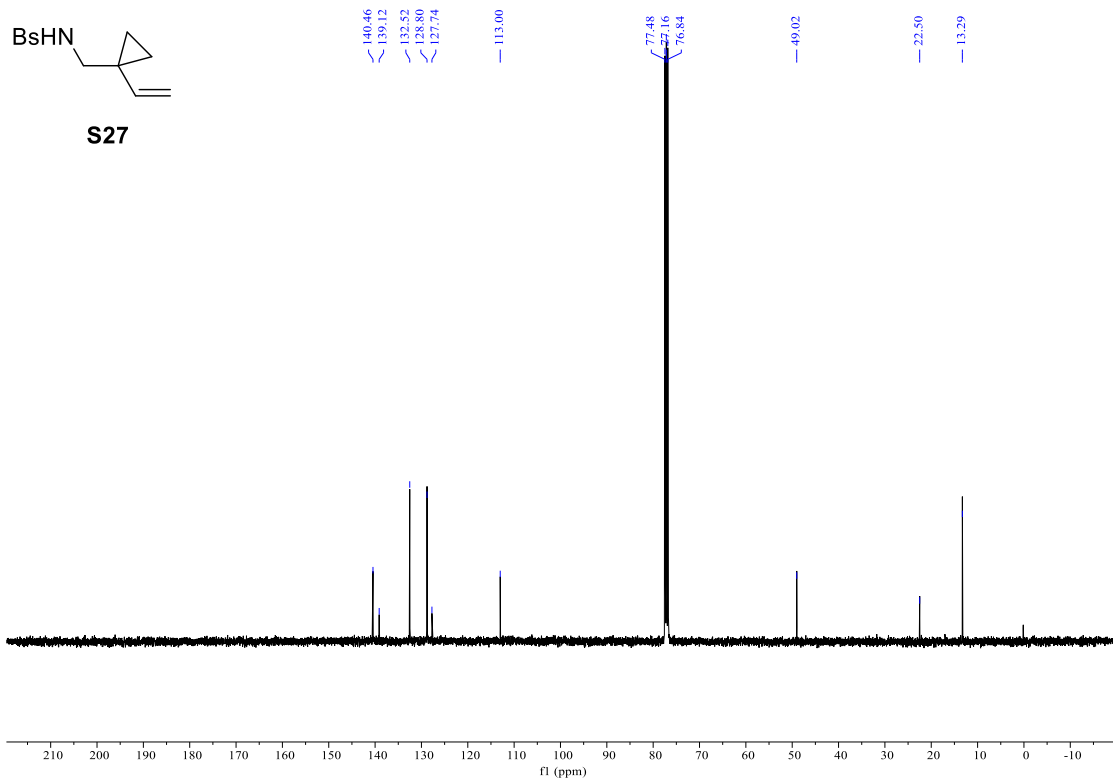
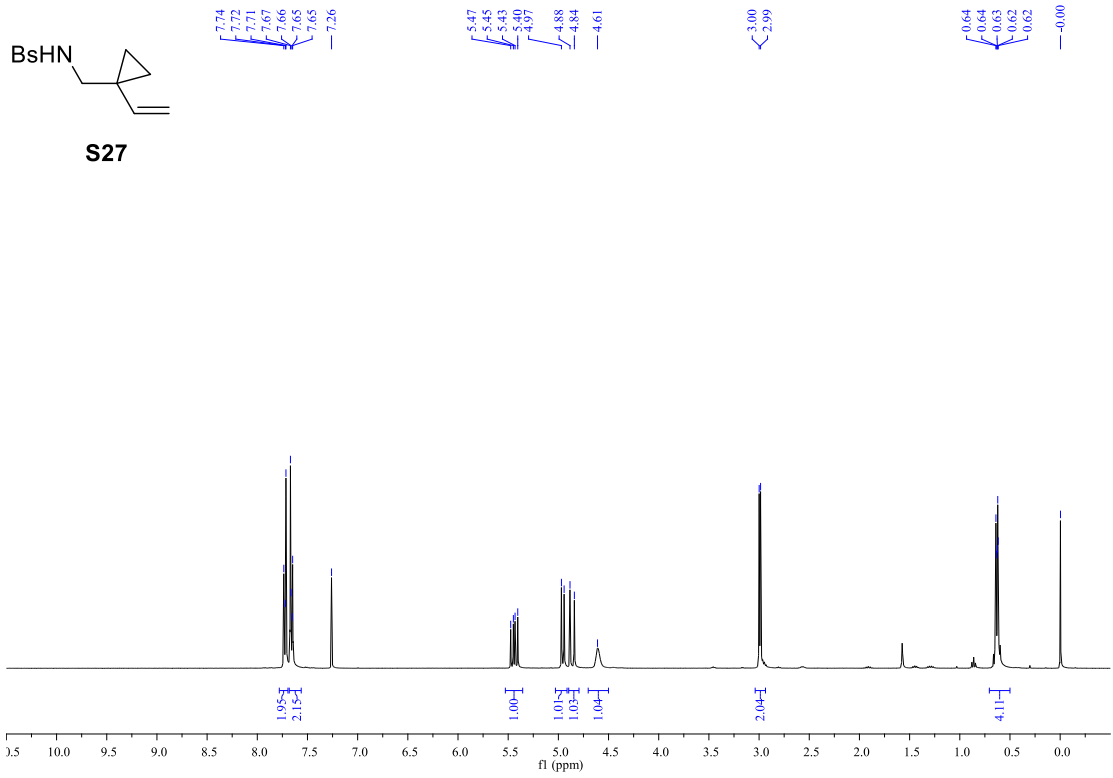
S26

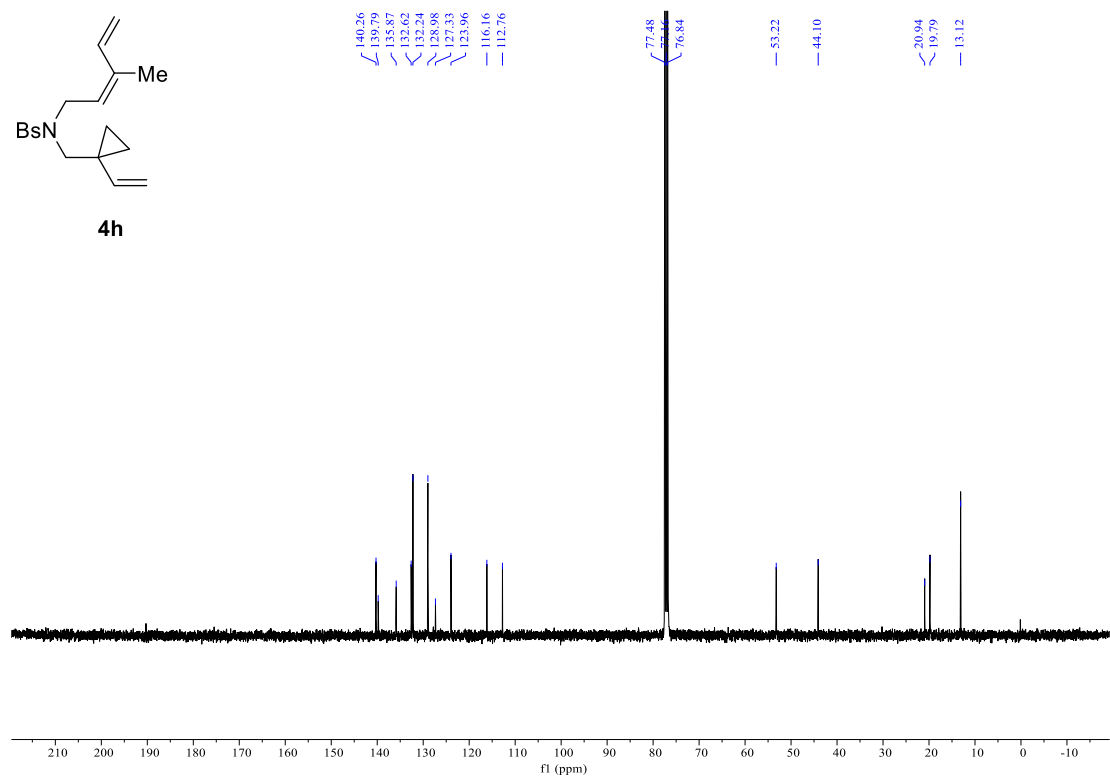
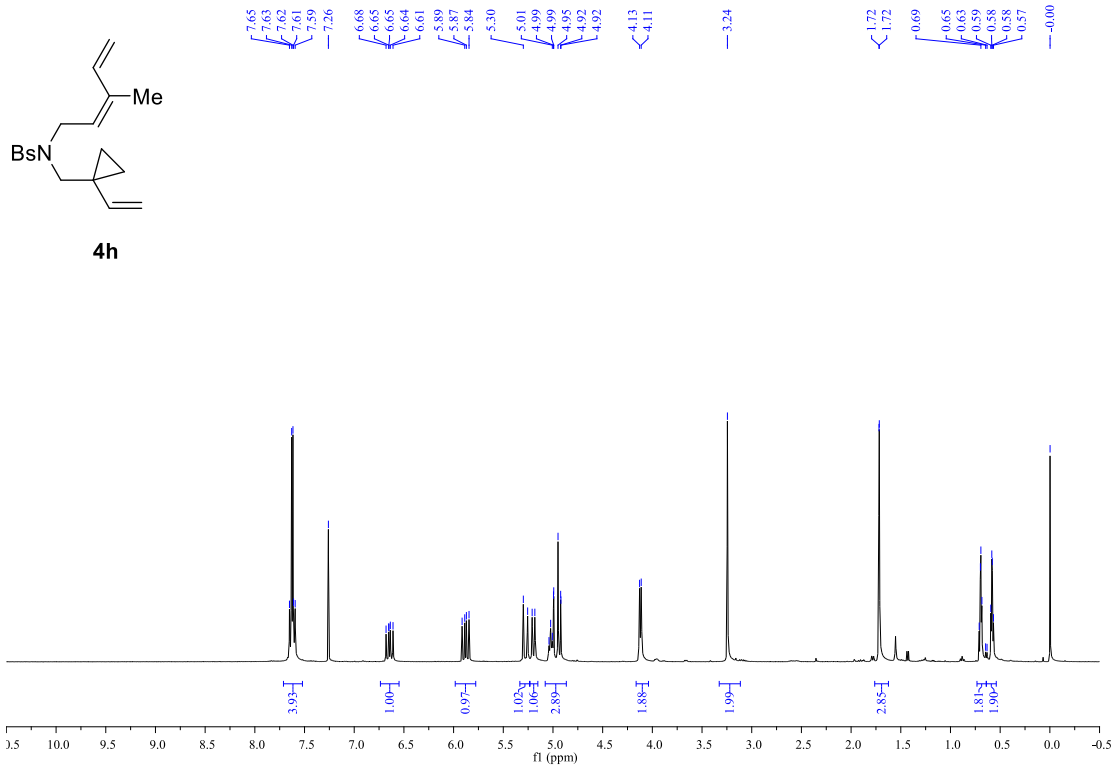


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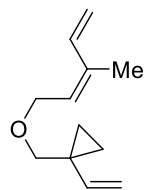




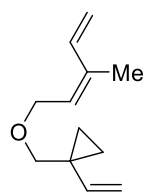
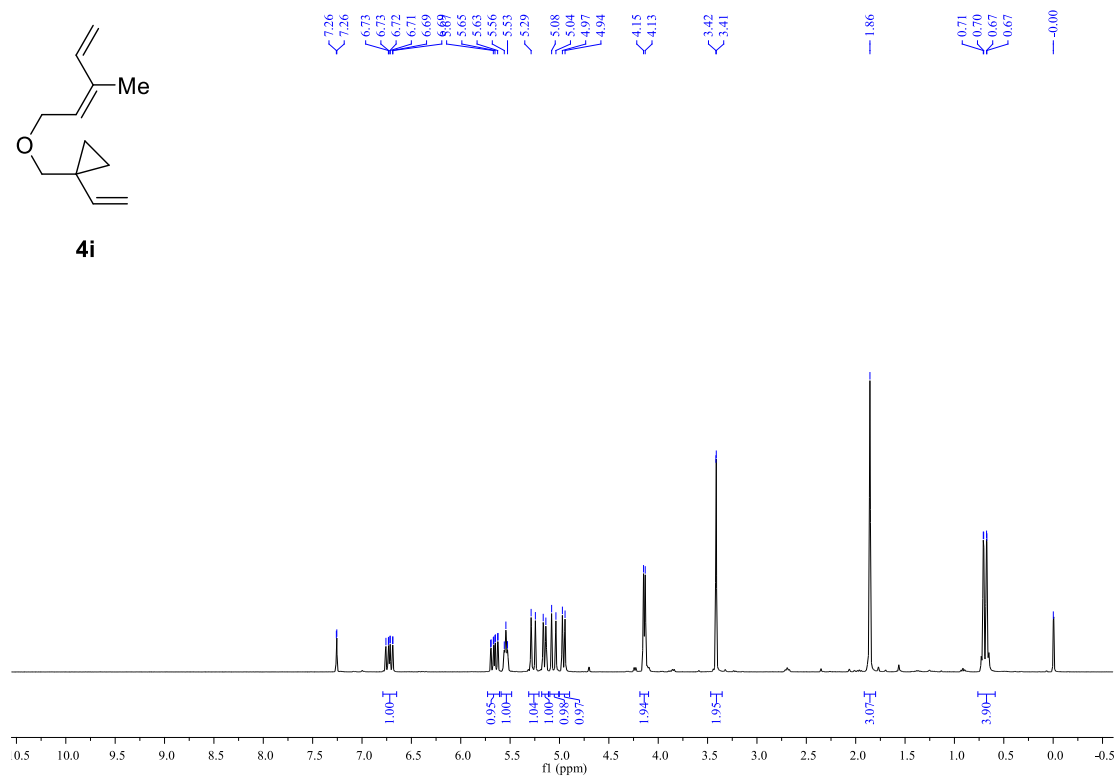




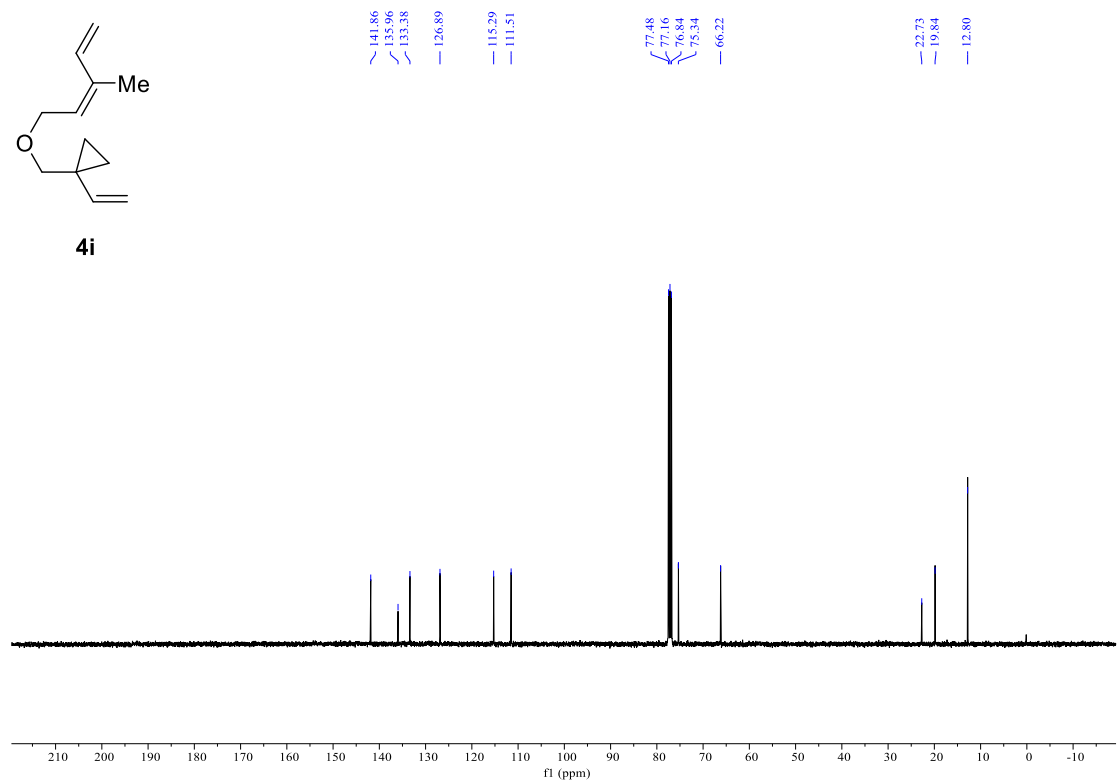


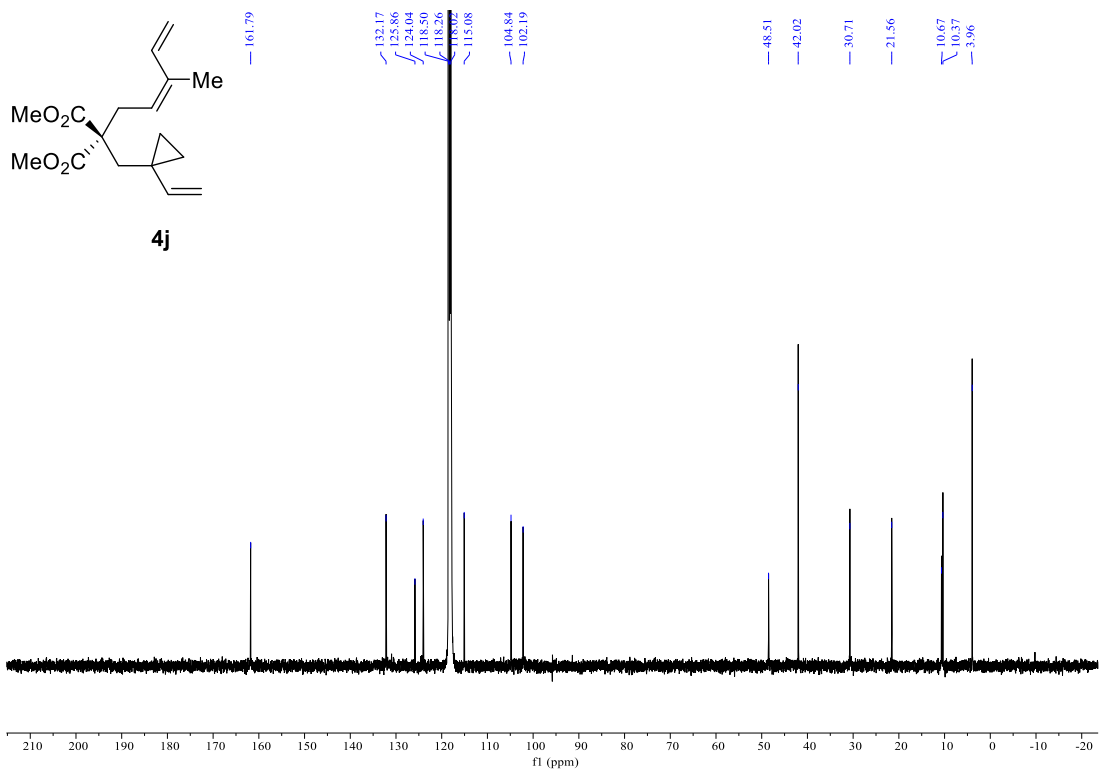
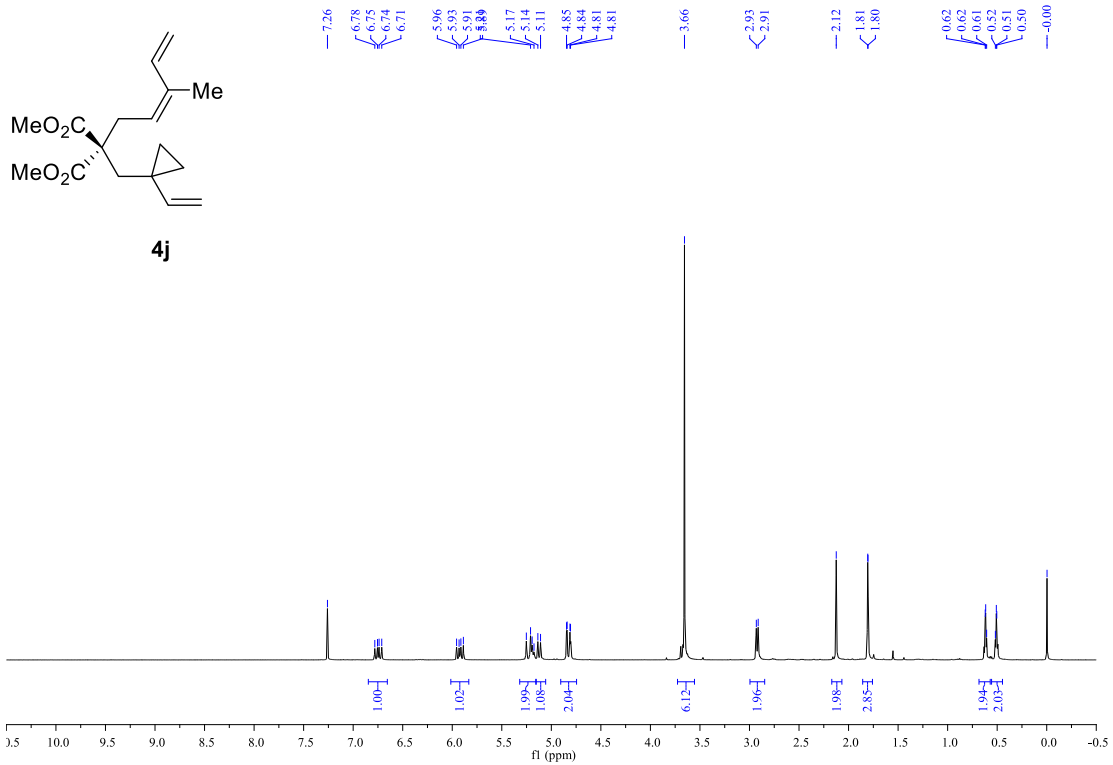


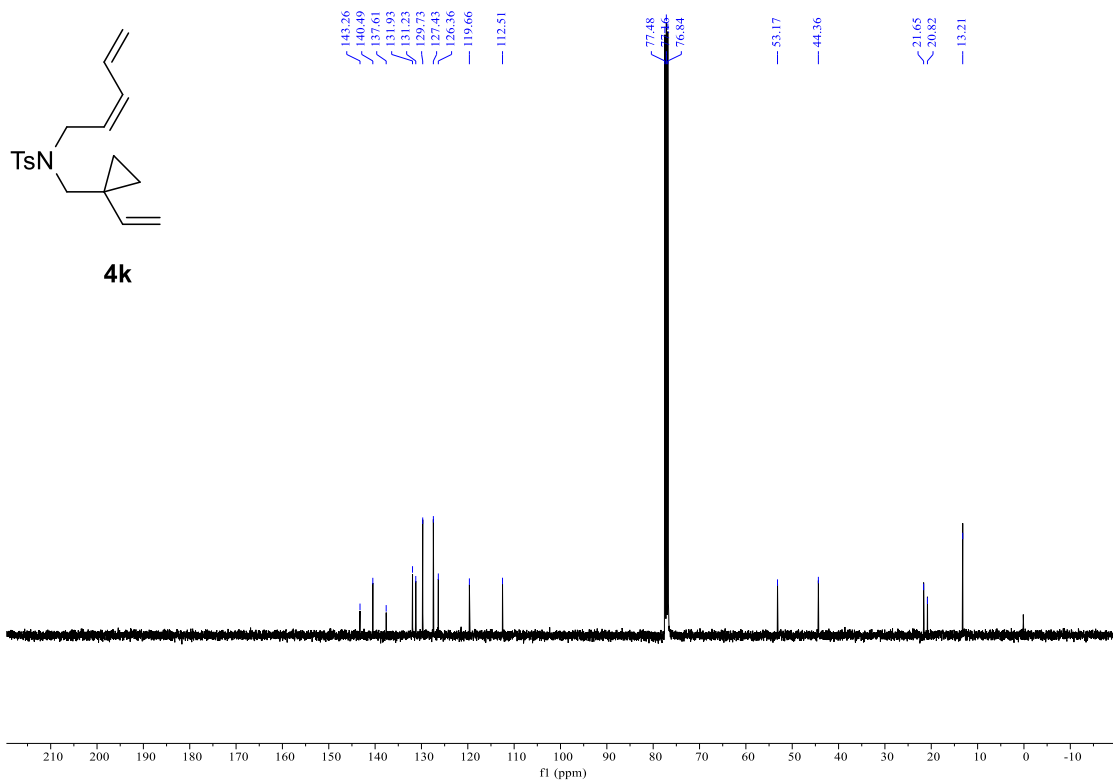
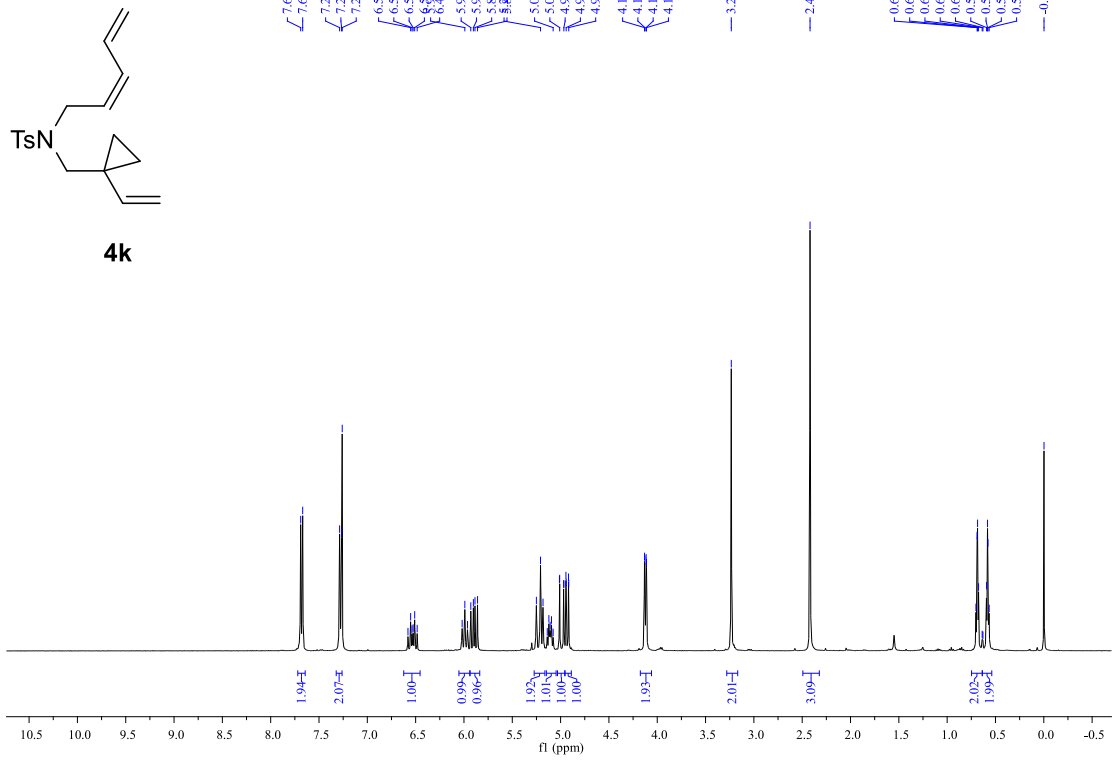
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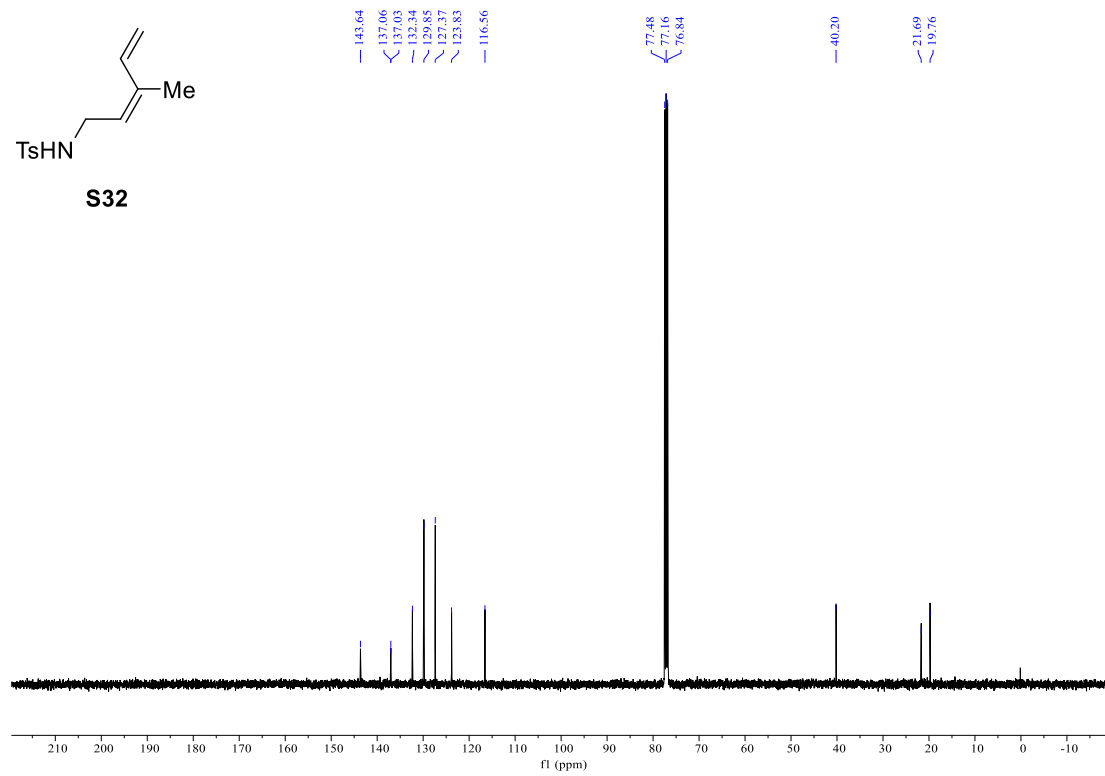
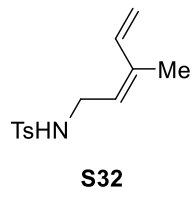
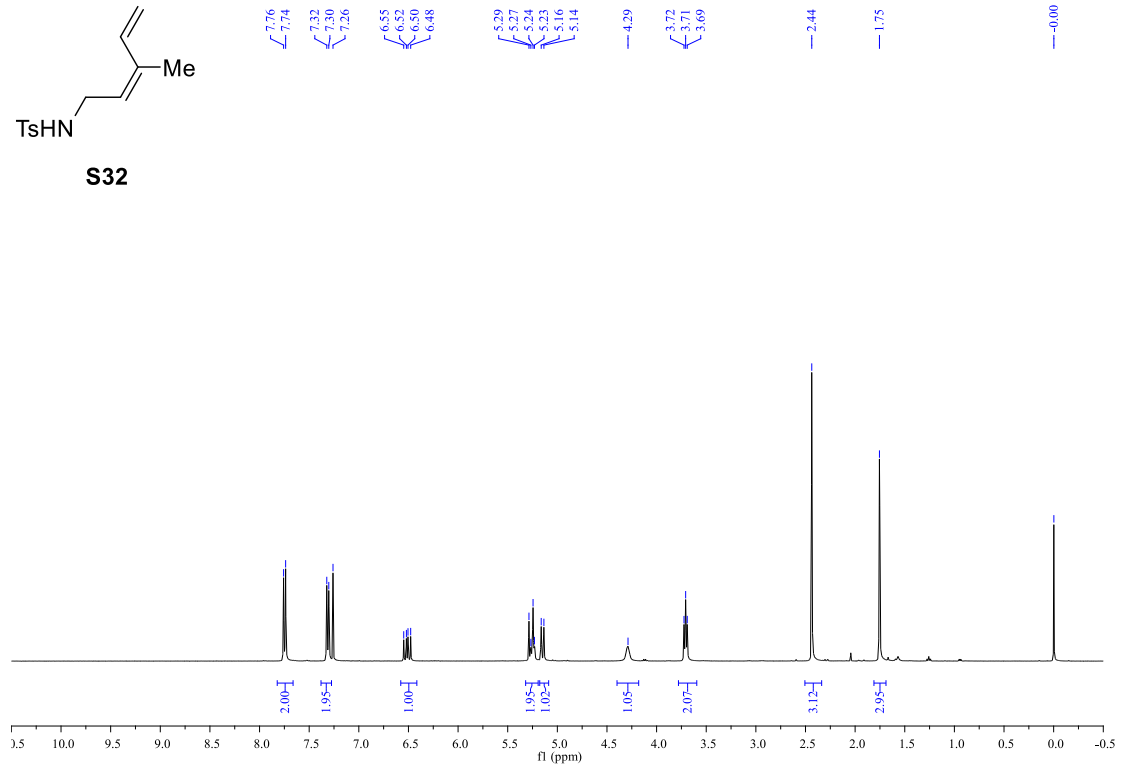
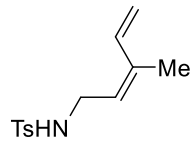


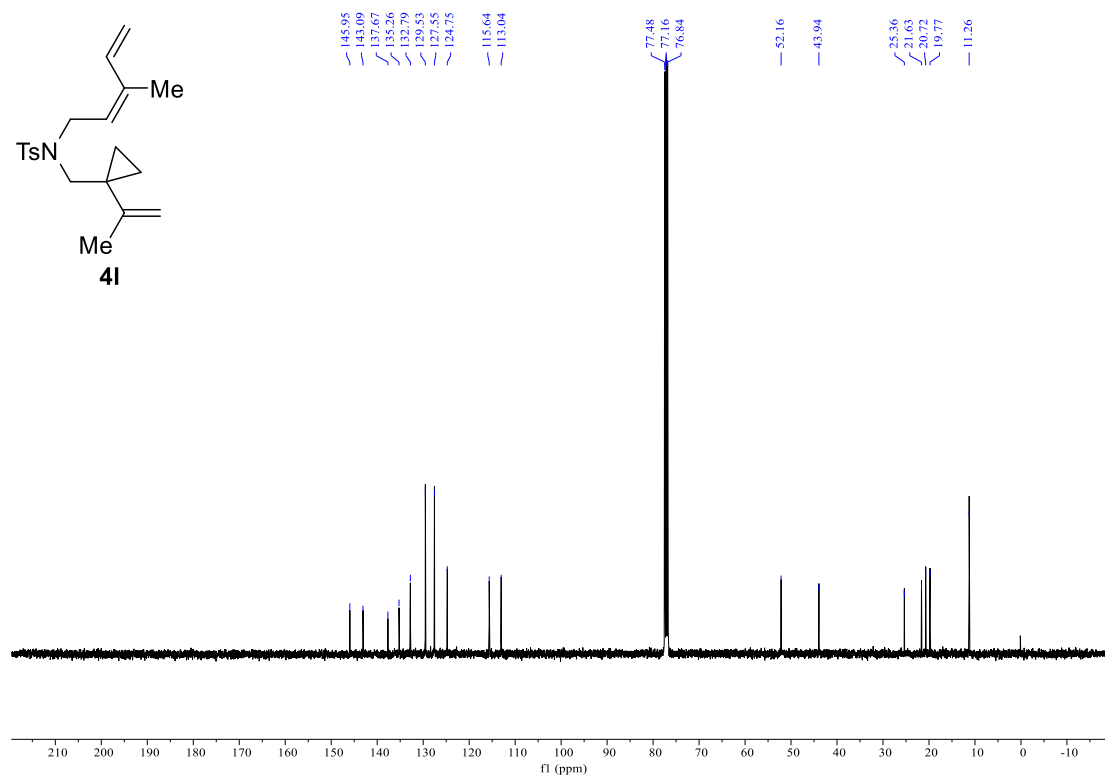
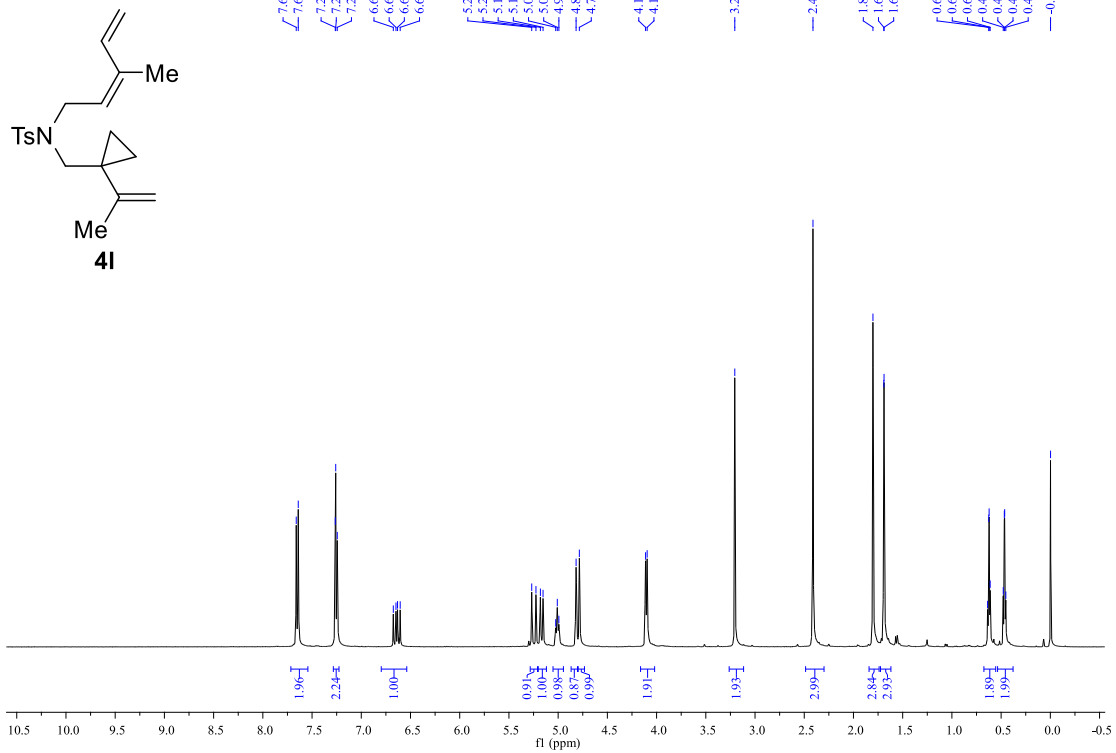
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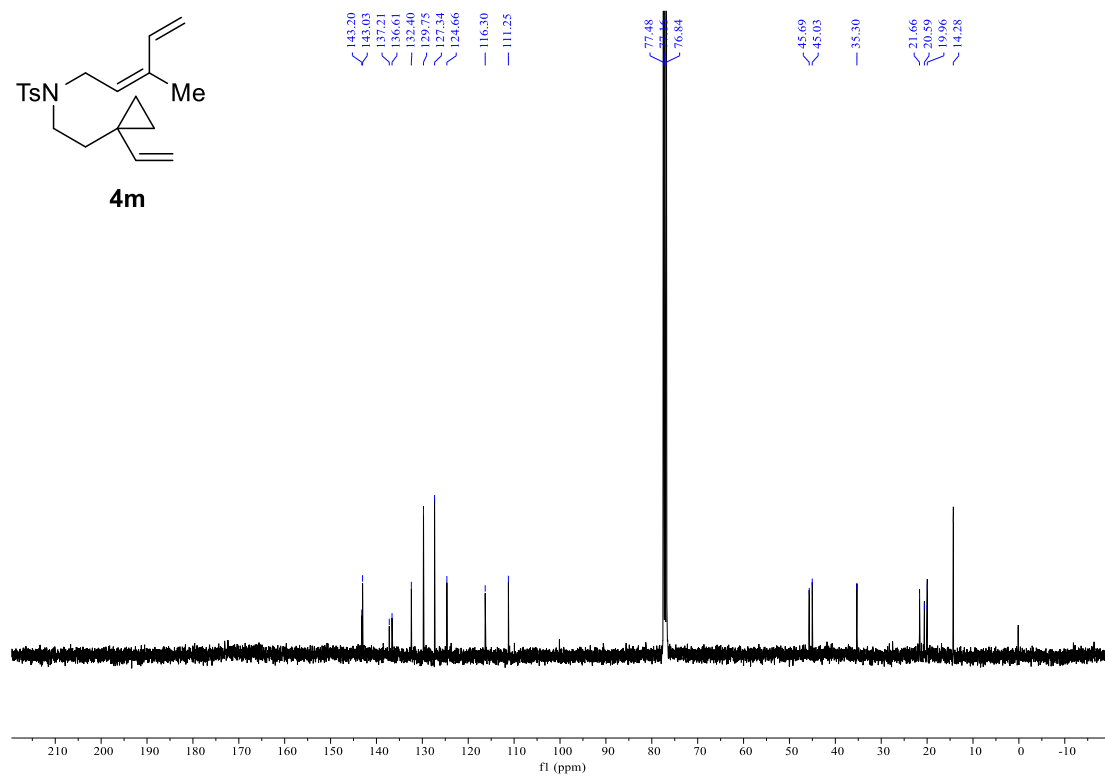
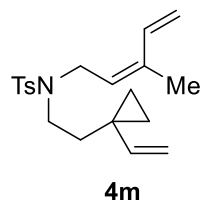
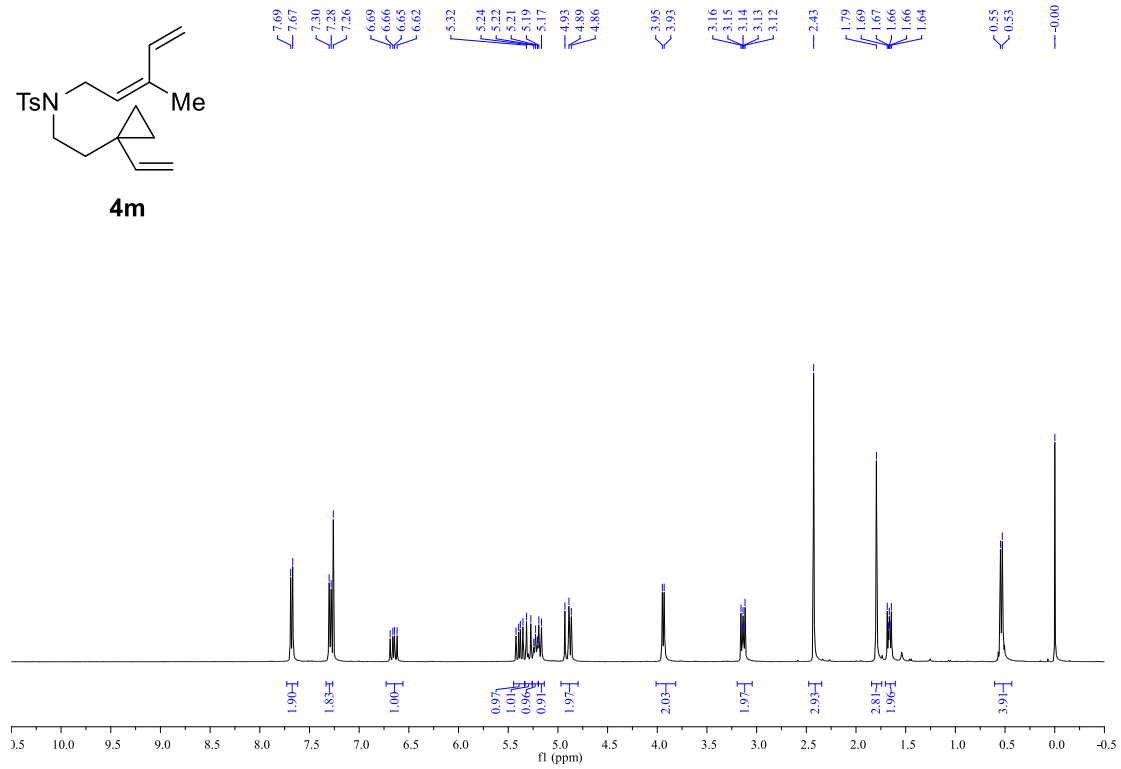
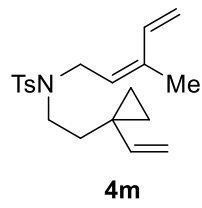


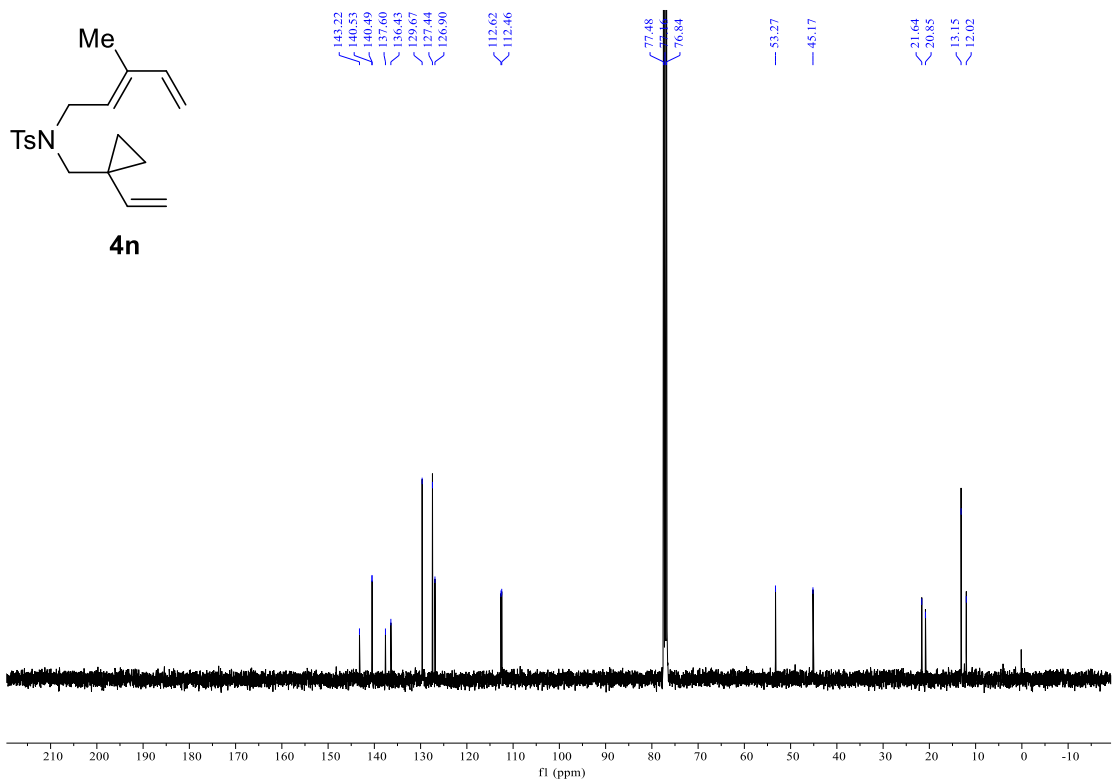
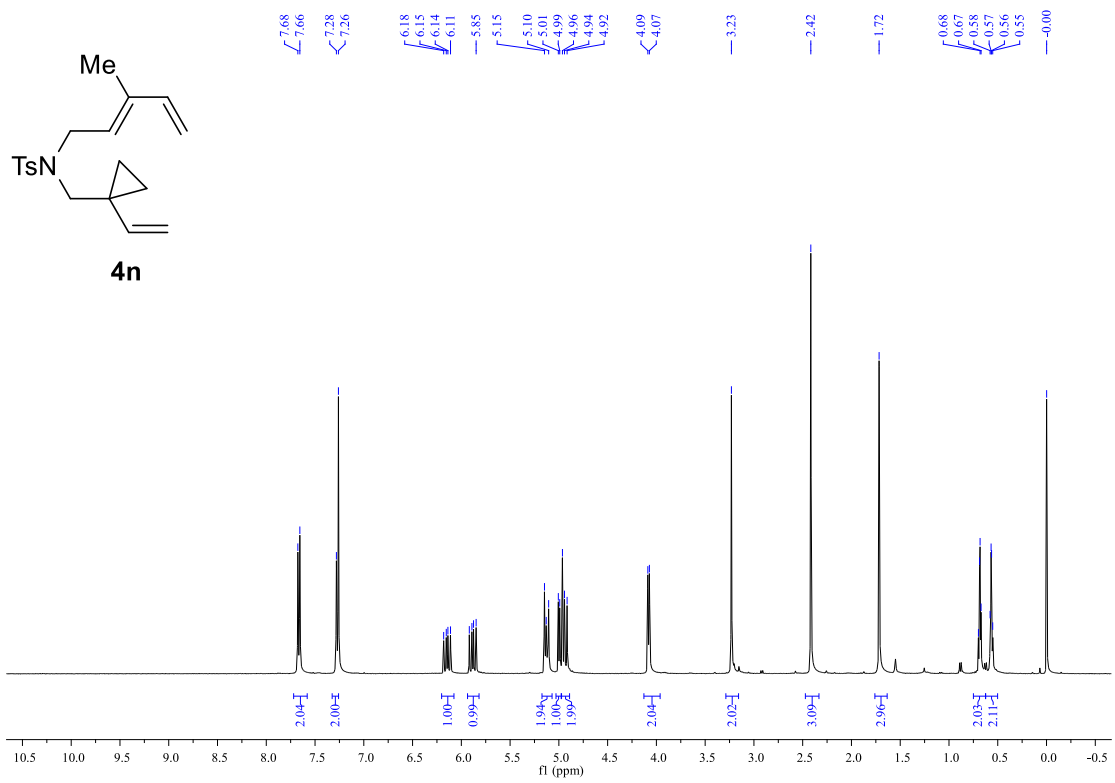


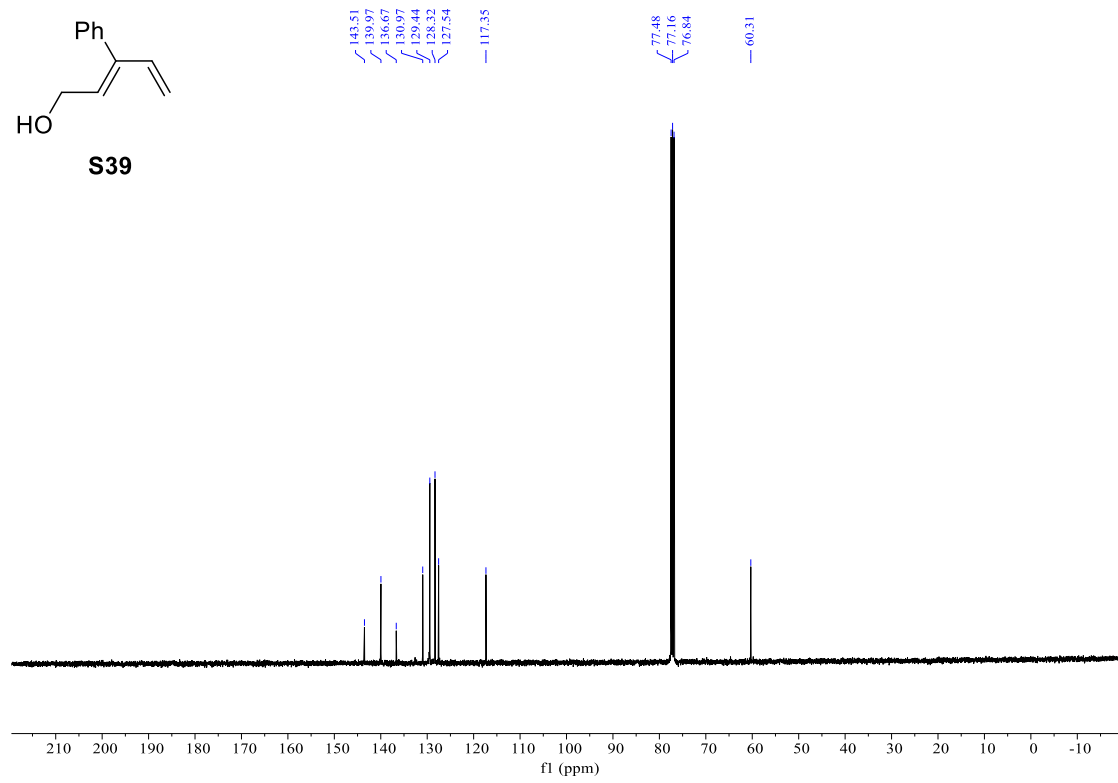
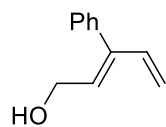
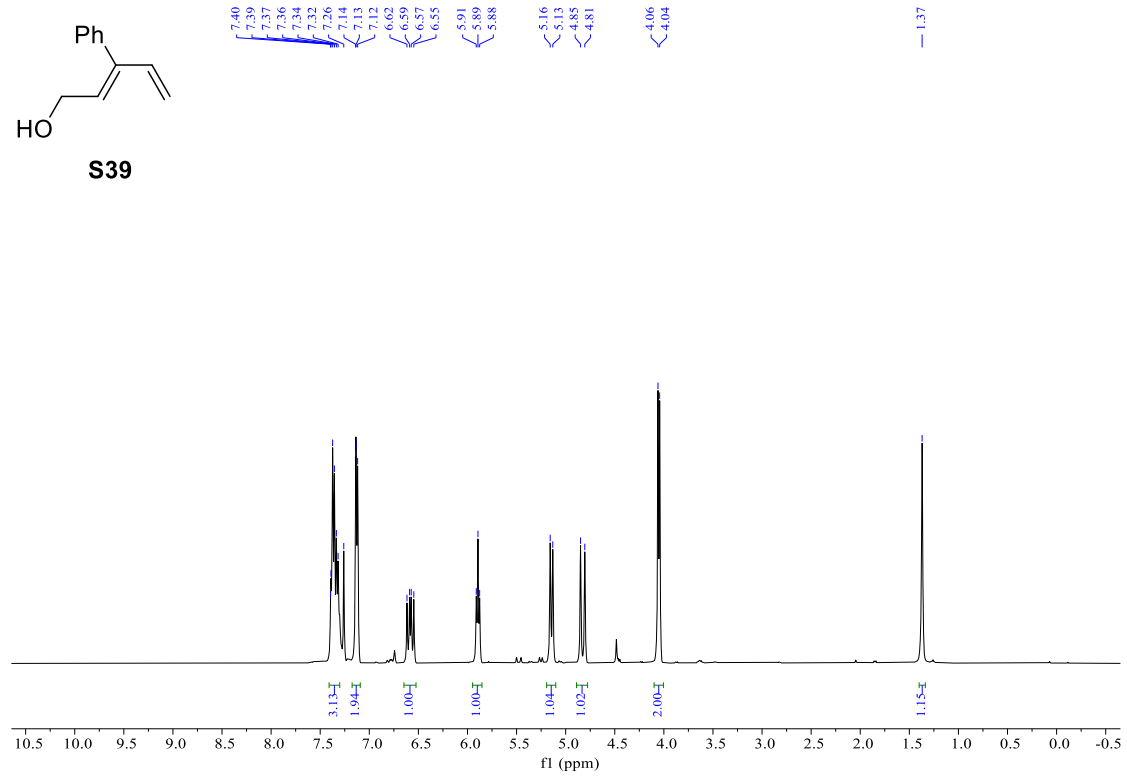
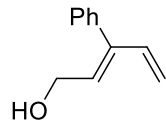




