

# Supporting Information

## Palladium-Catalyzed Selective C-C Bond Cleavage of Keto-Vinylidenecyclopropanes: Construction of Structurally Rich Dihydrofurans and Tetrahydrofurans

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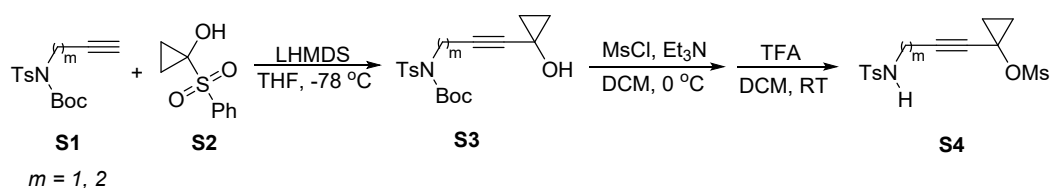
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## 1. General remarks

$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR spectra were recorded at 400 MHz or 600 MHz, 100 MHz or 150 MHz and 376 MHz, respectively. HRMS spectra were recorded by EI, ESI, FI method. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in  $\text{cm}^{-1}$ . Mass spectra were recorded by EI, ESI, and HRMS was measured on an Agilent Technologies 6224 TOF LC/MS instrument and a Waters Micromass GCT Premier. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. X-ray structure was determined on a Bruker Smart-1000 X-ray Diffraction meter. The employed solvents were dried up by standard methods when necessary. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC plate analysis with silica gel coated plates (Huanghai GF254). Flash column chromatography was performed by using 300-400 mesh silica gel eluting with ethyl acetate and petroleum ether at increased pressure. Chiral HPLC was performed on a SHIMADZU SPD-10A  $\nu\text{p}$  series with chiral columns (Chiralpak AD-H columns  $4.6 \times 250$  mm, (Daicel Chemical Ind., Ltd.)).

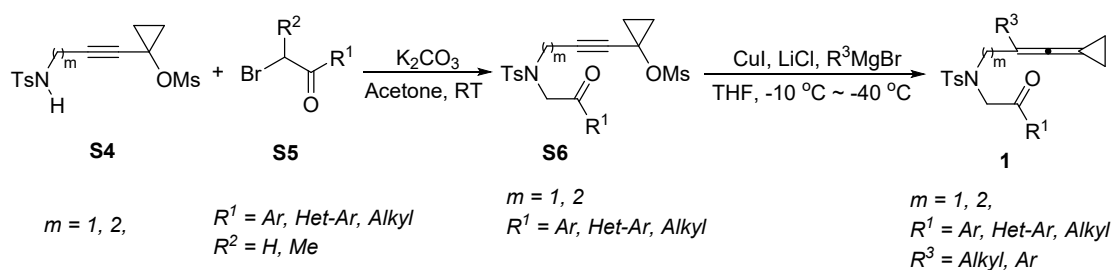
## 2. General procedures for the synthesis of substrates 1

Synthesis of substrates **1a-1q**, **1ad**, **1ae** and **1af**<sup>[1], [2], [3]</sup>



To the solution of compound **S1** (20 mmol) in THF (30 mL) was added LHMDS (22 mmol, 1.0 M in THF) within 20 min at  $-78\text{ }^\circ\text{C}$  under argon. The resulting solution was allowed to stir at  $-78\text{ }^\circ\text{C}$  for 0.5 h before a solution of **S2** (10 mmol) in THF (10 mL) was added into the above mixture. Consequently, the reaction mixture was allowed to warm up to room temperature and was stirred for 8 h. Then, saturated  $\text{NH}_4\text{Cl}$  solution was added to quench the reaction. Extracted with ethyl ether, dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, the organic phase was purified by a flash column chromatography on silica gel to give the corresponding product **S3** (PE/EA: 4:1~2:1).