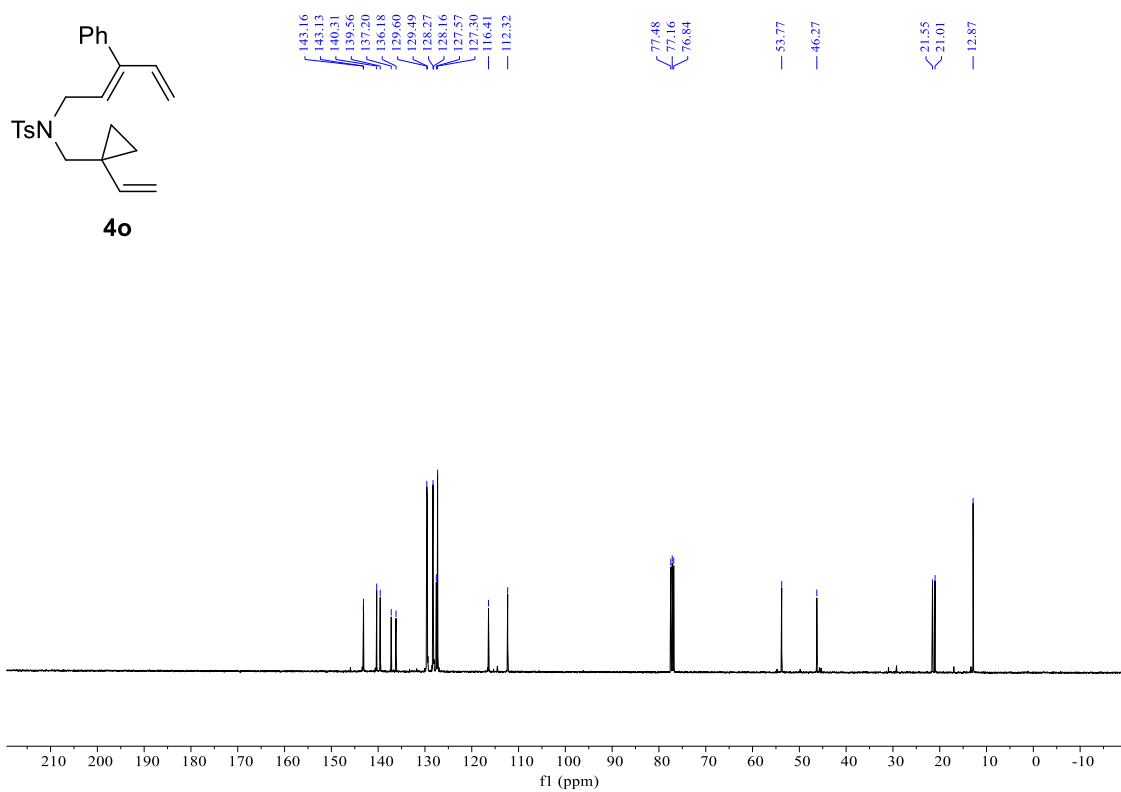
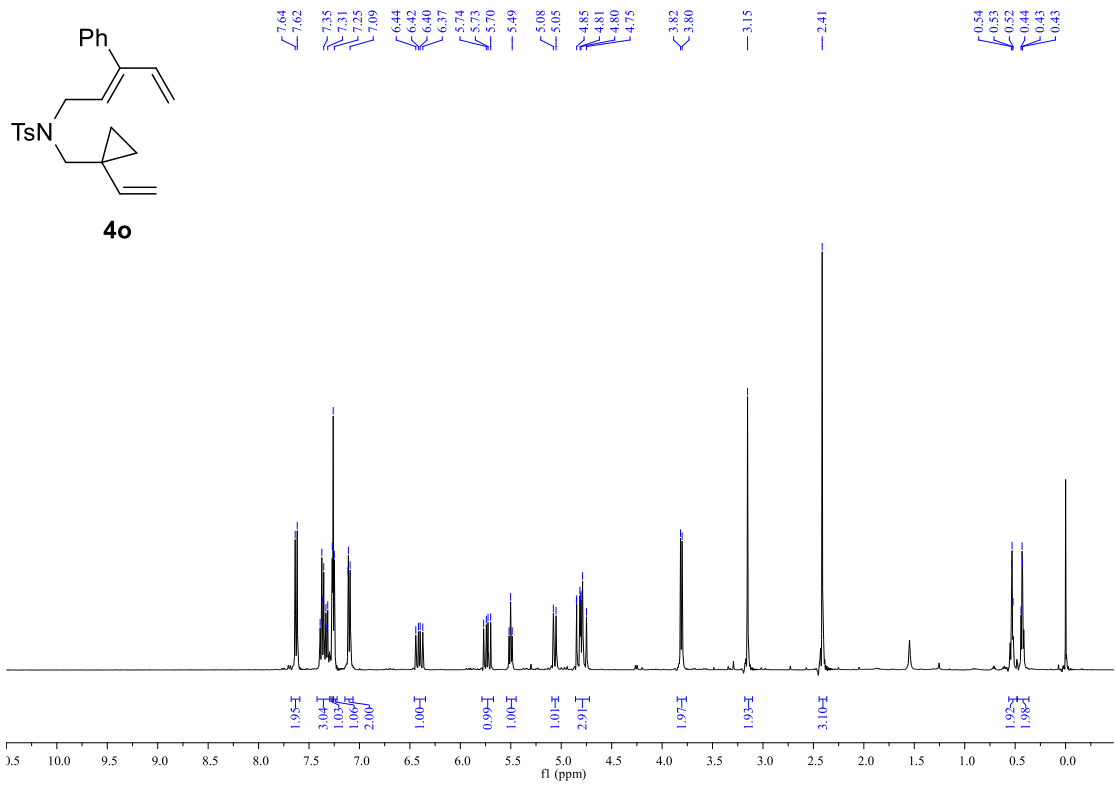


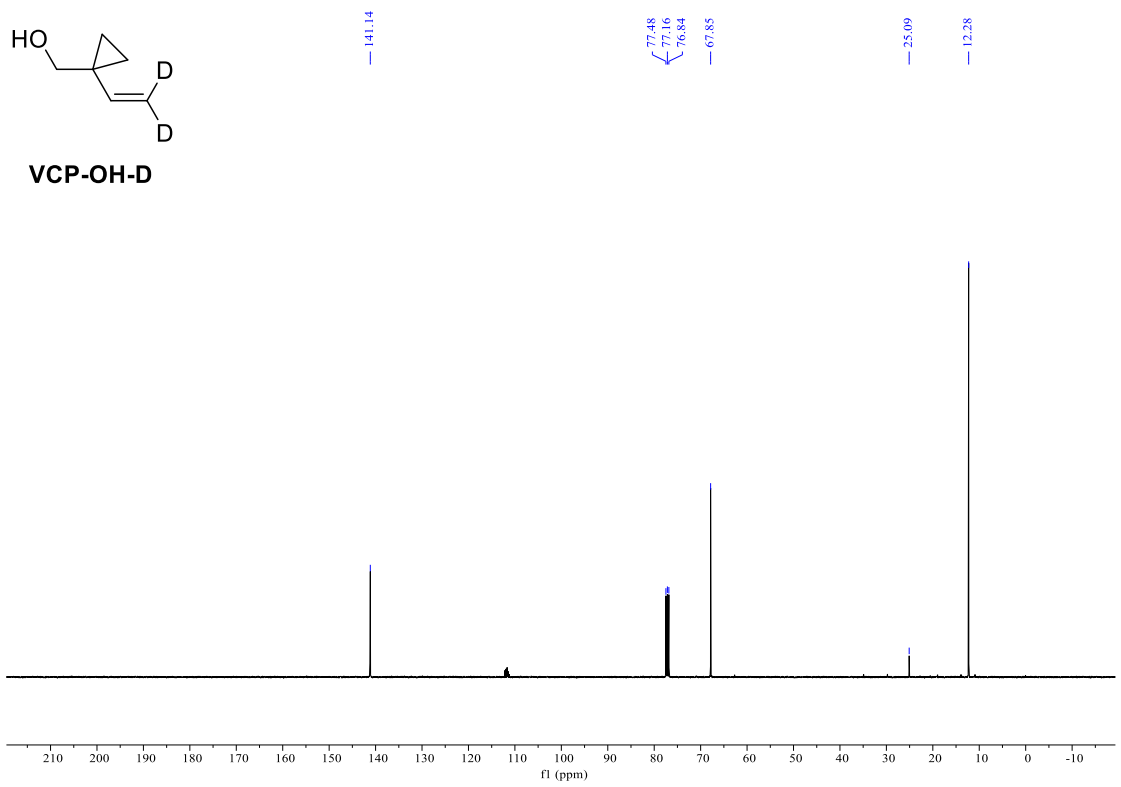
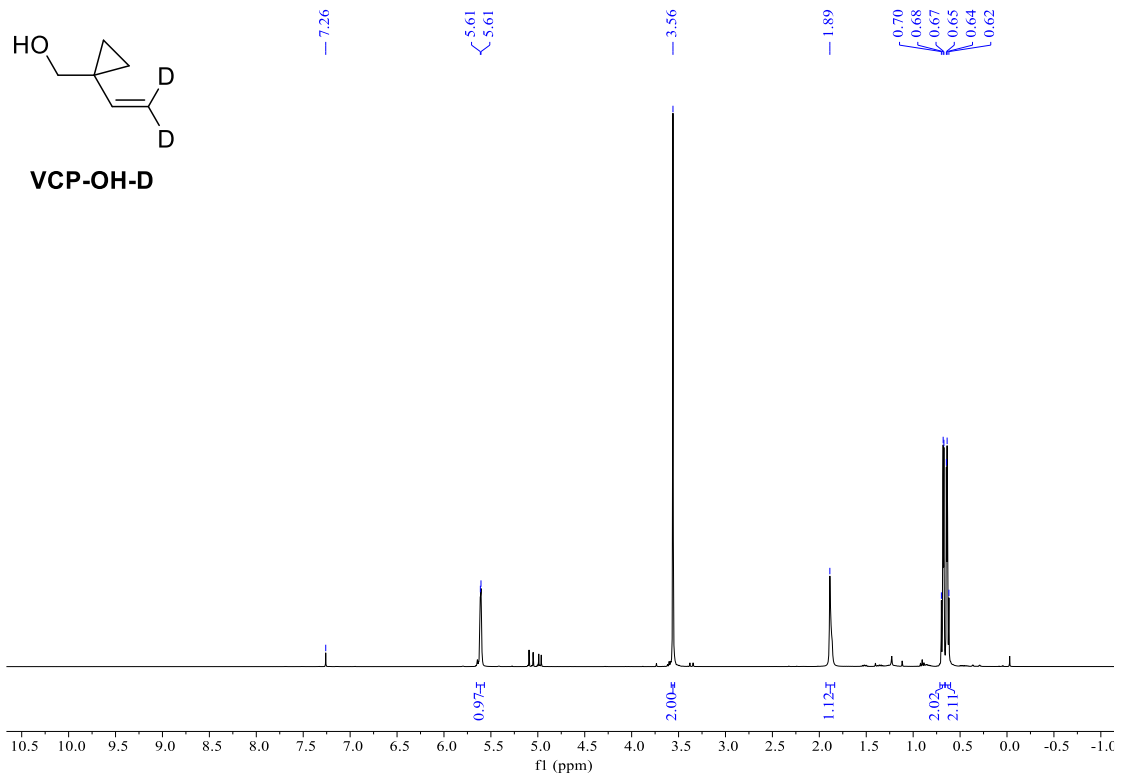


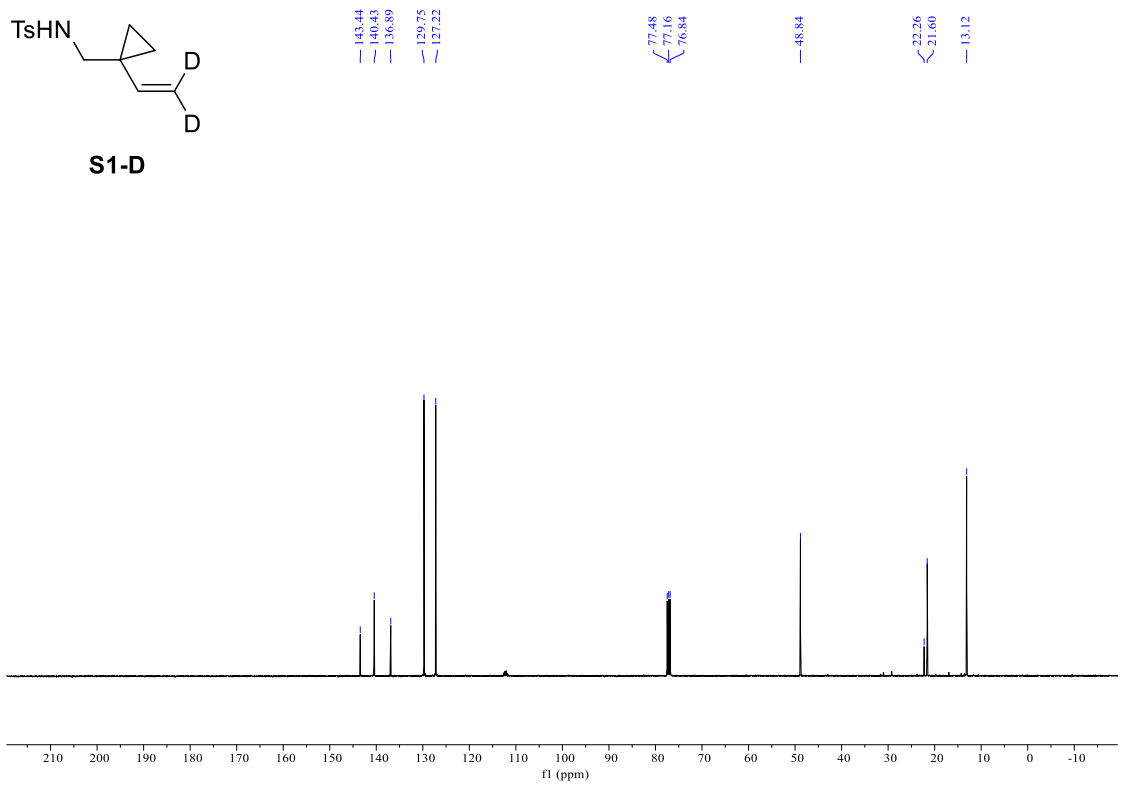
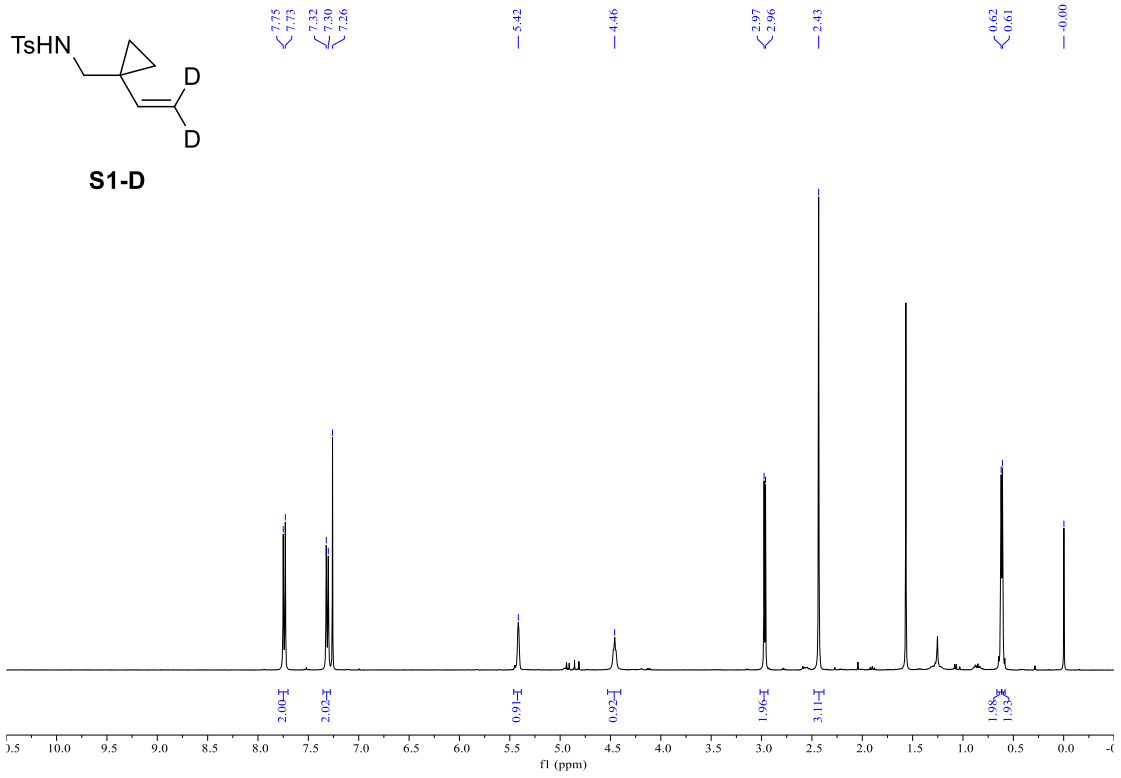


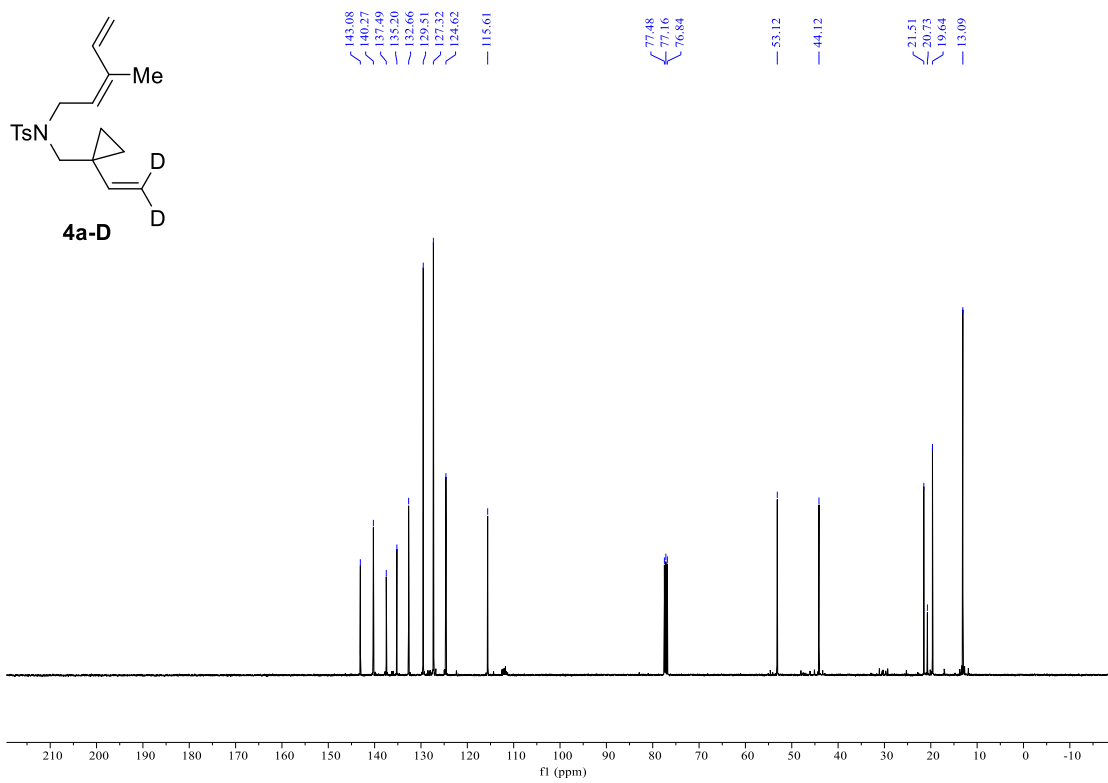
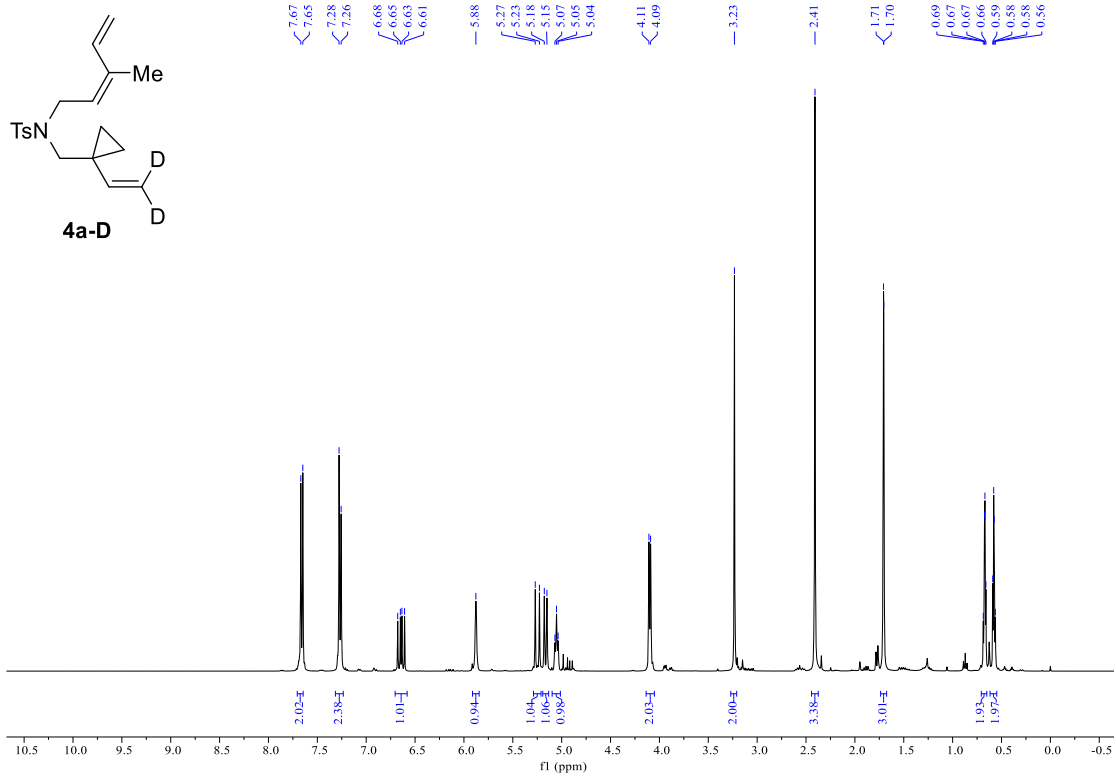


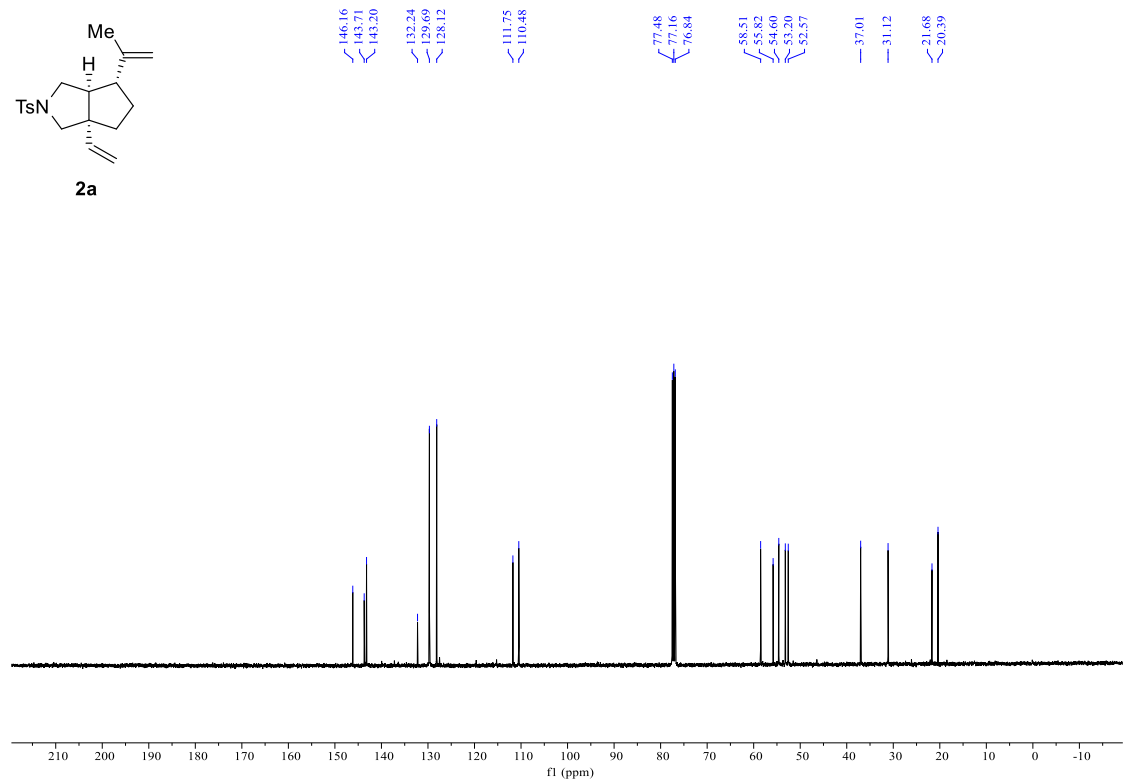
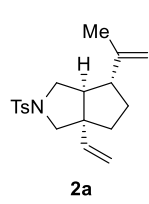
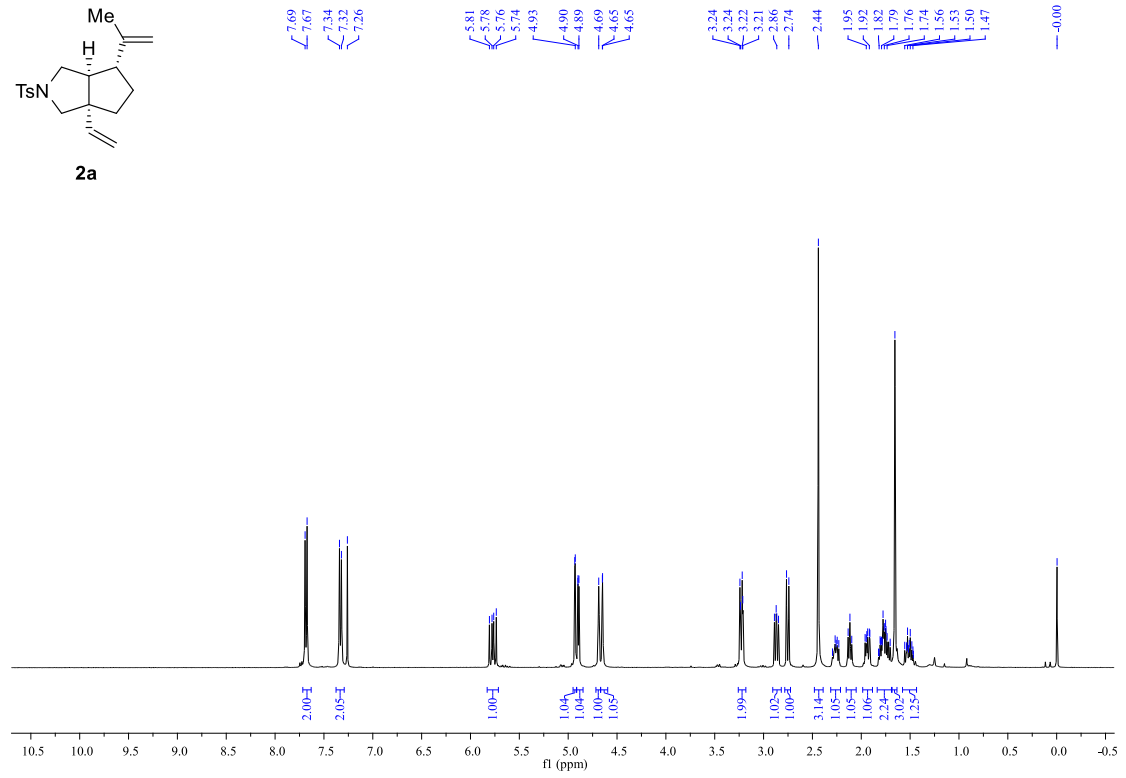
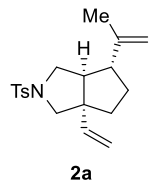


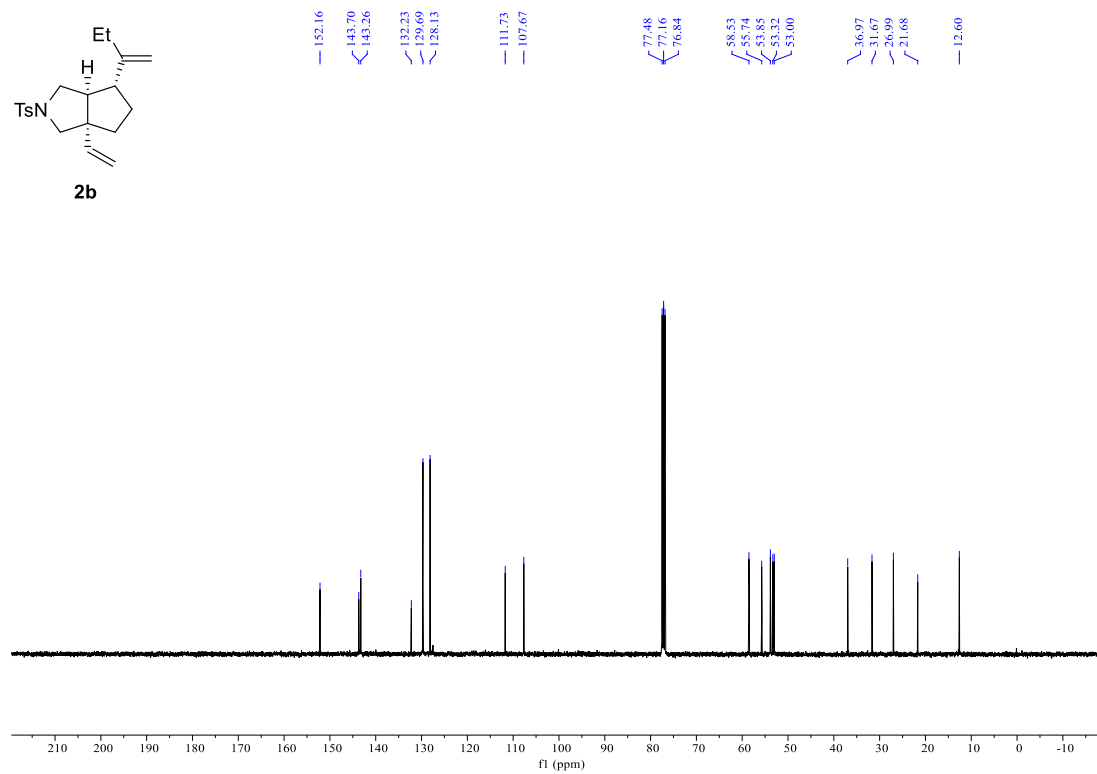
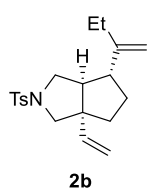
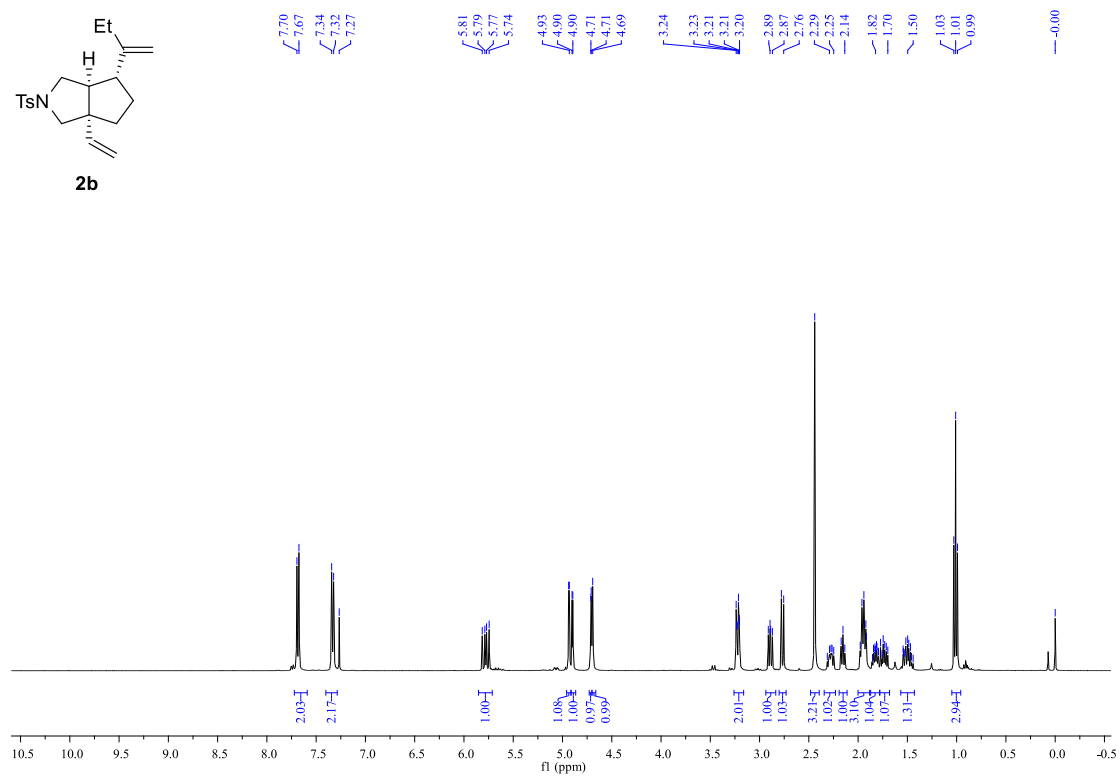
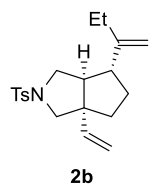


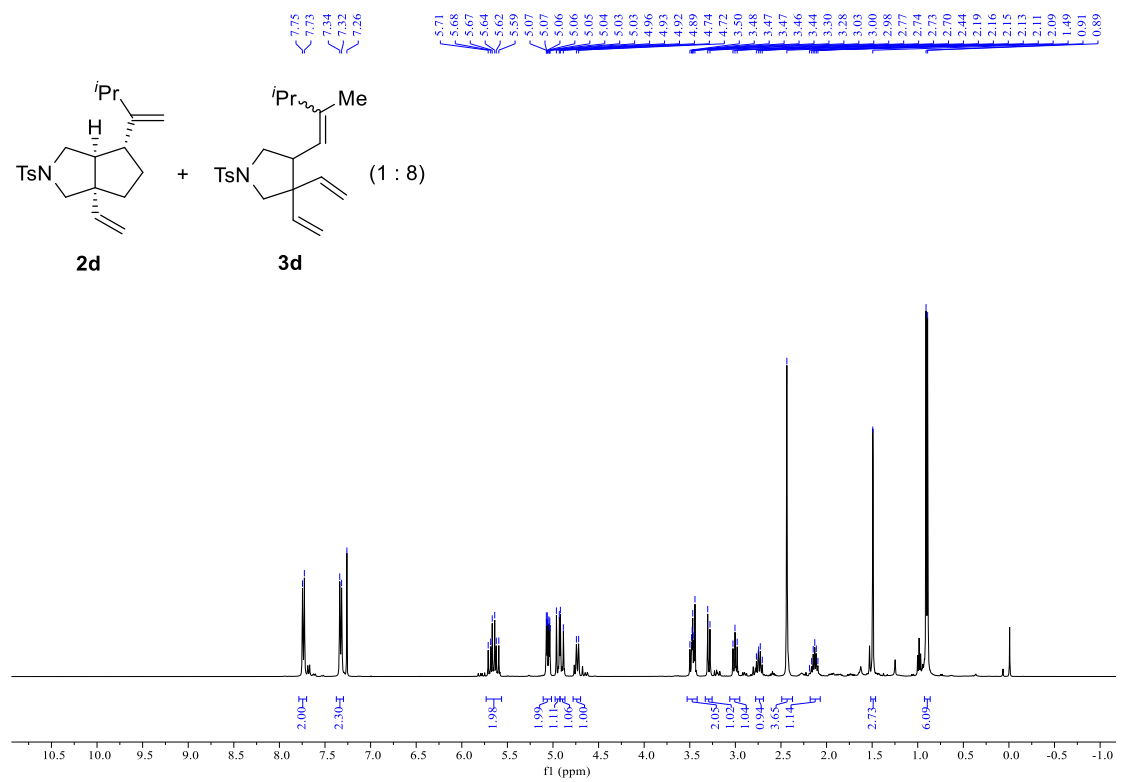
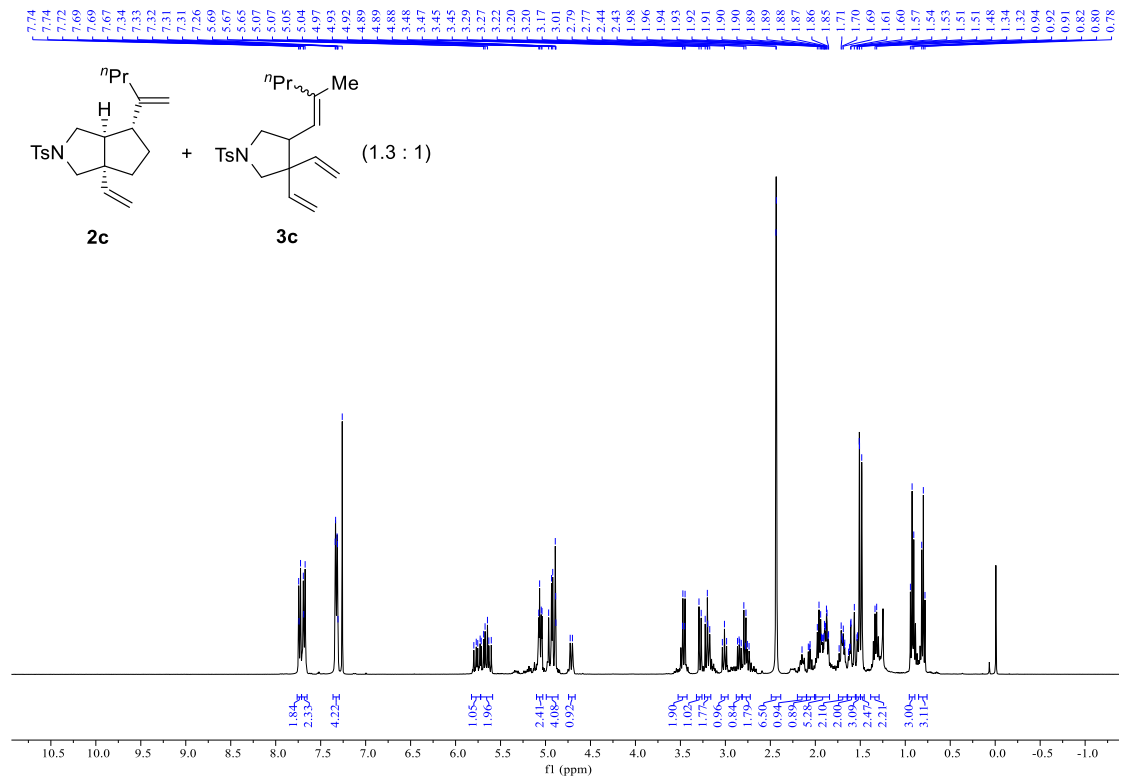


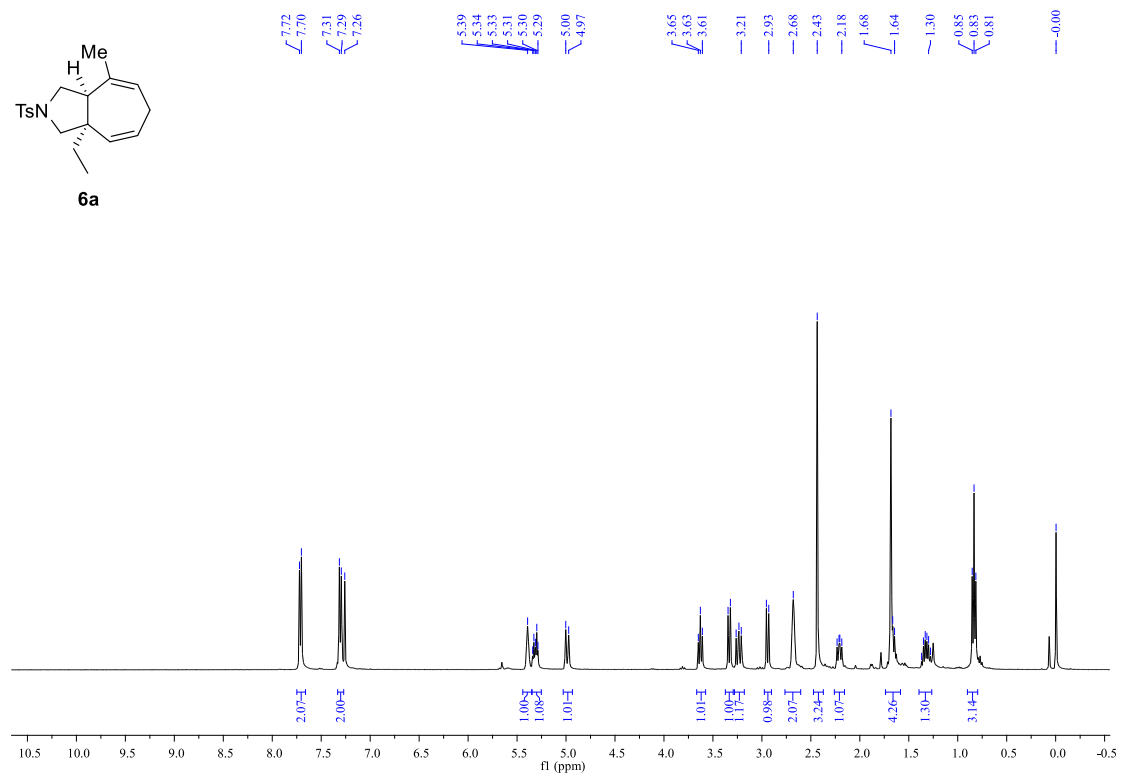
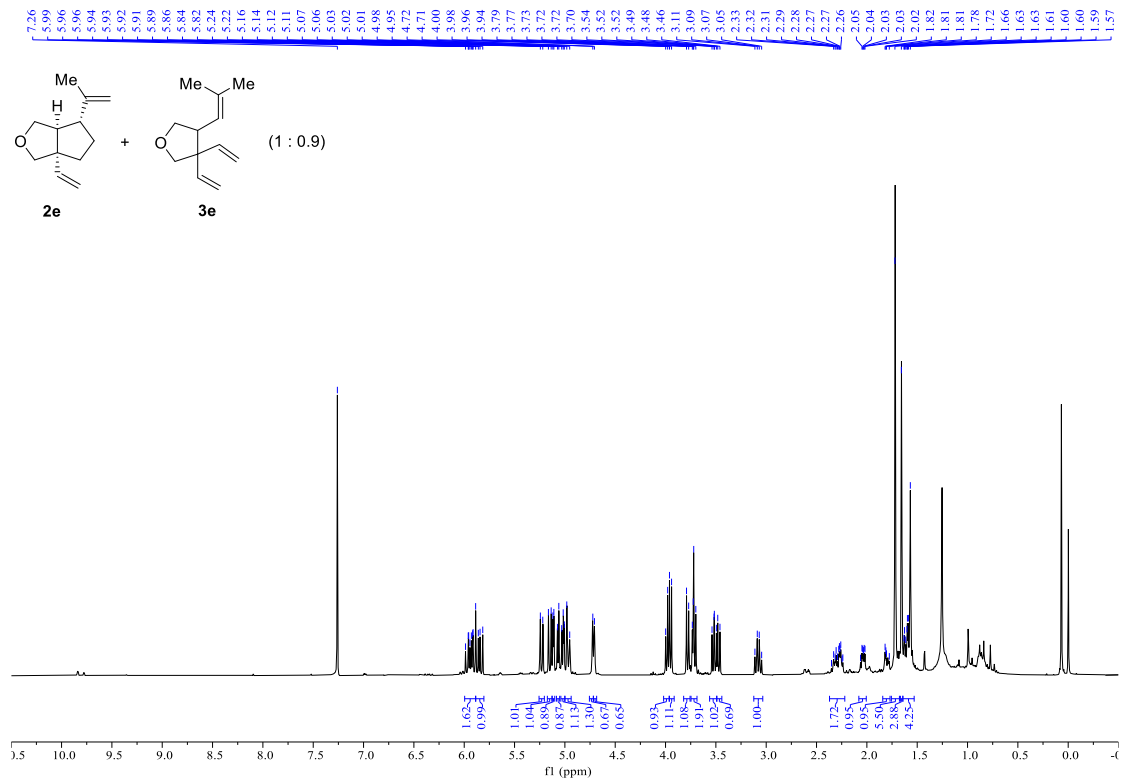




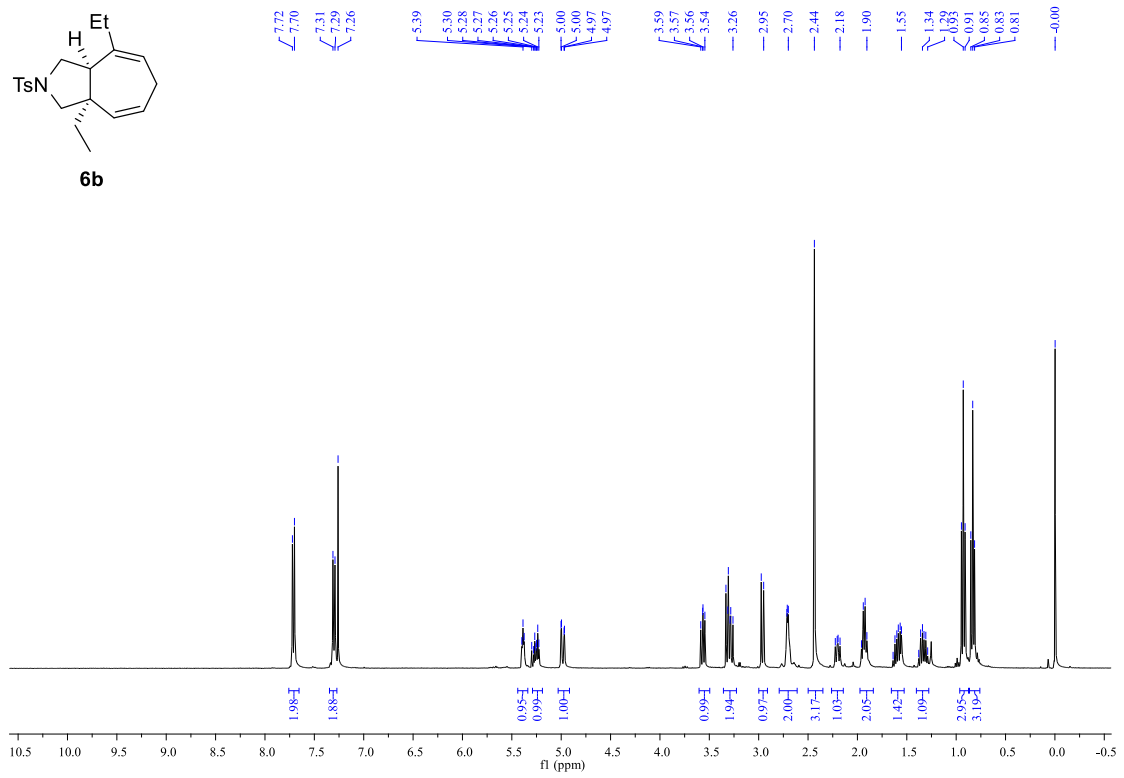
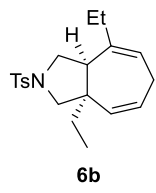
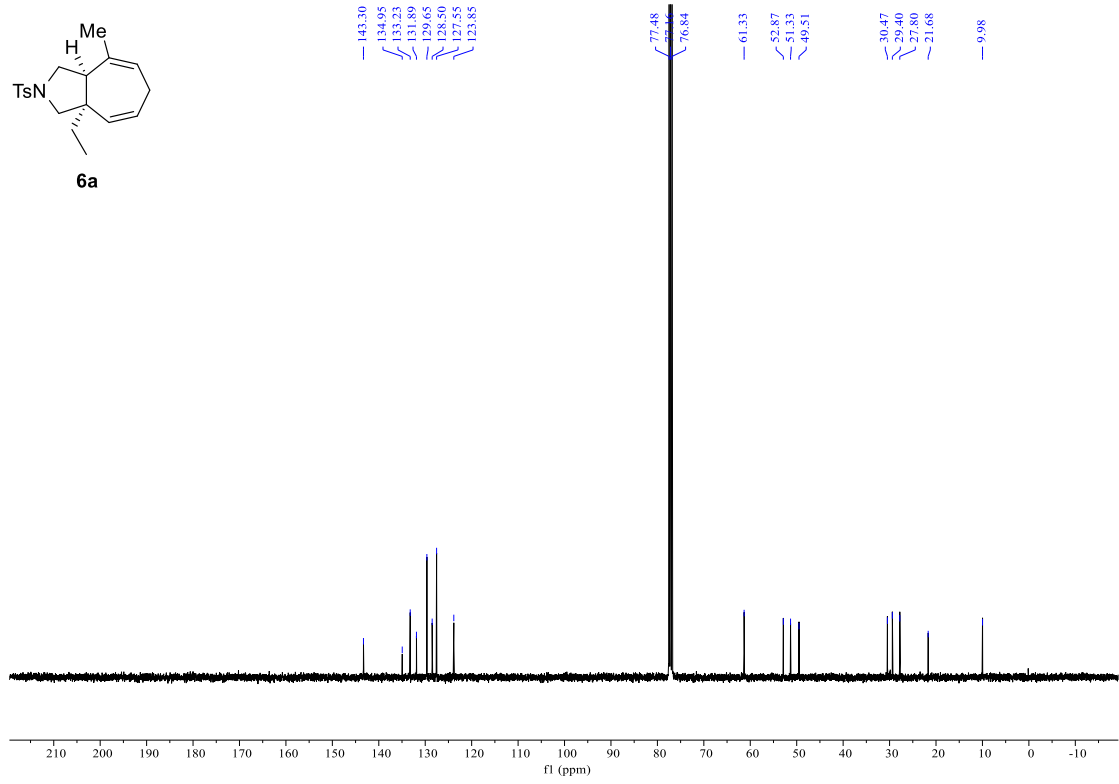
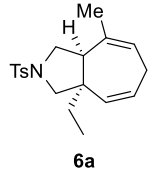


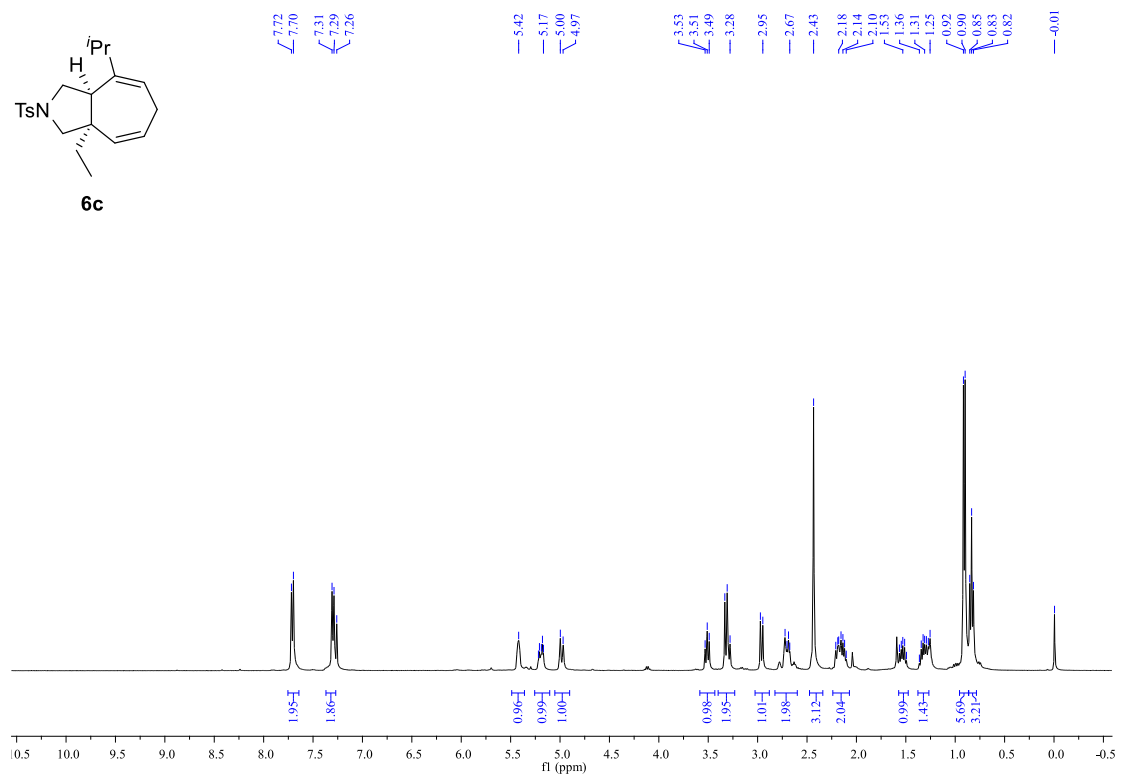
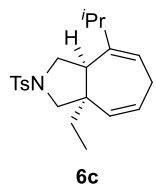
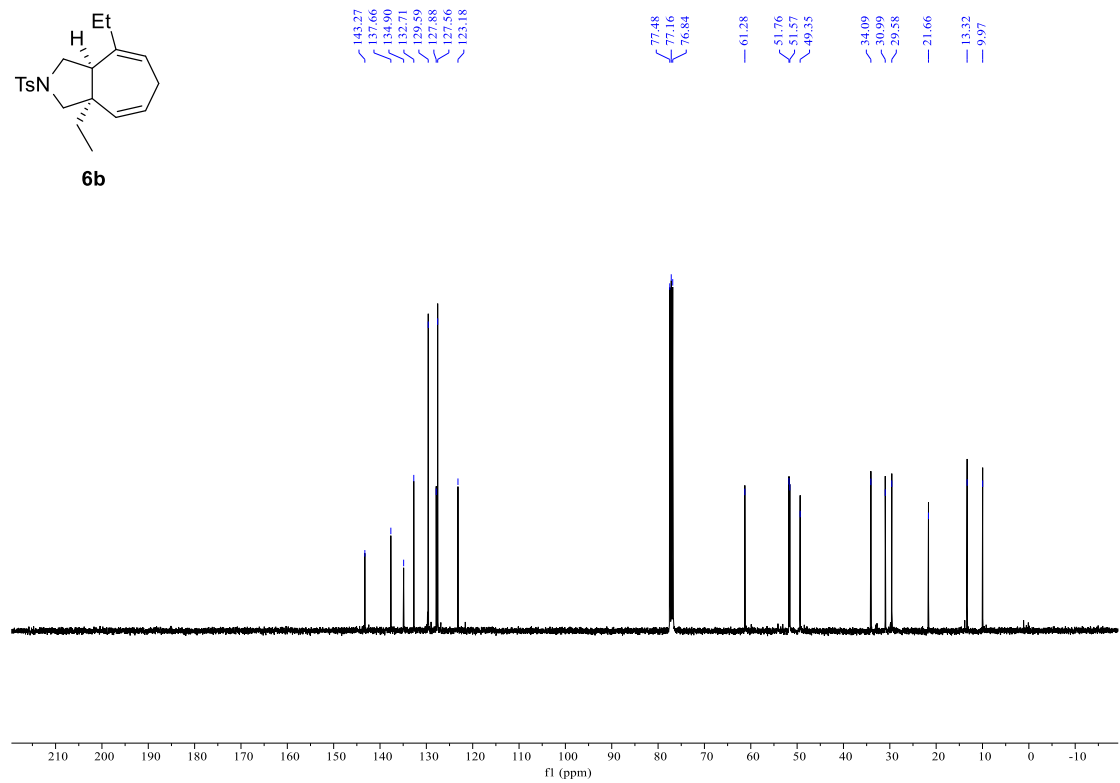
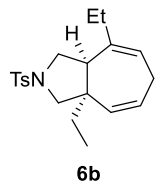


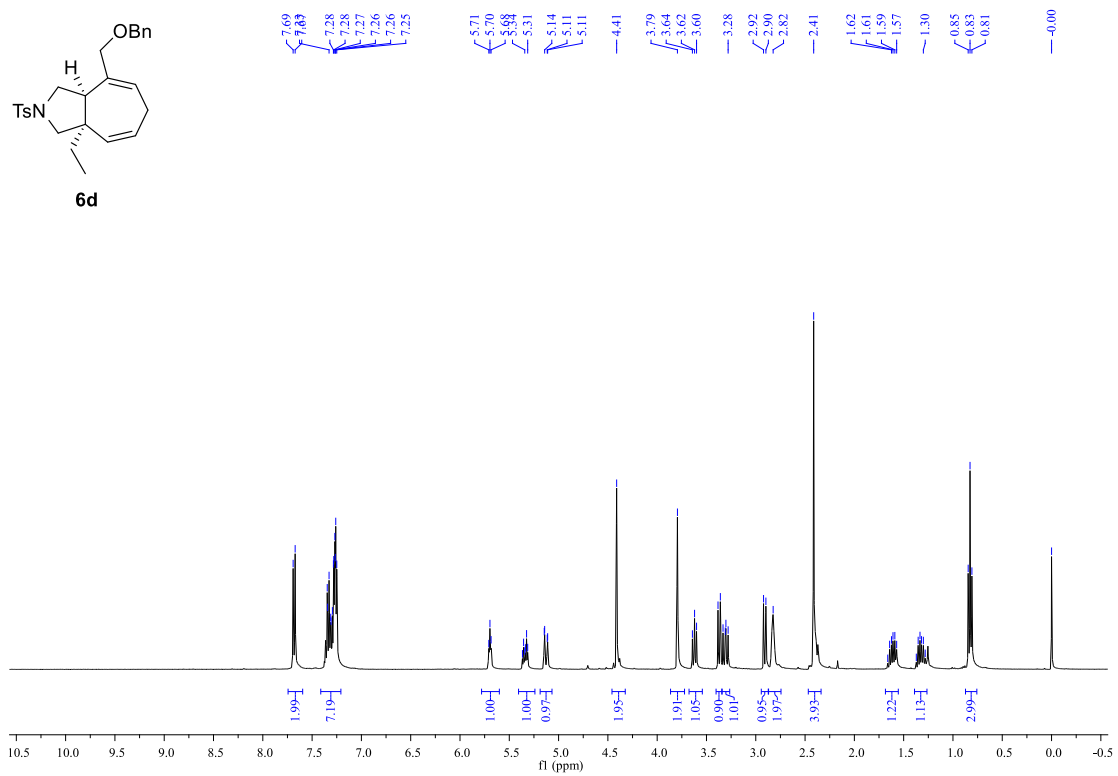
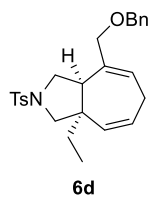
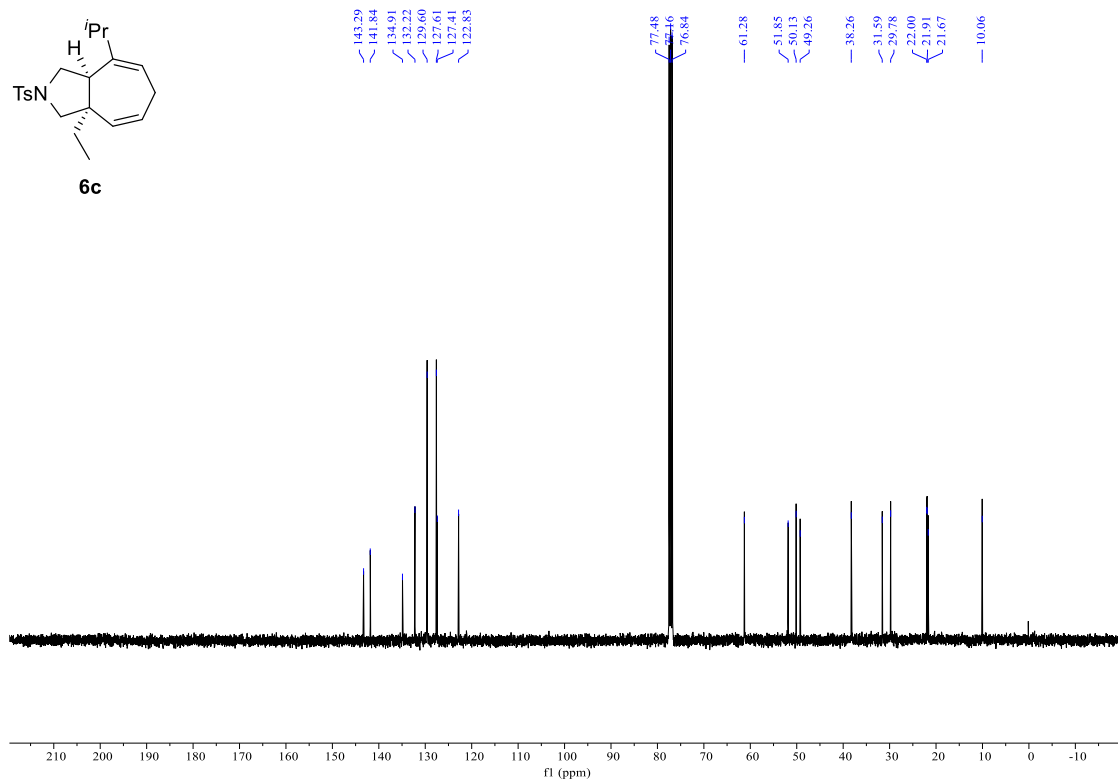
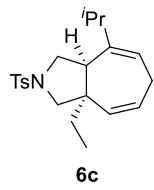


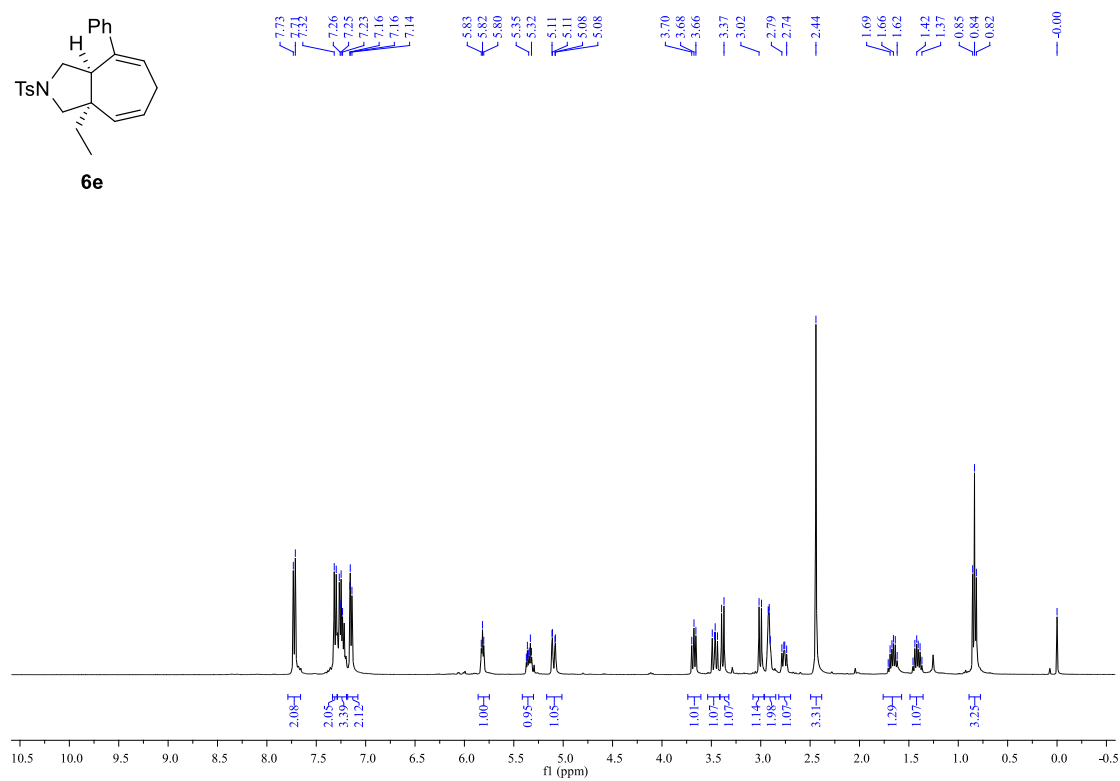
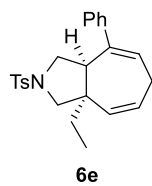
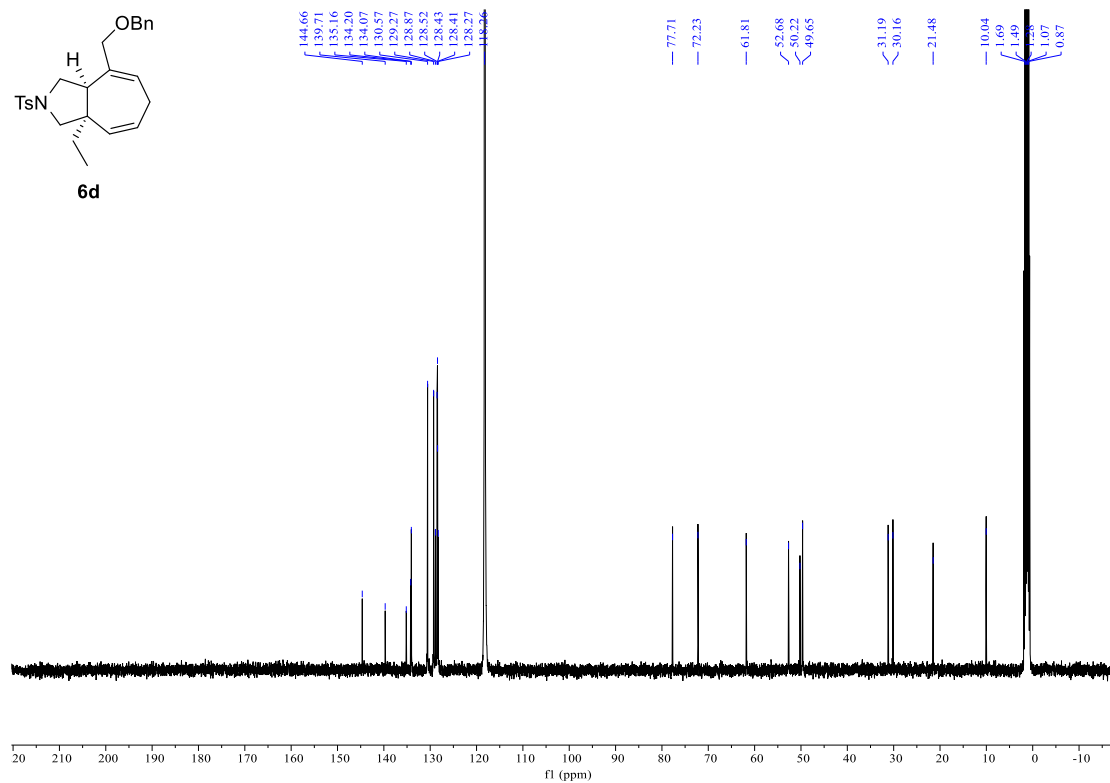
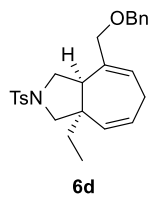


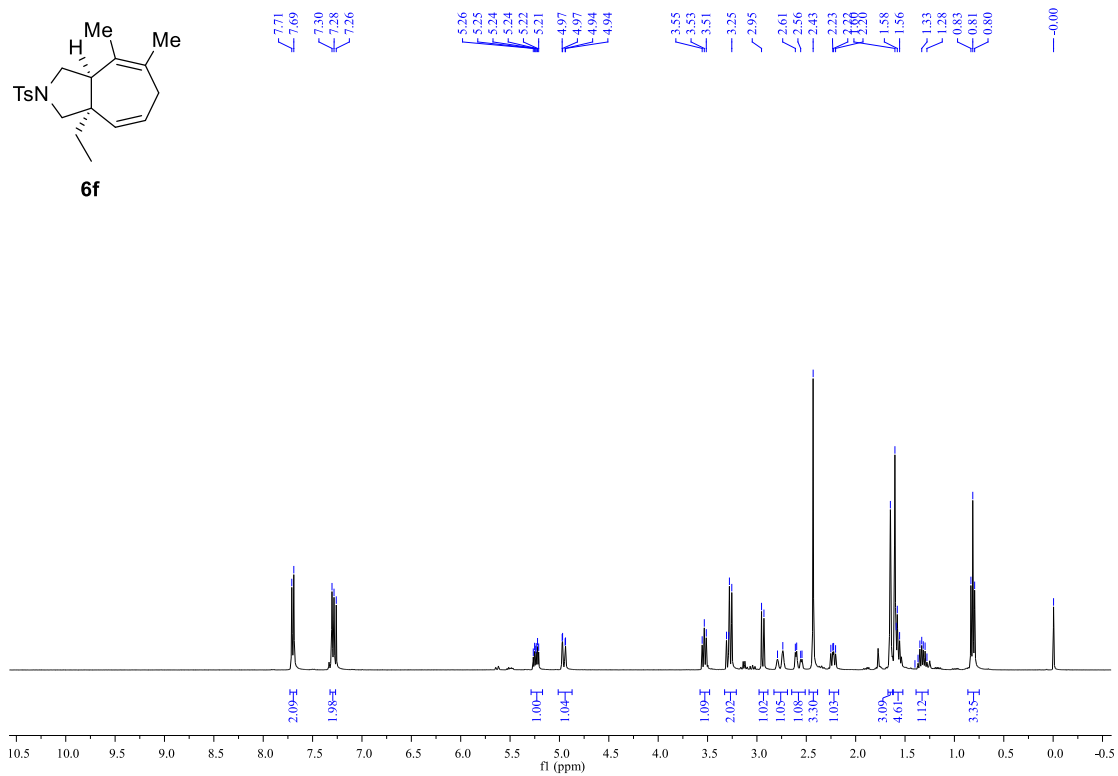
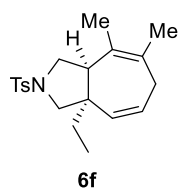
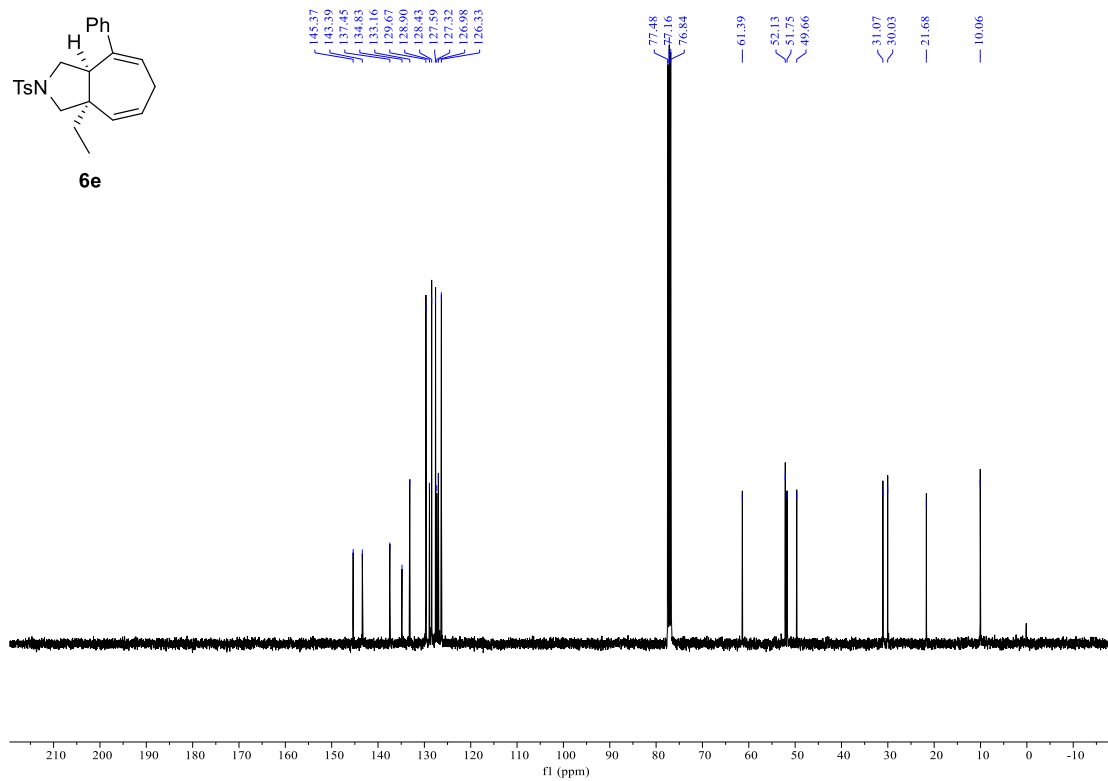
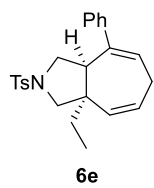


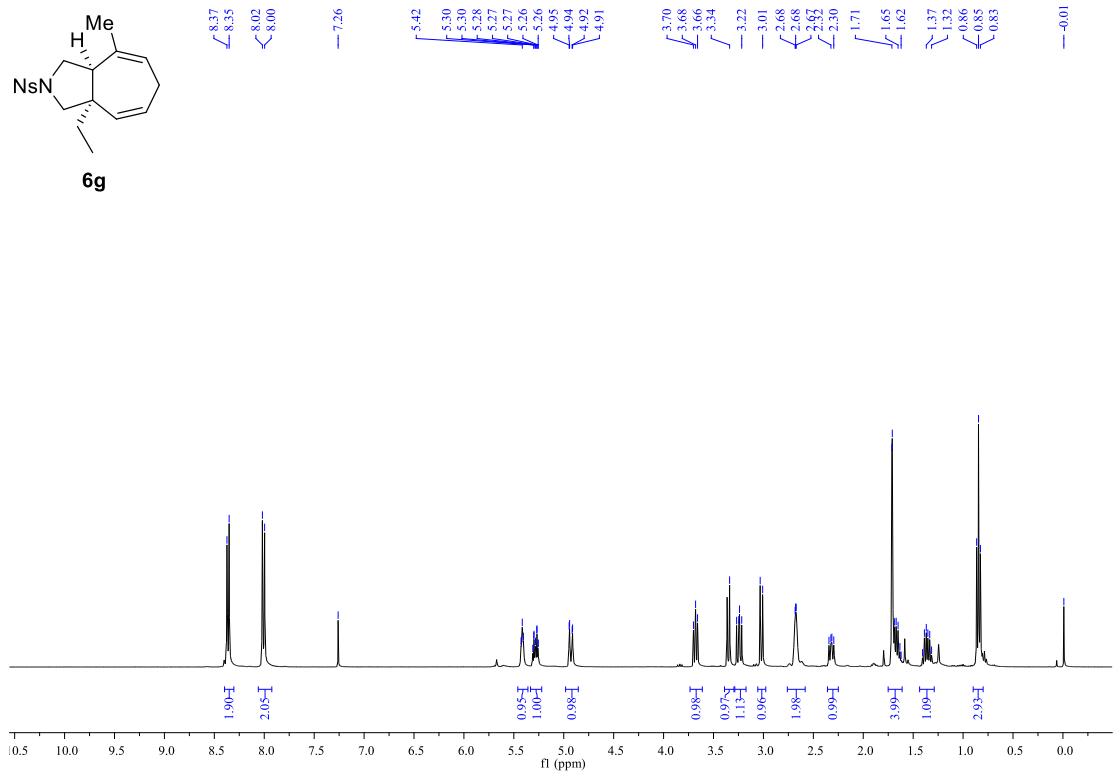
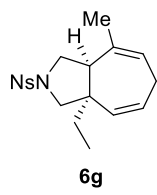
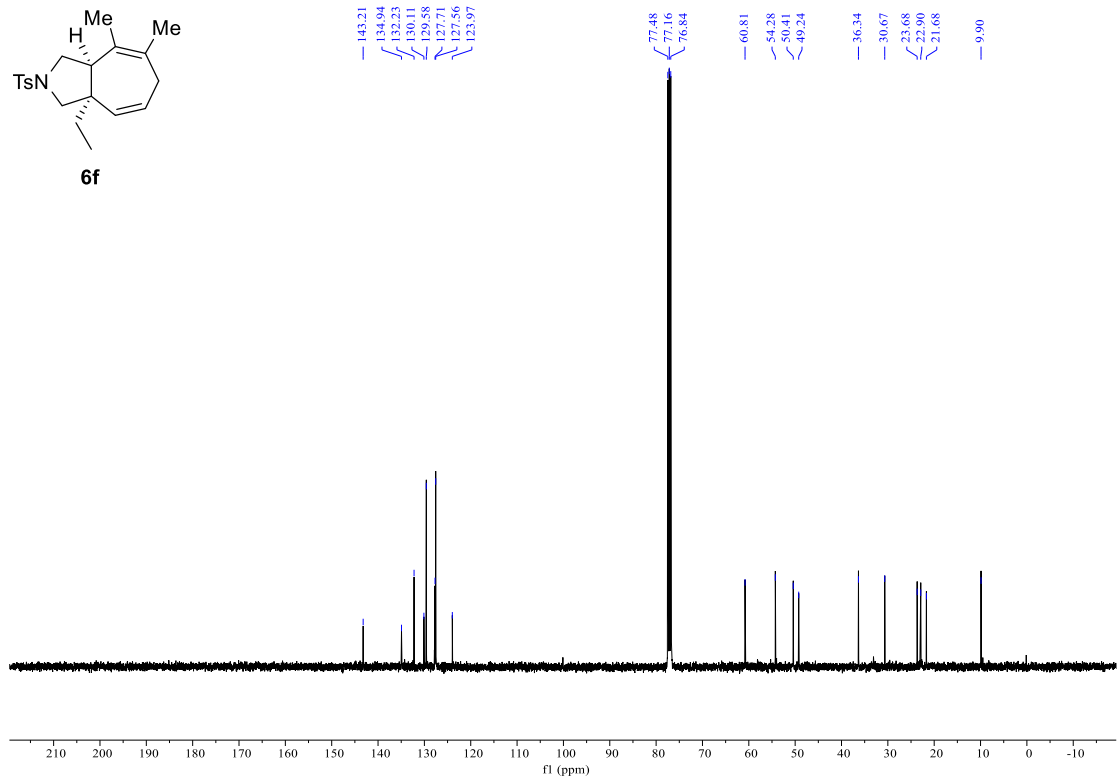
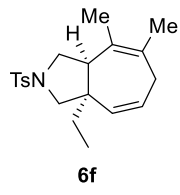


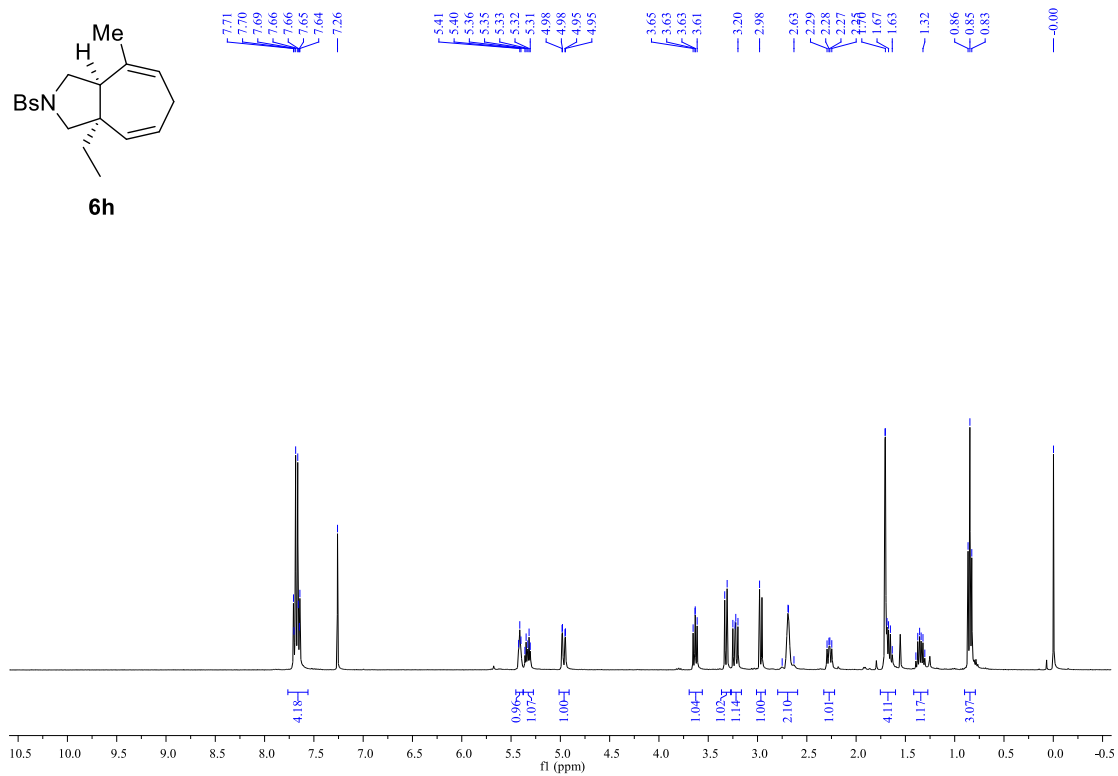
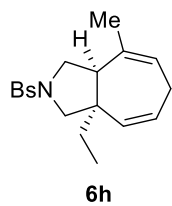
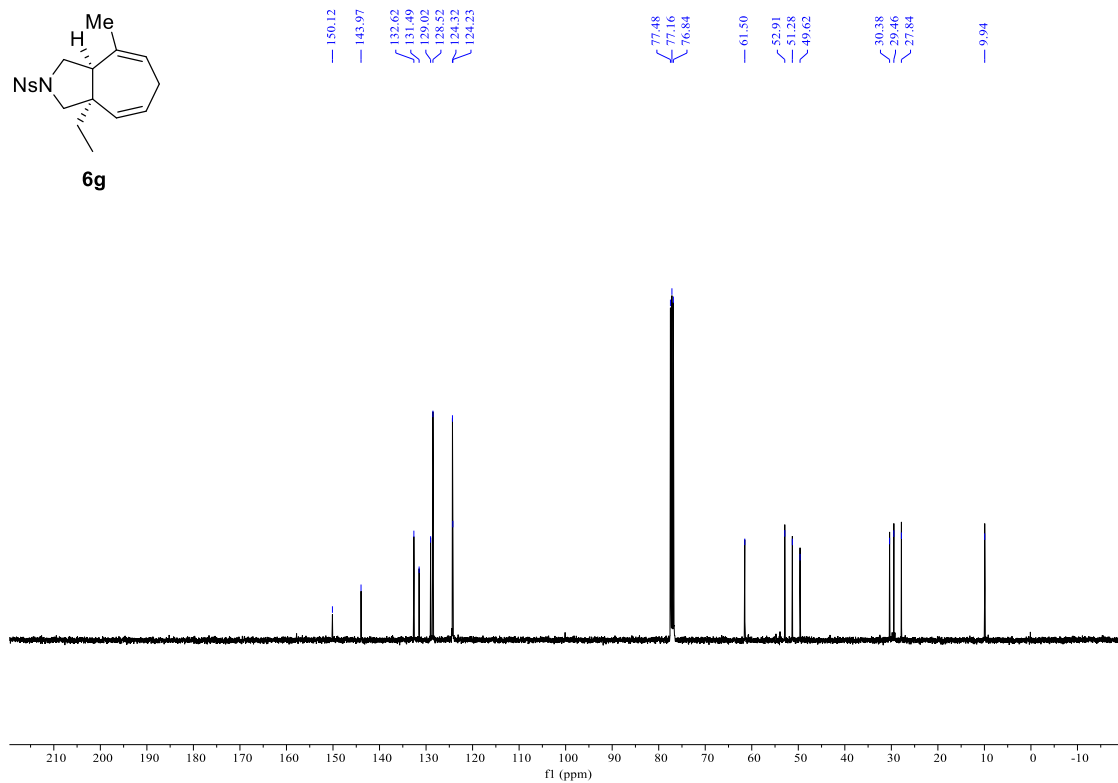
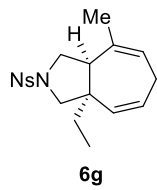


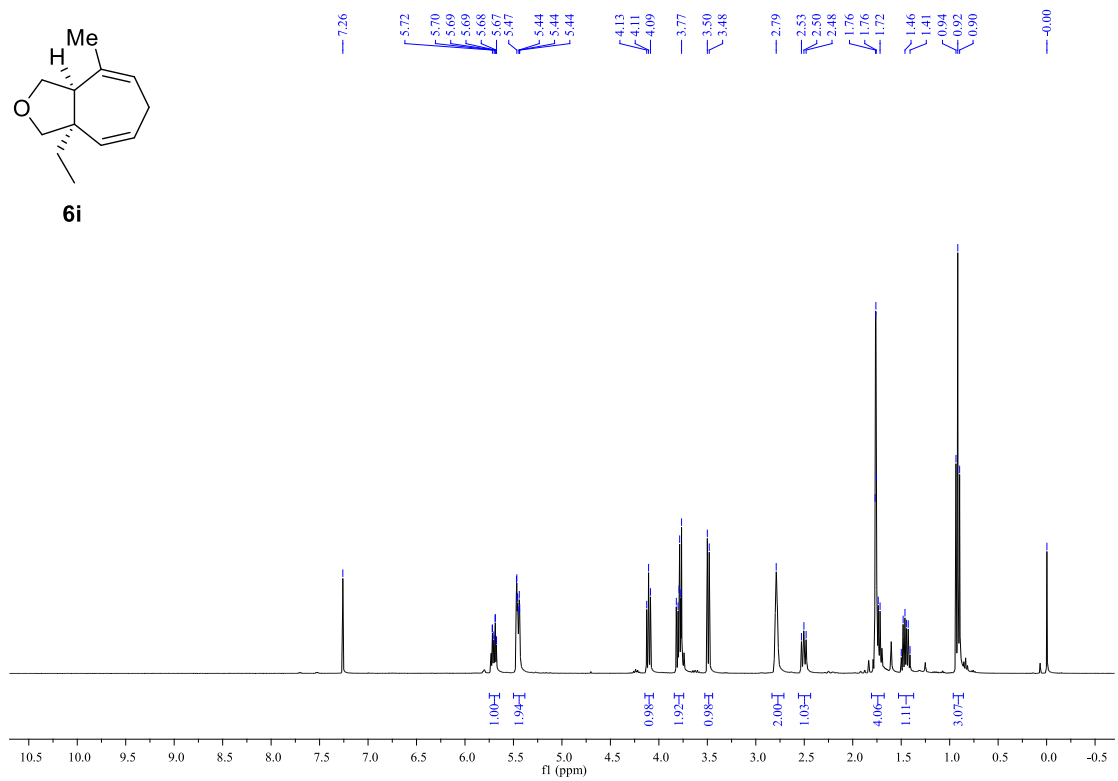
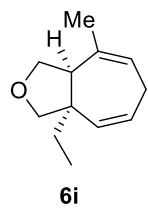
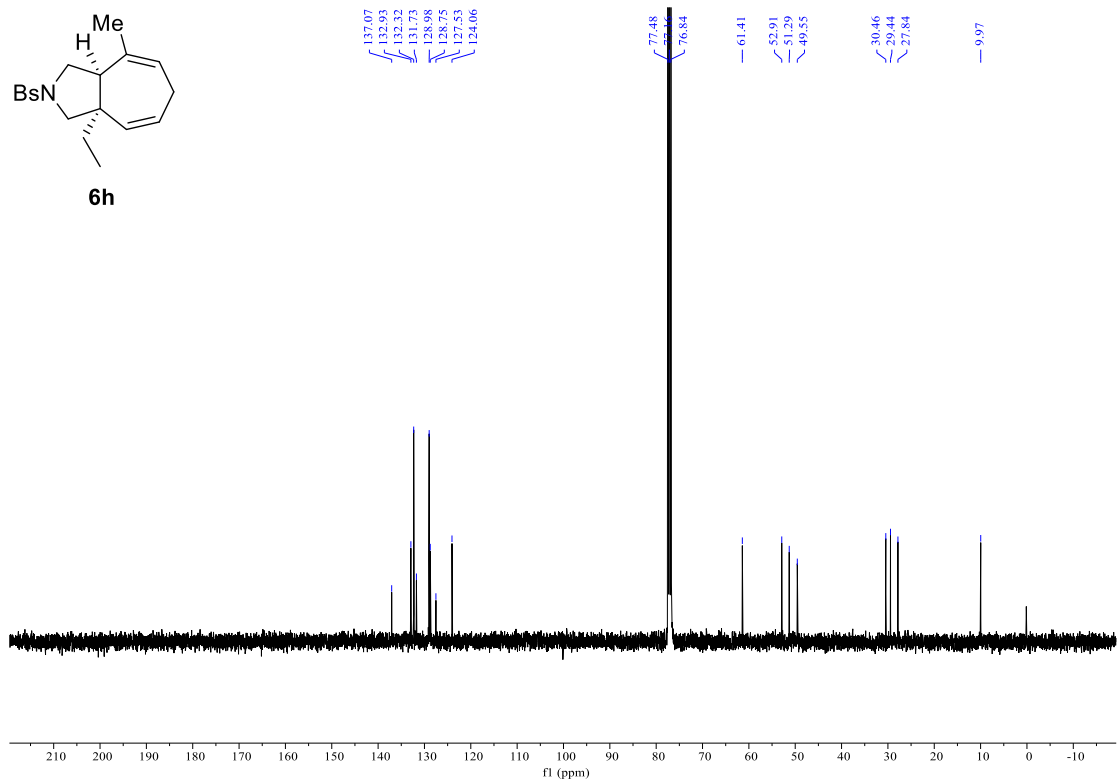
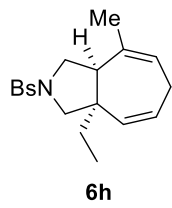




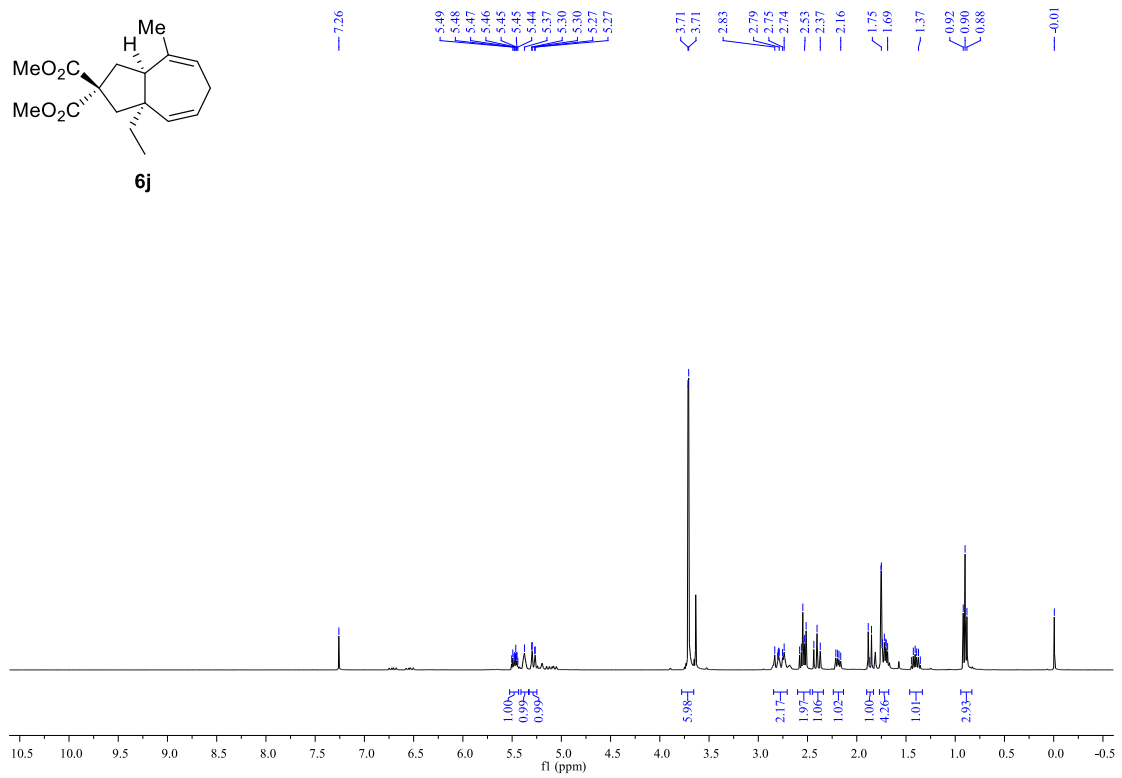
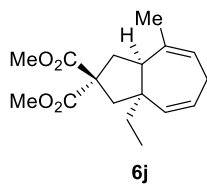
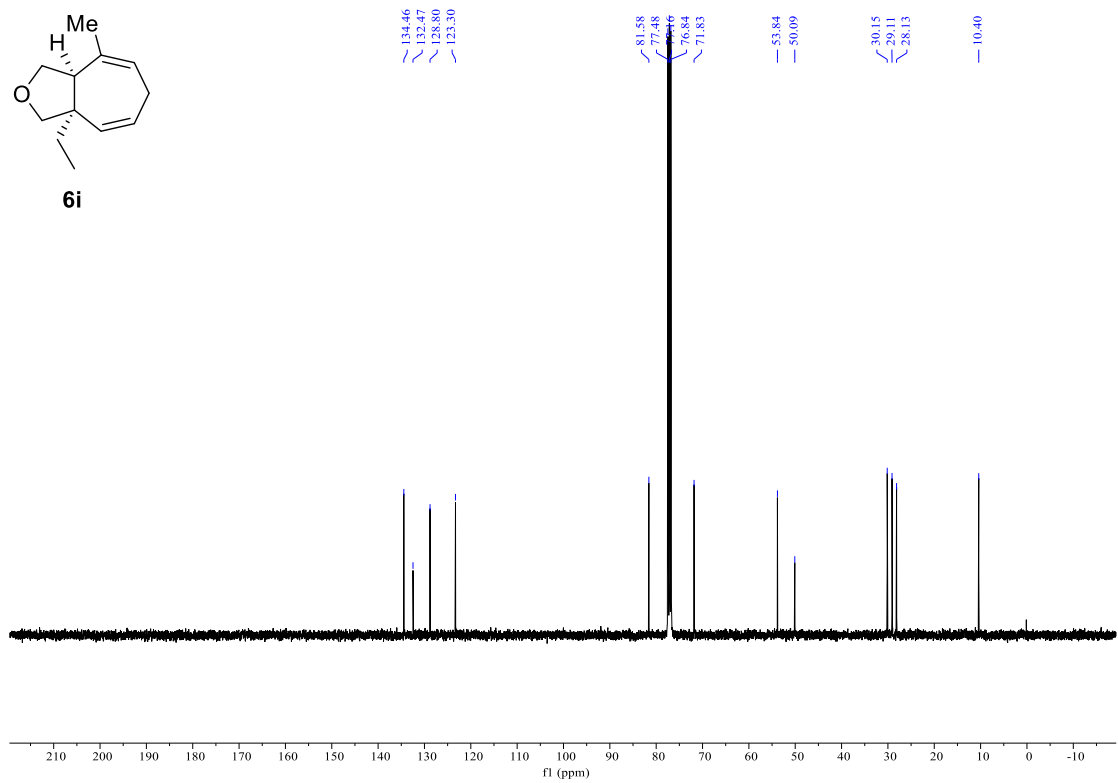
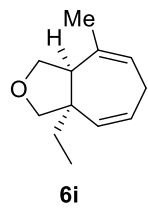


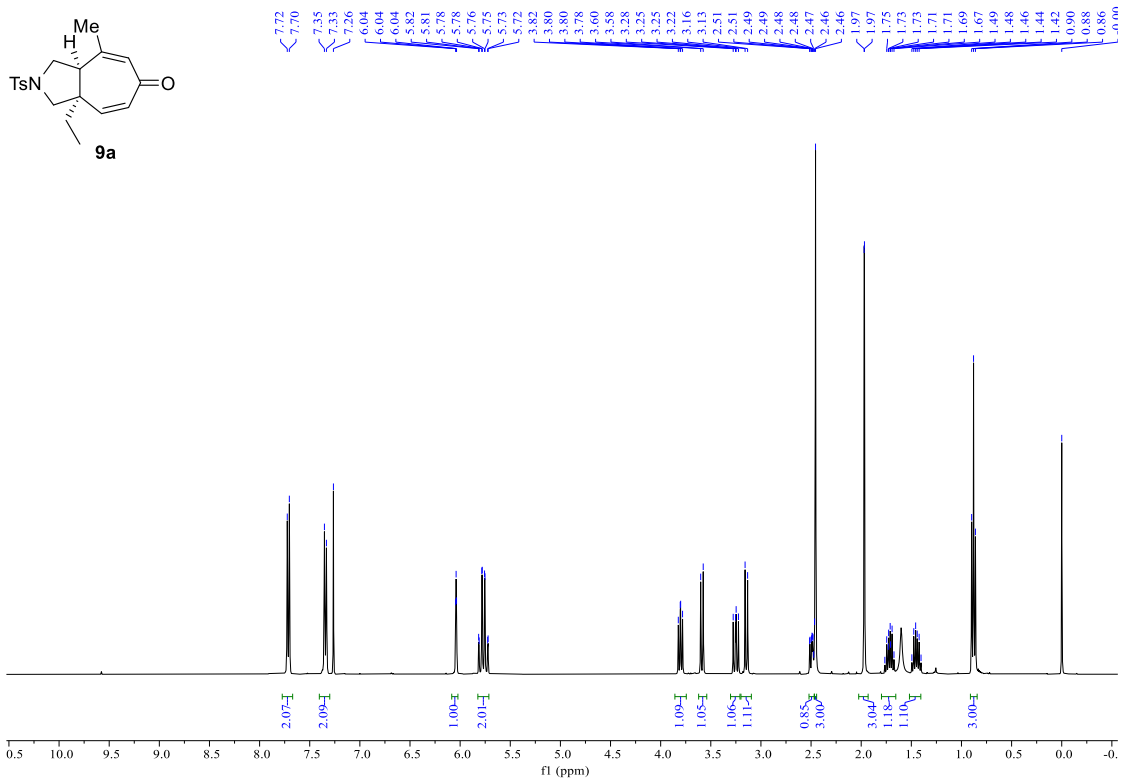
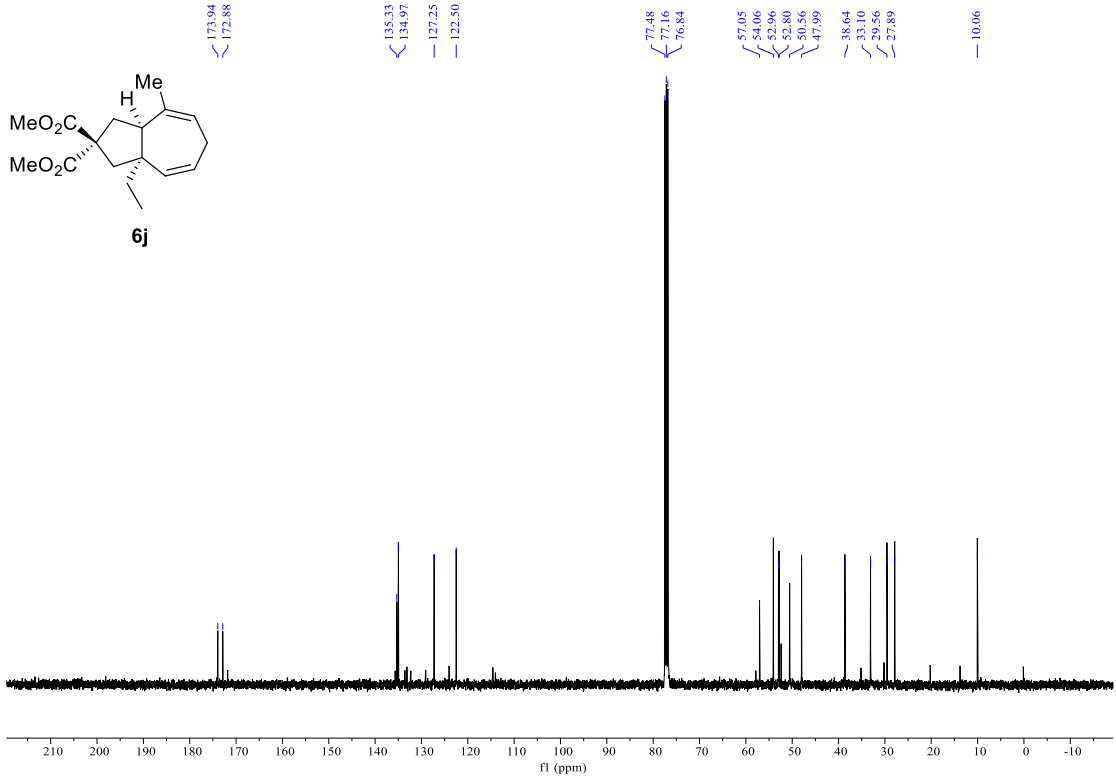


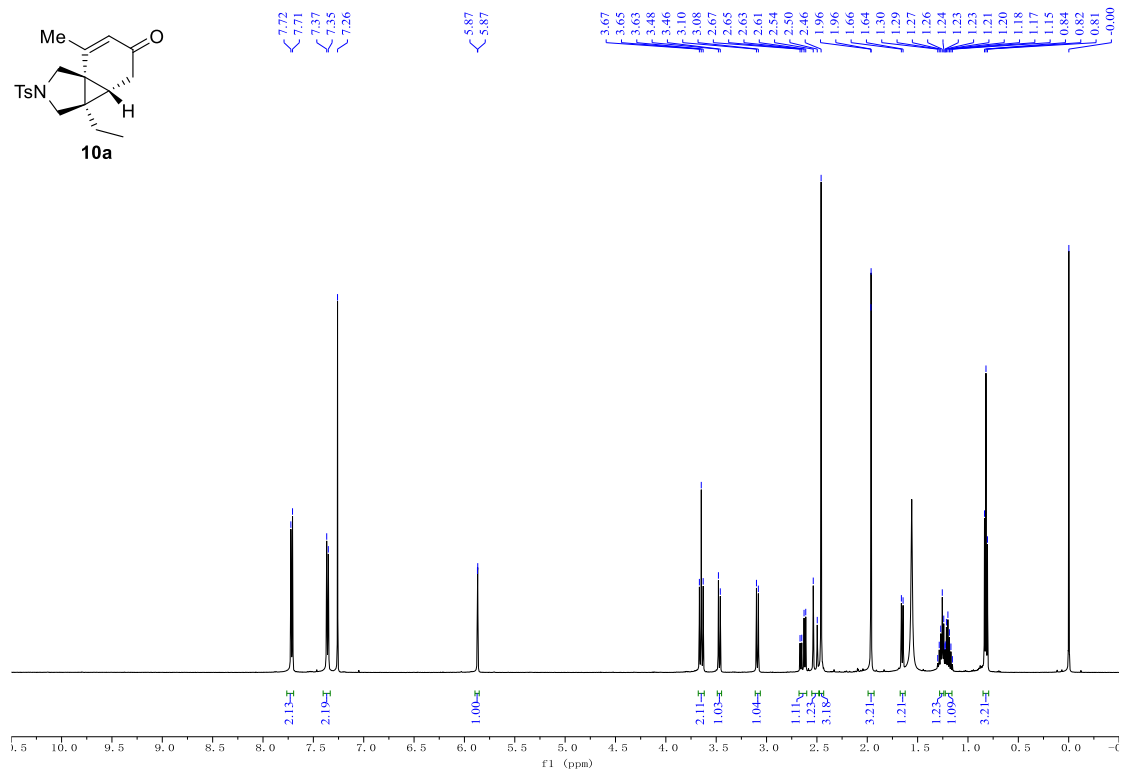
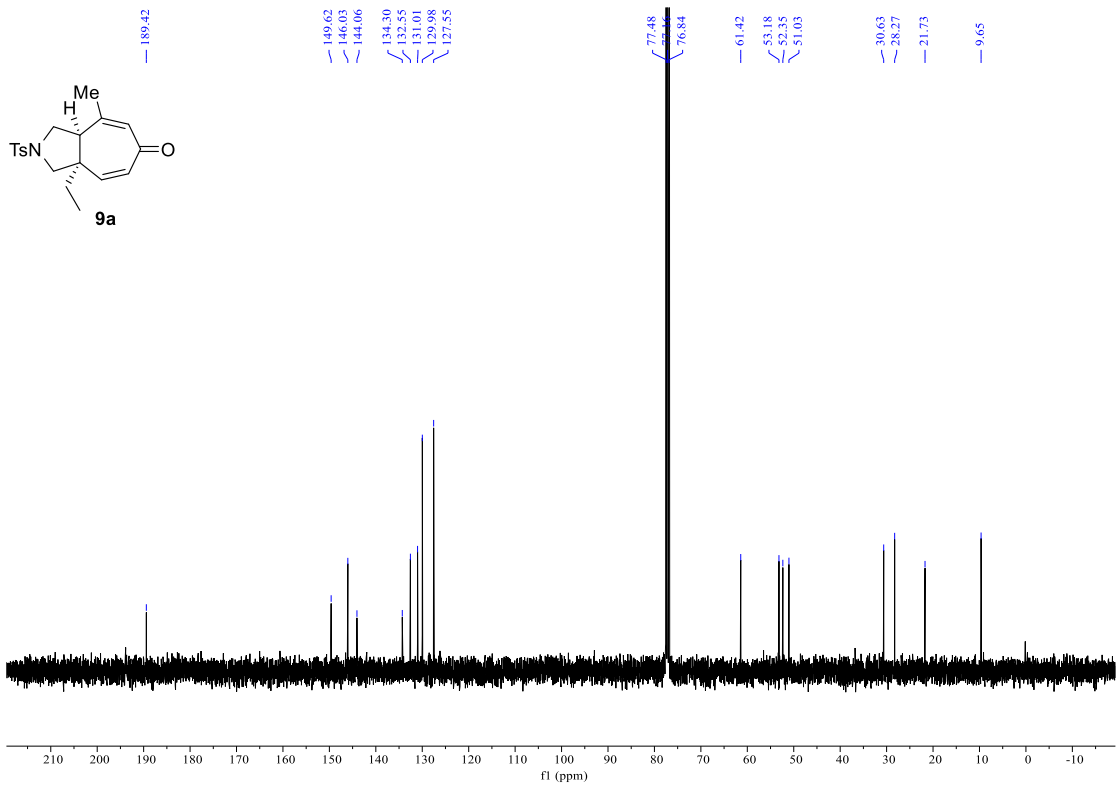


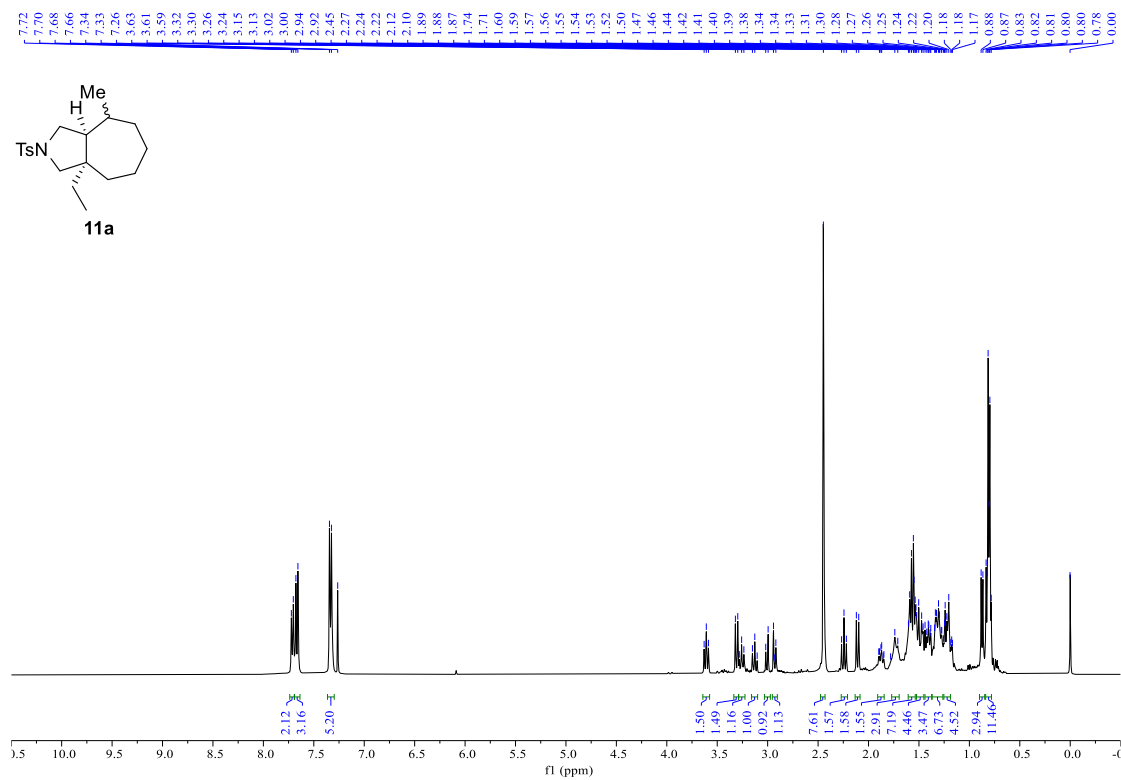
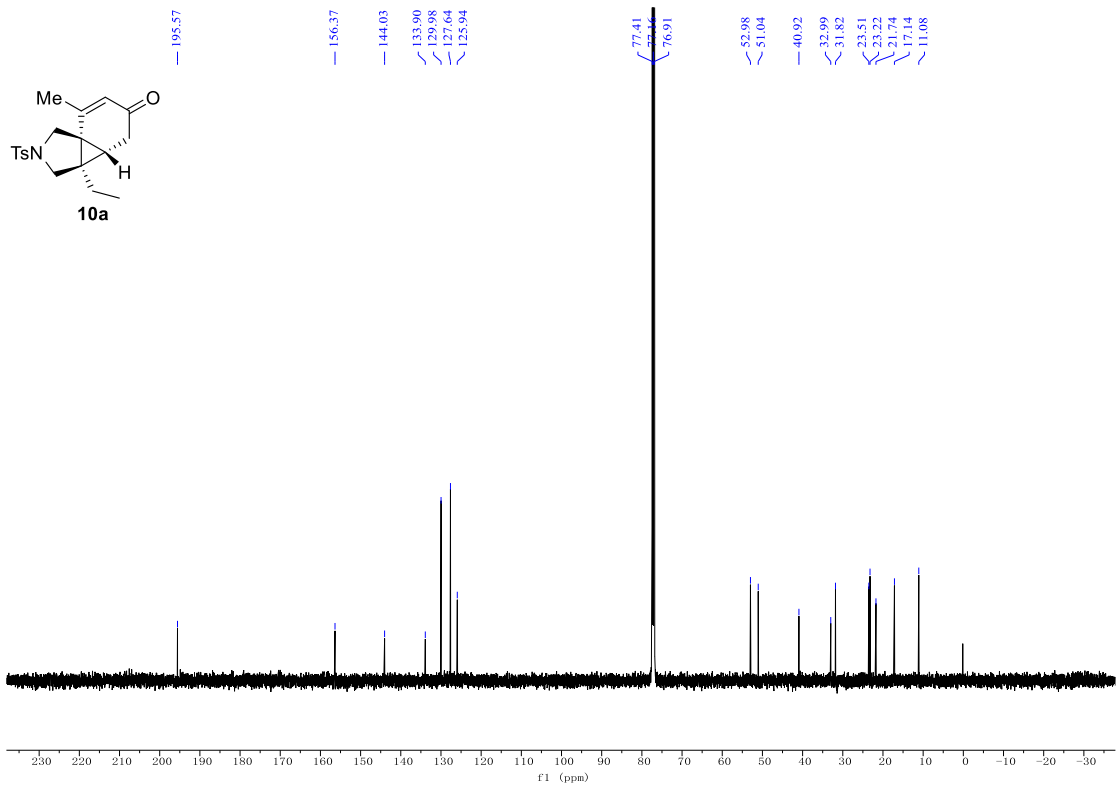


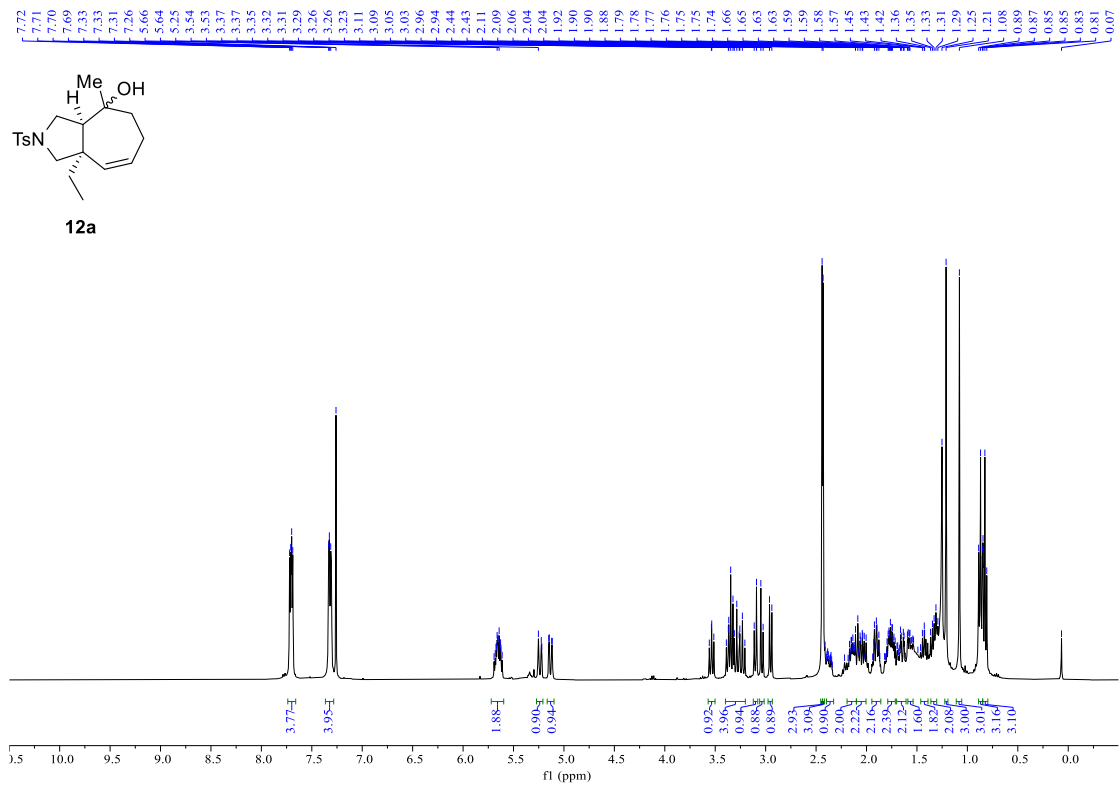
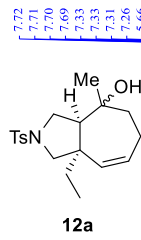
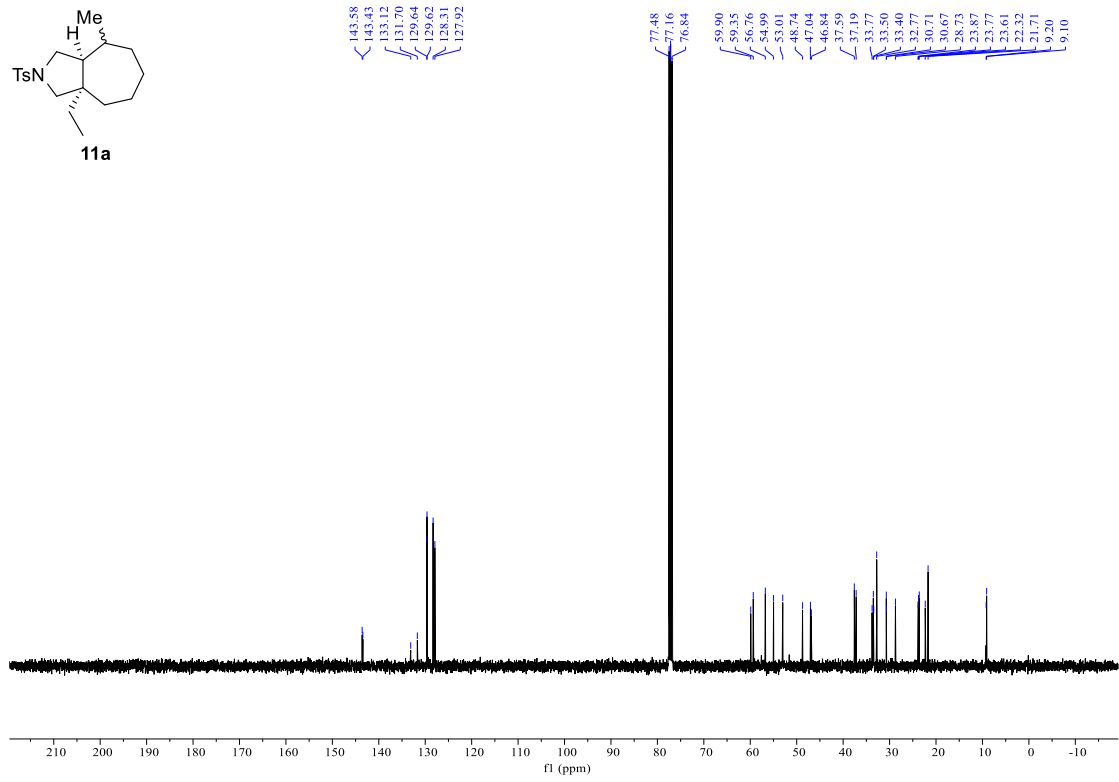
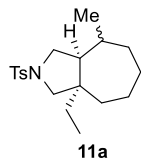