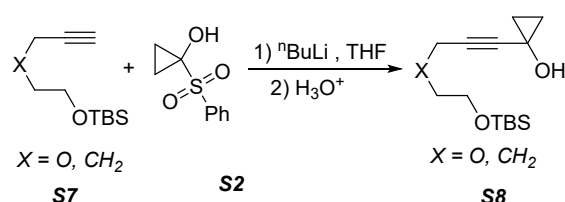
Under argon atmosphere, compound **S3** (4.0 mmol) was dissolved in DCM (10.0 mL) at  $0\text{ }^\circ\text{C}$ ,  $\text{Et}_3\text{N}$  (8.0 mmol) and MsCl (6.0 mmol) was added. After stirring for 1 h, the reaction was quenched with  $\text{H}_2\text{O}$  (10.0 mL), extracted with DCM (10 mL x 3), and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure and the residue was transferred into a 50 mL flask with 10 mL DCM. Then, trifluoroacetic acid (TFA, 40 mmol) was added dropwise. After stirring for 12 h, the reaction was quenched with saturated  $\text{Na}_2\text{CO}_3$  solution, extracted with DCM (10 mL x 3), and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography ( $\text{SiO}_2$ ) to give the corresponding product **S4** (PE/EA: 4:1~1:1).



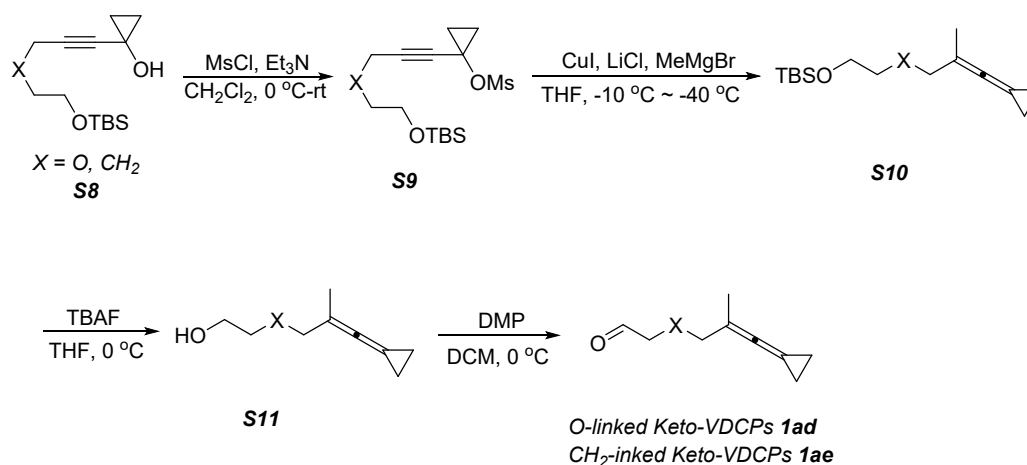
To the solution of **S4** (1.5 mmol) and  $K_2CO_3$  (1.8 mmol) in acetone (10 ml) was added **S5** (1.8 mmol). The resulting solution was allowed to stir at room temperature for 8 h. Then,  $H_2O$  was added to quench the reaction. The reaction mixture was extracted with EA twice, dried over anhydrous  $Na_2SO_4$ . The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography ( $SiO_2$ ) to give the corresponding product **S6** for two steps (PE/EA: 4:1~2:1).

Under argon atmosphere,  $CuI$  (2.2 mmol) and  $LiCl$  (2.2 mmol) in a three-necked bottle was dried upon heating. Then THF (10 mL) was added. At  $-5\text{ }^\circ C$ ,  $R^3MgBr$  (1.0 mol/L in THF, 2.0 mmol, 2.0 mL) was added to the reaction. 10 minutes later, the flask was moved into a  $-40\text{ }^\circ C$  bath and stirred for a while before a solution of **S6** (1.0 mmol) in THF (10 mL) was added dropwise into the above flask. After stirring at  $-40\text{ }^\circ C$  for 8 h, the reaction was quenched with saturated  $NH_4Cl$  solution, extracted with EA (10 mL x 3), and dried over anhydrous  $Na_2SO_4$ . The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography ( $SiO_2$ ) to give the corresponding product **1** (PE/EA: 10:1).