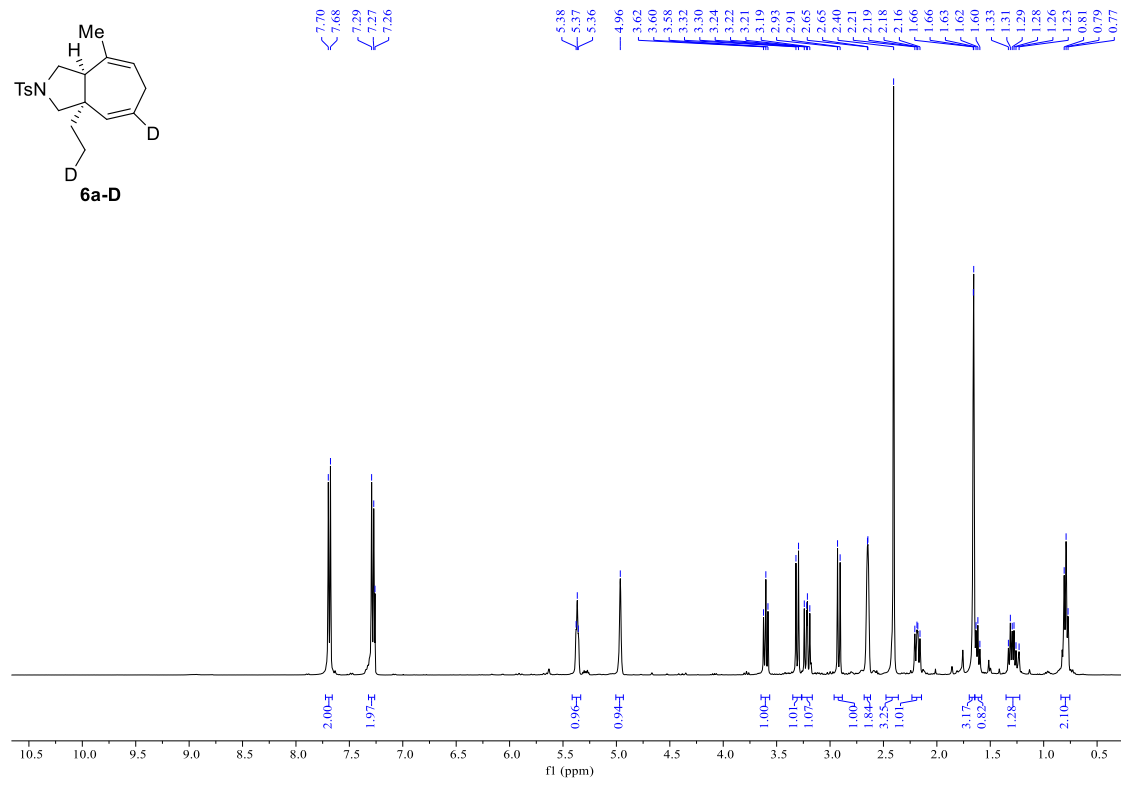
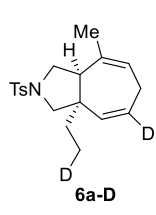
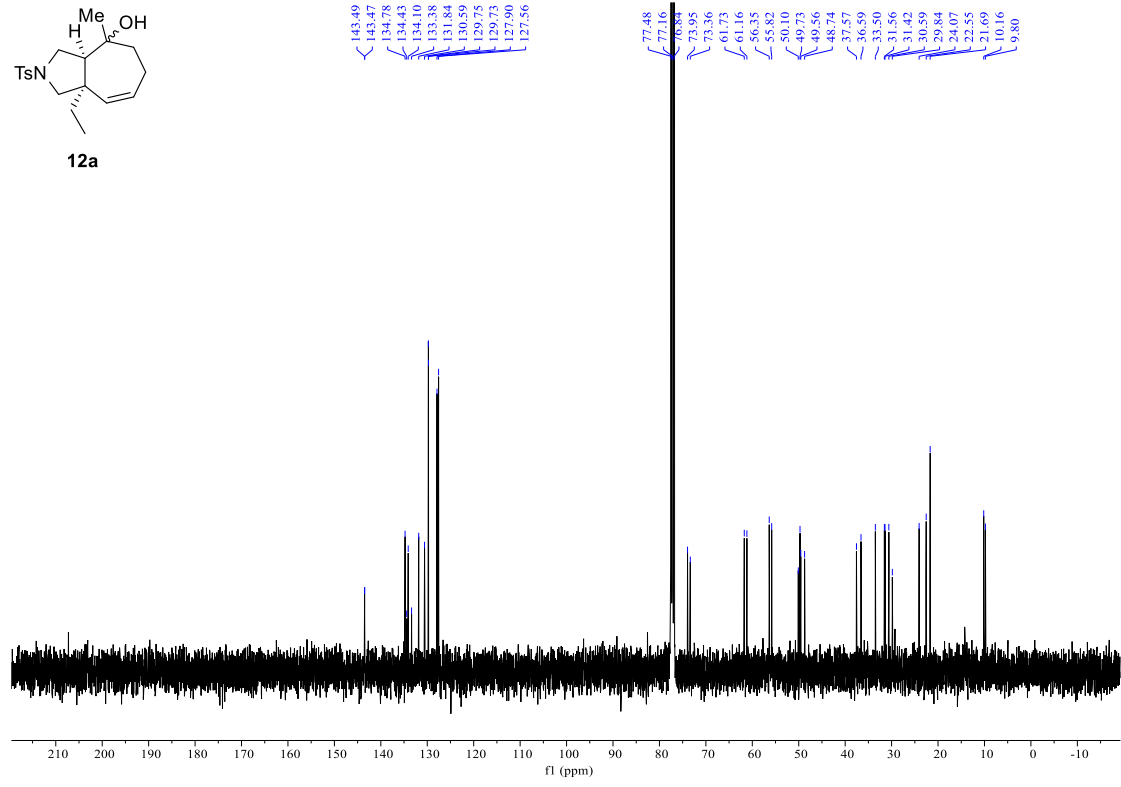
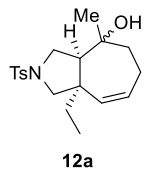


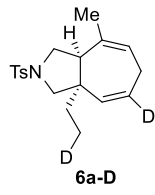




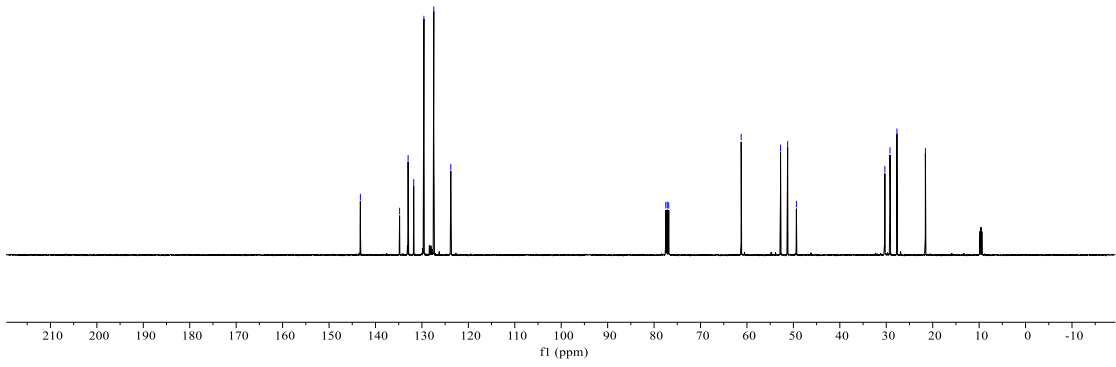




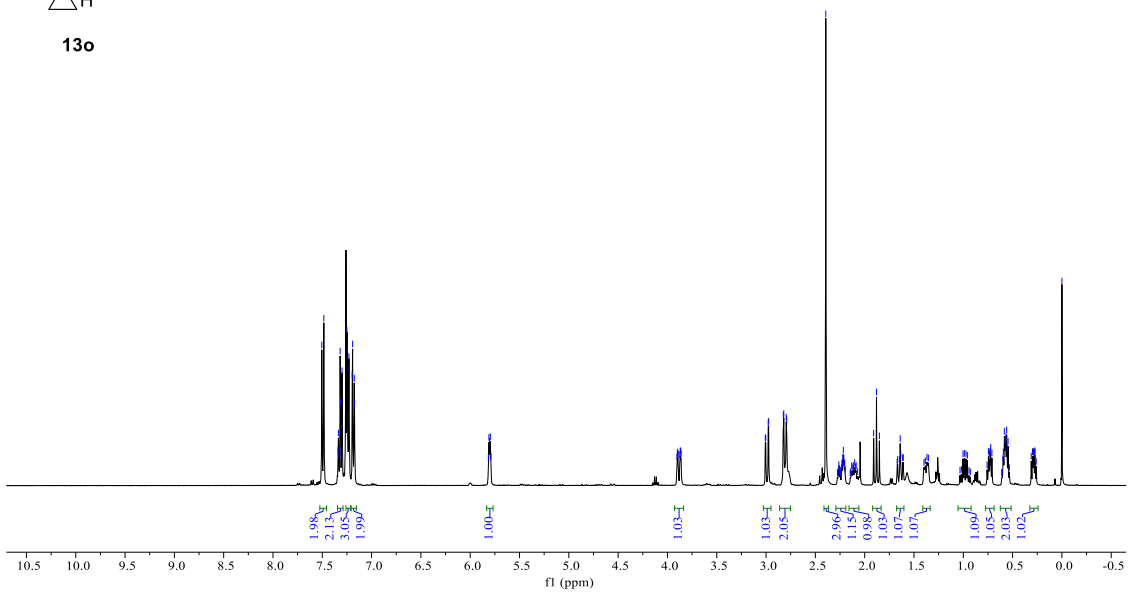
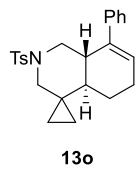


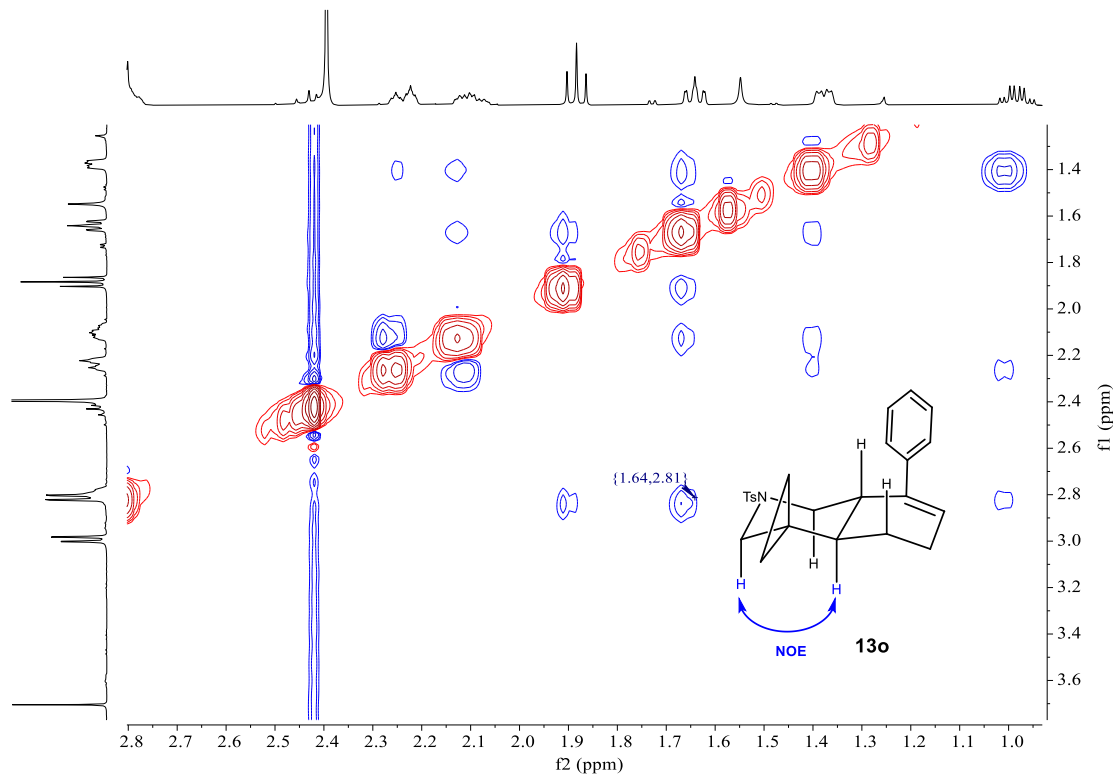
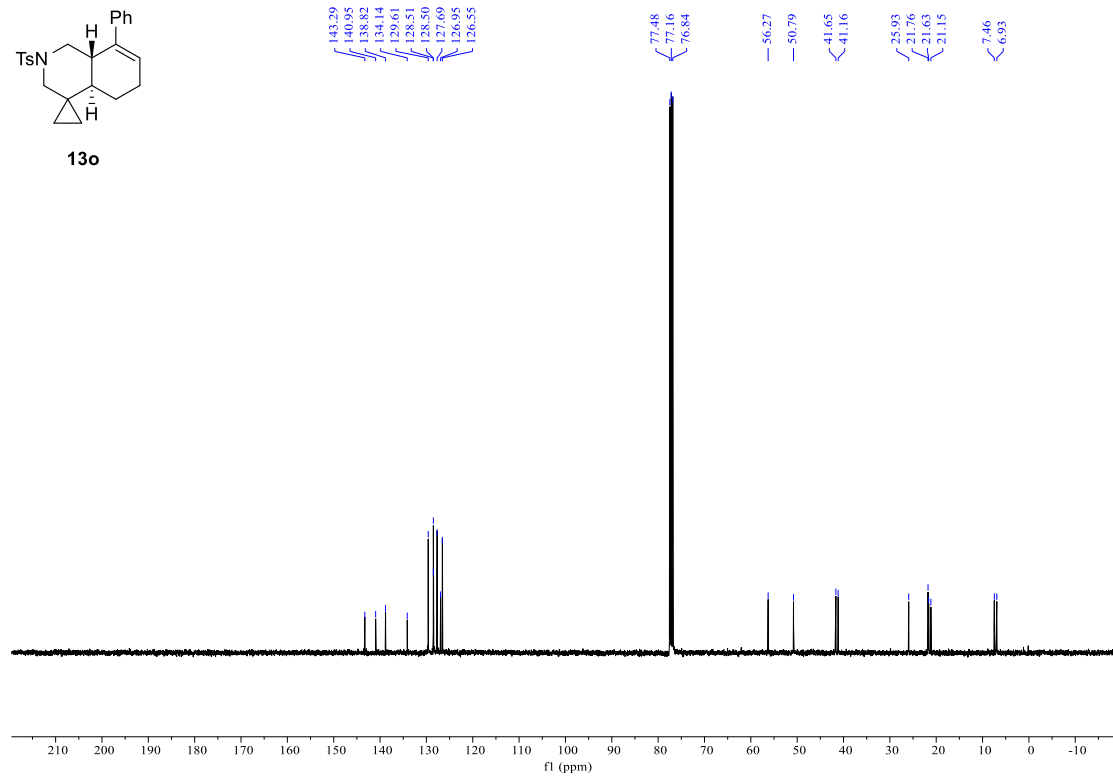
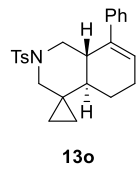


143.25  
 134.81  
 132.97  
 131.76  
 129.57  
 127.44  
 123.77  
 77.48  
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 61.24  
 52.77  
 51.24  
 49.35  
 30.30  
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 27.70  
 21.58

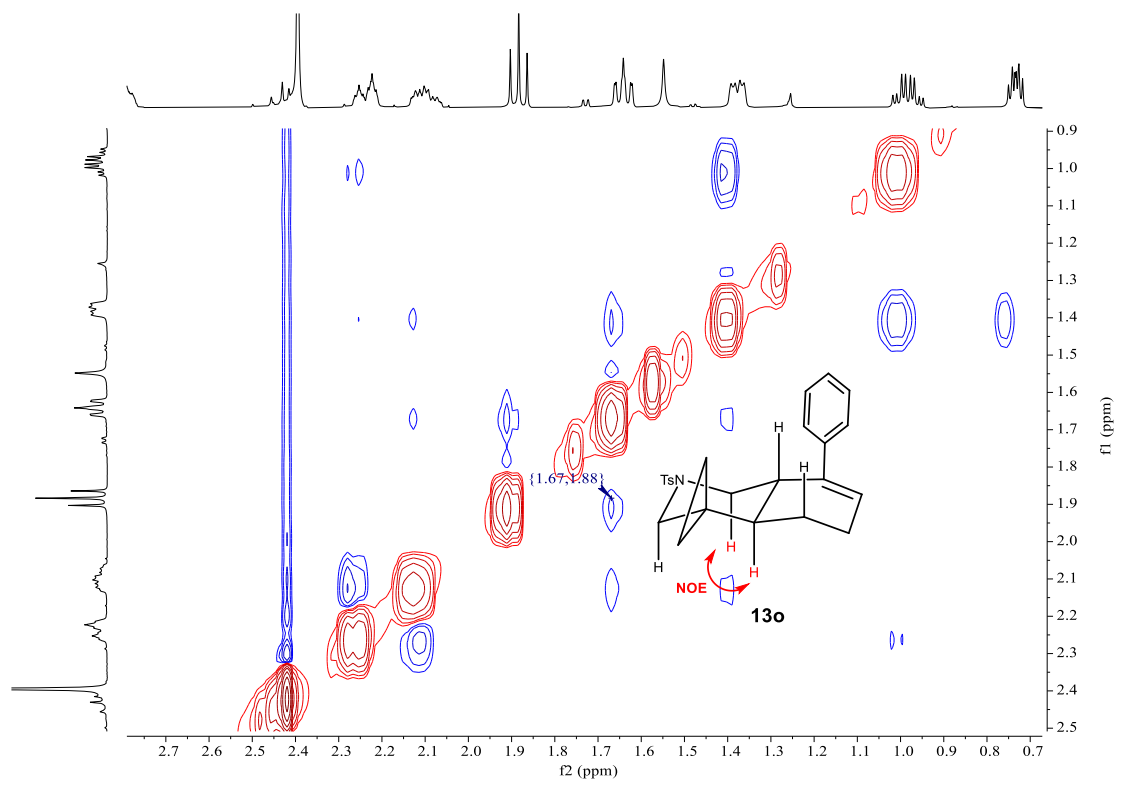
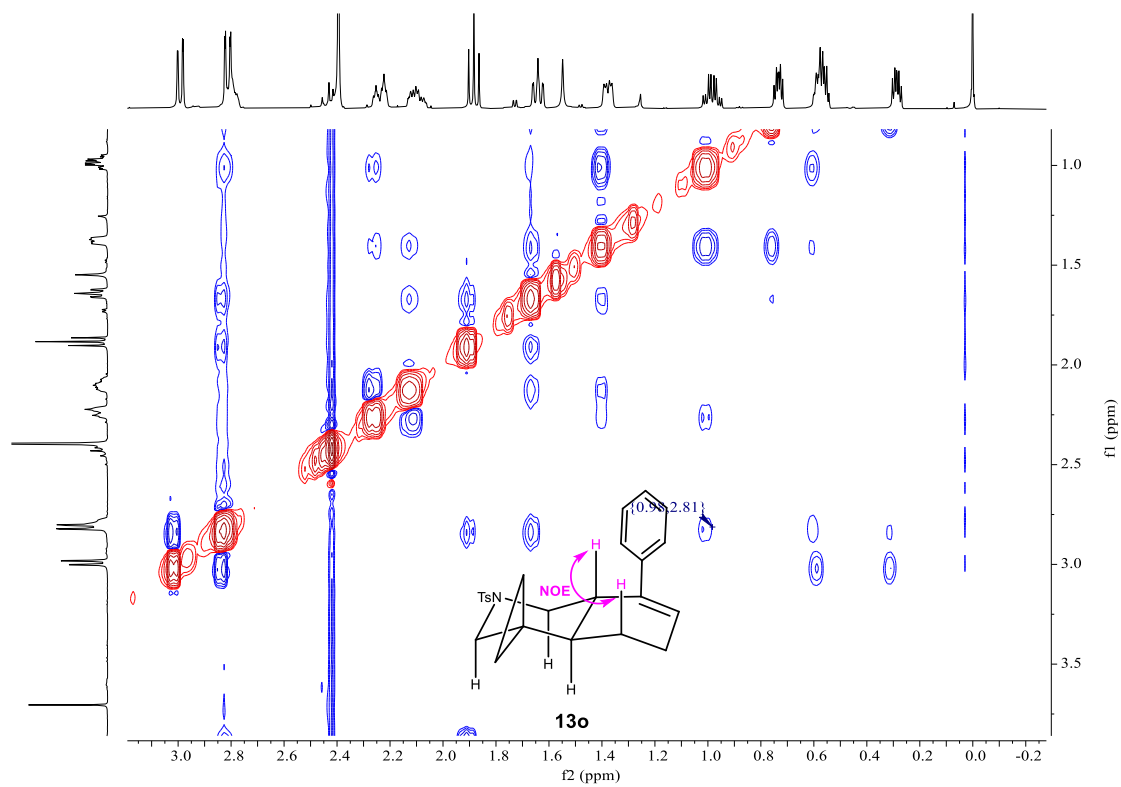


7.51  
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 7.34  
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 7.32  
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 7.30  
 7.30  
 7.25  
 7.25  
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 7.17  
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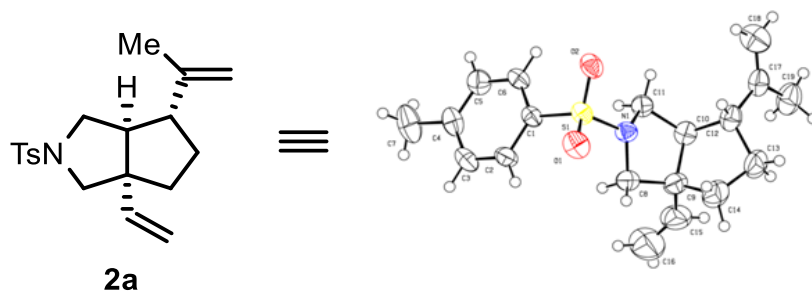






## 7. X-ray Data

### 7.1 X-ray Data of 2a



**2a**

CCDC: 1885512

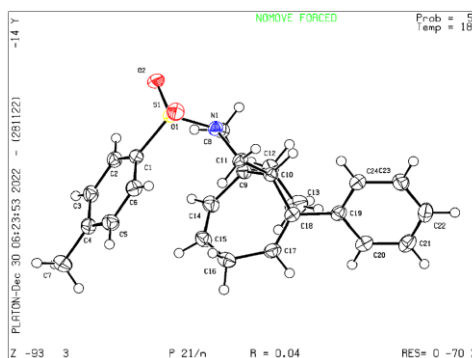
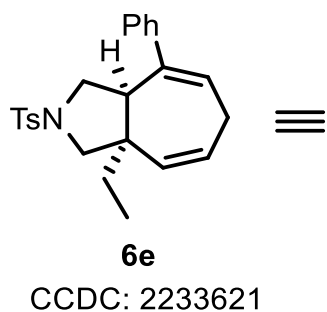
#### Crystal data

Chemical formula	C <sub>19</sub> H <sub>25</sub> NO <sub>2</sub> S
<i>M<sub>r</sub></i>	331.46
Crystal system, space group	Monoclinic, <i>Pn</i>
Temperature (K)	180
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.9893 (4), 6.3967 (2), 14.6868 (6)
β (°)	99.794 (4)
<i>V</i> (Å <sup>3</sup> )	924.79 (6)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.18
Crystal size (mm)	0.3 × 0.2 × 0.1

#### Refinement

$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.046, 0.124, 1.05
No. of reflections	2970
No. of parameters	210
No. of restraints	2
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.61, -0.26

## 7.2 X-ray Data of 6e



### Crystal data

Chemical formula	C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub> S
<i>M<sub>r</sub></i>	393.52
Crystal system, space group	Monoclinic, <i>P2<sub>1</sub>/n</i>
Temperature (K)	180
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.3221 (4), 9.4498 (3), 19.2347 (7)
β (°)	98.062 (3)
<i>V</i> (Å <sup>3</sup> )	2037.61 (12)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.18
Crystal size (mm)	0.24 × 0.11 × 0.10

### Refinement

<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.040, 0.107, 1.04
No. of reflections	5325
No. of parameters	255
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.36, -0.40

## 8. Data S2 (Cartesian Coordinates for the Stationary Points)

<b>4i</b>			C	-2.69726100	0.57063600	1.23428100	
H	-2.32530200	1.84914800	-0.04363400	C	2.79388200	-0.92575800	0.17186200
C	-3.14059300	1.13940400	-0.19558300	H	-1.43804300	1.20880100	-2.02958300
C	-4.34321400	1.58106500	-0.57426700	H	-0.30505400	3.19851400	-1.44193800
H	-4.53235000	2.64327400	-0.71909500	H	0.27889900	2.35843600	1.30106100
H	-5.17904000	0.90637300	-0.75499000	H	1.26632000	3.45615800	0.34266700
C	-3.82854200	-1.37238600	0.24040200	H	2.92450300	1.73906100	0.01730900
C	-3.03613900	-0.88283100	1.46032000	H	-0.69041300	-2.24348200	1.43770500
C	-1.45191900	-0.70988400	-0.59543200	H	1.05435600	-2.43100300	1.17865900
H	-3.61354800	-2.36689900	-0.14792000	H	0.41592900	-1.04080900	-2.01504800
H	-4.87347500	-1.08033200	0.16637300	H	-1.27534900	-1.62256900	-2.00672900
H	-3.55368000	-0.24734400	2.17579700	H	-2.93326500	-0.22404300	-0.76419700
H	-2.27801200	-1.53675300	1.88872100	H	-2.38379000	-1.41756300	0.40262700
H	-1.26614700	-1.78431500	-0.40697900	H	-3.76415800	0.43826600	1.45606500
H	-1.51410800	-0.56986000	-1.69128000	H	-2.14309900	0.37439800	2.16141000
C	0.82666700	-0.19116300	-0.69064300	H	-2.53321900	1.61935300	0.95322100
H	0.75036200	0.02464700	-1.77546800	H	3.69678400	-0.42744200	-0.19993500
H	1.08828000	-1.25925200	-0.59286600	H	3.05564100	-1.43654300	1.11070500
C	-2.75909000	-0.28775900	0.06090900	H	2.50134300	-1.70487900	-0.54667800
O	-0.40658500	0.06309100	-0.06966500				
C	1.86181200	0.70447000	-0.04960200	CO			
H	1.45887000	1.66442000	0.27596200	C	0.00000000	0.00000000	-0.64736900
C	3.17520000	0.45363200	0.12478100	O	0.00000000	0.00000000	0.48552700
C	3.80075000	-0.81578600	-0.30021000				
H	3.14252300	-1.56381500	-0.74165500	[Rh(CO) <sub>2</sub> Cl] <sub>2</sub>			
C	5.10574100	-1.10937200	-0.18711900	Rh	-1.64348300	0.00001500	0.09233000
H	5.82523300	-0.41093200	0.23580600	Rh	1.64350100	0.00000300	0.09217500
H	5.49335500	-2.07022400	-0.51888700	Cl	0.00000300	1.66392500	0.82400300
C	4.07273500	1.49406100	0.77173100	Cl	0.00007300	-1.66377700	0.82427500
H	4.55125600	1.09020300	1.67527300	C	-2.84138000	1.38477100	-0.46541900
H	4.87702500	1.80086300	0.08763500	C	-2.84111900	-1.38501400	-0.46532200
H	3.50098300	2.38536700	1.05280500	C	2.84110300	1.38492800	-0.46580400
				C	2.84130200	-1.38485900	-0.46551300
<b>6i</b>				O	-3.52708200	-2.23368300	-0.78571300
C	0.25912900	-0.41097700	0.70676300	O	-3.52757800	2.23323300	-0.78585300
C	-0.80138200	-0.14485700	-0.42408400	O	3.52703400	2.23354800	-0.78639000
C	-0.78639200	1.18792000	-1.15076000	O	3.52743600	-2.23338000	-0.78593000
C	-0.15312500	2.31758300	-0.81694800				
C	0.82399300	2.45356700	0.34741400	<b>IN1</b>			
C	1.91599400	1.39814000	0.25544400	H	-1.09638600	-2.32213100	0.10889300
C	1.67562200	0.08418600	0.36929600	C	-1.32007300	-1.36744400	0.58907400
C	0.15019200	-1.94997400	0.79048500	C	-0.71470300	-1.09169200	1.78965900
O	-0.07334200	-2.40441500	-0.53400700	H	-0.01445200	-1.79987400	2.22550500
C	-0.43271100	-1.31948300	-1.36897300	H	-1.03124700	-0.24323500	2.38794100
H	-0.05696500	0.04762600	1.65329600	C	-2.67792500	-0.68147700	-1.52176300
C	-2.26188900	-0.37047600	0.09545900	C	-3.61256400	-1.46500400	-0.60489600

C	-2.95444500	0.64519800	0.74896900	H	-0.65288500	-2.93326800	-0.12592200
H	-3.07166300	0.20490200	-2.01898200	H	-0.02305700	-1.96606700	-1.48384100
H	-1.94646100	-1.23811400	-2.10643100	O	-1.10172700	-0.91647400	-0.06537000
H	-3.50968000	-2.54765700	-0.56181000	C	-2.30978800	-0.94861900	-0.79747800
H	-4.63227100	-1.10360300	-0.47397900	H	-2.07534700	-0.97310400	-1.87818400
C	-1.33019700	2.27843000	0.09054800	H	-2.86993500	-1.86650600	-0.55878400
C	-2.47074200	-0.60552700	0.00274700	C	-3.07759500	0.30867800	-0.47553200
O	-1.97402000	1.57194900	1.12415700	H	-2.47607200	1.21318300	-0.57485300
C	-0.28081200	1.50169900	-0.73407000	C	-4.37344900	0.42719300	-0.11869500
C	1.15305300	1.82343700	-0.73252900	C	-5.27460500	-0.73337600	0.04269400
C	1.83885700	1.71719100	0.51732700	H	-4.83924100	-1.72218800	-0.09593000
H	2.92801500	1.69570600	0.50138600	C	-6.57957300	-0.65747900	0.34722200
C	1.11719100	1.29381200	1.68823100	H	-7.09191300	0.29110500	0.49466800
H	0.17384200	1.74856100	1.97385600	H	-7.18102000	-1.55754100	0.45557500
H	1.72609800	0.93474500	2.51700000	C	-4.96181000	1.80483500	0.13488100
C	1.92338900	2.07430700	-2.01339100	H	-5.35457500	1.87627300	1.15893800
H	2.97061100	1.76099000	-1.92560600	H	-5.79707600	2.00758000	-0.55030600
H	1.90266300	3.14876200	-2.24816200	H	-4.20701200	2.58660400	-0.00314100
H	1.46374900	1.54588400	-2.85745100				
Rh	0.72865400	-0.14935100	0.14592100	<b>IN2</b>			
H	-0.64614800	1.29155400	-1.74329000	C	0.34674600	-0.64497600	0.24310000
H	-3.42324600	0.33283900	1.69193600	C	-4.24090500	-0.22889700	-0.67445500
H	-3.73022000	1.13686700	0.13277500	C	-3.08860500	0.53612000	-0.06920600
H	-2.09312400	2.67391200	-0.60341100	C	-0.80580000	0.32385600	0.40309400
H	-0.86161900	3.13771600	0.58349200	C	0.61161200	-1.19754900	-1.17558300
Cl	2.40018200	-1.77493500	0.96715300	C	2.09891400	-0.93666000	-1.46732700
C	0.85026700	-1.25618100	-1.50922300	C	-5.54640300	-0.16636400	-0.34161200
O	0.99542400	-1.90490100	-2.43113700	Rh	2.53963200	0.01201400	0.28041200
				H	-0.03608800	-0.66818500	-1.88156500
<b>TS1</b>				H	0.35191200	-2.26483900	-1.21282000
Rh	1.95376200	0.33726200	0.15211200	H	2.70750900	-1.83329000	-1.61755100
Cl	2.02868200	1.44914400	-1.98650400	H	2.26833300	-0.20933900	-2.26582600
O	0.94031900	3.06797700	1.29911600	H	-3.31348800	0.89798900	0.94771600
C	1.33194400	2.07548600	0.91075500	H	-2.85418700	1.42490400	-0.68749000
C	2.72156600	-1.42726000	-0.79038000	H	-0.90301500	0.64125000	1.45725300
C	2.20095000	-2.69563000	-0.11322500	H	-0.60169500	1.22554500	-0.20211100
C	1.08557100	-1.80833400	0.34577600	C	0.99340200	-1.19683400	1.35343700
C	1.14301800	-1.00970400	1.54214800	C	2.25197200	-1.89784800	1.21118300
C	2.41556600	-0.57289900	2.02813300	H	2.34721100	-2.66353800	0.44004700
H	2.46179400	-1.33779800	-1.84499400	H	2.78218200	-2.13840600	2.13281500
H	3.77020600	-1.18052700	-0.57649300	H	-3.93878400	-0.88182400	-1.49466700
H	1.89662200	-3.50547100	-0.78284200	H	0.71029000	-0.82076400	2.33930900
H	2.82624800	-3.07920500	0.69597900	O	-1.97123400	-0.32097000	-0.03991600
H	0.20254300	-0.65912500	1.95811300	C	4.45842600	0.05739500	-0.05536400
H	3.30550300	-1.19055900	1.90694100	O	5.56887000	0.06956000	-0.28944400
H	2.42946500	0.06017600	2.91318900	Cl	2.13455700	2.25439400	-0.51771800
C	-0.22843800	-1.94419400	-0.39839500	C	-6.05150300	0.69314300	0.74934600

H	-5.31058200	1.25797900	1.31421700	C	-2.21388000	0.33423600	-0.27885700
C	-7.34343200	0.82647100	1.08826800	C	0.33288800	1.42524200	1.01114100
H	-8.13961900	0.30144800	0.56413600	C	-0.49276300	2.57408100	0.45021100
H	-7.64236700	1.47570100	1.90844500	C	-2.57350400	1.34029900	0.80097800
C	-6.56487900	-0.99658300	-1.10384600	C	-1.95652000	0.80190900	-1.72414500
H	-7.31647800	-0.35375000	-1.58389800	C	-0.50988700	0.32884800	-2.02705200
H	-7.10103900	-1.67540300	-0.42579300	C	1.62598900	1.12571700	0.61448200
H	-6.07937100	-1.59717400	-1.88088300	H	-2.07200700	1.89005800	-1.78144600

**IN3**

C	-2.29259100	0.24243500	-0.05592100
C	0.33763500	1.60827400	-0.71947800
C	-0.37106600	2.50577300	0.28856000
C	-2.57094400	1.64167200	0.48252800
C	-2.35047100	-0.01888800	-1.57443900
H	-2.38640200	0.95004300	-2.08734800
H	-3.27135900	-0.56189000	-1.83400600
H	0.04778200	3.51972700	0.21257700
H	-0.23800100	2.14632100	1.32132600
H	-3.58996400	1.94429600	0.20270900
H	-2.50048900	1.62778400	1.58312900
C	-2.20116700	-0.80817600	0.86102800
C	-1.66453800	-2.09997200	0.49511300
H	-2.00647300	-2.59990600	-0.40946800
H	-1.41773200	-2.76124100	1.32438400
H	-0.15481400	1.60864600	-1.69150400
H	-2.18965700	-0.54901700	1.91920700
O	-1.73330900	2.63931700	-0.04379800
C	2.49808200	1.36729100	0.50726100
H	1.99367800	1.62889600	1.43326300
C	3.83593400	1.27152600	0.48793100
H	4.41551500	1.47240300	1.38612000
H	4.39704200	0.99611100	-0.40283200
C	2.30453500	0.67237600	-1.96140800
H	2.93866700	-0.20630500	-1.79397400
H	2.95113100	1.47466900	-2.34536200
H	1.56538900	0.43439600	-2.73305300
C	1.63674300	1.14667400	-0.67637100
Rh	-0.16588200	-0.67865600	-0.03577100
C	-1.05200400	-0.79709600	-1.92052400
H	-1.24266600	-1.82495700	-2.24652300
H	-0.46381400	-0.29828100	-2.69855000
C	1.28929500	-1.91995600	-0.37945700
O	2.12219000	-2.66936300	-0.56778500
Cl	0.53583200	-0.41725900	2.37372600

**IN3-cis**

C	-2.21388000	0.33423600	-0.27885700
C	0.33288800	1.42524200	1.01114100
C	-0.49276300	2.57408100	0.45021100
C	-2.57350400	1.34029900	0.80097800
C	-1.95652000	0.80190900	-1.72414500
C	-0.50988700	0.32884800	-2.02705200
C	1.62598900	1.12571700	0.61448200
H	-2.07200700	1.89005800	-1.78144600
H	-2.70304300	0.35690700	-2.39623200
H	-0.45570700	-0.34268800	-2.89083300
H	0.17429600	1.16400100	-2.20395900
H	-0.33010500	2.67503700	-0.63097800
H	-0.12921300	3.50153400	0.91799400
H	-3.63083500	1.62769700	0.70693800
H	-2.43807400	0.86605600	1.78704800
C	-2.28902200	-1.03326100	0.00663600
C	-1.63689400	-1.99200100	-0.86034400
H	-1.75187200	-1.91567600	-1.94109200
H	-1.54978400	-3.00618900	-0.47409100
H	0.00905900	1.02776200	1.97490200
H	-2.50556800	-1.33979400	1.02952500
O	-1.87431800	2.55956200	0.72583400
C	2.25618200	1.78507800	-0.55795500
H	1.60946900	2.35880100	-1.21720300
C	3.56857200	1.74754900	-0.83520900
H	4.28359400	1.21197800	-0.21469400
H	3.96598500	2.27253000	-1.70134000
C	2.54863300	0.35835600	1.55132200
H	3.22759700	1.07692500	2.03398000
H	3.16660200	-0.37149300	1.01405200
H	1.97774800	-0.17489700	2.31486300
Rh	-0.11951200	-0.64015900	-0.21910100
C	1.46013700	-1.57665700	-0.87315600
O	2.36363100	-2.13532200	-1.27506200
Cl	-0.00613000	-1.81068700	2.01515400

**TS2**

C	-1.91036500	-0.20162100	-0.39223700
C	-0.79757300	1.36037800	-0.43530900
C	-1.41374800	2.07283100	0.76789200
C	-3.10279000	0.73383800	-0.08237200
C	-1.79094700	-0.82052700	-1.80188400
H	-2.05697900	-0.06664200	-2.55556200
H	-2.51012200	-1.64540000	-1.90799600
H	-1.43010100	3.15593100	0.57007300
H	-0.85489000	1.87938300	1.68959100
H	-3.37993300	1.27234000	-1.00746400

H	-3.97011800	0.15656200	0.25941200	H	0.83378000	-2.43913600	-1.07951400
C	-1.70982800	-1.17447600	0.72947200	O	3.52044000	0.40200200	-0.43847500
C	-1.27782000	-2.46922600	0.60716600	C	0.04768000	2.56604400	0.57533200
H	-1.25184800	-3.00157800	-0.33854800	H	0.78355000	2.38324600	1.35541300
H	-1.09396300	-3.04515900	1.51150100	C	-0.65256600	3.70764800	0.64188500
H	-1.28664400	1.64989500	-1.36813500	H	-1.40723000	3.97967400	-0.09223800
H	-1.81893400	-0.75890000	1.73106000	H	-0.48722500	4.40852100	1.45772300
O	-2.73974600	1.59912700	0.94807800	C	-0.93760000	1.96215900	-1.68475400
C	1.56476800	2.04763800	0.31362200	H	-0.51425300	2.89197000	-2.09476300
H	1.26935300	1.99555300	1.35686400	H	-1.97055600	2.16956700	-1.38036100
C	2.68957000	2.70705400	-0.00192400	H	-0.96796100	1.19725000	-2.46191700
H	3.27169000	3.19316900	0.77820600	Rh	-0.64818500	-0.43139300	0.21676800
H	3.07769400	2.78017200	-1.01537000	C	-2.44986000	-0.08588900	0.75656400
C	1.09067400	1.56567700	-2.13092400	O	-3.51867200	0.12485700	1.08090400
H	2.06580000	1.12002500	-2.36047500	Cl	-1.44006700	-1.24480700	-2.04070200
H	1.16316000	2.64738700	-2.31615800				
H	0.35536300	1.15791000	-2.82908500	<b>IN4</b>			
C	0.69028100	1.32420000	-0.66837800	C	1.88292400	-0.82748700	0.44491700
Rh	0.35592400	-0.66961400	-0.04437700	C	1.94676300	0.73658200	0.47822100
C	2.12374600	-1.37942900	-0.20890600	C	3.25814700	1.04990600	-0.31706200
O	3.17902200	-1.79069100	-0.30302500	C	3.38111200	-1.15556400	0.24949100
Cl	0.81440200	-0.26889100	2.40378600	C	1.17297000	-1.38456000	1.68850700
C	-0.30839200	-1.27902100	-1.93049300	H	1.73523100	-1.09306800	2.58757000
H	-0.21533700	-2.36486800	-2.04666300	H	1.18243300	-2.48270400	1.65479700
H	0.20473100	-0.81338300	-2.77344200	H	3.96617800	1.61244100	0.31229400
				H	3.08730100	1.62466100	-1.23544300
<b>TS2-cis</b>				H	3.91684300	-1.05716900	1.21232800
C	1.63049600	-0.89511000	0.25738500	H	3.57519100	-2.15115100	-0.16523000
C	1.13363400	0.72938900	-0.82547700	C	1.11116400	-1.23327100	-0.80276800
C	2.51637200	1.36655300	-0.62698200	C	0.09348600	-2.13839400	-0.87934800
C	2.98942000	-0.88662300	-0.45585500	H	-0.25449400	-2.72799800	-0.03637000
C	1.64267100	-0.44853700	1.73807000	H	-0.35432000	-2.37992000	-1.84051200
C	0.17298100	-0.11419200	2.10714400	H	2.10772100	1.02154900	1.52701000
C	-0.08770900	1.51578900	-0.48481600	H	1.48934600	-0.82957600	-1.73972700
H	2.30544700	0.41899500	1.84173100	O	3.82261800	-0.19715600	-0.68388300
H	2.07902100	-1.25347300	2.34958100	C	0.35268000	1.52591700	-1.42317300
H	-0.24750000	-0.80720300	2.84443900	H	1.07669300	1.11462800	-2.12620400
H	0.04897800	0.89504600	2.50153800	C	-0.84285800	1.92640000	-1.94776100
H	2.53241500	2.06390800	0.21747800	H	-1.03220700	1.85133700	-3.01590700
H	2.72165400	1.94177600	-1.54370900	H	-1.60151600	2.43540800	-1.35625800
H	3.68248600	-1.53732400	0.09444200	C	0.27416000	2.61768600	0.89115800
H	2.88376000	-1.27706100	-1.48236000	H	-0.63476400	3.12667800	0.54884400
C	0.83830000	-2.11865400	-0.03730900	H	1.09536700	3.35073700	0.84917300
C	-0.01987000	-2.75597700	0.82688100	H	0.13632500	2.33655600	1.94429000
H	0.00136400	-2.60811800	1.90145300	C	0.61534000	1.38641300	0.03345300
H	-0.62381000	-3.57648500	0.44582000	Rh	-0.88489500	-0.10328200	-0.10543000
H	1.03769400	0.25278000	-1.80525300	C	-2.22619800	0.92622300	0.82535000

O	-3.03305000	1.47560800	1.40299900	O	-3.75873900	-0.82882400	1.08441800
Cl	-2.88097500	-1.47496300	-0.62755000	C	-2.95752800	-1.79090000	0.45401500
C	-0.29356100	-0.85595800	1.75854100	C	-0.78159200	-0.79625400	1.12579400
H	-1.00180300	-1.64533700	2.03626500	C	-0.37845100	0.37020300	1.71302900
H	-0.36599900	-0.05595800	2.50565200	H	-2.94332900	-0.09702900	-1.52718100
<b>IN4-cis</b>				C	-0.91659000	-1.88968600	-1.10902400
C	1.85320200	-0.67692300	-0.50837000	C	0.57909000	-2.01067400	-0.72607400
C	2.03208100	0.82187900	-0.11415200	Rh	1.32904800	-0.28132500	0.20447900
C	3.37370300	0.78401400	0.63503000	C	0.70466600	0.76531100	-1.47301200
C	3.30245100	-0.90481400	-1.00158200	C	-0.41881500	1.73179500	-1.25630500
C	1.55982300	-1.65805500	0.66963700	C	-1.71954000	1.54226500	-0.95226400
C	0.09531400	-1.64543200	1.19604500	C	-2.65750300	2.74469100	-1.00186300
C	0.73247100	1.45004300	0.40060700	Cl	2.51022300	1.50124100	1.41431700
H	2.27821200	-1.45936000	1.47540400	H	-4.47280600	0.80675200	0.04312000
H	1.80802300	-2.66523400	0.30415800	H	-3.21256700	1.13256300	1.26143800
H	-0.38105700	-2.61281700	0.99434000	H	-2.71587000	-2.58116800	1.17711300
H	0.05340300	-1.50762200	2.28267300	H	-3.48298700	-2.25249600	-0.40160700
H	3.25844900	0.51037500	1.69533700	H	-0.51299100	-1.71808000	1.65017400
H	3.92306100	1.73253200	0.57903900	H	0.16701600	0.34464200	2.65414900
H	3.60225400	-1.95939100	-1.01124500	H	-0.65965700	1.35330400	1.35306800
H	3.45592000	-0.48354900	-2.00949200	H	-1.02245900	-1.42428200	-2.09727500
C	0.70156500	-0.65900400	-1.51237100	H	-1.36608300	-2.89169400	-1.19914500
C	-0.28372400	-1.59218600	-1.67980100	H	0.72576300	-2.82687500	0.00014900
H	-0.26334300	-2.55889000	-1.18301400	H	1.16068200	-2.28265200	-1.61768000
H	-1.03157400	-1.44116000	-2.45582800	H	1.58257500	1.33237000	-1.79842100
H	2.24343800	1.33937600	-1.06190300	H	0.46919500	0.01527100	-2.23334400
H	0.66531200	0.20960000	-2.17389700	H	-0.12466500	2.77193700	-1.41296800
O	4.11029500	-0.22737000	-0.04490500	H	-3.49840200	2.54925100	-1.68511100
C	0.17967000	1.06479100	1.63953200	H	-2.13307500	3.63807700	-1.35754600
H	0.76432100	0.41765000	2.28913400	H	-3.09254400	2.97545700	-0.01913700
C	-1.23739900	1.13894400	1.87342200	C	3.00755600	-0.54684800	-0.71074300
H	-1.82723200	1.95690900	1.46220200	O	3.99749100	-0.69373100	-1.24238900
H	-1.61225100	0.70411100	2.79883300	<b>IN5-cis</b>			
C	0.34683900	2.75561100	-0.27731000	C	2.23431200	0.15531700	-0.65585800
H	1.13660400	3.49010300	-0.04782100	C	1.50035600	-0.93182800	0.23540000
H	-0.61384900	3.14176400	0.07026800	C	0.91839400	-0.41427400	1.59151800
H	0.28164600	2.64761300	-1.36527000	C	-0.41055000	0.36986300	1.48720800
Rh	-0.94939600	-0.14976600	0.17037300	C	-0.29990700	1.60671900	-1.25490100
C	-2.62949700	-1.16111200	0.30129000	C	0.84500100	2.20998800	-0.49242400
O	-3.62504100	-1.69911200	0.38672300	C	2.00583000	1.59532300	-0.19684500
Cl	-2.29762200	1.31663300	-1.33977100	C	3.71403700	-0.33690000	-0.61522800
<b>IN5</b>				O	3.82839500	-1.13598100	0.53749500
C	-2.43026200	0.23380700	-0.60653100	C	2.67630900	-1.92875000	0.52864400
C	-1.70280500	-1.03806200	-0.06682200	C	0.33762400	-1.65115400	-0.40738500
C	-3.53802100	0.42995500	0.48130200	C	-0.17871800	-1.52097600	-1.65977800
				H	1.87420200	0.07132500	-1.68781800



C	3.07716700	2.28044500	0.63341300	H	3.18502100	3.43165900	0.95393600
H	0.73765000	-1.30612400	2.20702200	H	4.27682900	2.15169800	0.38795800
H	1.67999700	0.18475800	2.10823100	C	-2.42307600	-1.56037100	0.15150200
H	-0.24805400	1.44438800	1.58470200	O	-3.07517100	-2.45392700	0.40398100
H	-1.12228300	0.02054100	2.24423600	Rh	-1.34760700	0.02191900	-0.27158700
H	0.05663500	1.14969900	-2.18924000	Cl	-3.35469800	1.33870600	0.12775300
H	-1.00035700	2.40051100	-1.54657600	C	0.53717500	-1.25779100	1.57678600
H	0.69367300	3.21984900	-0.10145700	H	1.16508900	-1.22276400	2.48276700
H	3.92532700	-0.94561000	-1.51249400	H	0.05989900	-2.25038300	1.55421000
H	4.45708300	0.46194100	-0.55568100	C	-0.53398400	-0.16014200	1.60415900
H	2.58530100	-2.43279900	1.49661900	H	-1.34120600	-0.35598600	2.31850800
H	2.73679700	-2.68870400	-0.27282400	H	-0.10367800	0.82592100	1.80844800
H	-0.15392900	-2.38133600	0.24130600				
H	-1.00637900	-2.16515000	-1.95741500	<b>TS3-cis</b>			
H	0.27696400	-0.90259500	-2.42730200	C	-2.46693900	0.19452000	0.27216000
H	2.67891900	3.18332300	1.11195500	C	-1.44005000	-0.98406800	0.19675800
H	3.46471900	1.61124100	1.41650300	C	-0.82470200	-1.19398900	-1.21502500
H	3.94120200	2.58452700	0.02281100	C	0.33184100	-0.22275100	-1.46860500
Rh	-1.39130000	0.04642000	-0.30735300	C	0.36491600	1.97207700	0.64034500
C	-2.65964500	1.34822400	0.31782600	C	-0.98568100	2.31649000	0.05319400
O	-3.40768000	2.11050400	0.69707100	C	-2.13343900	1.63570900	-0.14567500
Cl	-2.87623300	-1.76981600	0.39424700	C	-3.66827800	-0.45076700	-0.47255500
				O	-3.61151300	-1.83328700	-0.18256900
<b>TS3</b>				C	-2.42375800	-2.13303800	0.51754500
C	2.44237700	0.06944800	0.43028100	C	-0.28307800	-0.88381500	1.19589200
C	1.39424500	-1.08583400	0.30512900	C	-0.12900200	0.32939700	1.93295500
C	3.53409100	-0.37033200	-0.60385600	H	-2.78397500	0.24597000	1.32897600
O	3.33807300	-1.74856500	-0.84312700	C	-3.32351300	2.40100400	-0.72173700
C	2.39331300	-2.24460500	0.07476300	H	-0.44540100	-2.22660300	-1.25299100
C	0.42164800	-0.98848400	-0.87947500	H	-1.58686600	-1.11383600	-2.00518300
C	0.44186400	0.14570700	-1.73936900	H	-0.00944700	0.78989200	-1.69805800
H	2.88628700	-0.10226300	1.42447700	H	1.00515200	-0.56410200	-2.26259000
C	-0.19689000	1.90482100	-0.69232400	H	0.53918300	2.52888900	1.56955000
C	1.11274400	2.28562400	-0.04827200	H	1.14842200	2.33495000	-0.04427300
C	2.17146700	1.57939300	0.39402800	H	-1.00754900	3.35871100	-0.28148400
C	3.36137900	2.35046800	0.96541900	H	-4.63252200	-0.04798500	-0.13597900
H	4.54687500	-0.19141300	-0.21248500	H	-3.59685600	-0.30263100	-1.56140300
H	3.43802200	0.17016700	-1.55686400	H	-2.05737100	-3.11342100	0.18513400
H	1.92591500	-3.13690200	-0.35989200	H	-2.61436900	-2.18171000	1.60460400
H	2.87257700	-2.53118300	1.02905600	H	0.05102600	-1.81319300	1.66163900
H	0.11020600	-1.93977100	-1.31583000	H	0.60013900	0.34628200	2.74890100
H	-0.15799400	0.09671600	-2.65307900	H	-0.96244900	1.00631900	2.08611600
H	1.31286000	0.78607000	-1.82430100	H	-3.06376700	3.44719900	-0.91652600
H	-1.01930100	2.34138700	-0.10110900	H	-3.67450300	1.95854900	-1.66429000
H	-0.29237300	2.37953600	-1.67745900	H	-4.17447500	2.38673700	-0.02401300
H	1.19923300	3.37054100	0.06947400	Rh	1.40913700	0.00283600	0.25868100
H	3.56658600	2.04514000	2.00231500	C	2.34617600	-1.65575700	-0.19491000

O	2.90866900	-2.60090000	-0.47312700	C	2.39465700	1.50023200	-0.39753700
Cl	3.37001500	1.19739900	-0.54560200	C	3.75752200	-0.72833700	-0.43543300
				O	3.45336700	-2.04817100	-0.06744200
<b>TS3-RE</b>				C	2.51362500	-1.91570900	0.96056400
C	2.38787400	0.12755600	0.71286900	C	0.25630600	-1.49029400	-0.08314900
C	1.75178600	-0.96620500	-0.23416600	C	-0.20042300	-1.43887500	-1.39665800
C	3.67613800	0.55711100	-0.08131200	H	2.00603200	-0.24685300	-1.55916800
O	3.78820100	-0.28675900	-1.20643700	C	3.72632900	2.20731400	-0.21063600
C	3.05123400	-1.44150200	-0.94257100	H	0.78504300	-0.68410100	2.51989600
C	0.78307500	-0.45503000	-1.29581400	H	1.85197300	0.65059700	2.07577600
C	0.44103100	0.83913300	-1.58668400	H	-0.10987700	1.93069600	1.61254200
H	2.72652200	-0.43974200	1.59644100	H	-1.09355900	0.53583400	2.03205500
C	1.06504900	-2.17256100	0.46422100	H	-0.28231300	1.28678900	-1.62358600
C	-0.44633600	-1.93185800	0.60104200	H	-0.87456100	2.49045600	-0.44678400
Rh	-1.28829500	-0.14650900	-0.26166600	H	1.31999300	3.28715300	-0.27419300
C	0.28204400	1.11667700	1.67500300	H	4.31952100	-0.74878100	-1.37506500
C	1.54375600	1.29879900	1.23685800	H	4.38152600	-0.25424400	0.34191600
C	2.15912400	2.68916900	1.26817800	H	-0.13091000	-2.28977900	0.55340500
H	4.56690800	0.46065200	0.56016900	H	-0.87814700	-2.20449900	-1.76820500
H	3.63374700	1.58497100	-0.45272300	H	0.31067200	-0.87472900	-2.17172500
H	2.86206500	-1.96428300	-1.88830400	H	3.59177700	3.29492200	-0.23097900
H	3.59566600	-2.12699900	-0.26453900	H	4.19605600	1.94460800	0.74904900
H	0.49191100	-1.22034600	-2.02174900	H	4.44254200	1.93719200	-1.00069600
H	-0.04905600	1.06323900	-2.53160100	Rh	-1.41336900	-0.04599400	-0.18982700
H	0.81446100	1.68357500	-1.01894200	Cl	-3.22178800	1.48380800	0.28906200
H	1.53916800	-2.36001400	1.43742200	C	-2.89392100	-1.36962700	-0.15585700
H	1.23290600	-3.07909300	-0.13972600	O	-3.76922100	-2.08674900	-0.05136900
H	-0.98006400	-2.29742500	-0.31048100	H	3.00832200	-1.58338800	1.89287600
H	-0.92978400	-2.42939300	1.44326900	H	2.04692300	-2.89102400	1.13843200
H	-0.30163500	1.98586700	1.98270200				
H	3.14750100	2.68153700	1.75123500	<b>TS4</b>			
H	1.51561900	3.37789300	1.82720400	C	-1.88787600	-0.71656500	-0.61918700
H	2.30254800	3.11157000	0.26129600	C	-2.22786700	0.59320300	0.14872500
C	-0.39193100	-0.20582200	1.80711600	C	-2.89157700	0.02744800	1.42067700
H	0.27706400	-0.90263100	2.31413000	C	-3.20838900	-1.47025200	-0.36316700
H	-1.34823400	-0.16738500	2.32885100	C	-1.45873300	-0.25702600	-2.01970400
Cl	-3.39331200	-0.65596800	0.75342800	H	-2.28741200	0.29275000	-2.48752800
C	-2.32470300	1.25696900	-1.17843300	H	-1.22373700	-1.10562100	-2.67357300
O	-2.95152000	2.10022900	-1.61678800	H	-3.64214200	0.70834600	1.84225100
				H	-2.15973100	-0.21136000	2.20644700
				H	-3.99990000	-1.10957900	-1.04181900
<b>TS3-RE-cis</b>				H	-3.12718300	-2.55918600	-0.45823100
C	2.37735200	-0.01754800	-0.55379900	C	-0.74715000	-1.48115100	0.06730100
C	1.50084400	-0.81118200	0.49550200	C	0.29977700	-2.08120500	-0.60422600
C	1.02832200	0.02406800	1.71254600	H	0.43062500	-2.01806100	-1.67998200
C	-0.23259900	0.86417900	1.43140300	H	0.93905000	-2.80081600	-0.09769300
C	-0.14533600	1.69336600	-0.59859200	H	-3.01971600	1.08936900	-0.43021200
C	1.25195200	2.20633300	-0.41616800				

H	-0.93234500	-1.77183300	1.10115100	H	-1.02391000	4.50973400	-0.57394200
O	-3.53173300	-1.16845600	0.99035000	C	0.17212500	1.49068400	1.72599200
C	-0.05355500	1.44099800	1.25223600	H	-0.44060300	2.11263900	2.40151800
H	-0.34994700	1.05336900	2.22413800	H	1.08280500	2.03516400	1.46940400
C	1.27887900	1.95459500	0.99270100	H	0.44798900	0.58027900	2.26680600
H	1.98360600	2.01038400	1.82044500	Rh	1.13318700	-0.41073000	-0.19706600
H	1.44318100	2.70130200	0.21906600	Cl	2.61531400	1.45043300	-0.58353900
C	-1.26792800	2.89065900	-0.45206400	C	2.57670500	-1.19943800	0.84831000
H	-0.34794300	3.45429700	-0.62849200	O	3.42982800	-1.62284400	1.47273800
H	-1.87015800	3.45353400	0.27959500				
H	-1.84103300	2.82944900	-1.38330800	<b>IN6</b>			
C	-1.01608700	1.52025100	0.16927000	C	-1.31427600	-1.03167900	-0.83603800
Rh	0.96365100	0.04511200	0.09840400	C	-1.82313900	-0.80382000	0.61793200
C	-0.21896300	0.65028500	-1.81218700	C	-0.61671300	-1.20239400	1.49638700
H	0.68944300	0.25060600	-2.27885700	C	-0.55757500	-2.33676200	-0.54980600
H	-0.33485200	1.66464500	-2.18616200	C	-2.65418600	-0.86674600	-1.58580300
Cl	2.96379600	-0.31142400	-1.34315700	H	-3.28114700	-1.75715100	-1.44190300
C	2.06949200	-0.72864400	1.48686500	H	-2.53487700	-0.70396700	-2.66304600
O	2.76688800	-1.17191700	2.26650300	H	-0.88749600	-1.91811800	2.28163500
				H	-0.03709600	-0.38966800	1.94149300
<b>TS4-cis</b>				H	-1.22265500	-3.14508100	-0.21439200
C	-1.74113500	-1.05649700	-0.14705700	H	0.11758600	-2.72230800	-1.31449800
C	-1.80345700	0.15135400	0.82362800	C	-0.29825700	0.00733300	-1.35345000
C	-3.31549700	0.52018500	0.78877300	C	0.76897600	-0.35983700	-2.21331100
C	-3.10591200	-1.70556400	0.14399900	H	0.91712400	-1.38111900	-2.55962300
C	-1.63396100	-0.45473600	-1.56735900	H	1.18905000	0.39206900	-2.87982900
C	-0.33308700	0.34570900	-1.61746100	H	-2.57716500	-1.59303300	0.76333500
C	-0.70601600	1.18710300	0.49171200	H	-0.65832500	1.03361400	-1.39108000
H	-2.51682800	0.16770700	-1.75871000	O	0.26726700	-1.89350000	0.55410000
H	-1.64250600	-1.25744900	-2.31873800	C	-1.80965700	1.76335100	0.79787900
H	0.46189000	-0.14962700	-2.22097100	H	-0.97933900	1.65280100	1.50006200
H	-0.37926000	1.36761200	-1.98086600	C	-2.05352200	2.97474800	0.28920200
H	-3.54237600	1.37279600	0.13836200	H	-1.43541500	3.82986200	0.55548800
H	-3.68272500	0.75664600	1.79787200	H	-2.87694400	3.16397000	-0.39944900
H	-3.46949900	-2.34502900	-0.66952600	C	-3.74879900	0.49802300	1.67839300
H	-3.06142000	-2.30573000	1.07090500	H	-4.39790100	1.37622400	1.57257000
C	-0.49713700	-1.85407200	0.21122000	H	-3.30429400	0.52769200	2.68266100
C	0.38601100	-2.40606400	-0.71999400	H	-4.36734700	-0.40747900	1.60130800
H	0.18506000	-2.37748500	-1.78894100	C	-2.65144700	0.50734900	0.58043300
H	1.09681800	-3.16755300	-0.40689200	Rh	1.49255500	-0.14950400	-0.20283900
H	-1.57983700	-0.23209000	1.82807100	C	2.34373600	1.46800200	-0.68669000
H	-0.44867700	-2.19878200	1.24624600	O	2.85431800	2.44289700	-0.97764800
O	-3.99518800	-0.61744300	0.27892400	Cl	2.81886300	-0.18791300	1.79631300
C	-1.15974000	2.44052400	-0.18821500	C	-3.29300000	0.38294700	-0.86834000
H	-2.00687700	2.34252100	-0.86612800	H	-3.09197900	1.28808800	-1.45139500
C	-0.61580700	3.65644300	-0.03563900	H	-4.38295800	0.27754400	-0.80523800
H	0.25055300	3.84266500	0.59290200				

**IN6-cis**

C	2.49794300	-0.44485700	-0.24941400
C	1.74414400	0.04616300	1.03881900
C	0.75098300	-1.08203600	1.29831200
C	1.41811600	-1.41459900	-0.86980000
C	2.80161900	0.85551300	-1.06230600
C	2.31622800	2.02973900	-0.16972600
C	1.15657100	1.45907400	0.70169200
H	2.29060900	0.85117100	-2.03007500
H	3.86994800	0.95634600	-1.27508800
H	3.13536500	2.33674300	0.49748700
H	2.00845600	2.90838200	-0.74962600
H	-0.10660700	-0.84006100	1.93264300
H	1.24609500	-1.98250000	1.69285000
H	1.10460000	-1.14989900	-1.88247600
H	1.77766500	-2.45184900	-0.87037400
C	3.72336100	-1.26995100	0.11921700
C	4.92978300	-1.25635800	-0.45269800
H	5.18422300	-0.60341800	-1.28511700
H	5.71685800	-1.92024500	-0.10026300
H	2.44952400	0.16401600	1.87164900
H	3.55275700	-1.97856900	0.93590400
O	0.26408600	-1.36540600	-0.01989500
C	-0.18164200	1.56652700	-0.08933500
H	-0.77138000	2.40229300	0.29315000
C	-0.42807300	1.25589400	-1.45907700
H	0.30345800	0.74689300	-2.07977100
H	-1.10932400	1.89011900	-2.02602700
C	0.96959300	2.26297300	2.00886800
H	0.16420100	1.83112800	2.62009000
H	0.70317600	3.30597500	1.79140800
H	1.89178700	2.26521200	2.60478300
Rh	-1.49010300	-0.12934900	-0.25659700
C	-3.08906100	0.89112700	-0.31952800
O	-4.04857000	1.50140500	-0.35526200
Cl	-2.80813500	-1.96437000	0.56687300

**TS5**

H	1.19765000	-1.97110700	-0.51252100
C	1.18901500	-0.88892600	-0.66454800
C	0.58748800	-0.50907400	-1.96128100
H	0.19013700	-1.36249900	-2.50770200
H	1.17064600	0.17682500	-2.57412000
C	3.04540400	-0.75612900	1.14391000
C	3.72445900	-1.10816500	-0.18169900
C	2.70777700	1.26349900	-0.45293000
H	3.53463800	-0.04172000	1.80394700

H	2.49774900	-1.54511900	1.65825400
H	3.61858300	-2.12469800	-0.55569300
H	4.67727200	-0.63634200	-0.41929500
C	0.70289000	2.53382800	-0.13440700
C	2.44805900	-0.21661800	-0.16218300
O	1.98583500	2.19135700	0.31513200
C	-0.38081200	1.71522300	0.57499000
C	-1.79457600	1.64781400	0.14394500
C	-2.06651000	0.97356200	-1.05253200
H	-3.08436100	0.65947600	-1.27393200
C	-0.99670300	0.58659300	-2.05384200
H	-0.48300700	1.46292100	-2.44173600
H	-1.45876900	0.00455900	-2.84954400
C	-2.91663400	2.03282500	1.08849400
H	-3.86266800	1.55053300	0.81618500
H	-3.06110000	3.12272200	1.06303800
H	-2.66405900	1.76080000	2.12092000
Rh	-0.66457800	-0.31697700	0.06352100
H	-0.29537600	1.90352300	1.65034900
H	0.65190900	2.46583300	-1.23059800
H	0.56439600	3.59412900	0.12704400
H	2.55744600	1.47321800	-1.52794600
H	3.76310800	1.46692900	-0.23050000
Cl	-1.63864100	-2.47295200	-0.61359100
C	-0.42903300	-0.97244700	1.83817700
O	-0.32036400	-1.37482500	2.89735200

**TS5-A**

C	-1.15255300	-0.55481900	0.90538400
C	-0.08609700	-1.55866800	1.03516400
H	-0.13522500	-2.42804500	0.37763200
H	0.20853700	-1.78547700	2.06056100
C	-2.54234200	-1.67843900	-1.04332500
C	-2.98522300	-2.33480900	0.26547800
C	-3.53134000	0.20411900	0.52725000
H	-3.31116300	-1.40029500	-1.76287600
H	-1.59123200	-1.97899800	-1.48271900
H	-2.33959900	-3.08739500	0.71269100
H	-4.05067900	-2.49087800	0.43189300
C	-1.94734400	1.93764100	0.36143900
C	-2.48348400	-0.87064200	0.25979700
O	-3.20195100	1.45749400	-0.01705400
C	-0.79624000	1.09612300	-0.25378600
C	0.47374600	1.90433400	-0.48369100
C	1.36726700	2.12629100	0.56834700
H	2.28747700	2.67380100	0.36319500
C	1.21561400	1.32785500	1.78798600

H	0.25876100	1.36219000	2.31149800
H	2.06328100	1.34302200	2.47339300
C	0.68881600	2.44717100	-1.88081900
H	1.64981500	2.97051900	-1.95541500
H	-0.11402200	3.14977400	-2.14847700
H	0.67825000	1.61811600	-2.60115400
Rh	1.11994000	-0.10118900	0.22589900
H	-1.13059500	0.70236700	-1.21697800
H	-1.85856100	2.01832200	1.46004900
H	-1.88345600	2.95148700	-0.05267000
H	-3.67113300	0.29972400	1.62174800
H	-4.49298800	-0.07849400	0.08340000
C	2.78611100	-0.98261300	0.56214500
O	3.77656800	-1.51250700	0.74105300
Cl	1.04005200	-1.13150800	-2.00783100
H	-1.28415700	0.00823600	1.83170100

**TS5-B**

H	-0.97406000	-1.41595800	-1.03684200
C	-1.18342900	-0.89742900	-0.09943800
C	-0.32231300	-1.39587800	0.98871100
H	0.05318500	-2.40754500	0.82791200
H	-0.64122400	-1.18527900	2.01116100
C	-3.57203000	-0.69656700	-1.12261800
C	-3.58046400	-1.89938800	-0.17048600
C	-3.02411300	0.19816800	1.29856700
H	-4.43914400	-0.03683100	-1.12100600
H	-3.10454800	-0.83111600	-2.09764900
H	-3.11399400	-2.82365400	-0.50631800
H	-4.44463400	-2.03754400	0.47883200
C	-1.80072300	1.82277700	0.11418500
C	-2.66600300	-0.69801000	0.12208600
O	-2.16213500	1.30584800	1.36623600
C	-0.78512700	0.95205400	-0.70941400
C	0.53783800	1.67178500	-0.97116100
C	1.28145300	2.14659200	0.12324900
H	2.22139400	2.66382300	-0.06962500
C	0.94837400	1.64284000	1.45407200
H	-0.07194000	1.69708700	1.82757000
H	1.70044300	1.81808500	2.22388000
C	0.95171700	1.90096800	-2.40963700
H	1.95083600	2.34966900	-2.46094000
H	0.24053400	2.57073400	-2.91465200
H	0.97633800	0.94319900	-2.94564900
Rh	1.08908400	-0.08905500	0.23118900
H	-1.19031700	0.68541600	-1.68709700
H	-1.35782800	2.80117800	0.31732800

H	-2.69545400	1.97801200	-0.50945200
C	2.57920500	-0.84830500	1.14366800
O	3.48425800	-1.29722200	1.66728600
Cl	1.53555300	-1.55390000	-1.70829100
H	-2.91014700	-0.33759700	2.24993100
H	-4.07592400	0.52544800	1.21116900

**TS5-C**

H	1.15947900	-1.06902100	1.47451300
C	1.16628600	-0.06166100	1.06712000
C	0.47640300	0.78106400	2.03477800
H	0.36695700	1.85322200	1.86096100
C	3.03062700	1.27548000	-0.30017900
C	3.73456300	0.44253500	0.78731700
C	2.33050700	-1.24319700	-0.74321800
H	3.46136800	1.27509300	-1.30157700
H	2.57356100	2.22011800	-0.00706900
H	3.73966700	0.83414900	1.80304200
H	4.62375100	-0.12164800	0.50818300
C	0.44672200	-2.67023700	0.08183400
C	2.38125800	-0.01158200	0.19683800
O	1.83348100	-2.42066000	-0.14369200
C	-0.56216700	-1.71152000	-0.56536000
C	-1.96136800	-1.51376100	-0.09776600
C	-2.20960300	-0.72600300	1.03855200
H	-3.21119700	-0.30857900	1.12949000
C	-1.23374800	-0.29041000	2.09389700
H	-0.69531300	-1.12333200	2.54594500
H	-1.72939300	0.35011000	2.82161800
C	-3.10811200	-1.84426900	-1.03598500
H	-4.02615000	-1.31177900	-0.76267100
H	-3.31118000	-2.92482700	-1.00800500
H	-2.84610400	-1.58727500	-2.07023300
Rh	-0.58790400	0.33327400	-0.06351600
H	-0.55281500	-1.86760300	-1.65036900
H	0.27346200	-2.73769400	1.16611400
H	0.26221600	-3.67697400	-0.32277300
Cl	-1.56179400	2.59933900	0.08614100
C	0.17988100	1.01570400	-1.68455400
O	0.56917800	1.46179400	-2.65748300
H	0.56550300	0.51998400	3.08909200
H	1.75587800	-0.99193900	-1.64663800
H	3.34774600	-1.50001800	-1.06603700

**IN8**

H	0.92175300	-1.61432900	-1.06007700
C	0.89032300	-0.52416100	-0.94482800

C	0.45845600	0.08027900	-2.29859600	H	-1.68510700	2.89438000	-1.66079500
H	-0.16625300	-0.66477600	-2.80769800	H	-2.00688200	2.31552800	-0.02895500
H	1.34643200	0.26454800	-2.92462300	H	-3.55572500	0.49891700	-0.01346000
C	3.05368400	-1.13147500	0.38599700	H	-3.53973400	-0.56593900	-1.43330900
C	3.45725100	-0.79842500	-1.05213300	H	-0.87549400	-1.28884900	1.79288200
C	2.51225900	1.36796800	-0.03270500	H	-2.14460700	0.42483200	2.89281600
H	3.68315400	-0.77376900	1.19946500	H	-2.20214500	1.46741900	1.48953300
H	2.60748800	-2.10947500	0.55945800	H	0.16218900	0.79890100	3.28962000
H	3.25384500	-1.54087900	-1.82159200	H	-0.41847800	2.41486300	2.88617300
H	4.35833200	-0.20887800	-1.21805800	H	1.83829700	1.49607900	1.88631200
C	0.61739600	2.49440700	0.88123000	H	2.41047000	2.21658100	-1.47678800
C	2.23742900	-0.08794000	-0.39876500	H	3.07928900	2.08276800	0.17580300
O	1.83272900	1.83430500	1.10356000	H	2.24406700	3.56290800	-0.34221000
C	-0.64064800	1.62050800	1.02817000	Rh	0.46307700	-0.21849400	-0.05611300
C	-1.75695300	1.57060000	0.07735500	C	-2.18721100	-2.36964900	-0.27936000
C	-1.58022000	1.16953400	-1.25513100	H	-3.10800500	-2.63914800	-0.79661400
H	-2.48638400	0.85726500	-1.77537200	H	-1.91207800	-3.05678000	0.52058700
C	-0.36672400	1.38035800	-2.15551600	C	-1.02836300	-1.89779100	-1.14097000
H	0.26417500	2.19227400	-1.78759200	H	-0.09505400	-2.42016100	-0.93037000
H	-0.72908900	1.68518500	-3.14686300	H	-1.23290900	-1.63785700	-2.17599400
C	-3.16415000	1.49853900	0.66548600	Cl	1.52870300	-2.13901400	1.11494100
H	-3.86607000	0.99945600	-0.01161500	C	2.12506600	-0.49925000	-1.32661800
H	-3.52116400	2.52306300	0.84723500	O	3.07871700	-0.73972300	-1.89043500
H	-3.17625900	0.97833000	1.63324400				
Rh	-0.76682900	-0.38629400	0.28709100	<b>TS6-RE</b>			
H	-0.99887900	1.65382500	2.06204400	H	-0.69923700	1.08150000	-1.28400000
H	0.63426900	3.00921600	-0.08862500	C	-1.12120500	0.18508800	-0.78561100
H	0.55844500	3.27653800	1.65068700	C	-1.29420700	-0.93063800	-1.83689700
H	2.30471000	2.02210500	-0.89773200	H	-1.62356100	-0.45422800	-2.77246800
H	3.58260000	1.46338700	0.19575100	H	-2.10567500	-1.60554800	-1.55838700
Cl	-1.73751900	-2.36479000	-0.73440400	C	-2.50865600	2.02292000	0.50737200
C	0.17941100	-1.33165200	1.69957300	C	-3.20757600	1.75491600	-0.82568600
O	0.67839100	-1.86926600	2.56605500	C	-3.30474900	-0.44897000	0.50780100
				H	-3.12848500	2.12161700	1.39739900
<b>TS6</b>				H	-1.61385100	2.63906800	0.50232500
C	-0.11170100	1.64399900	-0.93183400	H	-2.77316900	2.18873600	-1.72507100
C	-1.94869400	-0.91549300	-0.02313700	H	-4.29401200	1.66998400	-0.84544800
C	-1.58897500	2.02408000	-0.99728100	C	-1.59874800	-1.93830200	1.08644100
O	-2.35709200	1.01386100	-1.60839500	C	-2.41063000	0.62191900	-0.11149700
C	-2.90212100	0.03392000	-0.77385500	O	-2.68527100	-1.18935700	1.52864800
C	-1.17246300	-0.45235500	1.15225100	C	-0.28053300	-1.16188500	1.02911900
C	-1.56819400	0.75204700	2.01401600	C	0.92311300	-1.72960200	0.41780400
H	0.30518700	1.74871500	-1.93811600	C	1.05450300	-1.68817500	-1.00968200
C	-0.25328400	1.40576400	2.47443500	H	2.03262600	-2.02539300	-1.36152800
C	0.85382600	1.47096100	1.41393900	C	-0.00160200	-1.74279900	-2.11116600
C	0.89486300	1.95301600	0.07775200	H	-0.25839800	-2.79111400	-2.33323500
C	2.24347000	2.46561800	-0.42190100	H	0.48815400	-1.35359300	-3.01379400

C	2.04764900	-2.24607600	1.30069300	Cl	2.13613100	-1.24305000	1.48387100
H	3.00205000	-2.26494400	0.75891300	C	2.24028700	0.57503200	-0.79793800
H	1.82152700	-3.27375000	1.62181200	O	3.24378900	0.87424500	-1.23504500
H	2.16136600	-1.62925100	2.20104900				
Rh	0.98095700	0.26211600	-0.13518700	<b>TS7</b>			
H	-0.09993600	-0.71300900	2.01288900	C	-1.04650200	1.11600400	-0.59746900
H	-1.81702000	-2.47394500	0.15205300	C	-1.34885000	-1.15362900	-0.47961000
H	-1.42089700	-2.70570300	1.85681000	C	-2.57728100	1.28038100	-0.74699000
H	-3.68551200	-1.13851300	-0.26739000	O	-3.18890300	0.16603600	-1.33005200
H	-4.17328400	0.03380100	0.97057600	C	-2.85858800	-0.93322100	-0.54553100
Cl	0.92638800	2.60801700	0.51513000	C	-0.65744700	-1.60344500	0.71261200
C	2.93391100	0.59050900	-0.06144400	C	-1.16611800	-1.32851000	2.12494900
O	4.04877300	0.79302800	0.01762400	H	-0.55213700	1.44989100	-1.51623600
				C	-1.49811200	0.16146800	2.37761000
<b>IN9</b>				C	-0.48834600	1.19457500	1.86446400
C	-0.57492300	1.36956400	-1.08747400	C	-0.43088600	1.77021200	0.61451500
C	-1.22935900	-1.63437700	-0.18334500	C	0.26067000	3.11118700	0.42800400
C	-2.00505500	1.10136400	-1.58852000	H	-2.77667000	2.13289400	-1.40637000
O	-2.79236300	0.13683900	-0.93129100	H	-3.03316000	1.49156300	0.23461500
C	-2.35026200	-1.17299000	-1.10455800	H	-3.29803700	-0.84953700	0.46146800
C	-1.08313900	-1.30554600	1.14312300	H	-3.27800700	-1.82445800	-1.03378900
C	-1.95966500	-0.44201000	2.04855700	H	-0.15317600	-2.56729400	0.59844400
H	-0.03169000	1.79654200	-1.93728700	H	-0.37546200	-1.63469200	2.82324000
C	-2.00750100	1.07117600	1.73091700	H	-2.05118400	-1.94124600	2.36737200
C	-0.66852400	1.73049200	1.41072000	H	-1.59643900	0.31241100	3.46067700
C	-0.22701000	2.10975200	0.16147000	H	-2.48288600	0.39317000	1.95668800
C	0.84540000	3.19210600	0.06494500	H	0.08679700	1.70425200	2.63970900
H	-1.92419100	0.81702400	-2.65223000	H	0.80539700	3.16395600	-0.51704200
H	-2.59430800	2.02739000	-1.53809500	H	0.96029500	3.31772800	1.24679300
H	-3.21662200	-1.82644700	-0.91651000	H	-0.51568900	3.89243200	0.43510600
H	-2.03663700	-1.33481900	-2.15064600	C	2.31907900	-1.00079800	0.76750400
H	-0.33297400	-1.88580600	1.67940100	O	3.26009800	-1.48108900	1.18454600
H	-1.57237200	-0.57789500	3.06603700	Rh	0.74350900	-0.20005400	-0.01008900
H	-2.98930300	-0.83163100	2.04327500	Cl	2.36462800	1.23812600	-1.20679700
H	-2.41570300	1.58681200	2.61220500	C	-0.71978600	-1.66002200	-1.78951800
H	-2.70325600	1.23591800	0.90918900	H	-1.08089300	-1.03977100	-2.61882800
H	-0.13432100	2.15639700	2.26244000	H	-1.05697700	-2.69343100	-1.97850900
H	1.49687200	3.06342600	-0.80722900	C	0.80480400	-1.51372200	-1.60060600
H	1.46636500	3.23504500	0.96836200	H	1.30101900	-2.46329200	-1.37397900
H	0.34746500	4.16640100	-0.04899700	H	1.31522300	-1.01274700	-2.42537800
Rh	0.57563200	-0.09992100	-0.06807300				
C	-0.24927700	-2.62623700	-0.82503800	<b>TS7-RE</b>			
H	-0.74964400	-3.28662000	-1.54893800	C	-0.79311400	1.27140200	-1.26124100
H	0.22534700	-3.23979300	-0.05220200	C	-1.85915900	-1.29634500	0.54416200
C	0.77709000	-1.66379800	-1.44470500	C	-2.34360600	1.31139400	-1.06211100
H	1.79601000	-2.06046800	-1.44154700	O	-3.09673600	0.14151900	-0.99699100
H	0.49149500	-1.32901800	-2.44797200	C	-3.12574400	-0.51014400	0.25783100

C	-1.08704900	-1.17283100	1.63862500	H	-0.60441100	-1.02020000	2.92714500
C	-1.12483800	-0.04878100	2.66555000	H	-2.15368300	-0.54638700	2.25272500
H	-0.51824600	1.36891100	-2.31248900	H	0.24127700	1.10373800	2.90000700
C	-0.99375900	1.35384700	2.00219200	H	-1.40893600	1.64860200	2.68611700
C	0.17715300	1.57089300	1.02213500	H	0.56223700	2.46212200	1.01457500
C	0.12819700	1.94235800	-0.38429900	H	-0.23665800	2.05604800	-2.39916900
C	1.14587700	2.91577800	-0.96601900	H	0.63158700	3.02148900	-1.17855800
H	-0.24290900	-1.85963700	1.72423500	H	-1.09913400	3.32198400	-1.51910100
H	-0.29404800	-0.19626100	3.36715800	C	2.18702000	-1.69560600	0.21006700
H	-2.04598800	-0.05403100	3.26726600	O	2.82731600	-2.63093300	0.26830000
H	-0.87157000	2.10053000	2.80129600	Rh	1.09085900	-0.13290000	0.11002400
H	-1.93763400	1.59380300	1.51538600	Cl	3.01588200	1.33529900	-0.19273000
H	1.03159300	2.02098800	1.53218300	C	-0.90853200	-1.50799400	-1.62219200
H	1.44984300	2.61934600	-1.97755600	H	-1.48994800	-1.40156400	-2.55186900
H	2.04272900	2.98909900	-0.33911000	H	-0.78308900	-2.58514100	-1.43586400
H	0.69730700	3.91860500	-1.02508300	C	0.46644900	-0.82679100	-1.74025900
Rh	0.78975200	-0.06797700	-0.23229400	H	1.22562000	-1.47476900	-2.19139100
C	-1.38283200	-2.13445100	-0.63440800	H	0.42924400	0.09806700	-2.32730900
H	-2.23181800	-2.59163400	-1.16665500	H	-3.07502200	1.11105100	1.12171000
H	-0.71052200	-2.92591400	-0.29041100	H	-3.83949100	1.69068700	-0.37685700
C	-0.62216200	-1.19949700	-1.60492900				
H	0.19759000	-1.69988000	-2.12871300	<b>IN7-RE</b>			
H	-1.29108500	-0.73331100	-2.32249100	C	-1.42065600	1.16232400	-1.17411200
H	-3.37534700	0.20000100	1.06077900	C	-1.66492800	-1.44742700	-0.19922100
H	-3.96019100	-1.22117100	0.17784500	C	-2.88589000	1.23281700	-0.66794700
H	-2.56436400	1.95517100	-0.20098700	O	-3.26130800	0.35867900	0.35719600
H	-2.71451900	1.83767400	-1.95200800	C	-3.11254900	-1.00077500	0.04846400
C	2.59487500	0.34020600	0.36285100	C	-0.79119700	-1.62603500	0.81799600
O	3.67286700	0.59052900	0.63195200	C	-1.01268100	-1.13802100	2.23727100
Cl	1.93577900	-2.24604100	-0.22583300	H	-1.39014200	2.02411300	-1.85869100
				C	-1.07150100	0.42767700	2.28742300
<b>IN7</b>				C	-0.18095300	1.19448300	1.28324500
C	-1.91267000	0.63975000	-0.69210000	C	-0.32294500	1.51821800	-0.11130500
C	-1.63768300	-0.87570900	-0.42060400	C	0.36418100	2.82620100	-0.54320900
C	-3.24556800	0.87816100	0.05854500	H	-3.54534500	1.08605100	-1.54560000
O	-3.96432800	-0.31804200	-0.10203500	H	-3.07252500	2.23767900	-0.26920500
C	-3.07691100	-1.42170400	-0.17099100	H	-3.52469000	-1.54829000	0.90460600
C	-0.64955100	-1.08540200	0.75901500	H	-3.71389200	-1.25161000	-0.84427300
C	-1.06625500	-0.45781300	2.10557000	H	0.14623700	-2.15909000	0.59912500
H	-2.12548300	0.75422400	-1.76410600	H	-0.18579100	-1.49618200	2.86144600
C	-0.62144400	1.03204600	2.22378700	H	-1.94196300	-1.53906700	2.66929100
C	-0.20239500	1.68902000	0.91186200	H	-0.75832400	0.74190700	3.29096500
C	-0.75352800	1.56643500	-0.33906700	H	-2.10831500	0.74293900	2.14909200
C	-0.32450800	2.54506400	-1.42114000	H	0.44464900	1.92182500	1.80430900
H	-3.11758300	-2.00446800	0.76329200	H	0.80338200	2.73679100	-1.54638000
H	-3.41720400	-2.06974700	-0.99065200	H	1.14933000	3.13978800	0.15399600
H	-0.52843500	-2.17026900	0.88957500	H	-0.38385000	3.63411000	-0.58284700



Rh	1.08578800	-0.10304300	0.14016800
C	-1.24649100	-1.50630600	-1.64584700
H	-1.98885100	-2.04741400	-2.24769200
H	-0.28015200	-2.01539600	-1.74816900
C	-1.12795400	-0.02252800	-2.16533200
H	-0.10956800	0.12054500	-2.55123400
H	-1.81056100	0.11839300	-3.01477300
C	2.63659700	0.97991700	0.10891500
Cl	2.45700100	-1.94463200	-0.58698500
O	3.59414500	1.59698500	0.11645000

**IN10**

C	-2.66161600	-0.01397700	0.72912800
C	-1.16441400	0.47488100	0.49618100
C	-0.33026600	-0.29884400	-0.54598600
C	-0.13947900	-1.80624500	-0.30903500
C	-1.35956300	-2.56793200	0.29639800
C	-2.60983100	-2.18566000	-0.47143800
C	-3.19828400	-0.98650200	-0.32923400
C	-3.39267400	1.34557400	0.79050000
O	-2.76542700	2.12801700	-0.19388700
C	-1.38623100	1.95580000	0.01737900
C	1.09321700	0.84889700	1.52129800
C	-0.35365300	0.42405000	1.81125800
H	-2.71407900	-0.51352300	1.70742400
C	-4.38215300	-0.58067600	-1.18607800
H	-0.66040400	-0.09425500	-1.56912000
H	0.73004500	-1.99422300	0.39881200
H	0.15031100	-2.28416600	-1.25411500
H	-1.17028800	-3.64670400	0.24604000
H	-1.45943400	-2.30623600	1.35892200
H	-2.98581900	-2.88896500	-1.21548400
H	-1.03471700	2.66157000	0.79228800
H	-0.87095200	2.18386400	-0.92319000
H	1.17624700	1.93609900	1.40868100
H	1.81788200	0.51494100	2.27440700
H	-0.80192700	1.06841900	2.58506100
H	-0.36505200	-0.60130000	2.20843200
H	-4.19526400	0.39164900	-1.66307800
H	-5.29996800	-0.47869800	-0.58811600
H	-4.57032700	-1.32729400	-1.96624700
Rh	1.68738200	-0.12323700	-0.18614200
Cl	3.89804000	-0.97755900	0.24492500
C	1.98011600	1.54048200	-0.97381400
O	2.16568700	2.56404400	-1.43509600
H	-3.25454400	1.79772600	1.79064600
H	-4.46368400	1.30966200	0.57384800

**TS8**

C	-2.67731600	0.28762800	0.48521800
C	-1.12472100	0.59525900	0.39515500
C	-0.41048700	-0.11186200	-0.75669800
C	-0.31510800	-1.51917800	-0.80497200
C	-1.17176300	-2.44913000	0.05438600
C	-2.63739100	-2.16586500	-0.25488800
C	-3.27185800	-0.98953400	-0.10653400
C	-3.28208100	1.60759800	-0.06185600
O	-2.42580800	2.59854300	0.43253100
C	-1.12471900	2.14548000	0.14204100
C	1.09985200	0.22986600	1.62560700
C	-0.43151300	0.25254600	1.74349300
H	-2.92419700	0.27572400	1.56073400
C	-4.75484800	-0.89719100	-0.43815500
H	-0.34853700	0.42472800	-1.70423600
H	1.14123000	-1.94374900	0.01461800
H	-0.02587500	-1.94193300	-1.77107600
H	-0.92869500	-3.48970400	-0.18904100
H	-0.96331900	-2.31968700	1.12001500
H	-3.21353800	-3.00863200	-0.63838600
H	-4.29621200	1.81409500	0.29566100
H	-3.28507100	1.60298600	-1.16914800
H	-0.41401900	2.68399500	0.77768000
H	-0.87131200	2.36097000	-0.90890900
H	1.52748400	1.23853800	1.66455400
H	1.55472700	-0.39621400	2.40175100
H	-0.74176700	0.99799700	2.49395600
H	-0.78867300	-0.71395500	2.11587500
H	-4.94223100	-0.16898700	-1.24037700
H	-5.33117000	-0.56494600	0.43848500
H	-5.14954100	-1.86789800	-0.75918000
Rh	1.66199900	-0.39360700	-0.24429800
C	3.50359000	-0.69223600	0.41171300
O	4.54949300	-0.83177700	0.82667000
Cl	2.22420300	1.81379700	-1.07001300

**IN11**

C	2.83894000	0.43772200	-0.24071900
C	1.34433300	0.86985100	-0.27455600
C	0.49972700	0.04952400	0.69694100
C	0.27183400	-1.29433500	0.58303800
C	0.93037800	-2.19237100	-0.45575100
C	2.45363300	-2.10096100	-0.46387700
C	3.24900200	-1.02273900	-0.36672500
C	3.33428300	1.10767000	1.08120800

O	2.41198300	2.13835000	1.38437900	H	-3.15675800	-1.10440500	1.39681600
C	1.51263500	2.29071400	0.31251300	H	-2.68914500	-1.64157100	-2.34944800
C	-0.80748700	1.12172000	-1.58363700	H	-1.64393400	-2.78245200	-1.45852000
C	0.70905700	0.87396200	-1.68071500	H	-3.05243900	3.49655700	0.74656800
H	3.32274600	0.96799500	-1.07935000	H	-2.89238000	2.93753600	-0.93650400
C	4.76122600	-1.20094200	-0.40138400	H	-4.27686500	2.42041000	0.03054000
H	0.19457000	0.53262800	1.63034100	C	-0.63801200	0.03247200	-1.97721800
H	-1.50983500	-1.04542800	-1.34585800	H	0.00509000	-0.71716300	-2.46098000
H	-0.25264000	-1.78326900	1.40513300	H	-1.33056900	0.41174600	-2.74744700
H	0.64431900	-3.22855700	-0.24090600	C	0.22599900	1.19434500	-1.44082100
H	0.53992100	-1.97871100	-1.46021700	H	0.92668000	1.56241200	-2.19772100
H	2.95297100	-3.06430600	-0.58167800	H	-0.43275100	2.03239000	-1.17813500
H	1.91543700	2.97001800	-0.46035400	Rh	1.49293600	0.13011600	-0.04161300
H	0.58283800	2.71927300	0.70672300	Cl	2.90956300	-1.63739900	0.78153900
H	-1.00623700	2.13706600	-1.19696300	C	3.12018400	1.04826200	-0.56320400
H	-1.27444700	1.04857100	-2.57274000	O	4.08588300	1.58037500	-0.83390000
H	1.20010900	1.65013400	-2.29148500	H	0.71353200	1.50622900	0.04475000
H	0.90421600	-0.08167800	-2.18405200				
H	5.22172900	-0.85513600	0.53640900	<b>IN12</b>			
H	5.20669700	-0.60736900	-1.21399600	C	1.86921400	0.85824700	0.37761800
H	5.04091700	-2.25055900	-0.54708900	C	1.75876300	-0.42997600	-0.50242600
Rh	-1.67849900	-0.09200400	-0.13724300	C	0.60567900	-1.36793200	-0.16346000
C	-3.45938100	0.24310200	-0.82273800	C	0.04714100	-1.61663800	1.11463700
O	-4.49992800	0.40957500	-1.23821800	C	0.32659400	-0.71270400	2.32174600
Cl	-2.64485400	-0.61074800	2.04220100	C	-0.14156100	0.67625800	1.87104600
H	3.33947900	0.38820400	1.91270800	C	0.51033100	1.38159000	0.88711900
H	4.34666800	1.52311300	0.97099900	C	2.64740300	1.80248600	-0.57866900
				O	2.40039000	1.36568400	-1.90129900
<b>TS9</b>				C	1.55111100	0.24268400	-1.88703500
C	-2.63860900	0.17893700	-0.30928100	H	2.47955200	0.66395700	1.26921000
C	-1.44066800	-0.65567400	-0.84997700	C	3.09834300	-1.22863100	-0.53796300
C	-0.44256800	-1.14761600	0.19365700	C	3.57209000	-1.80402700	0.81012700
C	-0.17797900	-0.69084100	1.45892300	C	0.05960000	2.78214700	0.51766000
C	-0.83615800	0.38745800	2.29427700	H	0.50280700	-2.17814400	-0.89070000
C	-1.65875900	1.48035700	1.64432800	H	-0.41315000	-2.58538300	1.30634400
C	-2.42118400	1.41944600	0.54294900	H	1.38580100	-0.72224700	2.62512800
C	-3.48553600	-0.93507400	0.35968500	H	-0.27084700	-1.04509400	3.17632300
O	-3.26675900	-2.10268300	-0.40886600	H	-0.98367200	1.13998300	2.38573700
C	-2.25214200	-1.87386100	-1.36216000	H	3.72626900	1.72998700	-0.37531900
H	-3.18667100	0.49592200	-1.20997800	H	2.35818800	2.85445600	-0.47641000
C	-3.19957600	2.64043600	0.07826700	H	0.49745000	0.54654200	-2.01144700
H	0.06282300	-2.07912200	-0.07881700	H	1.82804100	-0.41595000	-2.72105100
H	0.51824400	-1.30562900	2.03237600	H	2.96070200	-2.05768100	-1.24857900
H	-1.45983900	-0.14276400	3.03948200	H	3.87781700	-0.58265600	-0.96602100
H	-0.03969800	0.85994800	2.88584100	H	4.46953800	-2.41846000	0.66467200
H	-1.63641900	2.42906200	2.18370100	H	3.83113700	-1.01306900	1.52645100
H	-4.55656900	-0.69196700	0.36946900	H	2.80002000	-2.43856000	1.26502300

H	-0.95585100	2.97050400	0.87732500
H	0.74394000	3.52034000	0.96297500
H	0.06803200	2.92988600	-0.56975700
Rh	-1.22067300	-0.25805200	0.07243600
C	-2.31669200	-1.48411500	-0.93679600
O	-2.97450000	-2.20664200	-1.51801700
Cl	-2.99474700	1.34383800	-0.14509600

**IN13**

H	-2.12163100	-2.52963900	-0.83940800
C	-2.04811200	-1.93221300	0.07183800
C	-1.49866700	-2.55978800	1.17397600
H	-1.22847300	-3.61055500	1.10881900
C	-3.47030000	-0.25794300	-1.27720000
C	-4.36062600	-0.87918800	-0.20465500
C	-2.46578600	0.46554200	1.04507000
H	-3.59512700	0.80345600	-1.47701700
H	-3.21791900	-0.87074900	-2.14201100
H	-4.70388400	-1.90316300	-0.33999000
H	-5.05999700	-0.22809000	0.31739700
C	-0.11595700	1.39443400	1.29774200
C	-2.84515100	-0.65743500	0.07272600
C	0.49236900	0.01555000	1.55027300
C	1.84774400	-0.29854100	1.07813000
C	2.22105100	-1.67359500	1.19523800
C	1.27196000	-2.58763300	1.78019800
H	0.80311800	-2.33365600	2.73058200
H	1.46366500	-3.64912600	1.63136200
Rh	0.28625100	-1.58891900	0.16687500
H	-0.27396300	1.91982500	2.25180400
H	0.58191400	2.00229800	0.71283500
H	-2.13288100	0.04654500	2.00250700
H	-3.35622600	1.06799300	1.24692500
Cl	0.57101600	-3.49086300	-1.36003900
C	-0.08544700	-0.52782000	-1.48885300
O	-0.27150500	-0.00265100	-2.47898500
H	-1.57507600	-2.12797900	2.17070500
H	0.22704500	-0.39468300	2.52674900
H	3.10918300	-2.02297900	0.67268300
C	2.76222400	0.65673400	0.37641900
C	3.12019500	1.85931000	1.01272400
C	3.33416200	0.34479400	-0.87037000
C	4.03345300	2.73395700	0.41326600
H	2.69244800	2.10158400	1.98467500
C	4.24442000	1.22189200	-1.46842600
H	3.05243400	-0.58129600	-1.37142300
C	4.59657600	2.41771200	-0.82867800

H	4.30436700	3.65894700	0.91853000
H	4.67434300	0.97143000	-2.43623600
H	5.30398500	3.09918000	-1.29703800
N	-1.38510500	1.34439900	0.53359700
S	-1.87855200	2.87958100	0.03980300
O	-1.40211800	3.88464900	0.97345300
O	-3.29396900	2.80257900	-0.27502600
C	-0.97139100	3.09882600	-1.51003300
H	0.10350800	3.02077500	-1.31915300
H	-1.21924900	4.10344300	-1.86893000
H	-1.30315200	2.33419300	-2.21692500

**TS14-A**

H	-0.04396100	-1.40125400	1.54346900
C	-0.18238100	-1.80927400	0.53824800
C	-1.53585200	-2.39916500	0.40730900
H	-1.99847800	-2.65770000	1.36068300
H	-1.67651200	-3.15022500	-0.37321500
C	0.94897900	-4.14696700	0.06575700
C	0.99907700	-3.36942100	-1.25446100
C	2.35401900	-2.02161100	0.54324800
H	1.84030800	-4.69204400	0.37278500
H	0.00865500	-4.60893300	0.35737500
H	0.08576000	-3.32469800	-1.84688100
H	1.91681300	-3.39255500	-1.83955100
C	1.45839000	0.26545500	0.24397900
C	1.02733500	-2.60549100	0.07654300
C	0.17348300	-0.18921300	-0.48856100
C	-0.71166600	1.00443000	-0.89001500
C	-1.66735700	0.76453400	-1.89371500
C	-1.98192200	-0.62150800	-2.20833400
H	-1.16344000	-1.30303700	-2.45170500
H	-2.86966400	-0.79084100	-2.81710400
Rh	-2.13354200	-0.50872300	-0.09792000
H	3.18552600	-2.64735400	0.20826900
H	2.35593900	-1.99219800	1.65003400
H	0.45498200	-0.71587700	-1.40248600
H	1.76819100	1.23224500	-0.15957700
H	1.26191700	0.38576300	1.32366000
Cl	-2.17759200	0.10131500	2.28916700
C	-4.00457200	-0.84513900	0.00146200
O	-5.12430700	-1.02960900	0.07348400
N	2.53948900	-0.68259600	-0.01253500
S	4.08835300	-0.08937000	-0.09268500
O	4.04655600	1.11810400	-0.88787200
O	4.93584200	-1.20539200	-0.45599500
C	4.52118500	0.39542000	1.60441300

H	3.84330200	1.19084900	1.93112800	C	2.88753300	0.79761900	0.51873600
H	5.55223600	0.76325400	1.57924100	C	3.00361900	2.09757200	1.04344000
H	4.44839500	-0.48203000	2.25544800	C	3.78825700	0.37738800	-0.47840100
H	-2.29640000	1.58959500	-2.22577300	C	4.00800500	2.95906000	0.58871300
C	-0.42957100	2.40504500	-0.44477300	H	2.31673800	2.42526600	1.82229900
C	-0.18857400	3.38089100	-1.43160300	C	4.78935200	1.24044300	-0.93153300
C	-0.39111400	2.77901800	0.91202300	H	3.68499300	-0.61678400	-0.91160200
C	0.07481100	4.70713400	-1.07111700	C	4.90326100	2.53190800	-0.39862300
H	-0.18911700	3.09260200	-2.48139000	H	4.08799900	3.96122300	1.00518300
C	-0.12829800	4.10617600	1.26563700	H	5.47460300	0.90779000	-1.70875600
H	-0.61625800	2.03909300	1.67722300	H	5.68296800	3.20185000	-0.75579800
C	0.10555400	5.07319400	0.27887500	N	-1.59772900	1.31230900	0.42720200
H	0.26366800	5.44777700	-1.84584000	S	-2.35803100	2.70587100	-0.11271400
H	-0.11903900	4.38623200	2.31725100	O	-3.78649600	2.44889600	-0.13158800
H	0.31167200	6.10371300	0.56178900	O	-1.83368700	3.85947700	0.59660600
<b>TS14-B</b>				C	-1.79934200	2.83061900	-1.82929300
H	-1.75423400	-2.79295800	-0.41630900	H	-0.70627800	2.87299100	-1.85679800
C	-1.51798300	-2.02097300	0.32066600	H	-2.22233300	3.76216200	-2.22017000
C	-0.84394600	-2.58181900	1.53252200	H	-2.17331700	1.96498100	-2.38145700
H	-0.83301100	-3.67114300	1.55547100	<b>TS14-C</b>			
C	-3.60746600	-0.93944200	-0.75024300	C	-0.88868700	1.88874600	0.87912700
C	-4.06440400	-1.59754500	0.55742600	C	-2.34835900	1.85107700	0.63987400
C	-2.43462400	0.33766600	1.16758000	H	-2.69941900	2.37129500	-0.25127700
H	-4.03112500	0.03249000	-0.99903600	H	-2.97102400	2.03141400	1.51758500
H	-3.40655400	-1.58832700	-1.60187900	C	-0.44663900	2.91703200	-1.55620900
H	-4.15244200	-2.68229800	0.57838900	C	-0.43869000	4.04095200	-0.52291100
H	-4.79528600	-1.07071800	1.16933300	C	1.49719200	2.50891200	0.11935300
C	-0.21093700	1.54811400	0.89615400	H	0.33203700	2.90074600	-2.31631700
C	-2.63566700	-0.99943900	0.43985900	H	-1.39920300	2.53261600	-1.90208400
C	0.42900700	0.22085300	1.25751000	H	-1.39676200	4.39761300	-0.14935300
C	1.84617900	-0.12009200	1.06293700	H	0.34407500	4.79773500	-0.56301800
C	2.07859300	-1.49444500	1.24512600	C	1.40869700	0.47191800	1.39529700
C	1.01128800	-2.39070200	1.86606700	C	-0.00200600	2.59864600	-0.12502300
H	0.83837400	-2.09448100	2.90322500	C	-0.09692100	0.11712500	1.36289000
H	1.33361600	-3.42795900	1.78868200	C	-0.39795800	-1.31577800	0.93663600
Rh	0.36823900	-1.38197300	-0.13281200	C	-1.53635400	-1.89643400	1.52701100
H	-0.21678300	2.24133500	1.75218500	C	-2.49575200	-0.99324100	2.15498500
H	0.34660500	2.03378500	0.08505500	H	-2.15649500	-0.30003800	2.92834900
H	-2.00643800	0.18834000	2.16727700	H	-3.47008100	-1.42278800	2.38931600
H	-3.42128800	0.78451800	1.31424800	Rh	-2.17019200	-0.15627800	0.23194200
Cl	0.89517600	-3.37866300	-1.43993800	H	1.57374500	1.13152400	2.26356300
C	-0.11274100	-0.45795100	-1.72628300	H	1.95845500	-0.45411600	1.59336300
O	-0.36507700	0.06148700	-2.70767900	H	1.75071600	3.03266300	1.06129500
H	-1.19900600	-2.14158300	2.46532600	H	2.03251500	3.00132200	-0.69558800
H	0.02432600	-0.18367600	2.18726900	C	-3.96504800	-0.39890400	-0.36096300
H	3.02588400	-1.95273900	0.97345600	O	-5.02942100	-0.55742200	-0.72674800

Cl	-1.79880800	-0.00586800	-2.21194300	Cl	1.44505800	-3.44651400	-0.22638300
H	-0.63512300	2.19525400	1.89825900	C	0.37792300	-1.25726900	-1.78614300
H	-0.43413700	0.20303200	2.39553200	O	0.46181000	-1.34727000	-2.92011500
N	1.95609900	1.10992700	0.19641200	H	-1.49292300	-2.08574400	2.71224200
S	3.65687100	1.03251900	0.17296500	H	-0.34896000	0.88970800	1.53708200
O	4.17185600	1.10003700	1.53143000	H	2.73483200	-1.06752200	2.00548300
O	4.10147100	1.99409800	-0.81533000	C	2.85606500	1.17799400	0.35373100
C	3.97433600	-0.62411500	-0.47027000	C	2.86320100	2.57665100	0.20464600
H	3.59037100	-0.67016200	-1.49090500	C	3.97595500	0.43668100	-0.06940000
H	3.49945000	-1.38307100	0.15902700	C	3.97487600	3.22613500	-0.34301200
H	5.06397300	-0.73552000	-0.45003600	H	2.00543800	3.15460100	0.54555600
H	-1.78251100	-2.93149600	1.29265600	C	5.08322100	1.08800900	-0.61933700
C	0.56904600	-2.16040800	0.16727400	H	3.95987800	-0.65008800	0.00260400
C	1.15482400	-3.26147700	0.82321000	C	5.08741700	2.48332100	-0.75488800
C	0.89188900	-1.91167700	-1.17862900	H	3.97267000	4.30993100	-0.44297300
C	2.03964500	-4.10793800	0.14399200	H	5.93929200	0.50447100	-0.95228400
H	0.91374600	-3.45151600	1.86844800	H	5.95109900	2.98741300	-1.18436000
C	1.75584100	-2.77724200	-1.85909800	N	-1.80203500	1.34796200	-0.62297100
H	0.43559200	-1.07034300	-1.69354400	S	-2.87767600	2.23490300	0.26570900
C	2.33586400	-3.87123200	-1.20377900	C	-3.14764000	3.73159800	-0.72378300
H	2.48532700	-4.95272300	0.66585000	H	-3.57008600	3.43620600	-1.68865900
H	1.97289900	-2.59386000	-2.91018700	H	-2.19374100	4.25228100	-0.85377800
H	3.01081200	-4.53656400	-1.73905500	H	-3.85165600	4.36190600	-0.17031700
<b>TS14-D</b>				O	-4.12367200	1.49626100	0.29179600
H	-1.75185900	-0.23159500	1.27557200	O	-2.22930800	2.65203200	1.49631700
C	-1.50623200	-1.14555600	0.73436900	H	0.13680000	1.52008300	-1.42958800
C	-0.99286900	-2.10889600	1.74161100	H	-0.29908800	2.74326700	-0.22745300
H	-0.77289600	-3.12817100	1.41472600	<b>IN14</b>			
C	-2.79223500	-2.45500300	-1.20052900	H	0.09236500	-0.66373600	-1.48121400
C	-3.83915100	-1.79415000	-0.28376100	C	-0.03198800	-1.22424900	-0.54066100
C	-2.29416200	0.12543000	-1.29501300	C	1.32602500	-1.82995500	-0.17183900
H	-2.93930600	-2.38104800	-2.27855400	H	1.79163700	-2.32278500	-1.03195200
H	-2.32418900	-3.38340100	-0.87549400	H	1.25434000	-2.52748100	0.67017800
H	-4.07306600	-2.28343200	0.66009300	C	-0.90872000	-3.59039300	-1.46808500
H	-4.67310600	-1.26189200	-0.73880100	C	-1.23068400	-3.56857500	0.03857500
C	-0.35793200	1.67224300	-0.46186000	C	-2.49828100	-1.58257300	-1.03336600
C	-2.43616800	-1.17730700	-0.44181100	H	-1.67475900	-3.95277000	-2.15256800
C	0.26910400	0.81733800	0.64291300	H	0.10883400	-3.83383700	-1.76735600
C	1.67005800	0.52676300	0.97484600	H	-0.43004800	-3.82063200	0.73009400
C	1.76670300	-0.61467300	1.80712900	H	-2.21784000	-3.89531200	0.36127700
C	0.54076400	-1.28212700	2.45802600	C	-1.85648800	0.38658000	0.26391800
H	-0.01589600	-0.54592600	3.04429900	C	-1.15717800	-2.25606300	-0.75533600
H	0.88417900	-2.11756000	3.06827100	C	-0.46339900	-0.21881100	0.56728100
Rh	0.49369300	-1.21117700	0.12947200	C	0.58382600	0.89081100	0.81282300
H	-3.26743200	0.35822100	-1.74043500	C	1.45864100	0.80656300	1.91253700
H	-1.59910600	-0.05345600	-2.12189600	C	1.96537200	-0.44038800	2.42270400

H	1.30257300	-1.30060200	2.51676900	C	1.69170700	0.08407000	1.26404100
H	2.72684100	-0.37783900	3.19938500	C	2.00746400	-1.31599400	1.35634500
Rh	2.57634000	-0.30215900	0.36360100	C	1.30196000	-2.40294200	2.18351400
H	-3.29148100	-2.32959700	-1.12858700	H	1.58622300	-2.32080500	3.24479300
H	-2.43606800	-1.00243000	-1.97467400	H	1.72302700	-3.34881900	1.81941700
H	-0.56995100	-0.79633600	1.49683400	Rh	0.70345100	-0.98989900	-0.33620400
H	-2.18249900	1.01732600	1.09645300	H	-0.72032600	2.20584600	1.83733600
H	-1.79878200	1.00646500	-0.64714600	H	-0.08070700	2.17991900	0.16786800
Cl	2.99413700	0.33996300	-1.93126100	H	-2.23215200	-0.05698500	2.18877700
C	4.05873000	-1.56634500	0.29455700	H	-3.54679300	0.01468000	1.02192100
O	4.91563500	-2.30666000	0.23842900	Cl	1.70126700	-2.61370800	-1.82223400
N	-2.82249000	-0.69691400	0.08895700	C	-0.61264700	-0.44881600	-1.83351600
S	-4.41565700	-0.36079600	0.38995700	O	-1.22493600	-0.15580300	-2.73861500
O	-4.46265600	0.39014600	1.62630500	H	-0.73366200	-1.85030200	2.80488800
O	-5.14368900	-1.60162600	0.22877400	H	-0.21432200	-0.23144700	2.06777000
C	-4.94845200	0.75854700	-0.93984300	H	3.04690600	-1.56298300	1.14142200
H	-4.33460400	1.66498000	-0.90958100	C	2.66414900	1.04997900	0.66399200
H	-5.99804300	1.00658100	-0.75020100	C	2.63468700	2.39578600	1.07562000
H	-4.84870500	0.24236000	-1.90043200	C	3.60394500	0.65002100	-0.30888300
H	2.03091600	1.70944200	2.14476600	C	3.53237600	3.32244600	0.53776700
C	0.35359900	2.25445000	0.21536200	H	1.91753200	2.70624600	1.83415100
C	0.08518100	3.34628100	1.06270300	C	4.48835600	1.58541500	-0.85606300
C	0.36248100	2.46342800	-1.17712700	H	3.62402300	-0.38155100	-0.66002200
C	-0.15938200	4.61961600	0.53465200	C	4.45902100	2.91977400	-0.43247700
H	0.05161300	3.19291500	2.14073300	H	3.50586400	4.35738500	0.87283100
C	0.11714500	3.73627800	-1.70144800	H	5.19690800	1.26874200	-1.61865200
H	0.61177300	1.63975300	-1.84200200	H	5.15018200	3.64333000	-0.86015800
C	-0.14508300	4.81750400	-0.84998700	N	-1.82671400	1.04215700	0.42918100
H	-0.36636800	5.45102000	1.20591600	S	-2.80042300	2.11406300	-0.37099700
H	0.14408800	3.88392100	-2.77944600	O	-1.93397400	2.94542500	-1.17946500
H	-0.33589700	5.80643200	-1.26244200	O	-3.88272900	1.35178600	-0.96021000
				C	-3.53880500	3.18304200	0.90087200
<b>IN16</b>				H	-4.11342000	2.56452200	1.59800500
H	-0.70183000	-3.00858800	-0.00745900	H	-4.20043100	3.88539600	0.38299800
C	-0.72428000	-2.10849400	0.62210100	H	-2.74121000	3.72712800	1.41695300
C	-0.24489300	-2.48012900	2.05010700				
H	-0.56732100	-3.50593800	2.28125300	<b>TS15</b>			
C	-2.98181500	-1.91103800	-0.67553200	H	0.16558500	-1.22849200	1.26031300
C	-3.29351900	-2.52102700	0.69288200	C	0.34699900	-1.54480300	0.21954200
C	-2.46318800	-0.10746400	1.11422400	C	-0.91945800	-2.28067100	-0.24982300
H	-3.66213400	-1.16562400	-1.08441400	H	-1.48151300	-2.73218200	0.57903900
H	-2.51670600	-2.56128900	-1.41583800	H	-0.74636200	-3.07868200	-0.97156600
H	-3.02678100	-3.56316000	0.85891000	C	1.64965400	-3.87554700	0.47579000
H	-4.19461400	-2.19861600	1.21366800	C	1.98464900	-3.32535600	-0.92393500
C	-0.54106300	1.56982300	0.94912000	C	2.80485500	-1.55696600	0.79945500
C	-2.12727100	-1.50200300	0.53902900	H	2.46037300	-4.29444300	1.07043800
C	0.28578300	0.35922300	1.31664900	H	0.69013800	-4.37235200	0.61073800