**Typical procedure for the preparation of compounds *O*-linked Keto-VDCPs **1ad** and  $CH_2$ -linked Keto-VDCPs **1ae**.**



To the solution of compound **S7** (20 mmol) in THF (30 mL) was added LMHDS (21 mmol, 1.0 M in THF) within 20 min at  $-78\text{ }^\circ C$  under argon. The resulting solution was allowed to stir at  $-78\text{ }^\circ C$  for 0.5 h before a solution of **S2** (10 mmol) in THF (10 mL) was added into the above mixture. Consequently, the reaction mixture was allowed to warm up to room temperature and was stirred for 8 h. Then, saturated  $NH_4Cl$  solution was added to quench the reaction. Extracted with ethyl ether, dried over anhydrous  $Na_2SO_4$ , filtered, the organic phase was purified by a flash column chromatography on silica gel to give the corresponding product **S8** (PE/EA: 8:1~4:1).



Under argon atmosphere, compound **S8** (4.0 mmol) was dissolved in DCM (10.0 mL) at 0 °C, Et<sub>3</sub>N (8.0 mmol) and MsCl (6.0 mmol) were added. After stirring for 1 h, the reaction was quenched with H<sub>2</sub>O (10.0 mL), extracted with DCM (10 mL x 3), and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **S9** (PE/EA: 10:1).

Under argon atmosphere, CuI (8.8 mmol) and LiCl (8.8 mmol) in a three-necked bottle was dried upon heating. Then THF (10 mL) was added. At -5 °C, MeMgBr (1.0 mol/L in THF, 8.0 mmol, 8.0 mL) was added to the reaction. 10 minutes later, the flask was moved into a -40 °C bath and stirred for a while before a solution of **S9** (4.0 mmol) in THF (10 mL) was added dropwise into the above flask. After stirring at -40 °C for 8 h, the reaction was quenched with saturated NH<sub>4</sub>Cl solution, extracted with EA (10 mL x 3), and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **S10** (PE/EA: 10:1).

Tetrabutylammonium fluoride (TBAF, 1.0 mol/L in THF, 6.0 mmol, 6.0 mL) was added dropwise into compound **S10** (4.0 mmol) was dissolved in THF (10.0 mL) at 0 °C. After stirring for 1 h, the reaction was quenched with saturated NaHCO<sub>3</sub> solution, extracted with DCM (10 mL x 3), and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **S11** (PE/EA: 4:1~1:1).

Then, **S11**, DMP and anhydrous DCM was added to the round bottom flask. After stirring for 1 h, the reaction was quenched with saturated NaHCO<sub>3</sub> solution and the organic phase was washed by

saturated  $\text{Na}_2\text{O}_3\text{S}_2$  solution. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography ( $\text{SiO}_2$ ) to give the corresponding *O*-linked Keto-VDCPs **1ad** and *CH*<sub>2</sub>-linked Keto-VDCP **1ae** (PE/EA: 4:1~1:1).

### 3. Optimization of the palladium-catalyzed 3+2 cycloaddition and tandem cyclization reactions of keto-vinylidenecyclopropanes **1** for products **2a**, **3a** and **4a**.

**Table S1.** Optimization of the palladium-catalyzed [3+2] cycloaddition and tandem cyclization reactions of keto-vinylidenecyclopropane **1a** for products **2a**, **3a** and **4a**

Entry <sup>a</sup>	Catalyst	L	Additive	Solvent	T (°C)	Yield/% <sup>b</sup>		
						<b>2a</b>	<b>3a</b>	<b>4a</b>
1	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	none	toluene	100	8	46	26
2	Pd <sub>2</sub> (dba) <sub>3</sub>	RuPhos	none	toluene	100	6	18	6
3	Pd <sub>2</sub> (dba) <sub>3</sub>	dppf	none	toluene	100	-	-	-
4	Pd <sub>2</sub> (dba) <sub>3</sub>	dppb	none	toluene	100	-	-	-
5	Pd <sub>2</sub> (dba) <sub>3</sub>	(rac)-BINAP	none	toluene	100	-	-	-
6 <sup>c</sup>	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	none	toluene	120	12	60	10
7	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	20 mol% AgOTf	toluene	100	-	40	8
8	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	20 mol% AgSbF <sub>6</sub>	toluene	100	-	32	8
9	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	20 mol% ZnI <sub>2</sub>	toluene	100	-	60	10
10	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	20 mol% LiCl	toluene	100	-	74	10
11	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	10 mol% LiCl	toluene	100	-	62	12
12	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	100 mol% equiv ZnI <sub>2</sub>	toluene	100	-	82	6
13	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	20 mol% ZnCl <sub>2</sub>	toluene	100	-	90	trace
<b>14</b>	<b>Pd<sub>2</sub>(dba)<sub>3</sub></b>	<b><sup>t</sup>BuXPhos</b>	<b>100 mol% ZnCl<sub>2</sub></b>	<b>toluene</b>	<b>100</b>	-	<b>92</b>	<b>trace</b>
16	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	100 mol% ZnCl <sub>2</sub>	dioxane	100	-	80	8
17	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	100 mol% ZnCl <sub>2</sub>	DCE	100	-	80	12
18	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	100 mol% ZnCl <sub>2</sub>	PhCl	100	-	40	8
19	Pd <sub>2</sub> (dba) <sub>3</sub>	<sup>t</sup> BuXPhos	100 mol% ZnCl <sub>2</sub>	MeCN	100	-	-	-
20 <sup>d</sup>	Pd <sub>2</sub> (dba) <sub>3</sub>	HP <sup>t</sup> Bu <sub>3</sub> BF <sub>4</sub>	none	toluene	100	80	-	12
21 <sup>e</sup>	Pd <sub>2</sub> (dba) <sub>3</sub>	HP <sup>t</sup> Bu <sub>3</sub> BF <sub>4</sub>	none	toluene	100	6	-	82
22	<b>Pd<sub>2</sub>(dba)<sub>3</sub></b>	<b>dtbpf</b>	<b>none</b>	<b>toluene</b>	<b>100</b>	<b>96</b>	-	-
23	Pd <sub>2</sub> (dba) <sub>3</sub>	dtbpf	none	toluene	90	72	-	6
24	Pd <sub>2</sub> (dba) <sub>3</sub>	dtbpf	none	toluene	120	86	-	-
25	Pd <sub>2</sub> (dba) <sub>3</sub>	dtbpf	none	dioxane	100	80	-	10
26	Pd <sub>2</sub> (dba) <sub>3</sub>	dtbpf	none	DCE	100	82	-	12
27	Pd <sub>2</sub> (dba) <sub>3</sub>	dtbpf	none	PhCl	100	48	-	6
28	Pd <sub>2</sub> (dba) <sub>3</sub>	dtbpf	none	MeCN	100	-	-	-
26	Pd <sub>2</sub> (dba) <sub>3</sub>	-	none	toluene	100	-	-	-
27	-	<sup>t</sup> BuXPhos	none	toluene	100	-	-	-
28	-	dtbpf	none	toluene	100	-	-	-