H	1.25942600	-3.48468300	-1.72100300	C	-2.51034500	-0.40366500	0.97412600
H	3.02041400	-3.35451400	-1.25776300	H	-2.02619400	-0.61774500	-1.76658000
C	1.76310800	0.55077400	0.04967500	H	-0.97553400	-2.13986400	-1.97781300
C	1.64575600	-2.36470900	0.22165500	H	-2.54460000	-3.48684400	-0.69797900
C	0.59455300	-0.23297900	-0.58881100	H	-3.72830300	-2.09561600	-0.69507300
C	-0.71144100	0.59091700	-0.76804300	C	-0.82969100	1.52611400	0.80199200
C	-1.61526300	0.16955900	-1.79900300	C	-1.84398800	-1.68447300	0.38248300
C	-1.59117800	-1.25396300	-2.08953000	C	0.07605200	0.39793100	1.23038400
H	-0.65038400	-1.70188700	-2.39385500	C	1.50449100	0.23137700	1.17395900
H	-2.45783900	-1.68749400	-2.59009400	C	1.91686300	-1.11583500	1.42143500
Rh	-2.37142900	-0.64173600	-0.06474400	C	1.34151300	-2.11631800	2.45108300
H	3.74210200	-2.11553200	0.72268300	H	1.70553500	-1.85023700	3.45710900
H	2.60376500	-1.33969700	1.86681100	H	1.80100000	-3.07967400	2.19502400
H	0.95111200	-0.51743300	-1.58944800	Rh	0.44337900	-1.12801800	-0.23647300
H	1.98214100	1.45310300	-0.52778100	H	-1.02741600	2.23584000	1.62074700
H	1.50132800	0.84761200	1.08172900	H	-0.41340300	2.08866900	-0.04386500
N	2.94958700	-0.30813200	0.04301100	H	-2.35043600	-0.39597400	2.06056500
S	4.43812900	0.41710900	0.01476800	H	-3.58766600	-0.48180100	0.81766800
O	4.35728800	1.51743900	-0.92166100	H	-0.71412700	-1.57072900	3.05466900
O	5.41501800	-0.63983800	-0.14058700	H	-0.35576200	-0.11854700	2.07188700
C	4.67630100	1.13285700	1.66876100	N	-2.10560800	0.88555200	0.38128700
H	3.88397800	1.86498500	1.85713500	S	-3.30070900	1.95126100	-0.08456700
H	5.65425800	1.62544900	1.66746400	O	-4.54795800	1.21298300	-0.14148100
H	4.65937200	0.32773700	2.41078000	O	-3.19732200	3.17066200	0.69447500
H	-2.32799100	0.84374000	-2.26969000	C	-2.83094100	2.37287900	-1.78359800
C	-0.71287800	2.04264000	-0.36636100	H	-3.53073200	3.14788600	-2.11383600
C	-0.69542200	3.05336000	-1.34478900	H	-2.92329200	1.47889300	-2.40636600
C	-0.72150800	2.41967700	0.99094800	H	-1.80845300	2.76260600	-1.79422600
C	-0.69368800	4.40469800	-0.97644200	H	2.96353900	-1.32354500	1.19812400
H	-0.67191900	2.77708600	-2.39780400	C	2.44175000	1.26997200	0.64032700
C	-0.71746000	3.76840400	1.35916200	C	2.21550500	2.61398400	0.98648800
H	-0.75271800	1.64648900	1.75857800	C	3.57003000	0.94984500	-0.14089000
C	-0.70433700	4.76630600	0.37496700	C	3.09131400	3.61879200	0.55704500
H	-0.67935700	5.17244700	-1.74779700	H	1.36400100	2.87103000	1.61376400
H	-0.73377400	4.04056600	2.41278100	C	4.43917100	1.95394900	-0.57299600
H	-0.70378500	5.81599200	0.66119800	H	3.74951000	-0.08329100	-0.43523300
C	-3.60511600	0.79824800	0.47677900	C	4.20285000	3.29225600	-0.22597500
O	-4.36316800	1.59396000	0.75851400	H	2.90331400	4.65294300	0.83877800
Cl	-3.89724000	-2.08786200	1.12547600	H	5.29771900	1.69237200	-1.18829100
				H	4.88063800	4.07271800	-0.56620700
				C	1.17890300	-0.01202800	-1.87578900
				O	1.54810600	0.42554000	-2.85430000
				Cl	1.34468100	-3.04199400	-1.51327200
<b>TS16</b>				<b>TS25</b>			
H	-0.51924300	-3.35984800	0.56505200	H	-0.94985700	-2.55985800	0.08136500
C	-0.64085000	-2.35189300	0.97588100	C	-0.97664400	-1.77655100	0.87077200
C	-0.19712800	-2.32348600	2.44914200				
H	-0.42464100	-3.28578800	2.92999700				
C	-1.67463700	-1.56532600	-1.37029500				
C	-2.68737700	-2.40928500	-0.62088800				

C	-0.43006600	-2.41197000	2.15954500				
H	-0.93664100	-3.37472600	2.31939300	<b>IN15</b>			
C	-3.38448800	-1.66614600	-0.15684700	H	1.11797400	2.03437800	-0.80131200
C	-3.52337800	-2.21247100	1.26849900	C	1.41580200	1.94133600	0.25722200
C	-2.59629400	0.22179100	1.40521000	C	0.88585500	3.20067700	0.95748700
H	-4.11372200	-0.93269600	-0.49977800	H	1.41578000	4.09304200	0.60195500
H	-3.01812000	-2.33161200	-0.93506600	H	1.02571100	3.13796000	2.04755300
H	-3.25166000	-3.25231400	1.44388700	C	3.95714800	2.83481500	0.35452300
H	-4.33963100	-1.85068900	1.89264700	C	3.73838400	1.91239800	1.57037500
C	-0.47269900	1.39505000	0.75233100	C	3.32122600	0.49859000	-0.58379100
C	-2.38957500	-1.21155900	0.91546200	H	4.87735300	2.71779300	-0.21683100
C	0.17018500	0.09243000	1.21343300	H	3.60374700	3.86139000	0.42057100
C	1.59075300	-0.24604100	1.00721200	H	3.22823300	2.33570300	2.43449100
C	1.84507600	-1.65845500	1.14309900	H	4.51060100	1.18471300	1.81534600
C	1.10005800	-2.64417400	2.05082400	C	1.07712900	-0.47076200	-0.22934000
H	1.55550000	-2.63596000	3.05351100	C	2.93170600	1.69747000	0.28424600
H	1.28376200	-3.64663600	1.64005400	C	0.73230200	0.64598800	0.79795900
Rh	0.62521000	-1.21267400	-0.55555500	C	-0.75546900	0.82685400	1.10817100
H	-0.32599100	2.15981300	1.53528300	C	-1.36684800	2.07004400	1.00711600
H	-0.00938600	1.76750800	-0.16773700	C	-0.61629200	3.33343400	0.62672200
H	-2.26378100	0.35732100	2.44817700	Rh	-2.17829500	0.44892900	-0.52985100
H	-3.66205100	0.46222300	1.38002200	H	4.38014800	0.25440200	-0.45904300
H	-0.67860700	-1.80135900	3.03826800	H	3.12969400	0.74245200	-1.64497100
H	-0.21046600	-0.20374800	2.18201700	H	1.22198900	0.36893100	1.74659600
H	2.87704900	-1.96279100	0.96607900	H	0.59263200	-1.42032500	-0.00770700
C	2.68028500	0.75251600	0.74079500	H	0.75607600	-0.14008400	-1.23106000
C	2.59229700	2.05593100	1.26160900	N	2.52653000	-0.66548600	-0.18401900
C	3.85278200	0.39352600	0.04484000	S	3.14387100	-2.18413100	-0.27832000
C	3.62846200	2.97857900	1.06996600	O	2.26847700	-3.04359100	0.49721900
H	1.72183000	2.35340900	1.83900800	O	4.55845700	-2.09036000	0.01662200
C	4.88663500	1.31126900	-0.14456200	C	2.98661900	-2.69438900	-2.01461600
H	3.96045600	-0.61100000	-0.35752200	H	1.92873000	-2.67348100	-2.29646400
C	4.77687300	2.61326700	0.36311500	H	3.38136200	-3.71285500	-2.09233500
H	3.53245900	3.98267400	1.47831100	H	3.57295400	-2.00892300	-2.63522100
H	5.77721300	1.00997200	-0.69251100	H	-2.33690900	2.22850700	1.47447300
H	5.58142400	3.32981600	0.21124400	C	-1.59784100	-0.34208000	1.50299300
N	-1.90319400	1.17570100	0.54008600	C	-3.03449500	-0.21069500	1.50471700
S	-2.73233200	2.38717200	-0.22865800	C	-1.04460100	-1.63101900	1.79836100
O	-4.13562000	2.22362000	0.10297900	C	-3.84370000	-1.37591000	1.66953000
O	-2.04710900	3.63934300	0.03866900	H	-3.53375000	0.74541300	1.64102300
C	-2.52827500	2.01968800	-1.98652800	C	-1.86211900	-2.72823800	1.97751300
H	-1.46218500	2.01426500	-2.23198100	H	0.03105200	-1.74705900	1.90073500
H	-3.05225400	2.81085400	-2.53354300	C	-3.27376100	-2.61588100	1.87352400
H	-2.95212400	1.03256200	-2.18866200	H	-4.92600500	-1.25866900	1.67239100
C	1.98182700	-1.24760700	-1.98353000	H	-1.41269600	-3.69268500	2.20566600
O	2.72538200	-1.26405300	-2.84176600	H	-3.89967300	-3.49613100	2.00211300
Cl	-0.90130100	-1.01865200	-2.43500400	C	-2.91364900	-0.92820400	-1.68239400



O	-3.30001200	-1.75913800	-2.35684200	H	-3.88736400	-0.04570400	0.25868700
Cl	-1.38042200	1.61764400	-2.44989100	C	-4.24205100	3.34582800	0.23614600
H	-0.74258800	3.52588700	-0.44940500	H	-2.82620800	4.73391000	-0.62549700
H	-1.05936600	4.18053300	1.16625600	H	-5.44334100	1.71923300	1.00626200
				H	-4.92423800	4.12232500	0.57647900
<b>IN17</b>				C	-1.27144900	-0.12682200	1.76815600
H	0.57142900	-3.35920500	-0.65702500	O	-1.70134600	0.34996400	2.70365700
C	0.80926200	-2.41792100	-1.15646200	Cl	-1.28985700	-3.16867500	1.31160000
C	0.18315900	-2.26099300	-2.53877700				
H	0.35724700	-3.18923900	-3.10252000	<b>TS17</b>			
C	1.19954300	-1.14431200	1.68479900	H	0.09217300	-3.40402400	-0.78399200
C	2.22489300	-1.95105800	0.87301100	C	0.15431900	-2.36298000	-1.10871700
C	2.47898900	-0.40524500	-1.17977500	C	-0.24266200	-2.09249300	-2.57115900
H	1.55104200	-0.13798300	1.92545700	H	-0.33391600	-3.04451500	-3.11057100
H	0.85574700	-1.67118400	2.57866200	C	0.19743700	-2.32424100	1.63088200
H	2.11128900	-3.02405700	1.06458400	C	1.54219300	-1.97746000	0.98146600
H	3.26561000	-1.65254100	1.05007700	C	2.41544000	-0.90076800	-1.14338400
C	0.88229200	1.55452700	-0.69507600	H	0.06959800	-1.92396000	2.63778900
C	1.76749800	-1.62092900	-0.54794700	H	-0.01476400	-3.39946800	1.61947200
C	-0.06815400	0.44994500	-1.09512500	H	2.30616700	-2.77499300	0.98898300
C	-1.51816400	0.30358400	-1.16714100	H	1.98876000	-1.11040100	1.48818400
C	-1.95427400	-0.97961800	-1.53193400	C	1.36419700	1.16829000	-0.21085500
C	-1.35544400	-2.06660200	-2.44410800	C	1.22600200	-1.59482700	-0.47368700
H	-1.75965000	-1.92276700	-3.46041600	C	0.26057500	0.34216300	-0.83583800
H	-1.77799700	-3.01114400	-2.07463200	C	-1.19048600	0.65803600	-0.94735600
Rh	-0.41564400	-1.09956600	0.31240700	C	-1.96577900	-0.28777300	-1.63028800
H	0.97249500	2.32925400	-1.47994100	C	-1.60206700	-1.34753200	-2.68667400
H	0.60860900	2.03913100	0.24685000	H	-1.68922100	-0.88447400	-3.68516400
H	2.28153300	-0.33325100	-2.25615500	H	-2.40222900	-2.09774900	-2.63572100
H	3.55199600	-0.59103400	-1.05801400	Rh	-0.98465400	-1.24227700	0.29964800
H	0.65205800	-1.46572600	-3.12821000	H	1.38139600	2.19163800	-0.61792600
H	0.35248800	-0.06151000	-1.94630200	H	1.28235000	1.22662300	0.88040400
N	2.19789900	0.88099200	-0.52424400	H	2.30978100	-0.85425500	-2.23399400
S	3.35702500	1.64952500	0.35538800	H	3.31221900	-1.48931800	-0.91767700
O	2.69792800	2.33569800	1.44802800	H	0.53821000	-1.53530200	-3.10413800
O	4.42159100	0.69437800	0.59579600	H	0.55493900	0.06155600	-1.84026800
C	4.02493200	2.93587600	-0.73895800	N	2.60529200	0.45396200	-0.59461100
H	4.77850400	3.48600700	-0.16576900	S	3.97643100	0.80468700	0.27837500
H	3.21167000	3.60671800	-1.03459600	O	3.59773300	1.23827200	1.60909800
H	4.48002400	2.45416600	-1.60984800	O	4.90213000	-0.29540200	0.09135600
H	-3.01971500	-1.15761600	-1.38506600	C	4.63872800	2.25061400	-0.58595300
C	-2.46880100	1.33153600	-0.63258400	H	5.52279700	2.57726100	-0.02833900
C	-2.18312200	2.68944900	-0.86285600	H	3.88007200	3.03971100	-0.58771200
C	-3.65912200	0.99698200	0.04335900	H	4.90625200	1.95274200	-1.60342200
C	-3.06395000	3.68923700	-0.43433400	H	-3.03749500	-0.08730700	-1.60497000
H	-1.27936200	2.96440300	-1.40281200	C	-1.78014800	1.95306100	-0.48162600
C	-4.53526500	1.99588700	0.47425300	C	-1.29178300	2.66621400	0.63065500

C	-2.78751400	2.54909800	-1.26751600	H	5.34347600	-2.15443100	-0.73247500
C	-1.81197800	3.92072600	0.95593600	H	-2.36331600	1.02738600	-1.83498400
H	-0.54418600	2.21740600	1.27382500	C	-0.58142800	2.33066600	-0.37779500
C	-3.31158100	3.80270600	-0.93666200	C	-1.78156700	2.70130300	0.26571100
H	-3.14451400	2.04422300	-2.16207100	C	0.43818600	3.29626100	-0.50032400
C	-2.82555800	4.49352600	0.17795600	C	-1.93927100	3.98831800	0.78712100
H	-1.43160800	4.44432200	1.83065600	H	-2.59213300	1.98120900	0.36878300
H	-4.08933800	4.24124000	-1.55898200	C	0.27038000	4.58664900	0.01251100
H	-3.22772800	5.47128000	0.43647900	H	1.35410500	3.06358100	-1.03300200
C	-2.42219600	-2.45994000	0.73194100	C	-0.91512400	4.93550000	0.66704100
O	-3.25605700	-3.17166600	1.02834900	H	-2.86911300	4.24601700	1.29024700
Cl	-1.83138300	0.00466700	2.25518400	H	1.07115600	5.31436900	-0.10282900

**IN18**

H	-0.23769600	-2.97769900	-0.21536000
C	-0.35015100	-1.96299400	-0.62289600
C	-0.58088100	-2.02356300	-2.14769000
H	-1.17551400	-2.91452600	-2.38673400
C	-0.77164900	-0.39720200	1.64128600
C	0.65367200	-0.88955700	1.34777800
C	2.27923700	-1.62707700	-0.43521800
H	-0.86089800	0.69508500	1.63740700
H	-1.14157300	-0.76045900	2.60638500
H	0.79794300	-1.87593700	1.81331900
H	1.41719700	-0.23283200	1.78999400
C	2.24970100	0.82915600	-0.55687500
C	0.84852000	-1.10265500	-0.17412000
C	0.90986100	0.21899400	-1.01172500
C	-0.41883200	0.98117100	-1.01052100
C	-1.45366700	0.43382900	-1.73657100
C	-1.34060000	-0.76072100	-2.69453200
H	-0.86597200	-0.40516700	-3.62396700
H	-2.36423200	-1.04205700	-2.97280600
Rh	-2.02625400	-0.95881400	0.10445900
H	2.68830300	1.51733100	-1.28582500
H	2.17035400	1.34833500	0.40517400
H	2.35491100	-2.14874900	-1.40067800
H	2.62403700	-2.29238100	0.36402200
H	0.37480200	-2.14442800	-2.68282900
H	1.07122200	-0.09715000	-2.05312800
N	3.09679600	-0.38904800	-0.47129600
S	4.44687200	-0.29272600	0.48676800
O	4.78800300	1.11403100	0.56547200
O	4.27417300	-1.07321900	1.70030300
C	5.69099200	-1.13833700	-0.51918300
H	6.61201600	-1.16970500	0.07235900
H	5.83471400	-0.56725000	-1.44023400

**TS24-trans**

C	1.14252400	-1.51214600	0.85933200
C	0.23513400	0.09406700	1.22172500
C	1.23348200	1.11314000	0.66627600
C	2.48416000	-0.88182000	1.30935900
C	0.47260900	-2.57229800	1.76330000
H	0.48769600	-2.22621200	2.80579100
H	1.05180400	-3.50602800	1.72941900
H	1.25193500	2.00897700	1.29824400
H	0.96011200	1.40822900	-0.35500700
H	2.50126300	-0.82607200	2.41029500
H	3.34314200	-1.47654700	0.98293500
C	1.28078600	-1.96045400	-0.57384600
C	0.78001300	-3.10561400	-1.12432000
H	0.36583900	-3.91906500	-0.53774900
H	0.91345800	-3.27447700	-2.19085600
H	0.38908900	-0.06853900	2.29171600
H	1.76351300	-1.24696900	-1.23879600
C	-1.26037800	0.28043600	0.96230100
Rh	-0.88762000	-1.32743900	-0.32740200
C	-2.63944300	-1.71998500	-0.96278800
O	-3.68396900	-1.97302300	-1.33293700
Cl	-0.30306100	0.06485100	-2.34204900
C	-0.98062100	-2.73227600	1.22246500
H	-1.17311600	-3.73638800	0.82841900
H	-1.73909800	-2.52760800	1.97845100
C	-2.10159900	-0.05679600	2.17188800
C	-3.34806000	0.37067200	2.40946800
H	-3.87522400	1.02778200	1.72101400
H	-3.87203200	0.06720400	3.31354700

H	-1.62452200	-0.69452800	2.91643500	C	-1.70891800	0.80563000	-2.08096900
C	-1.71402100	1.60813900	0.35066800	C	-2.47232800	1.83630900	-2.47139400
C	-1.39754400	2.79024500	1.05123000	H	-2.59296500	2.74501000	-1.88660600
C	-2.55567400	1.71060800	-0.76605500	H	-3.01757200	1.77473000	-3.41110600
C	-1.86311500	4.03552500	0.62141000	C	-0.82887300	2.09877700	-0.12896400
H	-0.79873000	2.73172600	1.95867400	C	0.02754800	3.08520200	-0.65877200
C	-3.03763600	2.95511600	-1.19096400	C	-1.71759400	2.49512600	0.88495700
H	-2.81135300	0.82370900	-1.33490900	C	0.04468500	4.38901200	-0.15231600
C	-2.68702500	4.12267600	-0.50719400	H	0.66655500	2.84443000	-1.50474800
H	-1.59070200	4.93231300	1.17473700	C	-1.71355900	3.80101500	1.39014800
H	-3.67913600	3.00564600	-2.06847600	H	-2.42381100	1.77649000	1.29017500
H	-3.05376100	5.08985300	-0.84545000	C	-0.82246700	4.75224400	0.88350300
N	2.52957100	0.43538500	0.70928300	H	0.72661000	5.12155300	-0.58009200
S	3.84536200	1.07546900	-0.03743400	H	-2.41098600	4.06952300	2.18149200
O	4.97565800	0.26184500	0.36435900	H	-0.81386300	5.76596100	1.27898100
O	3.80855700	2.50347700	0.19090500	N	2.72460500	-0.51490000	-0.66223800
C	3.56818200	0.81640900	-1.81374500	S	4.14765700	-0.08469500	0.10139100
H	2.55845600	1.14974000	-2.08303000	O	3.94201900	1.15373000	0.82839000
H	4.32240500	1.40976000	-2.34132500	O	4.65526100	-1.26469400	0.77285200
H	3.69851800	-0.24765300	-2.03384800	C	5.24459400	0.28312400	-1.28864800
<b>TS24-cis</b>				H	5.36260600	-0.62430700	-1.88714600
C	0.77992900	-1.53562400	0.35625200	H	6.20312800	0.59768000	-0.86253900
C	0.33145100	-0.13740300	-0.94186900	H	4.80514200	1.09342700	-1.87858200
C	1.71141700	0.52960900	-0.84905300	H	-1.65726800	-0.07696700	-2.71277100
C	2.11096400	-1.80267100	-0.35894800	<b>4i-H</b>			
C	0.86528300	-0.85046000	1.73731700	H	-2.06853600	1.77193000	0.53815800
C	-0.55918100	-0.30593900	2.02044600	C	-2.83074900	1.10475300	0.13190300
C	-0.90614600	0.73007900	-0.80322900	C	-4.03552000	1.58773600	-0.18426300
H	1.61439100	-0.04990500	1.72588700	H	-4.28055400	2.63701000	-0.02945300
H	1.20978200	-1.59063800	2.47398300	H	-4.81760900	0.96052500	-0.61007800
H	-1.01220900	-0.73631400	2.92152000	C	-3.39987200	-1.45143300	-0.19716700
H	-0.55852000	0.77883100	2.11936400	C	-2.66792000	-1.30150600	1.14432800
H	1.75041400	1.27000300	-0.04545900	C	-1.04062300	-0.48200600	-0.71387600
H	1.87972700	1.04890900	-1.80353000	H	-3.12445700	-2.28240500	-0.84509800
H	2.76630000	-2.38528500	0.29673600	H	-4.45557500	-1.19250000	-0.22801900
H	1.94257900	-2.37307300	-1.28295000	H	-3.23867600	-0.92123500	1.98879800
C	-0.08125200	-2.76001700	0.34230000	H	-1.89076200	-2.02072400	1.39888600
C	-0.88934200	-3.18065700	1.36681300	H	-0.79216100	-1.55642500	-0.80318900
H	-0.81399200	-2.79465900	2.37878500	H	-1.09398600	-0.06591900	-1.73771300
H	-1.53512400	-4.04036900	1.20211200	C	1.20484200	0.16038800	-0.59512400
H	-0.14653900	-3.28855100	-0.60844800	H	1.13052200	0.59980900	-1.61030600
Rh	-1.49125200	-0.99699800	0.28405900	H	1.55126500	-0.88083200	-0.72022700
C	-3.28603100	-0.56106500	0.77269100	C	-2.38226000	-0.31877800	-0.01305400
O	-4.36112500	-0.32292800	1.05419200	O	-0.05307300	0.18536300	0.02559300
Cl	-2.42319000	-2.28839200	-1.68841700	C	2.16280500	0.96863700	0.24758500
H	0.25109400	-0.76213100	-1.83628500	H	1.70861700	1.84023000	0.71962800

C	3.47331100	0.73017300	0.43103700	H	-5.25951400	0.85156100	-1.20955500
C	4.24676700	-0.38558400	-0.12905100	C	-4.16746600	-1.11734600	0.50067400
H	3.71421600	-1.12440100	-0.72891300	C	-3.40659800	-0.35679200	1.59446000
C	5.56720200	-0.52944200	0.06404500	C	-1.70780000	-0.87640100	-0.30587800
H	6.13479700	0.19267400	0.65114400	H	-4.01527100	-2.19271100	0.41974600
H	6.11979500	-1.36632200	-0.35726600	H	-5.17823900	-0.79163000	0.26677200
H	4.03978500	1.42805500	1.05073000	H	-3.90874600	0.48637000	2.06386600

**TS5-H**

H	0.45370100	-1.88828400	-0.99854200
C	0.73356800	-0.83537300	-0.91396100
C	0.14724100	-0.01423300	-1.99051200
H	-0.52386300	-0.57820800	-2.63537500
H	0.83204700	0.64385600	-2.52326600
C	2.70278800	-1.64817900	0.56116000
C	3.14667000	-1.77539900	-0.89753800
C	2.79516400	0.75037200	-0.43428900
H	3.42203500	-1.28278500	1.29235000
H	2.00800200	-2.39381000	0.94646600
H	2.73874500	-2.59341300	-1.48803100
H	4.16713200	-1.49553800	-1.15614400
C	1.24152400	2.35025900	0.43893200
C	2.16552000	-0.64423200	-0.46669300
O	2.40648600	1.59226400	0.61997300
C	0.03143200	1.68440500	1.10291900
C	-1.37276400	2.05382800	0.85341300
C	-1.92979400	1.78203100	-0.40091000
H	-3.01026300	1.76823700	-0.52383900
C	-1.08493700	1.43610000	-1.60311900
H	-0.37734500	2.22832900	-1.83435900
H	-1.73527800	1.21182100	-2.44676700
Rh	-0.82720600	-0.02804400	0.19450100
H	0.24539100	1.57394500	2.16985300
H	1.08516000	2.56403900	-0.62839200
H	1.42378000	3.31489400	0.93694100
H	2.63525000	1.26573300	-1.39917500
H	3.87898100	0.62378500	-0.31657800
Cl	-2.39785600	-1.64019300	-0.79914800
C	-0.61743200	-1.15676400	1.71730200
O	-0.52638000	-1.83778100	2.62417500
H	-2.05038200	2.24989400	1.68442800

**4i-CN**

H	-2.39986600	1.80166700	-0.53937500
C	-3.25283000	1.12090600	-0.56063500
C	-4.38929800	1.50368300	-1.14923800
H	-4.48498200	2.49198500	-1.59502400

H	-5.25951400	0.85156100	-1.20955500
C	-4.16746600	-1.11734600	0.50067400
C	-3.40659800	-0.35679200	1.59446000
C	-1.70780000	-0.87640100	-0.30587800
H	-4.01527100	-2.19271100	0.41974600
H	-5.17823900	-0.79163000	0.26677200
H	-3.90874600	0.48637000	2.06386600
H	-2.73203300	-0.91175800	2.24483300
H	-1.61906400	-1.85863900	0.19448200
H	-1.70415200	-1.05374900	-1.39750400
C	0.60719500	-0.57016300	-0.36488700
H	0.62159700	-0.70914400	-1.46464100
H	0.78410500	-1.56537100	0.08647100
C	-3.00389700	-0.19698600	0.11028300
O	-0.62352000	-0.05475100	0.04823300
C	1.68151800	0.40878900	0.04888700
H	1.31824600	1.38124900	0.37714600
C	3.00958800	0.16245600	0.01738900
C	3.61833100	-1.11333800	-0.41569500
H	2.91768200	-1.89513500	-0.70669200
C	4.93657200	-1.34718800	-0.46823500
H	5.66420800	-0.58655500	-0.18878500
H	5.31808000	-2.31171700	-0.79445900
C	3.91404100	1.21736800	0.42853600
N	4.66142400	2.04166400	0.74898400

**TS5-CN**

H	1.61013500	-1.83099600	-0.27002900
C	1.45391700	-0.78176300	-0.53353800
C	0.90515800	-0.62391900	-1.89685500
H	0.67259500	-1.57648600	-2.36949700
H	1.42211300	0.08227200	-2.54505400
C	3.10630400	-0.20691300	1.37919900
C	3.94150200	-0.55819400	0.14756800
C	2.61266500	1.59474200	-0.42559600
H	3.42380500	0.62853700	2.00098300
H	2.64327200	-1.02639900	1.92772500
H	4.02270700	-1.60581300	-0.13500000
H	4.82743200	0.03849700	-0.06536100
C	0.42370600	2.56280500	-0.36284900
C	2.54854400	0.12207500	-0.01291600
O	1.70149700	2.46131300	0.19901700
C	-0.56929400	1.63810200	0.35374200
C	-1.91036500	1.31017200	-0.18729400
C	-2.00568900	0.49279400	-1.32221500
H	-2.95204700	0.01798000	-1.57016200
C	-0.81047200	0.20468200	-2.19833600

H	-0.40715700	1.12264400	-2.61984500	C	0.50702000	-0.45495800	-1.97487200
H	-1.10964200	-0.49894200	-2.97340300	H	0.08865800	-1.28463700	-2.54183900
Rh	-0.51448900	-0.45142100	0.02068300	H	1.08586500	0.24444300	-2.57651900
H	-0.61554000	1.92688500	1.40691000	C	3.05221800	-0.86052900	1.04127300
H	0.46503200	2.39390100	-1.44890700	C	3.68039400	-1.17278000	-0.31853400
H	0.10040800	3.60312900	-0.21085900	C	2.70513900	1.22729700	-0.46351300
H	2.52736500	1.69149700	-1.52316700	H	3.57675700	-0.18292100	1.71281800
H	3.60380900	1.97359200	-0.14747000	H	2.50372600	-1.65796100	1.54148200
Cl	-1.10073500	-2.76844400	-0.51485300	H	3.54055400	-2.17114600	-0.72833100
C	-0.29784700	-0.92931500	1.86179300	H	4.63441500	-0.71068500	-0.56954700
O	-0.19255600	-1.23954500	2.94916600	C	0.74255100	2.53057400	-0.03693700
C	-3.09895300	1.54730500	0.60423300	C	2.42457300	-0.25725000	-0.22271500
N	-4.03376400	1.77537000	1.24826200	O	2.02325200	2.13505400	0.36397000
				C	-0.34695900	1.70753600	0.66172400
<b>4i-F</b>				C	-1.74000900	1.70761900	0.20688800
H	-2.34838100	1.79608300	0.45805500	C	-2.10418600	1.05036100	-0.96249500
C	-3.13658700	1.09683000	0.17270900	H	-3.14940200	0.81773200	-1.14797400
C	-4.38195700	1.54199300	-0.01572400	C	-1.06572700	0.65505300	-1.99664500
H	-4.63257300	2.59186600	0.12537500	H	-0.55567700	1.53162300	-2.39005200
H	-5.19378400	0.88218900	-0.31913200	H	-1.56619200	0.09317200	-2.78323100
C	-3.67303000	-1.48486500	0.01464200	Rh	-0.68227500	-0.30705000	0.08283700
C	-2.78865800	-1.26241800	1.24883700	H	-0.28973100	1.86589200	1.74254500
C	-1.41725800	-0.48255900	-0.81708100	H	0.65416000	2.49748600	-1.13350000
H	-3.45581300	-2.33498400	-0.63042100	H	0.63744400	3.58291200	0.26563500
H	-4.73160100	-1.25139200	0.10211100	H	2.52721700	1.48551400	-1.52357900
H	-3.26264400	-0.86078700	2.14193100	H	3.77016900	1.40233800	-0.26524300
H	-1.96543800	-1.95082900	1.43369800	Cl	-1.68916500	-2.42780800	-0.62224000
H	-1.17648500	-1.55604800	-0.93477600	C	-0.43003400	-1.01289400	1.83892400
H	-1.58545400	-0.06553800	-1.82800400	O	-0.30378500	-1.44722600	2.88225700
C	0.82062700	0.18008200	-0.95730100	F	-2.69999800	2.07175800	1.05245700
H	0.62877400	0.67137600	-1.93115000				
H	1.13168100	-0.85532200	-1.17854700	<b>4i-O</b>			
C	-2.67245200	-0.32169000	0.02897200	H	-3.29092100	-0.56419800	-1.60183900
O	-0.35421700	0.18468600	-0.18813100	C	-3.57738500	-0.49256600	-0.55109300
C	1.88677400	0.93574700	-0.20896600	C	-4.74196000	-1.00694800	-0.14593800
H	1.63423800	1.94790800	0.10244100	H	-5.42036500	-1.48383700	-0.85110900
C	3.10728800	0.47506800	0.10054500	H	-5.06073200	-0.97728600	0.89501100
C	3.69206500	-0.84128300	-0.17846300	C	-2.92112900	0.70642400	1.71021800
H	3.04940300	-1.56249900	-0.67773200	C	-2.73940500	1.71733700	0.56915300
C	4.94645700	-1.16972700	0.15959100	C	-1.13338900	-0.27167500	0.09036200
H	5.60311300	-0.46160100	0.65827500	H	-2.15047000	0.65291700	2.47788000
H	5.34158600	-2.15905900	-0.05795700	H	-3.92997800	0.53496200	2.07828100
F	3.94416700	1.29867600	0.75048000	H	-3.63326500	2.19180800	0.16952100
				H	-1.84392700	2.33685900	0.55951000
<b>TS5-F</b>				H	-0.44911200	0.26451300	0.76973400
H	1.12959600	-1.97307800	-0.59021700	H	-1.05767300	-1.35113300	0.32364400
C	1.13749800	-0.88655200	-0.70709100	C	0.49092600	-0.54724000	-1.59674500

H	0.52828500	-0.49592800	-2.69277700	Cl	-0.98241900	-2.79104600	-0.58799900
H	0.56820900	-1.60884900	-1.31366300	C	-0.16937200	-1.01759100	1.84552800
C	-2.56385300	0.20483800	0.30564500	O	-0.04658100	-1.35658500	2.92516100
O	-0.78173300	-0.04763700	-1.25059900	C	-4.13829700	1.03303600	0.54236900
C	1.62215200	0.27751100	-1.01758800	H	-4.53624300	1.34879800	-0.43210300
H	1.64510300	1.30494400	-1.37308900	H	-4.06597300	-0.06368400	0.57423600
C	2.55448800	-0.14033000	-0.12775600	H	-4.79593300	1.38616900	1.34020100
C	2.61014000	-1.49992700	0.45369300	O	-2.87483800	1.62020800	0.78843300
H	1.80478800	-2.17579100	0.17830200				
C	3.57272300	-1.91636700	1.28680000	<b>4i-N</b>			
H	4.38994300	-1.26316300	1.58079200	H	-2.65147400	1.64910700	-0.86667800
H	3.55985800	-2.92690100	1.68934600	C	-3.55599900	1.04247800	-0.79536400
O	3.55920800	0.63589600	0.33662900	C	-4.64725100	1.39699200	-1.47964800
C	3.66202300	1.95792000	-0.12285600	H	-4.65780300	2.29316100	-2.09723700
H	4.54009500	2.38578400	0.36941400	H	-5.56362600	0.80897500	-1.45355600
H	3.79831300	1.99049400	-1.21435300	C	-4.66125900	-0.90824400	0.59662400
H	2.77005700	2.54486100	0.14378300	C	-3.87552700	-0.02259100	1.57339200
				C	-2.16397800	-0.97381200	-0.14020700
<b>TS5-O</b>				H	-4.58696800	-1.98924500	0.70594600
H	1.73163600	-1.80312800	-0.39679700	H	-5.63951600	-0.55986700	0.27339000
C	1.54085600	-0.74641900	-0.60150800	H	-4.32719100	0.92076000	1.87285700
C	0.93051100	-0.53264300	-1.93210800	H	-3.26090100	-0.50217400	2.33378600
H	0.69049000	-1.46447100	-2.44101800	H	-2.15469300	-1.85510700	0.52908000
H	1.41381600	0.20770600	-2.56830900	H	-2.15123700	-1.34656900	-1.18192300
C	3.27280000	-0.23084000	1.25734800	C	0.16859700	-0.82589900	-0.17321300
C	4.05682700	-0.49653100	-0.02988900	H	0.17865900	-1.17179700	-1.22670100
C	2.65065500	1.64764900	-0.42038700	H	0.25774800	-1.73129000	0.45819200
H	3.60146800	0.57918700	1.90658100	C	-3.42233000	-0.15150700	0.10169800
H	2.85220000	-1.08786100	1.78244800	O	-1.04114000	-0.17004500	0.09703700
H	4.14821800	-1.52607000	-0.37026000	C	1.29543100	0.15035500	0.10105600
H	4.91904300	0.13178300	-0.24992300	H	0.96113300	1.12170800	0.45590900
C	0.45834700	2.58253700	-0.18113600	C	2.61142100	-0.13433500	-0.02429600
C	2.64295700	0.15370600	-0.08793600	C	3.04344200	-1.47325000	-0.50290800
O	1.76458100	2.45564500	0.30929600	H	2.31262900	-2.02479900	-1.09524400
C	-0.49722900	1.58490500	0.48590600	C	4.22697300	-2.03901600	-0.22944500
C	-1.86041900	1.32362400	-0.02578500	H	4.96754900	-1.52365500	0.37926400
C	-1.97449600	0.52884400	-1.17993000	H	4.47411100	-3.03393000	-0.59411300
H	-2.90917600	0.05175100	-1.45325200	N	3.64492500	0.75135800	0.36529300
C	-0.79653900	0.31195300	-2.11086600	C	4.54108400	1.16441300	-0.71456800
H	-0.40587800	1.25479000	-2.48418800	H	4.06823200	1.92033500	-1.36982300
H	-1.11689400	-0.33981200	-2.92185600	H	5.45287200	1.60002600	-0.28518800
Rh	-0.41029400	-0.47982500	0.03311900	H	4.81673100	0.29919200	-1.32315500
H	-0.53745600	1.80403200	1.55706900	C	3.24858200	1.88573300	1.17846400
H	0.45462300	2.51577200	-1.27933500	H	4.15248600	2.38420100	1.55089600
H	0.13418900	3.60147500	0.07818400	H	2.65425000	2.63404600	0.61824100
H	2.49076000	1.80187600	-1.50327900	H	2.65654500	1.53986600	2.03320500
H	3.65055200	2.03407600	-0.18553500				

**TS5-N**

H	-2.23965300	1.52865800	-0.04829300
C	-1.85008300	0.58295400	-0.43373600
C	-1.31679600	0.72013700	-1.81289400
H	-1.33705800	1.75179000	-2.16066300
H	-1.70494100	0.00979200	-2.54292600
C	-3.31452300	-0.55799900	1.37231800
C	-4.22283600	-0.26834600	0.17416600
C	-2.45499400	-1.98679100	-0.61877900
H	-3.43270300	-1.50525500	1.89627600
H	-3.03692900	0.27959100	2.01135100
H	-4.54062600	0.75936600	0.00934900
H	-4.95706900	-1.02041900	-0.11266700
C	-0.10471900	-2.43073100	-0.69993600
C	-2.71544900	-0.59461700	-0.03956300
O	-1.34808600	-2.68514100	-0.10739800
C	0.69400900	-1.39110500	0.09949100
C	1.97363800	-0.82721300	-0.44104500
C	1.77162900	0.21930200	-1.37717100
H	2.54913900	0.93877700	-1.60579700
C	0.50212500	0.33483000	-2.20620400
H	0.30220700	-0.58320300	-2.75332100
H	0.62897700	1.17739900	-2.88416200
Rh	0.15064400	0.64557300	0.06347700
H	0.81118000	-1.78226800	1.11232900
H	-0.23378500	-2.14951900	-1.75533900
H	0.44108300	-3.38758700	-0.68861800
H	-2.38377600	-1.93398700	-1.72063200
H	-3.32437200	-2.61398100	-0.38335700
Cl	0.16146300	3.10082500	-0.15022500
C	-0.06336000	0.78918500	1.94481500
O	-0.17381100	0.89321300	3.07495700
C	3.30409300	-1.91786000	1.30188700
H	3.01122900	-1.38172600	2.22070200
H	2.67889800	-2.80997500	1.20172400
H	4.34493100	-2.24171800	1.40579900
C	4.29342900	-0.17613500	-0.15581100
H	5.20262300	-0.56363900	0.31294300
H	4.46801600	-0.10308600	-1.23649000
H	4.09101600	0.83428800	0.23663000
N	3.19085300	-1.08662300	0.11383300

**TS-C1**

C	-1.17668700	-1.02038700	1.18853300
C	0.17712500	-1.65777700	1.07502400
H	0.23191700	-2.50409000	0.38577500
H	0.67873200	-1.84184600	2.02673200

C	-2.30927800	-1.74674600	0.44225600
C	-2.75616900	0.30945000	-0.28944100
O	-3.35286600	-0.82861100	0.26354900
C	-1.52320400	0.65574700	0.57497200
C	-0.61574400	1.72829500	-0.06291800
C	0.47889900	2.18442000	0.68110700
C	0.95698800	1.34589400	1.77358500
H	0.23373700	1.00807200	2.52088900
H	1.92213100	1.60934100	2.20508100
Rh	0.81287500	0.01819000	0.11690300
H	-3.49249200	1.12106200	-0.27408500
H	-2.43323200	0.11685400	-1.32401100
C	2.62091800	-0.52978000	0.00023700
O	3.71189700	-0.83737900	-0.10289600
Cl	0.26444300	-0.88125600	-2.09176500
H	-1.43576900	-0.84002500	2.23422600
H	-1.82332700	1.05697100	1.54807500
H	1.09458200	2.98661600	0.27458600
C	-1.01537100	2.37355800	-1.37613600
H	-0.31546000	3.18110800	-1.62060500
H	-2.02658000	2.80059400	-1.32054900
H	-0.98933900	1.63813400	-2.19073700
H	-1.92744600	-2.10992600	-0.52644400
H	-2.68945700	-2.58817600	1.03190000

**TS-C2**

H	-0.53548600	-2.29810200	-1.10154900
C	0.10296900	-1.42212900	-1.23522100
C	-0.45824700	-0.43912700	-2.23286000
H	-1.45104100	-0.72782400	-2.58034100
C	1.62454500	-1.74581000	-1.21301100
C	2.61861300	-0.03273900	0.16736000
O	2.29626900	-1.40991700	-0.00849000
C	1.48047800	0.81552000	-0.36118100
C	0.74713700	1.95624800	0.18149700
C	-0.48470100	2.10585000	-0.48183100
C	-0.77663800	1.31988000	-1.77960000
H	-0.15026900	1.73124800	-2.57524200
H	-1.83463900	1.43012300	-2.01900800
Rh	-0.41073400	-0.00698400	0.12369300
H	3.55572600	0.18719400	-0.37345900
H	2.79741800	0.10214600	1.24113700
H	2.13074000	-1.27336500	-2.07389300
H	1.75944500	-2.82934000	-1.30309300
Cl	-2.78229200	-0.46660200	0.44251300
C	-0.01943800	-1.10371100	1.63443900
O	0.15437600	-1.74040100	2.56015000

H	0.22218700	-0.24424300	-3.06518600
H	1.50259200	0.82508700	-1.45183200
H	-1.25424900	2.78527800	-0.12418400
C	1.12269900	2.71609600	1.43308100
H	0.24699400	3.19004500	1.89112700
H	1.85407300	3.49882000	1.18607500
H	1.58886300	2.05154300	2.17119300

**TS-C3**

H	-1.25948000	-1.04092200	-1.87453300
C	-1.20151100	-1.20625300	-0.79765900
C	0.04061500	-1.93790600	-0.42837400
H	0.62511500	-2.30414800	-1.27283700
H	-0.05415200	-2.65400600	0.39210800
C	-2.50586600	-1.75774900	-0.20292000
C	-2.87870000	0.38070700	0.31829500
O	-3.47519100	-0.75241200	-0.23522400
C	-1.48350900	0.58201700	-0.32913400
C	-0.65059500	1.61889300	0.43610300
C	-0.14286600	1.32687800	1.70542100
H	0.43966400	2.09076900	2.22066400
C	-0.08741400	-0.07366800	2.12491600
H	-1.00557800	-0.66248400	2.11532000
H	0.53801200	-0.28863400	2.99131200
C	-0.49454100	2.97193100	-0.22644500
H	0.14754900	3.62926800	0.37204500
H	-1.47161700	3.46082200	-0.35286700
H	-0.03867900	2.84224100	-1.21790800
Rh	0.72406800	-0.11035700	0.16980700
H	-1.58189900	0.96004900	-1.34794300
H	-2.78356900	0.28732700	1.41247300
H	-3.51458400	1.24526600	0.09600900
C	2.47905400	-0.68394000	0.62156700
O	3.53773600	-1.01023800	0.88101000
Cl	1.38952500	0.52251200	-2.10037000
H	-2.32558000	-2.10316200	0.83206500
H	-2.86855200	-2.60328100	-0.79782800

**TS-C4**

H	-0.33934100	-2.53836700	0.80241000
C	0.40218600	-1.90175000	0.31663600
C	0.40406800	-1.89333000	-1.14290000
H	-0.51192700	-2.23019600	-1.62509600
H	1.33082000	-2.18645100	-1.62973700
C	1.80079600	-1.84123700	0.93743200
C	2.66454100	0.34606700	0.47884900
O	2.64905200	-1.02813700	0.16004100

C	1.30543500	1.07995700	0.59115200
C	0.66082000	1.92914500	-0.44186100
C	0.23886000	1.29295900	-1.61726200
H	-0.47375600	1.78487700	-2.27603100
C	0.70240100	-0.08656200	-1.96763300
H	1.78157700	-0.19723100	-1.90848500
H	0.27766000	-0.41237600	-2.91574300
C	0.23112500	3.34697100	-0.12168800
H	-0.59291000	3.67678000	-0.76503900
H	1.08075600	4.02994900	-0.26735700
H	-0.08244500	3.43318800	0.92603000
Rh	-0.42297600	-0.00524000	0.05652800
H	1.24223000	1.57022100	1.56727100
Cl	-2.60164600	-0.70571500	-0.84590900
C	-1.30190000	0.15649900	1.74528300
O	-1.84870600	0.25197600	2.73872600
H	2.25723200	-2.84240000	0.92735900
H	1.76408400	-1.49690300	1.98326600
H	3.17512000	0.47322000	1.44815400
H	3.30001700	0.80560400	-0.28847900

**TS-C5**

H	-1.24386000	-1.13269700	-1.21643300
C	-1.12822500	-1.27952000	-0.13954700
C	0.13148300	-1.98932300	0.15739900
H	0.55045600	-2.53429100	-0.68985100
H	0.17945700	-2.52696800	1.10761700
C	-3.65964900	-1.10445000	-0.07653200
C	-2.53887900	0.93854000	-0.41385400
C	-2.41692600	-1.77187600	0.53478100
O	-3.66950300	0.28771800	0.09131500
C	-1.27498000	0.60266200	0.41506400
C	-0.24974600	1.72881400	0.43453700
C	0.69910400	1.69499300	1.46907000
C	0.84990000	0.44097600	2.20557300
H	-0.03723200	-0.02219200	2.64482800
H	1.72622000	0.36241200	2.84864300
Rh	0.95908500	-0.10888600	0.16061400
H	-4.57424600	-1.47650100	0.39943600
H	-3.70255100	-1.35682100	-1.15239400
H	-1.58292900	0.38968500	1.44074600
H	-2.75822900	2.00711900	-0.31995400
H	-2.37730000	0.71343500	-1.48232600
Cl	0.95158800	0.00742300	-2.29610100
C	2.77392000	-0.67700500	0.17391600
O	3.86272400	-1.00797700	0.16713400
H	1.43980300	2.49163400	1.53533900



C -0.30391900 2.85922700 -0.57238600  
H 0.60106200 3.47264300 -0.49399400  
H -1.17338800 3.50876700 -0.39947300  
H -0.35522300 2.45909600 -1.59290900  
H -2.38285100 -1.62234900 1.62295000  
H -2.48328900 -2.85546100 0.35812700

**TS-C6**

H 0.36426300 -2.57597300 0.32911100  
C -0.26189000 -1.75920600 0.69709300  
C 0.26836200 -1.17326100 1.97135400  
H 1.07502200 -1.76142100 2.41039000  
C -2.82820700 -0.97583700 0.57111600  
C -2.33163100 1.23733900 -0.20096300  
C -1.75577200 -2.09302200 0.53973900  
O -2.73651200 -0.07971300 -0.51616000  
C -1.02804700 1.22359500 0.57933800  
C 0.11577200 2.12352700 0.41702100  
C 1.25942500 1.62604600 1.05949300  
C 1.16965600 0.45677600 2.04907900  
H 0.62843300 0.77835800 2.94256300  
H 2.18139400 0.13271000 2.29037300  
Rh 0.50540200 -0.06178000 -0.12895100  
H -3.12863000 1.74401500 0.37298300  
H -2.23012200 1.75307400 -1.16361300  
H -2.81655300 -0.43669600 1.53090700  
H -3.80818200 -1.46955000 0.49803100  
Cl 2.66597400 -1.08607900 -0.64392900  
C -0.11322400 -0.41908100 -1.89506100  
O -0.42998400 -0.63223800 -2.96649600  
H -0.52012300 -0.95041700 2.69324100  
H -1.18543700 0.92128000 1.61691700  
H 2.24405200 2.05085200 0.87924100  
C 0.15563900 3.30878800 -0.52251500  
H 1.18619700 3.57530800 -0.78344600  
H -0.31854800 4.17751900 -0.04365800  
H -0.39554100 3.10225400 -1.44804700  
H -1.86927700 -2.61042300 -0.42336000  
H -2.04014200 -2.82582000 1.31502800

**TS-C7**

C -1.13409300 -1.20456800 0.66321400  
C 0.14923500 -1.91033400 0.73198700  
H 0.34368400 -2.65289600 -0.04336000  
H 0.47903500 -2.19034100 1.73332000  
C -3.61143600 -1.09045100 0.15708400  
C -2.59271600 1.01977900 0.46772400

C -2.27515800 -1.77630200 -0.18257800  
O -3.63194900 0.28772400 -0.11140800  
C -1.22950500 0.66834000 -0.18076400  
C -0.21863400 1.80414200 -0.19226300  
C 0.58665800 2.04875700 0.92407200  
H 1.34095200 2.83312400 0.85742600  
C 0.63683600 1.03987200 1.98363000  
H -0.30196500 0.74137000 2.45380900  
H 1.44766100 1.14719800 2.70432900  
C -0.13371500 2.62418700 -1.46266500  
H 0.69091800 3.34540900 -1.40969200  
H -1.07024000 3.17649600 -1.62941700  
H 0.03245300 1.95882700 -2.32015000  
Rh 0.91521600 -0.07274900 0.19869000  
H -1.41561600 0.38499100 -1.21970500  
H -2.57559900 0.91054700 1.56704800  
H -2.81289100 2.07035800 0.24017400  
H -3.83181600 -1.26513200 1.22768100  
H -4.42715800 -1.52436900 -0.43204600  
C 2.76225100 -0.51825700 0.43664500  
O 3.86075300 -0.78633800 0.55986600  
Cl 1.01914900 -0.73343800 -2.16484200  
H -1.47110500 -0.87466700 1.64761400  
H -2.03618700 -1.71856200 -1.25216000  
H -2.37113400 -2.84227400 0.07220600

**TS-C8**

H 0.01442800 -2.59224500 0.05540900  
C 0.66347800 -1.75653900 -0.21680500  
C 0.50809700 -1.37538500 -1.63555600  
H -0.28263000 -1.92730600 -2.14051600  
H 1.42562200 -1.28341500 -2.21577700  
C 3.15405800 -0.86080900 0.01907500  
C 2.26417400 1.35444000 -0.16538600  
C 2.05428000 -1.86718400 0.42099200  
O 3.04059200 0.43282300 0.55040800  
C 0.85003600 1.46692700 0.41473400  
C -0.28500800 2.13933800 -0.26112000  
C -0.80825200 1.50594700 -1.39477300  
H -1.79291100 1.78804200 -1.76165300  
C -0.09352800 0.39528000 -2.13226100  
H 0.87355500 0.72426600 -2.50343000  
H -0.73519200 0.03849800 -2.93614800  
C -1.03093100 3.27879800 0.40460600  
H -2.06300400 3.35702500 0.04338400  
H -0.51526400 4.22702400 0.19348000  
H -1.04469700 3.15096500 1.49417100

Rh	-0.53468600	-0.09679400	0.09399400
H	0.94021700	1.78426300	1.45903600
H	2.27509900	1.11167900	-1.23711900
H	2.76576100	2.32817400	-0.05320100
H	3.24622800	-0.80875900	-1.08104300
H	4.10702000	-1.25010800	0.40076300
Cl	-2.54573100	-1.38012600	-0.51263100
C	-0.88438700	-0.41129200	1.94179400
O	-1.11996600	-0.59966800	3.03894200
H	1.95743300	-1.84635600	1.51488600
H	2.44952800	-2.86625400	0.16614500

### TS-C9

H	-1.08025000	-0.17662400	-1.58178900
C	-1.13721300	-0.62450400	-0.58607100
C	-0.12937200	-1.70821900	-0.46408400
H	0.21226200	-2.09690800	-1.42471400
H	-0.31678500	-2.48250700	0.28334400
C	-3.14199800	-2.31233300	-0.24436900
C	-2.90430700	-1.64625100	1.11737500
C	-3.51789900	0.23492900	-0.61423100
H	-4.16984300	-2.42812000	-0.58627900
H	-2.46761000	-3.10838200	-0.55201400
H	-2.07676500	-2.01487100	1.72264700
H	-3.76912400	-1.31833900	1.69199400
C	-1.87643600	1.87941000	-0.27272700
C	-2.57845700	-0.88025800	-0.17248500
O	-3.19451500	1.47472100	-0.04164500
C	-0.86093400	0.96597600	0.46365200
C	0.41568500	1.71810400	0.85108100
C	1.18482600	1.16741000	1.88754700
C	0.93688200	-0.22950100	2.23674300
H	-0.08329700	-0.53830800	2.47599300
H	1.68229300	-0.70844300	2.87139900
Rh	1.15537100	-0.22841500	0.12204500
H	-4.54866800	0.01414800	-0.31188500
H	-3.48667500	0.30967100	-1.71761800
H	-1.33416600	0.58946100	1.37322700
H	-1.81422900	2.89354000	0.13375100
H	-1.64381900	1.92448700	-1.35136200
Cl	1.47196600	0.53185200	-2.19463300
C	2.72902000	-1.29053800	0.04353800
O	3.68403400	-1.90682700	-0.01496000
H	2.08454100	1.68798500	2.21488200
C	0.76325300	3.05369400	0.22493600
H	1.79108000	3.33069900	0.48638700
H	0.09598300	3.84991100	0.58425300

H	0.69552800	2.99914700	-0.86808100
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### TS-C10

H	-1.30602900	-1.98760800	0.18728800
C	-1.16419800	-0.98210100	0.59176500
C	-0.43240400	-0.99896200	1.89838800
H	-0.31107400	-2.00148900	2.30914200
C	-3.39406300	-0.64628300	-0.66287900
C	-3.74543200	-0.74696100	0.82564200
C	-2.34584700	1.41393100	0.48823300
H	-3.92500500	0.08547600	-1.26931800
H	-3.13452000	-1.56413800	-1.18826300
H	-3.70886100	-1.73001500	1.29142200
H	-4.51907900	-0.08952800	1.22127400
C	-0.37195000	2.62261400	-0.14457800
C	-2.39795500	-0.11698700	0.38353000
O	-1.59080100	2.02470900	-0.53889500
C	0.48095200	1.63821700	0.63755300
C	1.92762900	1.43396600	0.52318500
C	2.32818600	0.23714500	1.13831300
C	1.38014900	-0.52747600	2.06631200
H	1.19230900	0.06303400	2.96625300
H	1.82612100	-1.49260400	2.30310200
Rh	0.63223400	-0.33552000	-0.12779200
H	-0.57748500	3.52788700	0.45478700
H	0.11515500	2.93749900	-1.07542500
H	-1.98726800	1.73006000	1.48051600
H	-3.37605000	1.78475700	0.39018100
Cl	1.39595300	-2.59536300	-0.66913900
C	0.02211300	-0.07603800	-1.91766300
O	-0.30281300	0.03825300	-3.00138100
H	-0.84126500	-0.29519300	2.62534800
H	0.11480600	1.51406700	1.65885200
H	3.32013800	-0.17921700	0.97987600
C	2.85072400	2.25009700	-0.35492300
H	3.75642300	1.68726500	-0.60843500
H	3.14715800	3.16928200	0.17040600
H	2.35426800	2.54936000	-1.28605300

### TS-C11

H	-1.25515000	-1.33365100	-1.14706900
C	-1.22810500	-1.39073000	-0.05641400
C	0.00629100	-2.00049600	0.43600100
H	0.52594300	-2.63259700	-0.28449700
H	0.01620400	-2.36732600	1.46478700
C	-2.60286500	-1.69358100	0.52137600
C	-2.84080100	0.46800200	-0.31045000

O	-3.50920300	-0.70961900	0.07880800
C	-1.49875600	0.50392200	0.41810400
C	-0.61457900	1.69858300	0.20142000
C	0.38266800	1.91480100	1.17179100
C	0.66110400	0.82395100	2.10945400
H	-0.16245100	0.39943500	2.68866700
H	1.56947100	0.93060400	2.70266200
Rh	0.75769200	-0.05959000	0.18751400
H	-1.67734300	0.34911600	1.48440600
H	-3.45744000	1.32180800	0.00257300
H	-2.70580900	0.51232400	-1.40228200
Cl	0.83564700	-0.27771000	-2.26768800
C	2.61568400	-0.48304200	0.26297700
O	3.72748700	-0.72155600	0.29032600
H	1.04783200	2.77116000	1.06604600
C	-0.83965100	2.61904100	-0.97779900
H	-0.09093800	3.41935200	-0.98693300
H	-1.83805300	3.07744400	-0.93170000
H	-0.75160400	2.05591100	-1.91653300
H	-2.57754200	-1.74737900	1.62265600
H	-2.93746800	-2.66688700	0.13797700

**TS-C12**

H	1.79875000	0.47701800	-1.82223600
C	1.21785800	-0.38220500	-1.48766100
C	0.01673000	-0.38743000	-2.36282200
H	-0.68784100	-1.22168100	-2.32693200
C	2.27894900	-1.22141900	-0.76680400
C	2.29718200	0.56136700	1.02343900
O	2.96631100	-0.34835100	0.13801800
C	1.18603500	1.29063500	0.27096000
C	-0.07807800	1.94995300	0.61601100
C	-0.99075400	1.88233900	-0.47789500
C	-0.68541600	1.32734000	-1.87201200
H	0.13492900	1.86684400	-2.35300700
H	-1.59273100	1.34838100	-2.47676000
Rh	-0.36031700	-0.15261700	-0.04706200
H	3.10589100	1.23486600	1.33701700
H	1.90817800	0.04992300	1.91518500
Cl	-2.63029700	-1.03092300	0.10910900
C	0.00634500	-1.62972500	1.15264700
O	0.11208300	-2.45277200	1.93550400
H	0.18415200	-0.06032200	-3.39191500
H	1.58867300	1.72527500	-0.64062800
H	-2.03437500	2.11769100	-0.27851700
C	-0.47636600	2.46184400	1.98151600
H	-1.56484800	2.44776100	2.10928700

H	-0.12106300	3.49418200	2.11380900
H	-0.02183100	1.84889400	2.76939000
H	3.07172400	-1.51941200	-1.46703600
H	1.89762800	-2.12314300	-0.27714800