<sup>t</sup>BuXPhos

RuPhos

dppf

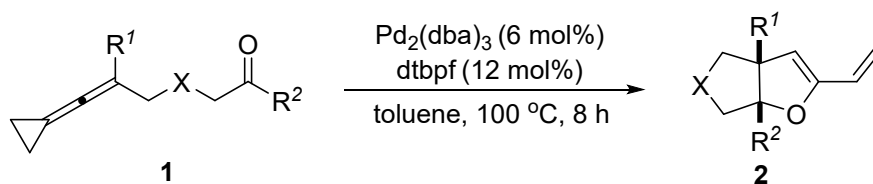
dppb

(rac)-BINAP

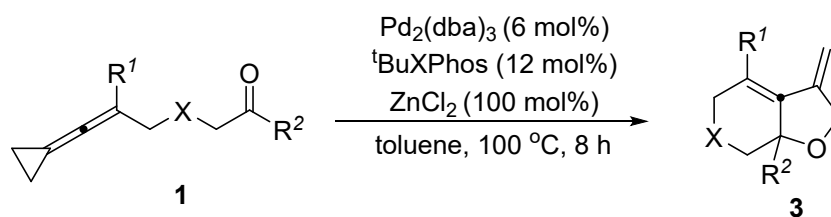
dtbpf

<sup>a</sup>Reaction condition: substrate **1a** (0.10 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (6 mol%) and L (12 mol%) in 1.0 mL anhydrous toluene under argon atmosphere for 8 h. <sup>b</sup>Isolated yield. <sup>c</sup>Pd<sub>2</sub>(dba)<sub>3</sub> (10 mol%), L (20 mol%) was added. <sup>d</sup>K<sub>2</sub>CO<sub>3</sub> (20 mol%) was added. <sup>e</sup>K<sub>2</sub>CO<sub>3</sub> (100 mol%) was added.

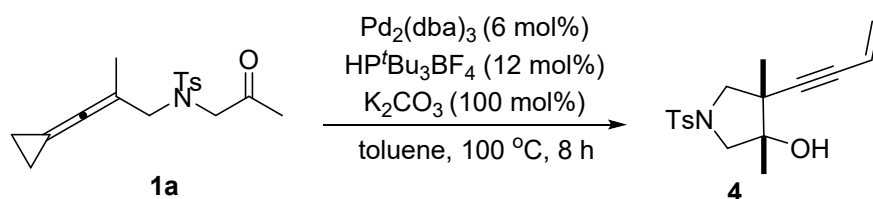
**4. General procedure for the palladium-catalyzed 3+2 cycloaddition and tandem cyclization reactions of keto-vinylidenecyclopropanes **1** for products **2**, **3**, **4** and **12-14**.**



To a 10 mL dried tube was charged with keto-VDCPs **1** (0.1 mmol, 1.0 equiv), Pd<sub>2</sub>dba<sub>3</sub> (6 mol%) and dtbpf (12 mol%). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (1.0 mL) was added into the tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **2**.



To a 10 mL dried tube was charged with keto-VDCPs **1** (0.1 mmol, 1.0 equiv), Pd<sub>2</sub>dba<sub>3</sub> (6 mol%), <sup>t</sup>BuXPhos (12 mol%) and ZnCl<sub>2</sub> (100 mol%). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (1.0 mL) was added into the tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **3**.