**TS-C13**

C	-1.26187700	-1.34101700	0.55665500
C	0.01621600	-2.02987500	0.41854200
H	0.19254400	-2.59571700	-0.49740400
H	0.40460100	-2.48474000	1.32989200
C	-2.52544700	-1.70086100	-0.20556600
C	-2.86661900	0.53281200	0.36913200
O	-3.48170300	-0.69097200	0.04098700
C	-1.45052900	0.52614400	-0.21026200
C	-0.56513600	1.74174300	-0.03351900
C	0.18929800	1.92808800	1.12973400
H	0.87113600	2.77787800	1.16669100
C	0.30549500	0.82437800	2.08330600
H	-0.61234200	0.40976700	2.50151200
H	1.09331100	0.92621700	2.82994000
C	-0.50180300	2.70234600	-1.20444800
H	0.22914000	3.49878500	-1.01996100
H	-1.48453800	3.16465500	-1.37721700
H	-0.21092600	2.15737100	-2.11305100
Rh	0.71567500	-0.07757900	0.19936700
H	-1.51608600	0.31096300	-1.28184500
H	-2.86916000	0.71184000	1.45708700
H	-3.44145900	1.33688400	-0.11010900
C	2.58300200	-0.42749900	0.46568500
O	3.69297100	-0.63323900	0.60303100
Cl	0.98089100	-0.41632100	-2.21939000
H	-1.51034800	-1.11816200	1.59489000
H	-2.92483700	-2.64368000	0.19130800
H	-2.32727400	-1.82742600	-1.28134500

**TS-C14**

H	-1.72292500	-1.29216700	-1.24551900
C	-1.62141800	-0.21974100	-1.07778900
C	-0.95436200	0.40222000	-2.21800900
H	-0.85028900	1.49104500	-2.22938800
C	-2.78430700	0.23208800	-0.21609900
C	-1.87901600	-1.50051000	1.17899800
O	-2.64549000	-0.32025500	1.08733600
C	-0.35172300	-1.24348500	1.22114000
C	0.80317900	-1.77381900	0.51960300
C	1.17171800	-1.51488700	-0.85403500
H	2.25784600	-1.43557600	-0.92633800

C	0.52069700	-1.14819400	-2.11050700
H	-0.30564400	-1.76144100	-2.45282000
H	1.23215300	-0.88755700	-2.89227300
C	2.02545800	-2.06505300	1.39561100
H	2.64758400	-2.83815500	0.92876400
H	1.72137000	-2.41847700	2.38591300
H	2.63234600	-1.15403900	1.50551600
Rh	0.22220800	0.30727500	-0.19887800
H	-0.06711000	-1.03538600	2.25660300
H	-2.15603200	-2.24362600	0.41924400
H	-2.15071800	-1.92373100	2.15322800
Cl	2.45292800	1.29491900	0.14180900
C	-0.39935300	1.89779100	0.72097000
O	-0.66738800	2.82560500	1.32097600
H	-1.03963100	0.01603600	-3.23174300
H	-2.84346200	1.32234500	-0.10936900
H	-3.73685300	-0.12152100	-0.64883800

#### TS-C15

C	-1.04271700	-0.88045400	1.35229700
C	0.33297000	-1.36162000	1.58222800
H	0.53987600	-2.36171300	1.19648200
H	0.76207300	-1.16295000	2.56554800
C	-3.27346300	-1.23648300	0.07563400
C	-2.71601500	0.98564900	0.38984300
C	-1.90511800	-1.79991500	0.48072200
O	-3.17624600	0.03571500	-0.51370400
C	-1.19051900	0.99188200	0.65761800
C	-0.38955500	1.74285300	-0.38450500
C	0.84361800	2.26669500	0.04377500
C	1.38099000	1.76355100	1.30998800
H	0.76490100	1.81371800	2.21018400
H	2.42479500	2.00551200	1.51175200
Rh	0.91140600	0.03254300	0.17025600
H	-3.22410400	0.85899400	1.36415500
H	-2.99809600	1.96940300	-0.00531100
H	-3.94441400	-1.17742500	0.95397200
H	-3.73901500	-1.89084700	-0.66909700
C	2.70984700	-0.56968700	-0.00402100
O	3.78256300	-0.92587400	-0.13096800
Cl	0.49579700	-1.32605200	-1.85034100
H	-1.54335000	-0.51319300	2.25205500
H	-1.02492200	1.45227800	1.63289600
H	1.45688200	2.82785600	-0.66088500
C	-0.93846000	1.95425600	-1.77864200
H	-0.13606800	2.25500700	-2.46151900
H	-1.70968800	2.73865800	-1.77977500

H	-1.38735200	1.02656800	-2.15021300
H	-1.33486900	-2.06009500	-0.41786900
H	-2.06845800	-2.72242300	1.05967600

#### TS-C16

H	1.14734000	-0.15235400	-2.14063200
C	0.73767800	-0.92117700	-1.47756200
C	-0.60750700	-1.23277300	-2.02296400
H	-1.18359100	-2.04280200	-1.57066400
C	2.98667800	-0.51776900	-0.48890500
C	2.01127400	1.63600500	0.20826500
C	1.96752500	-1.63540900	-0.92520900
O	2.57486000	0.36822400	0.53461800
C	0.65070800	1.54236400	-0.49665000
C	-0.65492300	2.10670200	-0.11019500
C	-1.71727900	1.43688600	-0.74881000
C	-1.52129600	0.42709400	-1.89485400
H	-0.95872200	0.89116600	-2.70990500
H	-2.50009900	0.07569300	-2.22143800
Rh	-0.43028900	-0.14847900	0.07758800
H	2.72750800	2.19133900	-0.42012300
H	1.93350700	2.15171400	1.17309200
H	3.27059700	0.05831500	-1.38729700
H	3.88978200	-1.01105900	-0.10724800
Cl	-2.19147200	-1.62665000	0.93840900
C	0.54420900	-0.77294100	1.62093000
O	0.97908000	-1.16699400	2.59590900
H	-0.69465800	-1.21899200	-3.11185700
H	0.76151300	1.52195000	-1.58137100
H	-2.73727800	1.58813800	-0.40266600
C	-0.88083400	3.11114600	0.99797300
H	-1.91741900	3.08556900	1.35289500
H	-0.66039800	4.12567800	0.63572200
H	-0.21798600	2.91364100	1.84944800
H	2.48006200	-2.20956900	-1.71601500
H	1.74896400	-2.32443100	-0.10267600

#### TS-C17

H	-0.65042100	-0.81065800	-2.03736500
C	-1.12215300	-0.98046900	-1.06861900
C	-0.31200900	-1.86874300	-0.22689400
H	0.37291500	-2.51220500	-0.78108500
H	-0.80332700	-2.34244900	0.62502700
C	-3.36802700	-1.17159300	0.16062300
C	-2.48907000	0.99935900	0.39867900
C	-2.63456900	-1.17248900	-1.19069100
O	-2.83874000	-0.20173600	1.02734800

C	-1.18999900	0.94746800	-0.47978300
C	-0.09640400	1.88240600	0.01916400
C	0.34490300	1.76042500	1.34969600
H	1.13057500	2.42892400	1.70127200
C	-0.00478300	0.54658400	2.08741900
H	-1.03856600	0.21885300	2.16698800
H	0.57408200	0.37065200	2.99466400
C	0.42591900	2.94606900	-0.92360300
H	1.26627000	3.48812000	-0.47425700
H	-0.36686300	3.66863800	-1.16603100
H	0.77530000	2.48017600	-1.85381900
Rh	0.75401000	-0.14170100	0.22597000
H	-1.38451400	1.21315100	-1.52101200
H	-2.34534100	1.72158200	1.20626700
H	-3.31870800	1.36298600	-0.23041000
C	2.27721300	-1.02147100	0.96336100
O	3.19959500	-1.53182600	1.39133000
Cl	1.85456200	-0.15227700	-1.98872700
H	-3.25198400	-2.13330100	0.67410000
H	-4.44616400	-0.99684400	-0.00173600
H	-3.04307000	-0.39539200	-1.85072400
H	-2.80115900	-2.13378700	-1.69772100

**TS-C18**

H	-1.51791500	0.05709800	1.69984200
C	-1.08672200	-0.81468000	1.20704300
C	0.05487000	-1.20354500	2.02542800
H	0.66356400	-2.06809800	1.75365300
C	-3.29827400	-0.46032200	0.18446800
C	-2.05542600	1.64339500	0.01842400
C	-2.25232100	-1.55507700	0.55363600
O	-2.82524800	0.61907900	-0.58679500
C	-0.60742900	1.50937200	-0.48653300
C	0.66457000	2.16662900	-0.05484700
C	1.41399400	1.62501100	0.98730900
H	2.47647100	1.86516300	1.00604700
C	0.95621100	0.64943800	2.03323800
H	0.10892600	1.02354600	2.60898800
H	1.79372000	0.33731200	2.65488600
C	1.32126900	3.16226200	-0.99451500
H	2.37385600	3.33099700	-0.73964600
H	0.79201400	4.12493500	-0.94383800
H	1.26118500	2.81296200	-2.03365100
Rh	0.47641600	-0.21834700	-0.06828400
H	-0.69356700	1.63925000	-1.57317300
H	-2.16716200	1.65749200	1.11067300
H	-2.46493300	2.59516700	-0.35342300

H	-3.73323400	-0.07948400	1.12635500
H	-4.11071300	-0.90418500	-0.40332700
Cl	2.54062200	-1.57578600	-0.21641500
C	-0.04048400	-1.09692100	-1.68968000
O	-0.31797900	-1.63339300	-2.65381800
H	0.01579500	-1.02914000	3.09979000
H	-1.96461000	-2.15575900	-0.31527300
H	-2.73841900	-2.23216600	1.27500300

**TS-C19**

C	-1.13901200	-0.49584100	1.01995500
C	-0.03883500	-1.51660900	0.95199500
H	-0.18818200	-2.32789400	0.23787900
H	0.29861800	-1.87116500	1.92783700
C	-2.49615400	-1.69243900	-0.94895900
C	-2.91834200	-2.34440200	0.36903700
C	-3.56103100	0.15178600	0.56763000
H	-3.27882700	-1.43697700	-1.66224200
H	-1.55150600	-1.97653400	-1.40685000
H	-2.25288000	-3.07732300	0.81959400
H	-3.97792000	-2.53053400	0.54125000
C	-1.97697000	1.56155000	-0.51701000
C	-2.45726300	-0.86909800	0.34909200
O	-3.21334900	1.44942600	0.13007300
C	-0.80836800	1.27302100	0.44990000
C	0.49292000	1.97991000	-0.00227200
C	1.57125800	1.99003200	0.88946300
C	1.58048800	0.98146000	1.94056400
H	0.69139500	0.88122600	2.56940100
H	2.50988700	0.85556700	2.49526600
Rh	1.19480600	-0.12096000	0.15871300
H	-1.92893300	2.60460100	-0.84283400
H	-1.89549900	0.91648200	-1.40448100
C	2.70779500	-1.26043300	0.16287300
O	3.62966700	-1.92757400	0.13341300
Cl	0.71090200	-0.64594200	-2.18278000
H	-1.32231400	-0.22544000	2.06403500
H	-1.04648600	1.70126800	1.42849500
H	2.47602500	2.53534000	0.62114600
C	0.52930000	2.77781200	-1.29194600
H	1.55700400	3.09735900	-1.49973600
H	-0.10114700	3.67562100	-1.22417600
H	0.18745200	2.16525100	-2.13516500
H	-4.47337300	-0.17286900	0.04339600
H	-3.80016900	0.21492200	1.64252300

**TS-C20**

H	-0.94787300	0.59889700	1.99184800	C	-3.60059400	-1.87584100	-0.42054700
C	-1.04847500	-0.20895000	1.26031400	H	-2.08879200	-1.85224300	-1.95938600
C	-0.33050200	-1.37023200	1.83907900	C	-3.24146000	-0.36287700	1.43621500
H	-0.36133300	-2.32492700	1.30874800	H	-1.44172000	0.82356100	1.36168900
C	-3.03962700	-0.90076600	-0.37373300	C	2.02658900	-2.57655100	1.31334900
C	-3.67620900	-0.48896900	0.96642800	H	0.12941400	-1.55118700	1.38499900
C	-2.33209100	1.61809300	0.16659100	C	3.34819800	-2.23215200	-0.68809500
H	-3.49966400	-0.53352700	-1.29040100	H	2.46757600	-0.95393300	-2.18860700
H	-2.60846000	-1.89854500	-0.45238700	C	1.68507600	3.07753200	0.99167600
H	-3.66489300	-1.21103200	1.78075400	H	2.02149500	0.95639900	0.78846200
H	-4.55338600	0.15781600	0.94141400	C	-0.15183600	3.99213400	-0.29161900
C	-0.10737000	2.64040400	-0.15417800	H	-1.23272400	2.59399300	-1.52401900
C	-2.31964100	0.10396600	0.51918800	C	-4.02324800	-1.33486000	0.79979100
O	-1.30491400	2.08455100	-0.69122100	H	-4.20680400	-2.62580700	-0.92575000
C	0.74438100	1.63105200	0.62900700	H	-3.56696800	0.06435400	2.38333000
C	2.14228100	1.20994300	0.43006400	C	3.18845300	-2.82365000	0.57062700
C	2.41022400	-0.02452700	1.05607500	H	1.89494700	-3.03893600	2.29028000
C	1.43944700	-0.72109300	2.02703700	H	4.24462200	-2.42584800	-1.27457100
H	1.19233800	-0.05072100	2.85565300	C	0.90512100	4.17413100	0.61104300
H	1.89872100	-1.64681200	2.37428300	H	2.51109300	3.21049600	1.68854300
Rh	0.54587400	-0.31836200	-0.09249500	H	-0.76235500	4.84025400	-0.59695800
H	-0.36921600	3.49594600	0.49083000	H	-4.95941600	-1.66260000	1.24836600
H	0.42574400	3.02497600	-1.03193900	H	1.12139600	5.16449800	1.00768200
H	-2.31882000	2.19527100	1.10863100	H	3.96236700	-3.47742100	0.96920300
H	-3.27319300	1.84246500	-0.35312500				
Cl	1.02321900	-2.54130800	-1.02170300	<b>IN19</b>			
C	-0.38924600	-0.07426700	-1.76243400	H	1.34198900	1.53198600	1.50075700
O	-0.83614900	-0.03596400	-2.80796900	C	2.14929000	0.84900600	1.23828800
H	-0.42326700	-1.49671000	2.92051300	C	2.39065300	-0.21517500	2.07291300
H	0.48368500	1.62904000	1.68816500	H	1.78474700	-0.34736400	2.96706500
H	3.32249200	-0.56395900	0.81110200	C	2.54950800	2.48077900	-0.74527400
C	3.12826700	1.87689600	-0.50356000	C	3.60827400	2.76294600	0.30458600
H	3.94166500	1.19570300	-0.77835400	C	3.98097300	0.28792900	-0.47868500
H	3.56333200	2.76239400	-0.01786300	H	2.84431500	2.47345500	-1.79292900
H	2.63293400	2.21424700	-1.42241500	H	1.53848000	2.84348100	-0.56478400
				H	3.32174300	3.30716400	1.20176900
PPh <sub>3</sub>				H	4.63446000	2.93045000	-0.01900800
P	-0.04728000	-0.00017900	-1.21968000	C	3.57615000	-2.10320900	-0.72026200
C	-1.59867500	-0.47419900	-0.36530100	C	3.05131300	1.31587900	0.13906000
C	1.17994600	-1.12890700	-0.45924100	O	3.22807000	-0.75811700	-1.08794700
C	0.35340800	1.60440000	-0.42709100	C	2.51372300	-2.62941700	0.24619700
C	-2.40322600	-1.44227000	-0.99987400	C	1.31009900	-3.17137100	-0.36054900
C	-2.03861900	0.06391900	0.86034200	C	0.09108000	-3.14124400	0.36194600
C	1.03105600	-1.73503400	0.80356800	C	0.14820800	-2.47616900	1.66577300
C	2.34731200	-1.39844900	-1.20096900	H	0.89017400	-2.79796600	2.39922700
C	1.40967500	1.80143600	0.48083600	H	-0.82285800	-2.23736700	2.10570600
C	-0.41676400	2.72307800	-0.81264500	Rh	1.05451600	-1.11605600	0.38560100

H	4.58148900	-2.12332200	-0.28227000	H	-2.45288700	1.31144800	-0.86117500
H	3.59998200	-2.68472700	-1.65098900	C	-1.96426000	0.59182900	-1.51608900
H	4.64998900	-0.13290700	0.28659200	C	-1.06792900	1.00465900	-2.50993600
H	4.60693500	0.76604500	-1.24470500	H	-0.83671200	2.06057700	-2.61827500
H	3.30540300	-0.79919700	2.01400700	H	-0.87791100	0.39203800	-3.39270800
H	2.83390200	-3.01143000	1.21652700	C	-1.39075400	-1.98108600	-1.95194800
H	1.27171800	-3.40492900	-1.42724200	C	-2.71051000	-1.66151200	-2.64593600
C	-1.19121300	-3.66882600	-0.23411600	C	-3.22124700	-1.15909300	-0.16724700
H	-1.25169600	-4.74278200	-0.00259400	H	-1.32425500	-2.87853600	-1.34365500
H	-1.21795000	-3.55408800	-1.32405900	H	-0.48747100	-1.74319600	-2.52339700
H	-2.06841100	-3.18480500	0.20456000	H	-2.66336300	-1.17039200	-3.61614100
P	-0.93425900	0.32050700	-0.03119600	H	-3.50788100	-2.39670400	-2.55278400
C	-0.85384600	1.11608900	-1.66297200	H	-3.25798100	-2.25447600	-0.01861600
C	0.28461000	0.92021800	-2.46785800	H	-2.72725300	-0.71679700	0.71976700
C	-1.93328800	1.86900000	-2.17728100	C	-5.34621600	-0.80874200	0.77090500
C	0.35223500	1.47948000	-3.75133500	H	-4.89079800	-0.32141700	1.65499000
H	1.12626000	0.33337300	-2.09818400	H	-5.45210500	-1.88379500	1.00125500
C	-1.85940500	2.43216600	-3.45323900	C	-2.43000600	-0.82365500	-1.42469500
H	-2.83729500	1.99315000	-1.58306100	Rh	-0.02811300	-0.04634300	-0.89204200
C	-0.71522600	2.23819000	-4.24156600	O	-4.49706900	-0.62628400	-0.34474600
H	1.23418200	1.31519100	-4.36701400	C	-6.68817200	-0.20138600	0.45909900
H	-2.69586600	3.01206200	-3.83771900	H	-6.67250400	0.84291100	0.14687400
H	-0.66463100	2.66911600	-5.23949500	C	-7.84418600	-0.87703600	0.55631700
C	-1.14303100	1.64328700	1.21194400	H	-7.82016800	-1.92505700	0.86513300
C	-1.02724400	1.28146800	2.57366200	C	-9.18526200	-0.32522100	0.27832800
C	-1.35955300	2.99600500	0.89135500	C	-10.26686400	-1.11061700	0.42159700
C	-1.16572600	2.23766400	3.58385500	H	-10.17882700	-2.14769400	0.74306700
H	-0.81648100	0.24541500	2.84200500	H	-11.27099600	-0.74175400	0.22137700
C	-1.48165600	3.95569700	1.90598000	C	-9.29293000	1.12039200	-0.16734600
H	-1.42567800	3.30900800	-0.14714000	H	-8.88811400	1.79701000	0.59891800
C	-1.39485500	3.57957000	3.25002000	H	-8.71892200	1.28901600	-1.08959200
H	-1.08602900	1.93857600	4.62705000	H	-10.33598300	1.39751900	-0.35427400
H	-1.64642900	4.99771200	1.63937400	P	0.89794400	1.93873400	-0.01662100
H	-1.49543600	4.32623200	4.03497100	P	1.63125600	-1.63828300	0.05500200
C	-2.55428700	-0.52833800	-0.07031700	C	2.81682500	-2.15721200	-1.22930400
C	-3.03238700	-1.05975100	-1.28657700	C	2.57731300	-1.81507400	-2.57421300
C	-3.29389200	-0.75917700	1.10629700	C	3.95469900	-2.93113100	-0.91844700
C	-4.22034800	-1.79707200	-1.32340100	C	3.44162200	-2.24498200	-3.58802900
H	-2.47899100	-0.89486600	-2.20839900	H	1.71747900	-1.19479400	-2.82649000
C	-4.47925300	-1.50412100	1.06581300	C	4.81835500	-3.35949700	-1.93178000
H	-2.96583100	-0.33881200	2.05406600	H	4.16561200	-3.19248400	0.11693200
C	-4.94484900	-2.02565900	-0.14712800	C	4.56197100	-3.01978500	-3.26729800
H	-4.57876700	-2.18996800	-2.27276500	H	3.24240800	-1.97082400	-4.62206300
H	-5.04468900	-1.66391300	1.98173500	H	5.69139700	-3.95762900	-1.67879700
H	-5.86894200	-2.59920900	-0.17634000	H	5.23571000	-3.35476100	-4.05350100
				C	0.69612700	-3.14912300	0.48541900
				C	-0.47273000	-3.00008500	1.26437300

C	1.06613800	-4.43885900	0.06512200	C	-1.77329900	4.93451600	-0.89283400
C	-1.23423400	-4.11246400	1.63442500	H	-1.64652200	3.27401500	0.47489900
H	-0.79232100	-2.00375600	1.57398600	C	-1.12295500	5.67338900	-1.89066400
C	0.29190700	-5.55158500	0.42258000	H	0.67694300	5.88087500	-3.06809700
H	1.95204900	-4.57803300	-0.54957900	H	-2.77002500	5.22022500	-0.56276400
C	-0.85300700	-5.39343900	1.21030200	H	-1.61552500	6.53289500	-2.34067900
H	-2.12382300	-3.98080600	2.24741800				
H	0.58859300	-6.54220000	0.08400100	<b>TS20</b>			
H	-1.44915100	-6.25999700	1.48873800	H	1.68233500	-2.31913500	0.46145100
C	2.68646800	-1.34419200	1.51906800	C	1.50516100	-2.05140100	-0.57957700
C	3.83903700	-0.54193900	1.38711300	C	0.49609500	-2.67352000	-1.33090500
C	2.35455700	-1.85260200	2.78994800	H	-0.09765500	-3.46054600	-0.87234800
C	4.63196200	-0.25374700	2.50221400	H	0.50179100	-2.66856300	-2.41992300
H	4.13141900	-0.15617900	0.41268900	C	1.26935600	0.09385600	-2.46392200
C	3.15153500	-1.55869600	3.90263200	C	2.49935200	-0.78736500	-2.59512600
H	1.48390300	-2.49189000	2.91408100	C	3.20717000	-0.18498000	-0.20064000
C	4.28950900	-0.75678800	3.76305300	H	1.50998400	1.15109800	-2.37961900
H	5.51930700	0.36378000	2.37889800	H	0.43908200	-0.12583900	-3.14995500
H	2.88571900	-1.96687200	4.87571200	H	2.36188600	-1.69827500	-3.18028300
H	4.91045500	-0.53378900	4.62829600	H	3.43434100	-0.28695400	-2.85195300
C	0.65984100	2.17010200	1.77339800	H	3.33068400	0.85126100	-0.55868200
C	0.38302800	1.06419400	2.59688500	H	2.80234800	-0.13955900	0.82679200
C	0.75050500	3.45073000	2.36242600	C	5.42674200	-0.25183100	0.53554600
C	0.21942500	1.22557400	3.97767400	H	5.06296400	-0.14635500	1.57585900
H	0.29827400	0.07352200	2.15792800	H	5.62848700	0.76337700	0.15075200
C	0.58382200	3.61057800	3.74101700	C	2.26865500	-0.94825200	-1.12058900
H	0.93397700	4.32270400	1.73741600	Rh	0.00360400	-0.51888300	-0.80522600
C	0.32041000	2.49745300	4.55116700	O	4.41970400	-0.87699600	-0.23918700
H	0.01215000	0.35875600	4.60152400	C	6.67147100	-1.09619400	0.49869000
H	0.65148600	4.60378100	4.18023000	H	6.55280800	-2.13066500	0.82177200
H	0.18931900	2.62379700	5.62403000	C	7.87068800	-0.62394400	0.12230800
C	2.68144100	2.11264700	-0.33913700	H	7.95061900	0.41647400	-0.20263900
C	3.56669400	2.76976300	0.53529600	C	9.12996700	-1.39453500	0.11095400
C	3.18656300	1.54959500	-1.52836100	C	10.26774000	-0.79681200	-0.28385000
C	4.92861100	2.85611200	0.22409400	H	10.28337100	0.24614500	-0.59763400
H	3.20311100	3.19456300	1.46772100	H	11.21534400	-1.33171100	-0.30535000
C	4.54749100	1.64037300	-1.84004800	C	9.09294900	-2.84547900	0.55058100
H	2.51017200	1.02415600	-2.20162100	H	8.73515900	-2.93172400	1.58650600
C	5.42146500	2.29181200	-0.95991400	H	8.40958600	-3.42928700	-0.08246500
H	5.60530900	3.36309600	0.90920000	H	10.08890500	-3.29759200	0.49242900
H	4.92273500	1.19507100	-2.75896800	P	-2.20862600	-1.34891300	-0.00838700
H	6.48184600	2.35808000	-1.19554000	P	-0.20252900	1.78605200	-0.01202700
C	0.15601100	3.45165300	-0.72068500	C	-2.24245900	-2.27417500	1.56252000
C	0.80130300	4.20107100	-1.72097400	C	-1.03583400	-2.72737500	2.12770300
C	-1.14079900	3.83104300	-0.31312200	C	-3.45411600	-2.58322300	2.21501600
C	0.16284900	5.30575100	-2.30063800	C	-1.03340900	-3.47903300	3.30855400
H	1.80303300	3.93078900	-2.04704300	H	-0.09323400	-2.48252700	1.64269200



C	-3.45142500	-3.33283400	3.39598600	H	3.53672800	4.40820500	-1.97521700
H	-4.39784500	-2.23270600	1.80213000	H	4.00486300	3.31941800	2.17120700
C	-2.24287700	-3.78280400	3.94420700	H	4.91375000	4.37862600	0.10489300
H	-0.09097800	-3.82316300	3.72991300	C	-1.29330100	2.90010500	-0.94857800
H	-4.39375500	-3.56550100	3.88799500	C	-2.26290600	2.34205400	-1.80143900
H	-2.24498300	-4.36580000	4.86300300	C	-1.21803800	4.30538300	-0.83101900
C	-2.72757800	-2.55598100	-1.28162200	C	-3.15476600	3.16149300	-2.50286200
C	-2.54630500	-2.21217600	-2.63834300	H	-2.32648400	1.26100500	-1.90824600
C	-3.29614900	-3.80343300	-0.97123900	C	-2.10532500	5.12268700	-1.53672000
C	-2.94151500	-3.08294600	-3.65759100	H	-0.45623700	4.75749600	-0.19825300
H	-2.09433800	-1.25314000	-2.89698600	C	-3.07730500	4.55163500	-2.37050400
C	-3.67861100	-4.68228400	-1.99416500	H	-3.90383700	2.71223800	-3.15130200
H	-3.43335500	-4.09658700	0.06681200	H	-2.03708900	6.20434800	-1.44019100
C	-3.50724700	-4.32443600	-3.33492900	H	-3.76725100	5.19110800	-2.91754900
H	-2.80476800	-2.79693900	-4.69869700				
H	-4.11022100	-5.64759800	-1.73742800	<b>IN23</b>			
H	-3.80772800	-5.00783300	-4.12653900	C	-2.21879900	1.11740400	0.40280500
C	-3.66004500	-0.24049600	0.12541500	C	-6.91592200	1.02144400	0.55383000
C	-3.82566400	0.55345900	1.27936300	C	-5.70603200	0.15194500	0.76780400
C	-4.59443100	-0.11549200	-0.92201000	C	-3.36284400	0.21398700	0.82098900
C	-4.89009600	1.45537000	1.37308100	C	-2.12725900	1.49994600	-1.08865600
H	-3.13510800	0.45710000	2.11441700	C	-0.64373700	1.36703500	-1.47833200
C	-5.65608800	0.79165000	-0.82383200	C	-7.87649800	0.74301000	-0.34196100
H	-4.50562900	-0.73517600	-1.81080500	Rh	0.07076800	0.72226600	0.31904500
C	-5.80497800	1.58207100	0.32083500	H	-2.76339400	0.81813700	-1.66350200
H	-5.00294000	2.05593800	2.27343400	H	-2.51546300	2.51748200	-1.23707200
H	-6.37291700	0.86753200	-1.63928100	H	-0.16501100	2.30581800	-1.77757900
H	-6.63457000	2.28201700	0.39830500	H	-0.45038500	0.60929400	-2.24385900
C	-0.78945200	1.82440600	1.71426200	H	-5.70886200	-0.26484400	1.79341000
C	-0.45308000	0.74215300	2.55127200	H	-5.70374400	-0.69883500	0.06312100
C	-1.55839100	2.87848100	2.24164100	H	-3.27068000	-0.07014900	1.88740400
C	-0.88138000	0.70683400	3.88321600	H	-3.36124600	-0.71281400	0.22319100
H	0.13087900	-0.08610000	2.15153900	C	-1.54695100	1.88754700	1.36341800
C	-1.98543200	2.84338700	3.57365200	C	-0.41036800	2.69265600	1.01421900
H	-1.84487000	3.71391600	1.60769200	H	-0.45036100	3.33055200	0.13105400
C	-1.65286600	1.75756800	4.39502600	H	0.17697600	3.11673800	1.82887900
H	-0.62510600	-0.14408800	4.51095500	H	-6.97989900	1.90488100	1.18900700
H	-2.58237300	3.66297300	3.96901400	H	-1.72219000	1.64554800	2.41506200
H	-1.99419300	1.73092900	5.42792000	O	-4.54156100	0.93456900	0.59173700
C	1.37913900	2.70335300	0.06649300	H	-7.77428800	-0.14743700	-0.96740600
C	1.89424700	3.32831300	-1.08994700	C	-9.09472800	1.54621000	-0.56901400
C	2.15606400	2.71493600	1.24089500	C	-9.98034400	1.15903000	-1.50364400
C	3.15970400	3.92464500	-1.07611300	H	-9.82318600	0.26126800	-2.10030300
H	1.29506800	3.37505200	-1.99794100	H	-10.88728000	1.72769800	-1.69993800
C	3.42210200	3.31340600	1.25218600	C	-9.30376900	2.79425900	0.26729300
H	1.77394300	2.25988100	2.15206200	H	-9.34962800	2.54533800	1.33703000
C	3.93114500	3.91139600	0.09355500	H	-8.47245900	3.50044100	0.13061100

H	-10.23525200	3.29958400	-0.00965800	C	-1.51552800	-2.44391900	-0.62019800
P	2.37932200	1.34262100	-0.09961600	C	-2.06277000	-1.97962500	-1.83563800
P	0.05952800	-1.73550000	-0.03849100	C	-2.23002700	-3.40065100	0.12366100
C	2.69080400	3.08948500	0.32457000	C	-3.29046600	-2.46359000	-2.29698000
C	3.25164000	3.46278800	1.55877600	H	-1.52806700	-1.23666000	-2.42602800
C	2.26822500	4.09787300	-0.56752200	C	-3.46656000	-3.87438800	-0.33428400
C	3.38512700	4.81660900	1.89470400	H	-1.82878800	-3.77188300	1.06356700
H	3.59355100	2.70111500	2.25631000	C	-3.99891700	-3.40837200	-1.54130800
C	2.40684200	5.44689200	-0.22986000	H	-3.69518300	-2.10131400	-3.23980900
H	1.85181000	3.82646600	-1.53742500	H	-4.00951500	-4.61144300	0.25392000
C	2.96264500	5.80944700	1.00491800	H	-4.95906000	-3.77929100	-1.89399100
H	3.82610100	5.09145700	2.85081100	C	1.34131100	-2.59879200	-1.01150900
H	2.08508900	6.21462200	-0.93081700	C	2.68335900	-2.55882500	-0.57535900
H	3.06849400	6.85978300	1.26827900	C	1.04952700	-3.20246300	-2.24917200
C	3.04944100	1.18262500	-1.78127300	C	3.70221200	-3.10119100	-1.36184700
C	4.14885100	1.95912800	-2.20794800	H	2.93451000	-2.11768300	0.38648200
C	2.50001700	0.23723000	-2.66656300	C	2.07671700	-3.73826700	-3.03762400
C	4.68368500	1.78256900	-3.48758100	H	0.02261700	-3.26720900	-2.59918300
H	4.57801300	2.70680200	-1.54380300	C	3.40388100	-3.68486100	-2.60023300
C	3.04019500	0.05998700	-3.94514000	H	4.72933900	-3.06417900	-1.00465600
H	1.65489200	-0.36796700	-2.35395300	H	1.83123500	-4.20698700	-3.98864000
C	4.13110100	0.83262000	-4.35744600	H	4.19939300	-4.10345400	-3.21330800
H	5.52872300	2.38933800	-3.80641200				
H	2.60548200	-0.68130000	-4.61235500	<b>IN24</b>			
H	4.54696300	0.70093100	-5.35446600	C	3.29570700	1.44461700	-0.36928000
C	3.48279500	0.39225200	0.99260300	C	2.95846300	-1.33451900	0.39796800
C	4.79041500	0.02197000	0.62798500	C	4.07185100	-0.78803800	1.27169800
C	2.96986000	-0.04397900	2.23122200	C	4.65123100	0.77750100	-0.49149200
C	5.56150900	-0.77401800	1.48317100	C	2.94710700	2.14703300	0.96113700
H	5.19746000	0.33495500	-0.33089300	C	1.63086000	1.48610700	1.41267600
C	3.73963000	-0.84206800	3.08400200	C	1.75554000	-1.77740000	0.92560600
H	1.95777700	0.22925000	2.53325600	H	3.76240500	1.99299800	1.67581300
C	5.03724700	-1.21145800	2.70674700	H	2.83859700	3.22726400	0.79446700
H	6.57077800	-1.05682400	1.19054400	H	0.79418200	2.17926200	1.54340900
H	3.32203000	-1.17895400	4.03052100	H	1.73980100	0.86032500	2.30553000
H	5.63733400	-1.83737000	3.36428600	H	3.63575800	-0.28630600	2.15031000
C	0.25965200	-2.34959200	1.66848800	H	4.64652100	-1.64856000	1.64433800
C	-0.30799800	-1.59301300	2.71709000	H	5.42971700	1.54673300	-0.59409600
C	0.96216900	-3.52688100	1.98982900	H	4.67995800	0.15262600	-1.40000400
C	-0.16221400	-1.99174400	4.05054900	C	2.48581200	1.66379700	-1.49928500
H	-0.89286700	-0.70076000	2.48926800	C	1.12554100	2.09254700	-1.33342400
C	1.10589200	-3.92518200	3.32405400	H	0.87181800	2.87199600	-0.61448600
H	1.40026800	-4.13072800	1.19886300	H	0.48668600	2.09821100	-2.21643800
C	0.55165200	-3.15733700	4.35595900	H	3.26148000	-1.69414500	-0.58859700
H	-0.60968100	-1.39884400	4.84580800	H	2.79673900	1.22750000	-2.45180900
H	1.64980700	-4.83874200	3.55585000	O	5.01805700	0.04622400	0.64825900
H	0.66497100	-3.47155000	5.39162300	Rh	1.33790300	0.27340100	-0.19723700

H	1.56904300	-1.59071600	1.98475100	C	4.32842600	-0.77657300	0.98648700
C	0.91453800	-2.83092500	0.29845000	C	4.80634000	0.92344700	-0.51602700
C	0.01662700	-3.49174900	1.04761100	C	2.90677700	1.89103600	0.93017600
H	-0.13378000	-3.26052300	2.10095200	C	1.49061900	1.41378600	1.29718400
H	-0.58669200	-4.29319400	0.62585600	C	1.88030100	-1.43399000	0.45590500
C	1.15195600	-3.16521800	-1.16212500	H	3.64236300	1.67867400	1.71274800
H	1.21029400	-2.25799700	-1.78342600	H	2.95140700	2.97025100	0.72849100
H	0.33378600	-3.77807600	-1.55614600	H	0.74377000	2.20937200	1.39642700
H	2.09433700	-3.71646500	-1.29433700	H	1.48018000	0.78223100	2.19162600
P	-1.08300600	0.11085500	0.00404200	H	3.98078000	-0.55177100	2.00578300
C	-1.89565300	-0.38842300	1.54860800	H	4.80007300	-1.76985200	0.99939300
C	-1.14171600	-0.61282800	2.71326100	H	5.30087800	1.90325900	-0.48654800
C	-3.30376200	-0.46468400	1.61918000	H	5.04568900	0.44366600	-1.48010200
C	-1.77374000	-0.93399100	3.92149100	C	2.58275000	1.58329000	-1.59164400
H	-0.05955200	-0.52087200	2.67778300	C	1.52148400	2.45849000	-1.61236300
C	-3.93196600	-0.79806300	2.82160200	H	1.26536600	3.08354200	-0.75973100
H	-3.90532800	-0.25405800	0.73611100	H	1.03762600	2.69200100	-2.55854800
C	-3.16762700	-1.03575800	3.97327400	H	2.88719100	1.11220300	-2.53056000
H	-1.17847600	-1.09838000	4.81723500	O	5.27097100	0.18032200	0.57130900
H	-5.01737700	-0.85953300	2.86326700	Rh	1.12560900	0.32017500	-0.37639400
H	-3.66083100	-1.28823800	4.90976200	H	3.47508000	-1.17605000	-0.97667300
C	-1.90510500	1.70511500	-0.34951500	H	1.73244400	-1.48477900	1.53828600
C	-1.91718400	2.67649500	0.67530100	C	1.35368400	-2.63064400	-0.28137900
C	-2.46484600	2.02897000	-1.59836700	C	0.59045400	-3.53792400	0.35157200
C	-2.46321600	3.94284700	0.44797000	H	0.34524900	-3.44667600	1.40877600
H	-1.52965500	2.43292800	1.66381600	H	0.19750300	-4.40728700	-0.17294700
C	-3.01363600	3.29946000	-1.82018900	C	1.70801100	-2.78821600	-1.75466100
H	-2.49438100	1.29098700	-2.39575900	H	1.51250900	-1.86891500	-2.33337300
C	-3.00829500	4.25960300	-0.80352100	H	2.77010600	-3.03751200	-1.89060000
H	-2.47238100	4.67699300	1.25114900	H	1.12145500	-3.59446500	-2.20906700
H	-3.45044900	3.53235800	-2.78923100	P	-1.20967700	0.10565700	0.05511600
H	-3.43399600	5.24506600	-0.98027900	C	-1.64602100	-1.12298600	1.32035100
C	-1.59786100	-1.03513800	-1.31329100	C	-1.00270700	-1.06051900	2.57485200
C	-1.07973400	-0.82190000	-2.61111100	C	-2.57041500	-2.15365800	1.07668700
C	-2.41136800	-2.16036700	-1.08657200	C	-1.27847200	-2.00992700	3.56203100
C	-1.39036400	-1.69404600	-3.65901400	H	-0.29545000	-0.25936200	2.78426400
H	-0.44056800	0.03963600	-2.80618400	C	-2.83717300	-3.11008600	2.06557400
C	-2.71323100	-3.03726500	-2.13627900	H	-3.07837100	-2.21279300	0.11723700
H	-2.80115000	-2.35743800	-0.09132400	C	-2.19167500	-3.04325400	3.30443200
C	-2.20878500	-2.80569300	-3.42160000	H	-0.78244900	-1.94697900	4.52855100
H	-0.99525700	-1.50671200	-4.65534800	H	-3.55108600	-3.90604600	1.86402100
H	-3.34794500	-3.90084500	-1.94815300	H	-2.40204300	-3.78690800	4.07036600
H	-2.45116500	-3.48700400	-4.23455400	C	-1.94591600	1.67731900	0.60184500
				C	-2.71346800	1.78406500	1.77584600
<b>TS21</b>				C	-1.73477400	2.83149300	-0.18432600
C	3.29108500	1.12954000	-0.36499500	C	-3.24914400	3.02145500	2.15878800
C	3.15616700	-0.83660700	0.01079000	H	-2.89620700	0.90770000	2.39209300

C	-2.27994600	4.06012200	0.19520800	C	-1.59253800	-3.02073200	-1.27883600
H	-1.16145300	2.75860300	-1.10721100	H	-0.80119200	-2.59237900	-1.91090100
C	-3.03373500	4.15803700	1.37395800	H	-2.56032300	-2.68442400	-1.67536400
H	-3.84013100	3.09068300	3.06960800	H	-1.54884900	-4.10981400	-1.38919400
H	-2.11951000	4.93892300	-0.42600900	P	1.17684100	0.14227400	0.04301700
H	-3.45254500	5.11643200	1.67359800	C	1.62224700	-1.17145200	-1.12956000
C	-2.10975400	-0.37177100	-1.45158000	C	1.59477300	-0.88385600	-2.51273300
C	-3.20334000	0.36378900	-1.94570500	C	1.90412400	-2.48658400	-0.71445900
C	-1.67355000	-1.51326600	-2.15938000	C	1.84611300	-1.88591600	-3.45343900
C	-3.83853500	-0.02912100	-3.13055400	H	1.39998300	0.13157700	-2.85340800
H	-3.56091600	1.23872400	-1.40888300	C	2.15522300	-3.48797400	-1.66166400
C	-2.31539700	-1.90337500	-3.33812500	H	1.92231800	-2.73491700	0.34278600
H	-0.85708100	-2.11568200	-1.76391600	C	2.12491700	-3.19232200	-3.02831400
C	-3.39493400	-1.15674500	-3.82968300	H	1.83217500	-1.64544600	-4.51446900
H	-4.68295900	0.54724800	-3.50272200	H	2.38107600	-4.49810700	-1.32625900
H	-1.97600700	-2.78894900	-3.87156500	H	2.32533400	-3.97260900	-3.75972500
H	-3.89129800	-1.45805000	-4.74987600	C	1.79158300	-0.36178400	1.67618300

**TS21-trans**

C	-3.34717600	1.08045600	-0.54200900	C	0.95890600	-0.23689900	2.80333900
C	-3.14983900	-0.71311700	0.31901400	C	3.59015300	-1.12480600	3.12969500
C	-4.15064100	-0.44796400	1.45133700	H	3.78452300	-0.88484600	0.99690500
C	-4.84784600	0.99618500	-0.18062500	C	1.43210500	-0.55599700	4.08204500
C	-2.92408400	0.85305600	-2.00762900	H	-0.06365600	0.12536000	2.69158000
H	-3.54623000	0.06913900	-2.45754000	C	2.74671900	-1.00562500	4.24362200
H	-3.08159200	1.77233600	-2.58900600	H	4.61565200	-1.46560300	3.25566800
H	-4.78418000	-1.34275600	1.56116100	H	0.77867400	-0.45062200	4.94546900
H	-3.63428700	-0.27535400	2.40440300	H	3.11669600	-1.25787200	5.23522600
H	-5.33755400	0.24497500	-0.82444400	C	2.22631300	1.56142100	-0.40988600
H	-5.33729000	1.96456200	-0.33461300	C	1.86833800	2.83733200	0.06793400
C	-2.69386100	2.24306400	0.12642400	C	3.42937900	1.41531900	-1.12919700
C	-1.65214500	2.98752000	-0.37262500	C	2.68780100	3.94433200	-0.17209700
H	-1.33153500	2.94472600	-1.40995000	H	0.95043700	2.95823100	0.64010200
H	-1.25611000	3.80592900	0.22413500	C	4.24316500	2.52694900	-1.37506600
H	-3.59122300	-1.18720200	-0.55935700	H	3.72901600	0.43892900	-1.50276900
H	-3.06268200	2.46635500	1.13036400	C	3.87442000	3.79101200	-0.89984900
O	-4.94592000	0.68049900	1.17124900	H	2.40102300	4.92354100	0.20580500
C	-1.83878900	-1.29704800	0.68517900	H	5.16578500	2.40285500	-1.93835900
Rh	-1.17263600	0.56794200	0.07974800	H	4.51053800	4.65251500	-1.09189600
C	-1.43776400	0.43625400	-1.93706500	<b>IN25</b>			
H	-0.75341700	1.13014000	-2.43771500	C	3.64839000	0.76525800	-0.19014700
H	-1.24827500	-0.57899900	-2.29031000	C	3.30267200	-0.74719100	0.06036600
H	-1.63749400	-1.21889500	1.76467800	C	4.13624300	-1.02571200	1.33183500
C	-1.38750300	-2.63056600	0.17341100	C	5.16471700	0.67618400	0.10604700
C	-0.79062700	-3.47198500	1.03560400	C	2.95571500	1.73245800	0.80485500
H	-0.61814100	-3.20267900	2.07711200	C	1.41101500	1.62425800	0.79167400
H	-0.45816400	-4.45963400	0.72126300	C	1.80020900	-1.07865300	0.06168400

H	3.34580000	1.52619000	1.80954300	H	-3.98992500	5.09316000	-0.11957400
H	3.27462700	2.75346700	0.55245400	C	-2.29735700	-1.00398300	-0.94813800
H	0.91467700	2.60386500	0.72442400	C	-3.62205800	-1.32465500	-0.58553200
H	1.04433900	1.11148400	1.68665800	C	-1.79488800	-1.45805000	-2.18029300
H	3.56437000	-0.80036500	2.24562100	C	-4.41849600	-2.09123700	-1.43901500
H	4.47857700	-2.06708500	1.38211500	H	-4.02638700	-0.97842400	0.36451600
H	5.60945100	1.64776200	0.35138400	C	-2.59783000	-2.21730800	-3.03984600
H	5.71043900	0.24163300	-0.74882700	H	-0.77149700	-1.22490000	-2.47405100
C	3.22976100	1.02770300	-1.61207900	C	-3.90805100	-2.53574900	-2.66727200
C	2.39051200	2.01084900	-2.04242800	H	-5.43725700	-2.33884800	-1.14874500
H	2.11276900	2.85534700	-1.41316100	H	-2.20124500	-2.55861900	-3.99352800
H	2.12216400	2.07377200	-3.09659200	H	-4.53350400	-3.12671600	-3.33323500
H	3.77882500	-1.29655400	-0.76337100				
H	3.58602600	0.30532800	-2.35182900	<b>IN29</b>			
O	5.25213800	-0.15450400	1.24458500	C	4.10327800	0.55976500	0.72579000
Rh	0.86891500	0.53400000	-0.83183000	C	3.69955400	-0.71415000	-0.12083400
H	1.40655600	-1.13880900	1.08433100	C	2.94452500	-0.39517300	-1.45459400
C	1.41566600	-2.31111300	-0.71981900	C	1.42577900	-0.14676500	-1.27713400
C	0.76537200	-3.32857100	-0.13031300	C	1.21452400	1.18865900	1.45968000
H	0.52690900	-3.30840300	0.93134400	C	2.08879900	2.11234300	0.65275100
H	0.47934900	-4.22038700	-0.68619600	C	3.36853900	1.82875000	0.34851000
C	1.78721200	-2.36957000	-2.19704500	C	5.64545800	0.65726500	0.47185900
H	1.47910400	-1.45795000	-2.73813900	O	5.92216600	-0.18554600	-0.62176400
H	1.31037100	-3.22547900	-2.68781300	C	5.11559800	-1.30785300	-0.43824000
H	2.87264500	-2.46545700	-2.34124500	C	2.82359200	-1.72188500	0.57689300
P	-1.27790700	0.06414900	0.10356100	C	2.36772100	-1.73913800	1.86478400
C	-1.37423400	-0.60909000	1.78403400	H	3.93833500	0.35245800	1.79104600
C	-1.12089800	0.21527200	2.90276900	H	3.08225300	-1.26502700	-2.11200200
C	-1.62725100	-1.98031200	1.99116100	H	3.42703100	0.45743800	-1.94682700
C	-1.12271300	-0.32263200	4.19353800	H	1.14330400	0.89501200	-1.45118200
H	-0.94624400	1.28116700	2.77127700	H	0.84535600	-0.76973000	-1.97566900
C	-1.62676100	-2.51241400	3.28606300	H	1.71333500	0.88360700	2.39156000
H	-1.83337900	-2.63066000	1.14476300	H	0.26875900	1.67972000	1.71877300
C	-1.37313600	-1.68726000	4.38726200	H	6.20012900	0.31690200	1.36197200
H	-0.93668200	0.32631200	5.04668100	H	5.97581200	1.66875500	0.21534300
H	-1.83384500	-3.57075700	3.43128500	H	5.14044500	-1.91670500	-1.34831400
H	-1.37805700	-2.10169600	5.39322900	H	5.46809000	-1.91483000	0.41691500
C	-2.13837800	1.66628000	0.12088500	H	2.55623100	-2.58120200	-0.05099800
C	-3.14338100	1.99995700	1.04890100	H	1.81978800	-2.60732300	2.23439800
C	-1.81946400	2.58569700	-0.90029400	H	2.68230400	-1.01076100	2.60723700
C	-3.80269200	3.23113100	0.95974700	Rh	0.71668400	-0.62120800	0.59203700
H	-3.40571600	1.30645100	1.84489600	H	3.92698400	2.54675500	-0.25513400
C	-2.48108800	3.81406700	-0.98932600	C	1.43789600	3.38897900	0.15273700
H	-1.06395800	2.33540900	-1.64962500	H	2.15515600	4.02339800	-0.38051500
C	-3.47283900	4.13806600	-0.05491300	H	1.01515500	3.96883300	0.98560300
H	-4.57689300	3.48004100	1.68254600	H	0.61205200	3.15629300	-0.53666200
H	-2.22789000	4.51144700	-1.78506900	P	-1.50965100	-0.00866200	-0.07737100

C	-2.50714900	0.76956100	1.21883400	H	4.45064800	0.34704200	-1.34291200
C	-2.12368700	0.59160800	2.56424800	H	1.25368300	1.76379800	1.11883700
C	-3.69233200	1.47753500	0.93204600	H	2.73325300	1.21048900	1.90088500
C	-2.90312600	1.11327700	3.60111900	H	2.02843700	-1.12852400	1.78073100
H	-1.21467800	0.04058300	2.80863700	H	0.49924200	-0.26020500	2.11418000
C	-4.46784000	2.00070200	1.97224900	H	2.43064200	-3.07181900	-1.47386300
H	-4.00662200	1.62127400	-0.09953500	H	1.66239100	-3.04639200	0.10419100
C	-4.07411000	1.82168300	3.30448800	H	5.97713600	1.44114600	0.06878200
H	-2.59464100	0.97212600	4.63467400	H	4.96420900	1.24098500	1.52112700
H	-5.37876900	2.54869200	1.74074100	H	2.39042100	3.18301000	-0.33639200
H	-4.67865400	2.23344000	4.10995300	H	3.36673400	2.53469700	-1.68971200
C	-2.21268800	-1.66987800	-0.32157600	H	1.00536800	1.07011600	-1.76906700
C	-3.50499200	-2.01673200	0.11827900	H	1.47860900	-1.14431700	-2.82213400
C	-1.40583300	-2.66385300	-0.92194500	H	3.15394100	-1.08778700	-2.09959300
C	-3.97860000	-3.32256000	-0.04791100	Rh	0.61422800	-1.12141600	-0.36122400
H	-4.13756600	-1.27154100	0.59497700	H	5.30344500	-1.17650900	0.76554300
C	-1.88449400	-3.96839900	-1.08704100	C	4.18807100	-3.51488100	0.71141300
H	-0.40946800	-2.41633600	-1.29077500	H	3.51834300	-3.89080600	1.49953500
C	-3.17197100	-4.29831600	-0.64735700	H	5.18122500	-3.36623500	1.14956400
H	-4.97930200	-3.57842000	0.29387400	H	4.26266700	-4.30374200	-0.05105400
H	-1.25615400	-4.72129300	-1.55825300	P	-1.49438500	0.01436500	0.03429000
H	-3.54454000	-5.31310600	-0.77029200	C	-1.36229300	1.75913300	0.50704400
C	-1.78494000	0.93272900	-1.60241800	C	-0.98717500	2.72459800	-0.45267500
C	-1.94257800	0.28084500	-2.83988900	C	-1.46733800	2.14188600	1.85793900
C	-1.75227400	2.34288900	-1.56546400	C	-0.72950300	4.04337300	-0.06564400
C	-2.06748000	1.02763500	-4.01765900	H	-0.92197900	2.45303800	-1.50547500
H	-1.98329200	-0.80526800	-2.88722700	C	-1.20157600	3.46263500	2.24084200
C	-1.87984100	3.08242800	-2.74491100	H	-1.76018100	1.41114800	2.60917200
H	-1.65093900	2.86389500	-0.61494600	C	-0.82977400	4.41274200	1.28320900
C	-2.03485000	2.42559500	-3.97296400	H	-0.45720400	4.78286800	-0.81611200
H	-2.19749400	0.51277500	-4.96727800	H	-1.28832000	3.74736700	3.28727000
H	-1.86427100	4.16948300	-2.70393300	H	-0.62510000	5.43804600	1.58379800
H	-2.13635500	3.00346800	-4.88915300	C	-2.46390500	-0.04204300	-1.49898500
				C	-2.29866000	-1.16567900	-2.33530500
				C	-3.39369100	0.95094600	-1.86460800
<b>TS26</b>				C	-3.04498500	-1.29671800	-3.51085400
C	4.10864200	0.32469200	-0.29453600	H	-1.60199500	-1.95954900	-2.05411800
C	2.69666000	0.98892900	-0.28192700	C	-4.13761400	0.81911800	-3.04202200
C	2.00792200	0.96723800	1.11128700	H	-3.52715100	1.82874100	-1.23540600
C	1.32776200	-0.37585400	1.40341900	C	-3.96431200	-0.30128000	-3.86494000
C	2.31269700	-2.44301400	-0.58210200	H	-2.91226400	-2.17065800	-4.14495900
C	3.64951800	-2.22109900	0.10740800	H	-4.85293100	1.59187100	-3.31600100
C	4.35025200	-1.07865900	0.24028700	H	-4.54677900	-0.39984500	-4.77856000
C	4.94166000	1.41251500	0.43386000	C	-2.51704900	-0.77844600	1.30609000
O	4.29847600	2.64458100	0.16579200	C	-1.99176300	-1.84983700	2.05260700
C	3.14441600	2.43428000	-0.61177100	C	-3.84299700	-0.36043100	1.54306500
C	1.72576800	0.39361300	-1.30375000	C	-2.77291900	-2.49262600	3.02110700
C	2.11491800	-0.79276000	-2.00252700				

H	-0.96568900	-2.18092200	1.88576000	C	3.81086600	-3.45477400	1.22931700
C	-4.61978800	-1.00062400	2.51078400	H	3.54319400	-2.33691900	-0.59528100
H	-4.26573800	0.46038300	0.96565400	C	3.49144500	-3.55573200	2.59039900
C	-4.08529400	-2.06677600	3.24989900	H	2.40298100	-2.68569800	4.24424000
H	-2.35697200	-3.31874200	3.59373200	H	4.46901200	-4.18730300	0.76679000
H	-5.64191300	-0.67264900	2.68747300	H	3.90209000	-4.36941400	3.18455200
H	-4.69437800	-2.56426100	4.00182800	C	1.31215000	-0.58587000	-1.54460500

**TS27**

C	-4.34265000	0.43313700	0.34999300
C	-3.37637500	-0.61063000	-0.27522000
C	-2.51292500	-1.37896100	0.75259400
C	-1.48516800	-0.49801600	1.48869100
C	-1.34785400	1.51694900	1.38113600
C	-2.74447500	1.95817000	1.77952800
C	-3.92998700	1.48831800	1.35565500
C	-5.46120800	-0.49388800	0.91462800
O	-5.42703000	-1.68107000	0.14522900
C	-4.44873000	-1.57362600	-0.85621400
C	-2.45849100	-0.08265800	-1.35865600
C	-2.24329300	1.25406000	-1.61821800
H	-4.78677500	0.97645700	-0.50192100
H	-1.98642200	-2.17394100	0.20696800
H	-3.16932100	-1.86613400	1.48776200
H	-1.89027400	-0.19630100	2.45307700
H	-0.54823600	-1.02946300	1.68938000
H	-0.94656300	2.30792700	0.68837900
H	-0.68335000	1.54192900	2.24973000
H	-6.45064000	-0.02149000	0.84348900
H	-5.27365900	-0.74675000	1.96894000
H	-4.05453100	-2.57559900	-1.06900100
H	-4.86922300	-1.15517700	-1.78808800
H	-2.08724000	-0.82490500	-2.07331800
H	-1.73955500	1.56644800	-2.53069800
H	-2.74782800	2.02776000	-1.04210300
Rh	-0.51917500	0.45996800	-0.30846000
H	-4.80529800	1.98916000	1.77852900
C	-2.70110700	3.09729600	2.79298000
H	-2.11821700	3.94597400	2.40557400
H	-2.21559500	2.77356400	3.72557300
H	-3.70703100	3.45588000	3.03692700
P	1.75645300	-0.05393600	0.14318700
C	2.42836000	-1.45911100	1.05157700
C	2.11568300	-1.56826100	2.42157500
C	3.28718600	-2.41089400	0.46069200
C	2.64821900	-2.61138200	3.18708400
H	1.46669000	-0.83103400	2.89280900

C	3.81086600	-3.45477400	1.22931700
H	3.54319400	-2.33691900	-0.59528100
C	3.49144500	-3.55573200	2.59039900
H	2.40298100	-2.68569800	4.24424000
H	4.46901200	-4.18730300	0.76679000
H	3.90209000	-4.36941400	3.18455200
C	1.31215000	-0.58587000	-1.54460500
C	0.97846400	-1.92128800	-1.90627400
C	1.01755900	0.46335100	-2.45742500
C	0.41678500	-2.18995800	-3.14980600
H	1.16832200	-2.73560400	-1.21096200
C	0.44156500	0.17147400	-3.71451600
H	1.34362800	1.48038100	-2.24089600
C	0.14498800	-1.14345600	-4.05751600
H	0.18527400	-3.21698600	-3.42496800
H	0.25643600	0.98112200	-4.41781600
H	-0.28504100	-1.37093900	-5.03074700
C	3.03847500	1.22007200	0.04240100
C	2.64211300	2.57231700	0.01240300
C	4.41030900	0.89989100	-0.00507800
C	3.60025800	3.58726400	-0.08713400
H	1.58473300	2.82880700	0.07510500
C	5.36293500	1.91763400	-0.10015400
H	4.73386100	-0.13748700	0.04495000
C	4.95978000	3.25930000	-0.14438600
H	3.28575500	4.62839100	-0.10870600
H	6.42012900	1.66364300	-0.13544900
H	5.70574500	4.04834900	-0.21449800

**TS22**

C	3.49361700	-0.81278900	0.06640500
C	3.53759100	0.73447800	0.29899900
C	5.06366500	1.00060100	0.41901500
C	4.69083600	-1.23463600	0.94253900
C	3.74290400	-1.02664200	-1.44544000
C	2.65777800	-0.25357900	-2.21585500
C	2.75552800	1.38495700	-0.83554700
H	4.74760300	-0.66477400	-1.69198200
H	3.71946100	-2.09618600	-1.69326100
H	1.89915600	-0.91091900	-2.68662300
H	3.02852400	0.38803000	-3.01591900
H	5.48938800	1.40908800	-0.50876100
H	5.28347500	1.70011400	1.23717900
H	5.10505700	-2.21390600	0.67849800
H	4.40753600	-1.24382700	2.01003000
C	2.11432600	-1.29973500	0.48128500
C	1.28089600	-2.09940300	-0.26042000

H	1.60272200	-2.56462700	-1.19091700	H	0.33893900	-0.04026800	4.69781100
H	0.37138700	-2.49157300	0.19121600	H	-0.82902000	-2.13856800	5.36546400
H	1.80214600	-1.04567400	1.49756200				
O	5.66879400	-0.25634900	0.67266900	<b>IN26</b>			
C	1.48427700	2.10478700	-0.61074100	C	-3.29167300	-1.05225500	0.22590800
C	0.63429400	2.12771400	-1.75412200	C	-3.44871100	0.35433200	-0.42785700
H	1.05609200	2.08057700	-2.75926900	C	-4.92701200	0.32540200	-0.92555900
H	-0.32795800	2.62904800	-1.67006200	C	-4.29392100	-1.87318800	-0.62035900
Rh	0.87752300	0.12727900	-0.95603700	C	-3.81719500	-0.78874400	1.65558300
C	1.12524500	2.82036000	0.67312100	C	-3.17862200	0.56321700	2.02755100
H	1.51564400	3.84806700	0.63045700	C	-3.08482700	1.39218700	0.69262100
H	0.03501400	2.88204900	0.78011500	H	-4.90876800	-0.69751800	1.60994100
H	1.54925800	2.33998200	1.56098800	H	-3.58031100	-1.58442000	2.37133000
H	3.04809400	0.94869500	1.25647700	H	-2.18417200	0.37169400	2.51405900
H	3.36304900	1.77881600	-1.65047800	H	-3.70777500	1.10417300	2.82178400
P	-1.33340400	-0.06511200	0.04525000	H	-5.58798600	0.97296400	-0.33379200
C	-2.35210900	1.44105800	0.19080000	H	-4.98940700	0.64147400	-1.97718200
C	-2.79636100	2.04785000	-1.00465000	H	-4.64886400	-2.78228200	-0.12193100
C	-2.70459700	2.02236800	1.42217200	H	-3.84265200	-2.15129400	-1.58988700
C	-3.56920100	3.21084400	-0.96591400	C	-1.84557700	-1.53313000	0.15552600
H	-2.55203600	1.59735500	-1.96645100	C	-1.10988100	-2.10988800	1.20196000
C	-3.47682800	3.19235100	1.45525700	H	-1.56994900	-2.29625900	2.17340900
H	-2.39534600	1.56004100	2.35631700	H	-0.23475100	-2.71252800	0.97368400
C	-3.90752200	3.78853300	0.26623500	H	-1.47377100	-1.66652000	-0.86408800
H	-3.91097100	3.66271400	-1.89481900	O	-5.38729500	-1.00667900	-0.78644700
H	-3.74830600	3.62729400	2.41497200	C	-1.69770500	2.02867200	0.46659200
H	-4.51059700	4.69353100	0.29658800	C	-0.79964100	2.26876000	1.50510700
C	-2.40822500	-1.19864900	-0.88676400	H	-1.09188000	2.21567300	2.55598100
C	-3.78730400	-1.28567800	-0.59851000	H	0.08584700	2.86865600	1.29948200
C	-1.87450800	-2.00341100	-1.91056700	Rh	-0.67963200	0.05325700	1.13719100
C	-4.60246800	-2.17145500	-1.30736400	C	-1.47034700	2.70671100	-0.87117400
H	-4.22050600	-0.65605300	0.17704600	H	-2.15543400	3.56759200	-0.92706500
C	-2.69430700	-2.88696800	-2.62394700	H	-0.44607800	3.08190300	-0.95877500
H	-0.81535300	-1.93818900	-2.15893600	H	-2.77754500	0.44674700	-1.28704800
C	-4.05665700	-2.97390800	-2.31970200	H	-3.82438300	2.20830600	0.70862000
H	-5.66350700	-2.23171200	-1.07426800	P	1.32052700	-0.06448400	-0.08273300
H	-2.26969200	-3.50072200	-3.41558000	C	1.20411600	0.81551500	-1.66783000
H	-4.69480000	-3.66127700	-2.87128600	C	1.93153200	1.98908600	-1.93744600
C	-1.22436400	-0.75281900	1.73176700	C	0.28888200	0.34293500	-2.63402300
C	-1.87740400	-1.93687400	2.12072600	C	1.75024500	2.67005300	-3.14903400
C	-0.41144700	-0.08512400	2.67542500	H	2.63548400	2.37782700	-1.20573700
C	-1.72873500	-2.43362700	3.42336200	C	0.12204100	1.01589500	-3.84696700
H	-2.50368000	-2.47316400	1.41218200	H	-0.28896700	-0.56061700	-2.44152300
C	-0.27723800	-0.57499800	3.97751200	C	0.85049300	2.18597800	-4.10421900
H	0.10421200	0.83167600	2.39049400	H	2.31982700	3.57625600	-3.34442100
C	-0.93552100	-1.75473100	4.35299000	H	-0.57440200	0.63041100	-4.58902100
H	-2.23978600	-3.35095200	3.70838300	H	0.71689700	2.71558300	-5.04524500



C	1.95516200	-1.73012300	-0.46559900	Rh	-0.83482500	-0.61834600	-0.31148400
C	2.26846800	-2.56827400	0.62769900	H	-2.61329900	-1.57893600	-1.86709800
C	2.18937600	-2.19635200	-1.77128400	C	-2.03786900	-2.48773200	0.00401900
C	2.78764900	-3.84659400	0.41589200	C	-0.73605700	-2.82070900	-0.46337600
H	2.11789600	-2.21307600	1.64719500	H	-0.54163700	-2.82768300	-1.54355700
C	2.70868900	-3.48228100	-1.97859800	H	-0.08780400	-3.47192300	0.11889300
H	1.98666200	-1.56110200	-2.62886000	C	-2.50876000	-2.92077200	1.37645000
C	3.00349300	-4.30851900	-0.89088200	H	-2.96767100	-2.10113200	1.93963400
H	3.02696600	-4.48017600	1.26730600	H	-1.68234300	-3.33528400	1.96436700
H	2.88722300	-3.82978100	-2.99404100	H	-3.26288400	-3.71210700	1.25103700
H	3.40536800	-5.30593700	-1.05637800	P	1.47740100	0.07519900	0.02108700
C	2.68051200	0.68119600	0.86099800	C	2.28438300	-0.35759000	-1.55003300
C	3.99175300	0.67944500	0.33707400	C	1.60486300	-0.02193600	-2.74368500
C	2.45725700	1.20655700	2.14692000	C	3.49440900	-1.06923600	-1.62991400
C	5.04573000	1.21919600	1.07717300	C	2.13166300	-0.38208900	-3.98734700
H	4.18524200	0.25056000	-0.64531300	H	0.67368900	0.54652100	-2.69903100
C	3.51871200	1.73728800	2.89105700	C	4.01512100	-1.43341100	-2.87860300
H	1.45443400	1.19529900	2.57155300	H	4.02744800	-1.34420800	-0.72280200
C	4.80973700	1.74988100	2.35414200	C	3.33821100	-1.09236700	-4.05481900
H	6.05234400	1.21802200	0.66442000	H	1.60459700	-0.10933600	-4.89941500
H	3.33497200	2.13495900	3.88687500	H	4.95127400	-1.98573600	-2.92901900
H	5.63431600	2.16393900	2.93073400	H	3.74703100	-1.37809300	-5.02171800
H	-1.67490500	2.06583600	-1.73292700	C	2.47253100	-0.64061700	1.35617200
<b>TS23</b>				C	1.99907800	-1.76867000	2.05126200
C	-3.64660200	0.60132700	0.52517100	C	3.72124100	-0.08640100	1.70984700
C	-3.95899200	-0.71635700	-0.30985100	C	2.76401700	-2.34394500	3.07301100
C	-4.83521000	-0.17330600	-1.48880100	H	1.02843500	-2.18861100	1.79271900
C	-4.60505000	1.62628000	-0.17910600	C	4.48314500	-0.66489500	2.72838200
C	-2.20384300	1.11972700	0.33848900	H	4.09020100	0.79802000	1.19252100
C	-1.60290100	1.28663800	-0.94820300	C	4.00577800	-1.79394600	3.40957200
C	-2.71320900	-1.48148200	-0.77938700	H	2.38895300	-3.21419600	3.60765100
H	-1.87411000	1.82566300	1.10754900	H	5.44556000	-0.23341400	2.99541500
H	-1.43370700	0.06688400	1.02356400	H	4.60002300	-2.23865000	4.20526300
H	-0.81659700	2.03577600	-1.04269100	C	1.67092400	1.87397600	0.21846900
H	-2.20532000	1.09908500	-1.83587000	C	2.34603300	2.68599500	-0.70938600
H	-4.55117200	-0.57677200	-2.46672700	C	1.07823000	2.47285000	1.35152700
H	-5.89680900	-0.40622100	-1.30599700	C	2.42540700	4.07148700	-0.50691400
H	-4.24739800	2.66024700	-0.13074200	H	2.81268600	2.24165400	-1.58584900
H	-5.60794700	1.57038500	0.28028500	C	1.16595400	3.85229200	1.55326300
C	-4.02053900	0.42820800	1.98569700	H	0.56851000	1.85103900	2.08921900
C	-3.25053600	0.60199700	3.06466800	C	1.83721500	4.65514100	0.61912400
H	-2.20526700	0.90291500	3.01412700	H	2.95152200	4.69008300	-1.23117200
H	-3.65319800	0.44703900	4.06331000	H	0.71592000	4.30163700	2.43635500
H	-4.57333500	-1.37914900	0.31291200	H	1.90101700	5.73034000	0.77290900
H	-5.06075600	0.12711200	2.13393500	<b>IN27</b>			
O	-4.64141300	1.22023600	-1.51671100	C	3.74414500	0.57931400	-0.64886900

C	3.96337300	-0.63138500	0.35671900	H	-0.50842000	1.84327300	-2.13384600
C	4.74211600	0.03440300	1.54132500	C	-3.13776800	3.89407900	-0.13004200
C	4.72002800	1.63608300	-0.01699100	H	-3.33490000	2.14961300	1.12419500
C	2.33530000	1.19333500	-0.62168700	C	-2.49893800	4.46459600	-1.23739900
C	1.65617100	1.64683400	0.48116300	H	-1.05259500	4.16739800	-2.81863300
C	2.66657500	-1.31544800	0.79310200	H	-3.87174000	4.46761800	0.43225900
H	1.96592300	1.52668800	-1.59088900	H	-2.73710700	5.48273100	-1.53799700
H	0.78234800	-0.68673000	-1.44495800	C	-1.92575600	-0.12773900	1.68517400
H	0.81784200	2.32966500	0.35281800	C	-1.32629400	0.72559500	2.64061000
H	2.07502000	1.53803200	1.48254800	C	-2.69849500	-1.21833700	2.12947500
H	4.34180000	-0.22221600	2.52842300	C	-1.50847500	0.49617600	4.00880300
H	5.80354300	-0.25922100	1.50509700	H	-0.74777800	1.58851100	2.31096600
H	4.44581600	2.67138500	-0.24166300	C	-2.87686200	-1.44141500	3.49977000
H	5.74955200	1.44636400	-0.37034400	H	-3.16559800	-1.88361000	1.40640500
C	4.18994000	0.19944000	-2.05086800	C	-2.28199200	-0.58952100	4.43937500
C	3.45783800	0.11778700	-3.16612600	H	-1.05364400	1.16676300	4.73504700
H	2.38932400	0.32404800	-3.19781400	H	-3.48495000	-2.27995400	3.83301700
H	3.91874700	-0.17273200	-4.10791400	H	-2.42504600	-0.76794000	5.50317700
H	4.61281900	-1.36926400	-0.13082000				
H	5.25418900	-0.04268300	-2.11304400	<b>TS24</b>			
O	4.61568200	1.42459900	1.36202500	C	3.40957000	0.77135500	-0.38135800
Rh	0.81176300	-0.50441600	0.08774000	C	3.97054100	-0.55615600	0.28780200
H	2.42331300	-1.21334900	1.86023100	C	4.87305800	-0.01519100	1.44805100
C	2.01645400	-2.38759400	0.11205900	C	4.40282500	1.81570700	0.23687200
C	0.65225700	-2.60477100	0.52008700	C	2.00516700	1.11535700	0.10909900
H	0.40026600	-2.55029600	1.58481500	C	1.59438400	1.00706700	1.41833400
H	0.04061800	-3.30313200	-0.04817400	C	2.85952400	-1.49640700	0.73789400
C	2.55907500	-3.01708700	-1.15211400	H	1.41170400	1.74876300	-0.55363100
H	3.14303400	-2.31212300	-1.75198800	H	-0.09014500	-1.94327400	-0.55613300
H	1.74707200	-3.41891000	-1.76831400	H	0.69635600	1.51977900	1.75525800
H	3.21159200	-3.85565500	-0.86657700	H	2.25413600	0.61844400	2.19044300
P	-1.50052900	0.10452400	-0.06567900	H	4.65250800	-0.47029700	2.42098100
C	-2.65614300	-0.89664100	-1.03647300	H	5.93363900	-0.19263600	1.20925700
C	-2.18128200	-1.95838500	-1.82733400	H	3.99868000	2.83233300	0.27413300
C	-4.03808900	-0.61163400	-1.02026400	H	5.34215200	1.81896000	-0.34584000
C	-3.07283000	-2.73106200	-2.58208100	C	3.51845200	0.72556400	-1.89377300
H	-1.11473800	-2.17192300	-1.85660900	C	2.51979300	0.70610200	-2.78269600
C	-4.92423800	-1.38701800	-1.77076600	H	1.46897700	0.71182300	-2.49370200
H	-4.41781800	0.21835500	-0.42640800	H	2.73023900	0.67685300	-3.84998700
C	-4.44206800	-2.44786500	-2.55165500	H	4.59781400	-1.07101000	-0.44950900
H	-2.69657100	-3.54812400	-3.19412300	H	4.54775800	0.70235400	-2.26185100
H	-5.98836400	-1.16139200	-1.75270700	O	4.61739000	1.36565000	1.54270800
H	-5.13551900	-3.04707700	-3.13830300	Rh	0.81561000	-0.85744800	0.20534500
C	-1.88923100	1.83140800	-0.46210500	H	2.68994700	-1.57897500	1.81383700
C	-1.24479300	2.41793100	-1.57056300	C	2.29738500	-2.50130700	-0.07812200
C	-2.83742000	2.58323600	0.25846700	C	1.03991700	-3.03606300	0.40567300
C	-1.55174700	3.72568100	-1.95865300	H	0.86069700	-3.10323800	1.48131800

H	0.54657000	-3.81263500	-0.17616600	C	-2.85752200	-1.31248800	-0.16841300
C	2.78965200	-2.85454200	-1.46676800	H	-1.00262600	1.90729900	0.51595800
H	3.17840500	-1.98381500	-2.00249100	H	-0.36638400	0.70749200	2.57335600
H	1.98449200	-3.29843700	-2.06330500	H	-1.99254600	-0.13939800	2.61984200
H	3.59412600	-3.59998100	-1.37889700	H	-2.21275600	1.63391500	-1.62551100
P	-1.41566500	0.03990400	0.01625600	H	-3.58684300	2.68004200	-1.17632200
C	-1.98296400	0.23013700	-1.70053700	C	-3.88889400	2.12930800	1.26170500
C	-1.36132100	-0.48867000	-2.73999600	C	-3.46721300	2.77879800	2.34933400
C	-3.06641600	1.08130900	-2.01292200	H	-2.45416800	2.68697300	2.73538000
C	-1.81853900	-0.37317300	-4.05843300	H	-4.13966100	3.44173100	2.88993200
H	-0.51443900	-1.13494400	-2.51709000	H	-4.29718500	-0.46788700	1.23720500
C	-3.52106900	1.19246400	-3.32982900	H	-4.91714500	2.28684000	0.92668700
H	-3.54459900	1.66400400	-1.22767800	O	-4.04274300	0.75648000	-1.80179000
C	-2.89919600	0.46452300	-4.35365900	Rh	-0.70395400	-0.74342700	0.31611200
H	-1.32865000	-0.93486600	-4.85098400	H	-2.71643700	-1.35166000	-1.25412500
H	-4.35785800	1.84972600	-3.55690600	C	-2.40542400	-2.38226000	0.58107200
H	-3.25339900	0.55559600	-5.37846300	C	-1.73013500	-3.56629900	-0.10312200
C	-1.61411700	1.70269400	0.73297500	H	-2.44070800	-4.40545600	-0.15401300
C	-1.14333000	2.82319200	0.01461700	H	-0.86499800	-3.92302100	0.47469100
C	-2.11706500	1.88606500	2.03492300	C	-2.77180300	-2.63921800	2.03158700
C	-1.17874800	4.09760200	0.58853400	H	-3.32648100	-1.81795200	2.49241900
H	-0.77845300	2.70349800	-1.00511300	H	-1.87358900	-2.83565200	2.63276200
C	-2.14776600	3.16527800	2.60579000	H	-3.39906900	-3.54158500	2.08362300
H	-2.49274700	1.03564000	2.60001500	P	1.48076400	0.16552000	-0.00679200
C	-1.67710000	4.26993500	1.88721200	C	1.66219000	-0.77124800	-1.55286200
H	-0.82334100	4.95504500	0.02077600	C	1.29236900	-2.13587400	-1.46822600
H	-2.54398700	3.29514900	3.61081100	C	2.00717400	-0.23185200	-2.80562800
H	-1.70310000	5.26227800	2.33246200	C	1.26668400	-2.94086400	-2.61446900
C	-2.62102200	-1.01358400	0.87633900	H	1.09568100	-2.58960500	-0.49131500
C	-2.20714700	-1.66957100	2.05406100	C	1.98904100	-1.04397500	-3.94510100
C	-3.94410900	-1.17965900	0.42692600	H	2.29075100	0.81499500	-2.88875500
C	-3.10372500	-2.46329200	2.77658800	C	1.61375800	-2.39208400	-3.85442300
H	-1.18050400	-1.55196100	2.40236800	H	0.99384900	-3.99141600	-2.53599900
C	-4.83489200	-1.98400200	1.14659500	H	2.26963000	-0.62351700	-4.90864200
H	-4.27558500	-0.69512300	-0.48845300	H	1.60006700	-3.01354900	-4.74714200
C	-4.41872100	-2.62249800	2.32098400	C	2.81508200	-0.37808400	1.08519900
H	-2.77613900	-2.96084900	3.68717400	C	2.50915800	-0.79988600	2.39302800
H	-5.85419600	-2.11147800	0.78804400	C	4.15431800	-0.40577900	0.64109900
H	-5.11580700	-3.24674000	2.87627000	C	3.52832500	-1.23559700	3.24913200

**IN28**

C	-3.08352400	1.17889400	0.37461300	H	4.39933500	-0.09096300	-0.37253600
C	-3.80605600	-0.21541700	0.29227300	C	4.85398700	-1.25458200	2.80288400
C	-4.81098500	0.06142200	-0.85059400	H	3.28531200	-1.56114200	4.25833400
C	-3.19007500	1.65539700	-1.12478200	H	6.19798600	-0.86044500	1.15297100
C	-1.63526800	1.07726700	0.84023900	H	5.64609900	-1.59521200	3.46665300
C	-1.24428800	0.37571900	2.01863000	C	1.73592300	1.91851900	-0.37400300

C	0.87875700	2.54852700	-1.30412300	P	-1.23896400	0.17498000	-0.00728600
C	2.71388600	2.68460400	0.28696900	C	-1.69672600	1.83517900	0.58931600
C	1.01515100	3.91041500	-1.58138500	C	-1.45631900	2.16431900	1.94202800
H	0.11447300	1.96580700	-1.81898400	C	-2.27247800	2.80606400	-0.25206500
C	2.83874700	4.05257500	0.01207200	C	-1.81172000	3.41888900	2.44459100
H	3.37475300	2.21733000	1.01307100	H	-0.99031100	1.43505500	2.60257400
C	1.99578400	4.66483000	-0.92074200	C	-2.61505600	4.06673100	0.25279000
H	0.35782600	4.38381000	-2.30763600	H	-2.45283300	2.58363600	-1.30034800
H	3.59790200	4.63642400	0.52816400	C	-2.39227700	4.37380300	1.59879800
H	2.09733900	5.72704800	-1.13346300	H	-1.62991200	3.65366100	3.49145400
H	-1.41286400	-3.33230800	-1.12689600	H	-3.05968800	4.80656700	-0.40952800
H	-5.20129900	-0.84587400	-1.32455600	H	-2.66390900	5.35303400	1.98742400
H	-5.66024000	0.66434000	-0.48921900	C	-2.50861400	-0.96600300	0.63963900

**TS18-A**

C	2.95066300	0.69796600	1.20408400
C	1.59441600	1.05514200	1.66162600
H	1.19639800	2.01372600	1.32368500
H	1.39027800	0.86808600	2.71843500
C	2.47793600	1.89300700	-1.12396400
C	3.25492100	2.88576500	-0.24856900
C	4.81616300	0.85638300	-0.55828500
H	2.77230700	1.78017100	-2.16611700
H	1.40081800	1.83762500	-0.95547700
H	2.70499500	3.43221700	0.51405800
H	4.06423800	3.44892900	-0.71200700
C	4.64946600	-1.21880800	0.45971300
C	3.47269700	1.37801100	-0.05075200
O	4.83287700	-0.53576500	-0.73992200
C	3.16677000	-1.26335500	0.90058700
C	2.38781700	-2.15291000	-0.02913700
C	1.17702000	-2.75093900	0.34410300
C	0.57285700	-2.14279000	1.53717900
H	1.16481900	-2.08970500	2.45520500
H	-0.47809600	-2.37141100	1.71936100
Rh	1.01899700	-0.47797900	0.40960100
H	5.25856800	-0.77061200	1.26394500
H	4.99499000	-2.24806000	0.30434500
H	5.60776600	1.14288200	0.15802800
H	5.05534400	1.30408100	-1.52899300
H	3.69865500	0.59829600	1.99558500
H	3.08146900	-1.57791900	1.94432400
H	2.82670500	-2.35245200	-1.00734700
C	0.48842300	-3.79539100	-0.50256000
H	-0.60012500	-3.68577000	-0.44716700
H	0.73642900	-4.79358300	-0.11375300
H	0.80908200	-3.74879900	-1.54995900

C	-1.69672600	1.83517900	0.58931600
C	-1.45631900	2.16431900	1.94202800
C	-2.27247800	2.80606400	-0.25206500
C	-1.81172000	3.41888900	2.44459100
H	-0.99031100	1.43505500	2.60257400
C	-2.61505600	4.06673100	0.25279000
H	-2.45283300	2.58363600	-1.30034800
C	-2.39227700	4.37380300	1.59879800
H	-1.62991200	3.65366100	3.49145400
H	-3.05968800	4.80656700	-0.40952800
H	-2.66390900	5.35303400	1.98742400
C	-2.50861400	-0.96600300	0.63963900
C	-3.14833700	-0.75026100	1.87402000
C	-2.79747300	-2.14499300	-0.08049400
C	-4.05033200	-1.69543800	2.37906000
H	-2.96506300	0.16008700	2.43860400
C	-3.69968200	-3.08538400	0.42731500
H	-2.33665600	-2.31538300	-1.05183600
C	-4.32482600	-2.86459900	1.66150400
H	-4.54432700	-1.50867500	3.33037100
H	-3.92044000	-3.98345100	-0.14615900
H	-5.02750800	-3.59553800	2.05610500
C	-1.52725300	0.18300500	-1.80272300
C	-2.83389400	0.24571000	-2.33512700
C	-0.43439900	0.13104000	-2.68865500
C	-3.03348800	0.26714100	-3.71787700
H	-3.69245700	0.26880600	-1.66578700
C	-0.63679300	0.15150900	-4.07444600
H	0.58283800	0.06763400	-2.30277500
C	-1.93535500	0.22143300	-4.58876800
H	-4.04529000	0.31365900	-4.11517700
H	0.21726400	0.10794000	-4.74693000
H	-2.09454000	0.23441600	-5.66512800

**TS18**

H	3.11217200	-0.49139100	1.59586200
C	2.93285900	-0.59800100	0.52388400
C	1.64474600	-1.28201500	0.23664400
H	1.22556600	-1.83017200	1.08731900
H	1.58027100	-1.87021900	-0.68179700
C	4.39689700	-2.56768000	-0.41627100
C	4.16120100	-1.62458800	-1.60403300
C	5.44019300	-0.21129900	0.22365400
H	5.39899700	-2.96997200	-0.27405500
H	3.59065400	-3.24057600	-0.13069300
H	3.20999800	-1.68814800	-2.13034400

H	5.01053100	-1.39878700	-2.24853800	C	-3.72294000	-0.08757300	3.46994500
C	4.24944500	1.66037600	0.92230500	H	-4.06408000	0.05972900	1.34385400
C	4.20620300	-1.05848700	-0.17717400	C	-1.41625600	-0.36977400	4.16807200
O	5.11368400	0.63344000	1.29670300	H	0.04398300	-0.48523300	2.59293300
C	3.08049800	1.22761700	-0.01248300	C	-2.77194100	-0.23462900	4.48888500
C	2.08203700	2.37070000	-0.06874400	H	-4.77662200	0.01838000	3.71962800
C	1.14441400	2.50878000	-1.09818400	H	-0.67556900	-0.48260700	4.95690400
C	0.92362200	1.26521300	-1.84760900	H	-3.08774900	-0.24160800	5.52992800
H	1.78346000	0.77641600	-2.31629900				
H	0.01943400	1.22689000	-2.45915800	<b>TS18-B</b>			
Rh	0.82105000	0.57635600	0.09455600	H	-3.79613800	-0.22445000	-1.20902100
H	4.80257700	2.45438600	0.38783400	C	-2.81233900	0.25511100	-1.26081500
H	3.84667800	2.08221500	1.85161300	C	-2.01614200	-0.28474800	-2.38085000
H	5.80604400	0.38241800	-0.63318200	H	-1.10712300	0.26415000	-2.63767800
H	6.25920400	-0.85057900	0.56945000	C	-1.93571200	2.76436500	-0.97635800
H	2.16227600	3.14976700	0.69147700	C	-3.41600600	2.85872600	-1.34877700
C	0.29416500	3.74364500	-1.27789300	C	-3.32561400	1.41645700	0.85173200
H	-0.74172900	3.47412800	-1.51489800	H	-1.56474000	3.39492600	-0.17097900
H	0.68603200	4.32998200	-2.12140900	H	-1.22243700	2.59145100	-1.78180400
H	0.30792700	4.38004000	-0.38498400	H	-3.69718100	2.73120700	-2.39213800
H	3.42900800	1.01212500	-1.02554100	H	-4.04337400	3.55183000	-0.78946000
P	-1.39168800	-0.20394800	0.06959700	C	-3.26146700	-0.92820200	1.75624600
C	-1.62727300	-1.87958200	-0.58496900	C	-2.87596200	1.61228000	-0.60340400
C	-0.99057500	-2.22316000	-1.79623900	O	-2.57383800	0.35035700	1.50170000
C	-2.43074800	-2.83417500	0.06434200	C	-2.93664000	-1.83011600	0.55258500
C	-1.16423800	-3.49401100	-2.35141700	C	-1.80797100	-2.77457200	0.51900100
H	-0.36152500	-1.49040500	-2.30207600	C	-1.07378000	-2.77040500	-0.68371800
C	-2.59110500	-4.11090700	-0.48899000	C	-1.64409500	-2.05927500	-1.94119500
H	-2.92484800	-2.58638800	1.00114700	H	-2.66024300	-2.41880400	-2.12395500
C	-1.96207800	-4.44130600	-1.69408700	H	-0.99497000	-2.28905200	-2.78946500
H	-0.67430400	-3.74846800	-3.28913100	Rh	-1.40488100	-0.65719600	-0.07730600
H	-3.20848200	-4.84543900	0.02388500	H	-4.33155100	-0.73212600	1.88845800
H	-2.08868600	-5.43482900	-2.11929100	H	-2.83817900	-1.29255900	2.69794500
C	-2.57959700	0.84944400	-0.81676300	H	-4.39149100	1.15114300	0.89344100
C	-3.29462700	0.39817500	-1.94095600	H	-3.16115700	2.32065300	1.44817100
C	-2.77023200	2.17375900	-0.36600500	H	-2.56645600	-0.56834400	-3.28083600
C	-4.18163900	1.25780200	-2.60353700	H	-3.73847900	-1.98252300	-0.17309300
H	-3.17054900	-0.62308900	-2.29359900	H	-1.38990400	-3.26176000	1.40092900
C	-3.66228500	3.02349200	-1.02502800	C	0.22817700	-3.52997300	-0.83643400
H	-2.23236700	2.53405700	0.51101300	H	0.06972500	-4.44541600	-1.42456100
C	-4.36716000	2.56675200	-2.14870800	H	0.64128900	-3.80445200	0.14177800
H	-4.73218600	0.89646800	-3.46960300	H	0.97712100	-2.92142400	-1.36018600
H	-3.81061800	4.03874400	-0.66243900	P	0.95264900	0.24529400	0.06077200
H	-5.06179300	3.22919800	-2.66101400	C	1.98322600	0.49946200	-1.41907100
C	-1.96097900	-0.21367400	1.79358100	C	1.67415200	-0.22211700	-2.58887800
C	-3.32286900	-0.07156400	2.13009800	C	3.12624400	1.32572300	-1.41568600
C	-1.01392200	-0.36189100	2.82811100	C	2.47897900	-0.11941100	-3.72950800

H	0.80532900	-0.87711500	-2.60050100	C	-2.43844200	-2.35141200	0.56058500
C	3.92634600	1.43276500	-2.55787300	C	-3.45395700	-1.49201200	-0.22047500
H	3.38924100	1.88388700	-0.51974800	H	-4.34156500	-1.34455300	0.39930800
C	3.60408600	0.71256200	-3.71603900	H	-3.72182700	-2.01904400	-1.13771900
H	2.22761200	-0.68499500	-4.62446400	Rh	-1.31933500	-0.55749600	-0.10264500
H	4.80390600	2.07582400	-2.54139400	H	-1.82514700	0.75433700	3.65771900
H	4.22895700	0.79937100	-4.60244200	H	-0.27177900	0.17561300	2.99471700
C	1.85360200	-1.03731100	1.01017200	H	-4.16625300	0.67940700	-0.10085300
C	1.21125800	-1.63141900	2.11901200	H	-3.06870500	-0.06165100	1.71972700
C	3.13681800	-1.49153700	0.65473600	H	-1.11771000	-2.38219400	2.28993000
C	1.83959800	-2.63755400	2.85949200	C	-2.21395400	-3.77030800	0.08325300
H	0.21566600	-1.29667400	2.40983200	H	-3.13189400	-4.36421200	0.19730400
C	3.75873900	-2.51044700	1.38854400	H	-1.41789800	-4.25755300	0.65871300
H	3.65632200	-1.05853700	-0.19630400	H	-1.93884400	-3.78671700	-0.97975400
C	3.11540600	-3.08475000	2.48968400	P	0.96277100	-0.02842400	-0.10140900
H	1.33519800	-3.07183300	3.72070600	C	1.20602900	-1.09165900	-1.56361700
H	4.75008300	-2.85148700	1.09708500	C	0.37747900	-0.83591800	-2.68444200
H	3.60332400	-3.87296600	3.05928100	C	2.09622400	-2.18323400	-1.61267200
C	1.16171200	1.77585100	1.03921400	C	0.43347100	-1.66024700	-3.81614400
C	1.06086000	3.03138100	0.40284100	H	-0.26648200	0.04254700	-2.69377600
C	1.35009600	1.74130200	2.43342500	C	2.15145200	-2.99739900	-2.74866800
C	1.14939200	4.21578000	1.14105800	H	2.75213400	-2.38888300	-0.77060500
H	0.93702400	3.08513600	-0.67717100	C	1.31679000	-2.74464900	-3.84659600
C	1.42885500	2.92916100	3.17129200	H	-0.19983800	-1.44427100	-4.67418700
H	1.45515700	0.79004300	2.94873000	H	2.85195300	-3.82959600	-2.77887300
C	1.32826700	4.16771800	2.52975200	H	1.36684300	-3.38296600	-4.72621200
H	1.08742200	5.17437600	0.62927800	C	1.74974600	1.55727600	-0.49216300
H	1.58146700	2.88234400	4.24767600	C	2.61916400	1.67901600	-1.59456000
H	1.39867500	5.08891100	3.10442200	C	1.54773200	2.66273900	0.36023200
				C	3.27157400	2.89170300	-1.84327900
<b>TS18-C</b>				H	2.79028600	0.83103000	-2.25358200
H	-1.85922900	1.31039100	-1.88612600	C	2.21639600	3.86577300	0.11130300
C	-2.18293200	1.13218800	-0.85405300	H	0.86622800	2.57450200	1.20428300
C	-3.42920700	0.28603100	-0.80239800	C	3.07371700	3.98395100	-0.99060500
H	-3.87265000	0.08942100	-1.77902400	H	3.93758300	2.97894600	-2.69913000
C	-1.36780600	3.59293600	-0.72741000	H	2.06437700	4.71382300	0.77631200
C	-2.89455000	3.63094700	-0.69405200	H	3.58781900	4.92367800	-1.18274000
C	-2.13057100	2.44744700	1.47750000	C	1.93392600	-0.75668000	1.25344400
H	-0.82675900	4.28108200	-0.08124700	C	1.66059100	-2.08399100	1.65540500
H	-0.87118900	3.39779800	-1.67668500	C	2.92334000	-0.03024000	1.94114300
H	-3.43657400	3.44656700	-1.61974500	C	2.36235700	-2.66731200	2.71245200
H	-3.37712000	4.34472600	-0.02731400	H	0.91511500	-2.66917200	1.11897900
C	-1.25640600	0.57767800	2.72818800	C	3.61641700	-0.61571100	3.00939400
C	-2.13054900	2.43332300	-0.05938700	H	3.15857000	0.98873200	1.64590400
O	-1.01379300	1.80108200	2.06514400	C	3.33888900	-1.92942800	3.39742800
C	-2.02516600	-0.36922200	1.82260600	H	2.15085000	-3.69464700	3.00224800
C	-1.83687400	-1.81430400	1.70257700	H	4.37724100	-0.04010700	3.53224400

H	3.88283000	-2.38107500	4.22437900	H	2.41085300	3.22063900	3.76019800
H	-2.08999700	3.49764900	1.79626100	H	1.84782500	5.25985900	2.44386600
H	-3.07079500	2.03774600	1.87858500	C	2.31309600	0.22075600	-1.58851000
<b>IN20-A</b>				C	3.47525900	1.01133200	-1.71507200
C	-2.95207700	0.76838900	-1.19419800	C	1.86372900	-0.52697400	-2.69358100
C	-1.44271200	0.62972400	-1.37145500	C	4.17171600	1.04461700	-2.92663200
H	-0.91403600	1.57866200	-1.20592300	H	3.82650200	1.60327500	-0.87193500
H	-1.17845000	0.25244900	-2.36737300	C	2.56498100	-0.49030600	-3.90386900
C	-2.43326900	1.43673000	1.34982400	H	0.96780100	-1.13650600	-2.60229400
C	-2.67574700	2.75332800	0.58669300	C	3.71740700	0.29548000	-4.02066800
C	-4.86487400	1.38245900	0.35973400	H	5.06560600	1.65789800	-3.01813800
H	-2.87669400	1.29164400	2.33336600	H	2.20936000	-1.06986000	-4.75309600
H	-1.39173800	1.06637100	1.29158300	H	4.26076600	0.32715500	-4.96289500
H	-1.84531800	3.15572700	0.00890300	C	2.28321000	-1.11279200	1.01874100
H	-3.29109700	3.51087700	1.07098500	C	3.54623100	-1.64275300	0.70125900
C	-5.11368800	-0.53072600	-0.95578700	C	1.59969100	-1.59701800	2.15753500
C	-3.35642700	1.47121400	0.11160400	C	4.11601800	-2.63215300	1.51206800
O	-5.34498800	0.06194900	0.29565900	H	4.07952600	-1.28899600	-0.17839300
C	-3.59083100	-0.65977900	-1.21458300	C	2.17351700	-2.58306200	2.96654400
C	-3.00046800	-1.54973800	-0.12466800	H	0.62678300	-1.18048600	2.43351800
C	-2.00028600	-2.51922000	-0.24085700	C	3.43363000	-3.10264000	2.64045500
C	-0.91936800	-2.31317900	-1.20132300	H	5.09455900	-3.03500100	1.25934000
H	-1.17208400	-1.96498600	-2.20457400	H	1.64288700	-2.94176900	3.84605900
H	-0.09301000	-3.02587300	-1.17638500	H	3.88155300	-3.87254600	3.26516600
Rh	-0.83609500	-0.65812700	0.06796500	<b>IN20</b>			
H	-5.57304600	0.06995900	-1.76113400	H	-3.08987900	0.22112500	1.64428000
H	-5.59772100	-1.51337100	-0.93477900	C	-3.07402000	0.31684800	0.54306900
H	-5.38137400	2.00396100	-0.39525900	C	-1.63885300	0.62393000	0.10487500
H	-5.12409100	1.76391500	1.35400100	H	-1.19990200	1.45284100	0.68202800
H	-3.37737700	1.34174100	-2.03705000	H	-1.55974100	0.86897500	-0.96202100
H	-3.41792400	-1.10247700	-2.20633700	C	-3.87623200	2.86700500	0.23885900
H	-3.59367000	-1.57496400	0.79155000	C	-4.06060800	2.17870500	-1.12610100
C	-1.79323900	-3.54023500	0.86829600	C	-5.52841600	0.87172600	0.58848500
H	-0.74180800	-3.59522000	1.18306200	H	-4.67628500	3.50868700	0.60590500
H	-2.06682600	-4.53384300	0.48483100	H	-2.87621200	3.20727600	0.50192200
H	-2.42305400	-3.32886200	1.73989600	H	-3.18557400	2.08504900	-1.76544100
P	1.42973900	0.11193300	-0.01413100	H	-4.98939500	2.34798000	-1.66841000
C	1.64572700	1.73443500	0.78065300	C	-4.95879000	-1.38015200	0.38255000
C	1.33247200	2.89576200	0.03996600	C	-4.14294100	1.35981800	0.17102400
C	2.03217600	1.86507500	2.12731700	O	-5.83726800	-0.36823500	-0.00332100
C	1.40822500	4.15720500	0.63686300	C	-3.50024800	-1.06096000	-0.04510600
H	1.06223300	2.81729800	-1.01261900	C	-2.57270400	-2.16443400	0.42461500
C	2.10176200	3.13243700	2.72074800	C	-1.56118800	-2.77028900	-0.31582400
H	2.29241200	0.98586900	2.71238900	C	-0.86367300	-1.95367200	-1.31442100
C	1.78900600	4.27718200	1.98065200	H	-1.44542800	-1.29682800	-1.96375000
H	1.17956500	5.04529300	0.05124600	H	-0.00069800	-2.40895900	-1.80615000

Rh	-0.47474500	-0.99718200	0.46513900	C	3.52746800	-0.42321800	0.89522800
H	-5.30730300	-2.30535800	-0.09078100	C	2.69577000	-0.88292600	2.11718100
H	-4.98298800	-1.51945900	1.48214300	H	2.36550200	-0.05737800	2.76716200
H	-2.86931000	-2.67172200	1.34798400	H	3.24202400	-1.55387700	2.77774600
C	-0.92501300	-4.07585100	0.13182600	C	2.05812800	1.87249400	0.96518200
H	0.17288100	-4.02655600	0.10823400	C	3.44558700	2.15926700	1.56940000
H	-1.22297400	-4.87012900	-0.56815300	C	3.84205900	1.40585600	-0.86647700
H	-1.25395800	-4.36705600	1.13593100	H	1.62849500	2.57981400	0.25672800
H	-3.47824500	-0.98050900	-1.14135300	H	1.30437100	1.47542300	1.65457000
H	-6.30431300	1.57444100	0.26477900	H	3.61820100	1.86485600	2.60416500
H	-5.57698600	0.78313600	1.69081800	H	3.94257400	3.08573600	1.28356500
P	1.52548900	0.23484800	0.02680800	C	3.80160200	-0.77413700	-1.63518900
C	2.74912600	-1.01372400	-0.46379800	C	3.29859300	1.06157700	0.51966600
C	2.84577100	-2.16956300	0.34240900	O	3.34311500	0.53550300	-1.85212300
C	3.56551900	-0.89828100	-1.60220900	C	3.22930200	-1.36532500	-0.33043000
C	3.74435700	-3.18829000	0.01607800	C	1.72256500	-1.65354600	-0.48018900
H	2.23698600	-2.25935900	1.24507900	C	1.02657300	-2.62196600	0.34595400
C	4.46441700	-1.92372700	-1.92624200	C	1.67158100	-2.74270500	1.64884500
H	3.49985200	-0.01505800	-2.23377600	H	2.70742700	-3.06868400	1.67075500
C	4.55351500	-3.06575900	-1.12286900	H	1.08499300	-3.15060900	2.47631400
H	3.81973000	-4.07043100	0.64839100	Rh	0.72907700	-0.74835100	1.11661100
H	5.09579300	-1.82521900	-2.80678400	H	4.90551700	-0.78361900	-1.59554700
H	5.25250100	-3.85906200	-1.37951700	H	3.48478600	-1.37307600	-2.49696600
C	1.45193900	1.47514900	-1.28879000	H	4.94652700	1.35470600	-0.85277400
C	0.91996000	1.09706900	-2.54093600	H	3.55141700	2.42201100	-1.15646600
C	1.87739300	2.80133600	-1.09214400	H	4.59954400	-0.52869200	1.13062800
C	0.83365900	2.02624700	-3.57984000	H	3.75122800	-2.31878900	-0.15013000
H	0.58605300	0.07215500	-2.70219300	H	1.30215100	-1.45653100	-1.46650300
C	1.77876900	3.73140100	-2.13528100	C	-0.11273900	-3.49736500	-0.12876500
H	2.28297600	3.10953000	-0.13143700	H	-0.76403900	-3.79854200	0.70021300
C	1.26114800	3.34673300	-3.37610300	H	0.29274900	-4.41264600	-0.58401700
H	0.43249000	1.72466400	-4.54513000	H	-0.71417200	-2.98058500	-0.88847000
H	2.10934100	4.75532400	-1.97446700	P	-1.20310100	0.10754300	-0.08204800
H	1.18840800	4.07088400	-4.18491500	C	-1.17955300	-0.08504600	-1.88575700
C	2.20855600	1.03463900	1.50183700	C	-0.03473300	0.35717900	-2.58726700
C	1.35289500	1.36838600	2.57007000	C	-2.23911500	-0.67377000	-2.60045400
C	3.58571600	1.32013000	1.60682000	C	0.03004400	0.23370500	-3.97791500
C	1.86104200	1.98224700	3.72077000	H	0.81544200	0.78065200	-2.05024800
H	0.28503400	1.15575800	2.50666800	C	-2.16226500	-0.80309900	-3.99359500
C	4.08876000	1.93739500	2.75500400	H	-3.12251500	-1.02787200	-2.07431300
H	4.25980600	1.05197900	0.79459800	C	-1.03466800	-0.34538300	-4.68323400
C	3.22799300	2.26751900	3.81174700	H	0.91430700	0.58386200	-4.50624400
H	1.19313300	2.23302800	4.54201300	H	-2.98761900	-1.25846800	-4.53691700
H	5.15196200	2.15634300	2.82809400	H	-0.98244300	-0.44196900	-5.76577000
H	3.62451900	2.74337000	4.70632500	C	-1.31835900	1.89939700	0.24144000
				C	-1.25886300	2.88198200	-0.76172000
				C	-1.42227100	2.30110800	1.59115000

**TS19-A**



C	-1.29568300	4.24124700	-0.41807800	H	-0.52695900	2.94473400	2.38580400
H	-1.18871900	2.59243400	-1.80740800	H	0.44410400	2.37392300	3.75479800
C	-1.45791600	3.65579500	1.92912900	H	-0.76740100	1.29387500	3.02443400
H	-1.49876800	1.55089400	2.38032100	H	3.64162900	0.63872100	1.91185100
C	-1.38973300	4.62979800	0.92202700	H	6.19304700	-1.76029300	0.16407400
H	-1.25541000	4.99333100	-1.20353600	H	4.59718700	-2.44978300	-0.24589500
H	-1.54328400	3.95263300	2.97239500	P	-1.67877500	-0.23784500	-0.00113000
H	-1.41712500	5.68538200	1.18394900	C	-1.83952300	-2.01053700	-0.30762900
C	-2.79379600	-0.52390400	0.52012200	C	-1.13123300	-2.90456700	0.51871600
C	-4.00295500	0.11987900	0.17871300	C	-2.65905000	-2.51664900	-1.33786000
C	-2.83055300	-1.64199500	1.37323700	C	-1.24791300	-4.28549100	0.32464500
C	-5.21922400	-0.36344400	0.66615100	H	-0.48988400	-2.51874200	1.31009600
H	-3.98644600	1.00126300	-0.46079300	C	-2.76471100	-3.89679400	-1.53296700
C	-4.05124000	-2.12047700	1.86678700	H	-3.20516900	-1.83229800	-1.98555500
H	-1.90077300	-2.13426500	1.65454700	C	-2.06152100	-4.78015100	-0.70169500
C	-5.24455000	-1.48405300	1.51004300	H	-0.70202400	-4.97205400	0.96821800
H	-6.14671300	0.13704300	0.39581500	H	-3.39322900	-4.28330900	-2.33252100
H	-4.06832900	-2.98411300	2.52826800	H	-2.14484500	-5.85382500	-0.85740500
H	-6.19412500	-1.85325000	1.89203900	C	-1.64408700	0.57516600	-1.63446000
				C	-0.55969800	0.20985200	-2.47602700
<b>TS19</b>				C	-2.47857100	1.64421200	-2.02397300
H	2.65412700	-0.94686100	-0.48841300	C	-0.32826900	0.89564700	-3.68008600
C	3.18426700	-0.06446200	-0.09178700	H	0.04401300	-0.66931100	-2.23435700
C	2.52071200	1.17409500	-0.72007800	C	-2.24442600	2.31336400	-3.22776900
H	2.10122600	0.97026000	-1.71821100	H	-3.31407300	1.93847200	-1.39251600
H	3.17548400	2.03696400	-0.84328200	C	-1.16889900	1.94697700	-4.05319400
C	5.34668600	0.15041600	-1.67113900	H	0.49244300	0.59108300	-4.32651700
C	5.66991700	0.87701000	-0.35197000	H	-2.90499500	3.12457300	-3.52730600
C	5.11184700	-1.61393900	0.26616800	H	-0.99683400	2.47747500	-4.98730800
H	6.11032000	-0.49581100	-2.10190500	C	-3.16241400	0.31403600	0.87333600
H	4.74454500	0.68102200	-2.40777000	C	-4.23477400	-0.55636200	1.14578000
H	5.29760300	1.89380600	-0.22825500	C	-3.23171400	1.65461700	1.30853900
H	6.64219500	0.70460400	0.10619600	C	-5.35980100	-0.08658800	1.83362200
C	3.47884500	-1.48565600	1.95354100	H	-4.19228700	-1.59466000	0.82549500
C	4.67654000	-0.29100100	-0.36725900	C	-4.36201300	2.12025000	1.98459800
O	4.83425800	-1.65706500	1.64683000	H	-2.40134800	2.33034900	1.10898700
C	2.98025000	-0.11323000	1.45446400	C	-5.42659800	1.24769300	2.24989300
C	1.52814700	0.19485700	1.83634000	H	-6.18429500	-0.76519800	2.04158600
C	1.04613000	1.54874400	1.86848500	H	-4.40980100	3.15713300	2.31037600
C	1.77254900	2.39806100	0.92147900	H	-6.30340400	1.60771300	2.78411200
H	2.84839200	2.48058800	1.04670000				
H	1.30756900	3.33989400	0.62131000	<b>IN21</b>			
Rh	0.50072800	0.76443200	0.04745400	H	-2.92293900	0.34526700	-0.89277400
H	3.39353000	-1.56214100	3.04407500	C	-3.38384100	-0.18738300	-0.04046200
H	2.86633700	-2.28843900	1.49624800	C	-2.91033300	-1.67688200	-0.09406300
H	1.01610700	-0.53114700	2.47270600	H	-2.17359000	-1.80575800	-0.92447500
C	-0.02042800	2.06766800	2.80612700	H	-3.72400700	-2.35119400	-0.39128400

C	-5.83770900	-0.72279200	-1.00086200	H	-0.49010400	-0.20986100	-4.36754900
C	-5.91219000	-0.81141000	0.53482700	H	2.78639500	-2.96005700	-3.81602500
C	-5.11091700	1.62121400	-0.10246900	H	0.87834300	-2.12646000	-5.17737800
H	-6.63617800	-0.19555900	-1.52143400	C	3.02516000	-0.64399000	0.90733400
H	-5.44611500	-1.57960000	-1.54783800	C	4.07098500	0.07547400	1.51751400
H	-5.56204100	-1.73064900	1.00503000	C	2.96352800	-2.04628000	1.06705700
H	-6.75879300	-0.34945400	1.03973600	C	5.04577400	-0.60097200	2.26047200
C	-3.15300900	2.02018500	1.13339600	H	4.12466700	1.15668300	1.41685900
C	-4.88336300	0.10634600	-0.13775100	C	3.94636300	-2.71522100	1.79921800
O	-4.53245100	2.23858400	1.02378200	H	2.14519300	-2.60762500	0.61776300
C	-2.86711900	0.51261300	1.24708800	C	4.98853400	-1.99201300	2.39735900
C	-1.42423100	0.12680100	1.54984200	H	5.84915500	-0.03721500	2.72953600
C	-1.12971200	-1.25793100	1.66368100	H	3.89790900	-3.79648700	1.90907800
C	-2.26590600	-2.18836900	1.22637800	H	5.74972100	-2.51354400	2.97386600
H	-3.02878000	-2.22944000	2.02148400				
H	-1.89219500	-3.21087500	1.08504700	<b>TS22'</b>			
Rh	-0.42074600	-0.53454100	-0.22190400	C	2.22291900	-0.86517000	0.24101500
H	-2.82219500	2.55482700	2.03235500	C	2.20288800	0.65177700	0.61866600
H	-2.61459400	2.43828100	0.25855900	C	3.71709200	0.99282900	0.66825600
H	-0.82147600	0.83788500	2.12030700	C	3.48885800	-1.29781100	1.01242300
C	-0.11085600	-1.81058600	2.63918900	C	2.39384000	-0.93437700	-1.29367600
H	0.35585600	-2.72822700	2.26004200	C	1.23437700	-0.15165400	-1.93306800
H	-0.61531800	-2.06503300	3.58464800	C	1.31538900	1.36253800	-0.39202600
H	0.67787300	-1.08176800	2.85983700	H	3.36697600	-0.50595000	-1.55852800
H	-3.48369800	0.14911000	2.08742000	H	2.40170400	-1.97888400	-1.63224400
H	-6.18099000	1.85444400	-0.06698500	H	0.49240500	-0.80118300	-2.44239100
H	-4.69115700	2.06562800	-1.02617400	H	1.53474900	0.58946300	-2.67449200
P	1.73402200	0.18201600	-0.04133500	H	4.06123600	1.49659600	-0.24633800
C	2.11235900	1.94199000	-0.13090100	H	3.95271100	1.63671900	1.52641100
C	1.27320700	2.86456600	0.52190000	H	3.93759100	-2.22478400	0.63886100
C	3.23089700	2.40637700	-0.85602900	H	3.26828000	-1.41681600	2.08801300
C	1.55598000	4.23422700	0.46353000	C	0.89154400	-1.45860500	0.68236400
H	0.39901500	2.51068700	1.06554900	C	0.05480600	-2.23281900	-0.08144900
C	3.50419200	3.77497600	-0.91492400	H	0.33762200	-2.60014400	-1.06631100
H	3.87990500	1.69974100	-1.37193000	H	-0.80074900	-2.72111000	0.38115400
C	2.66927400	4.68745300	-0.25294100	H	0.63491200	-1.30730900	1.73434200
H	0.90631000	4.94377600	0.97125900	O	4.39674600	-0.24524500	0.78119500
H	4.36430400	4.13095900	-1.47788800	C	0.01526200	1.95350600	-0.02467500
H	2.88701800	5.75247800	-0.30022900	C	-0.87614100	2.07571200	-1.13710500
C	1.70296900	-0.48268100	-1.73138800	H	-0.48183300	2.19923300	-2.14710600
C	0.62258200	0.00324100	-2.52283600	H	-1.85813600	2.51477700	-0.97091200
C	2.46910900	-1.56972400	-2.20524100	Rh	-0.50151500	0.01871000	-0.59332000
C	0.32485500	-0.59938800	-3.76098900	C	-0.33041600	2.45162200	1.36282100
H	0.10272600	0.92362500	-2.23535700	H	0.09875200	3.45378900	1.51001200
C	2.17577000	-2.13954000	-3.44444200	H	-1.41789700	2.54067600	1.46912700
H	3.29377800	-1.95186000	-1.60739800	H	0.04868100	1.80098100	2.15818900
C	1.09912100	-1.66651400	-4.21652200	H	1.77471700	0.74681600	1.62346900

H	1.83981000	1.87356600	-1.19884900
P	-2.69609300	-0.35141800	0.35395400
C	-3.88194900	1.03596600	0.36454500
H	-4.84669800	0.71477300	0.77960700
H	-3.50491600	1.87036400	0.96940300
H	-4.04458400	1.39669600	-0.65916300
C	-3.62167400	-1.64416100	-0.54924000
H	-4.60527700	-1.81658500	-0.09131400
H	-3.76944600	-1.33558800	-1.59237900
H	-3.06612900	-2.59052100	-0.55035800
C	-2.72021100	-0.93537000	2.08462700
H	-3.74326700	-1.16557200	2.41193800
H	-2.10918000	-1.84107200	2.19537800
H	-2.30593100	-0.16153700	2.74412700

**TS24'**

C	-2.15835900	-0.74471900	-0.60736700
C	-2.56408700	0.42836000	0.38472400
C	-3.46640800	-0.29220700	1.44197700
C	-3.22127700	-1.82092800	-0.18624000
C	-0.77654100	-1.32205400	-0.30036900
C	-0.32651800	-1.60082800	0.97063400
C	-1.35421000	1.14680900	0.97078600
H	-0.27443600	-1.80201600	-1.14273900
H	1.58841500	1.59248000	-0.28099000
H	0.50469500	-2.28240600	1.12674600
H	-0.92582600	-1.36668600	1.84760700
H	-3.16409800	-0.09939100	2.47822200
H	-4.51369400	0.02447600	1.31818800
H	-2.91359900	-2.84770500	-0.40824800

H	-4.17821400	-1.60891200	-0.69661500
C	-2.32377700	-0.33831500	-2.05943800
C	-1.35820500	-0.16074300	-2.96639800
H	-0.30190400	-0.28645600	-2.73082000
H	-1.59921200	0.13610800	-3.98496400
H	-3.17049200	1.15112900	-0.17390400
H	-3.36193900	-0.17339200	-2.35933600
O	-3.33977100	-1.67277200	1.19860000
Rh	0.62277200	0.42862900	0.28321100
H	-1.15143500	0.98744900	2.03301600
C	-0.70848800	2.23211000	0.34679000
C	0.61522400	2.54257800	0.86776000
H	0.82496100	2.38643900	1.92976700
H	1.15174200	3.38555100	0.43421500
C	-1.18904100	2.91707700	-0.91525600
H	-1.76524400	2.25000800	-1.56091200
H	-0.34435300	3.31066600	-1.49235500
H	-1.82560600	3.76755500	-0.62838100
P	2.78026400	-0.56892000	-0.04683100
C	4.14368800	0.32690000	0.76789300
H	5.10740100	-0.15649500	0.55775600
H	3.98801900	0.34653700	1.85420000
H	4.18106700	1.36256700	0.40749200
C	3.27742100	-0.62137100	-1.80138300
H	2.56712100	-1.22966500	-2.37612600
H	4.28119900	-1.05400900	-1.91102300
H	3.27747800	0.39177900	-2.22178200
C	3.03329700	-2.29188800	0.50266100
H	4.06307700	-2.60897300	0.28868300
H	2.34948200	-2.97200500	-0.02174000
H	2.85855700	-2.38164700	1.58257500

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