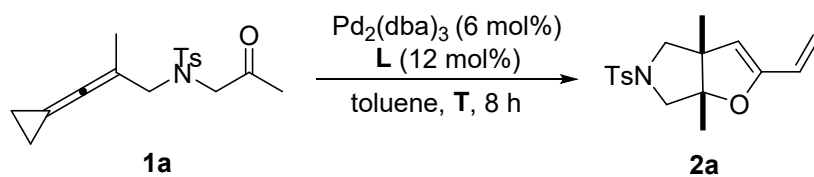






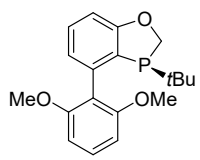
## 5. Asymmetric studies

**Table S2.** Studies of the enantioselective tandem cyclization reactions

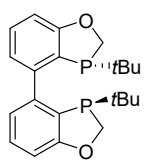


Entry <sup>a</sup>	Catalyst	L	T (°C)	Yield <sup>b</sup> (%)	ee <sup>c</sup> (%)
1	$\text{Pd}_2(\text{dba})_3$	<b>L1</b>	100	-	-
2	$\text{Pd}_2(\text{dba})_3$	<b>L2</b>	100	-	-
3	$\text{Pd}_2(\text{dba})_3$	<b>L3</b>	100	86	15
4	$\text{Pd}_2(\text{dba})_3$	<b>L4</b>	100	-	-
5	$\text{Pd}_2(\text{dba})_3$	<b>L5</b>	100	90	0
6	$\text{Pd}_2(\text{dba})_3$	<b>L6</b>	100	82	7
7	$\text{Pd}_2(\text{dba})_3$	<b>L7</b>	100	-	-
8	$\text{Pd}_2(\text{dba})_3$	<b>L8</b>	100	-	-
9	$\text{Pd}_2(\text{dba})_3$	<b>L3</b>	90	-	-
10	$\text{Pd}_2(\text{dba})_3$	<b>L5</b>	90	56	0
11	$\text{Pd}_2(\text{dba})_3$	<b>L6</b>	90	-	-
12	$\text{Pd}_2(\text{dba})_3$	<b>L9</b>	90	34	11
13	$\text{Pd}_2(\text{dba})_3$	<b>L10</b>	90	32	0
14	$\text{Pd}_2(\text{dba})_3$	<b>L11</b>	90	66	12
15	$\text{Pd}_2(\text{dba})_3$	<b>L12</b>	90	42	12
16	$\text{Pd}_2(\text{dba})_3$	<b>L13</b>	90	52	16
17	$\text{Pd}_2(\text{dba})_3$	<b>L14</b>	90	62	12
18	$\text{Pd}_2(\text{dba})_3$	<b>L15</b>	90	40	20
19	$\text{Pd}_2(\text{dba})_3$	<b>L16</b>	90	80	14
20	$\text{Pd}_2(\text{dba})_3$	<b>L17</b>	90	42	3
21	$\text{Pd}_2(\text{dba})_3$	<b>L18</b>	90	30	16
22	$\text{Pd}_2(\text{dba})_3$	<b>L19</b>	90	60	2
23	$\text{Pd}_2(\text{dba})_3$	<b>L20</b>	90	40	9
24	$\text{Pd}_2(\text{dba})_3$	<b>L21</b>	90	34	16
25	$\text{Pd}_2(\text{dba})_3$	<b>L22</b>	90	15	20
26	$\text{Pd}_2(\text{dba})_3$	<b>L23</b>	90	-	-
27	$\text{Pd}_2(\text{dba})_3$	<b>L24</b>	90	32	4
28	$\text{Pd}_2(\text{dba})_3$	<b>L25</b>	90	50	12
29	$\text{Pd}_2(\text{dba})_3$	<b>L26</b>	90	-	-
30	$\text{Pd}_2(\text{dba})_3$	<b>L27</b>	90	-	-

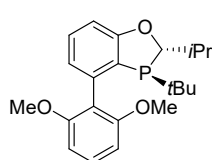
<sup>a</sup>Reaction condition: substrate **1a** (0.10 mmol),  $\text{Pd}_2(\text{dba})_3$  (6 mol%) and **L** (12 mol%) in 1.0 mL anhydrous toluene under argon atmosphere for 8 h. <sup>b</sup>Isolated yield. <sup>c</sup>Determined by HPLC on a chiral stationary phase.



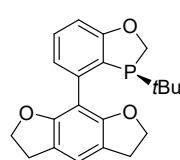
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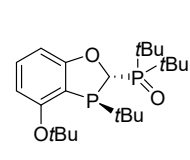
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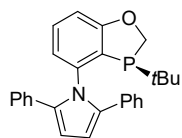
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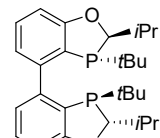
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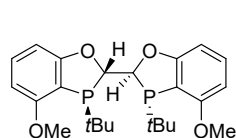
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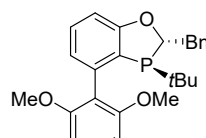
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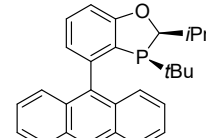
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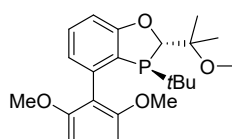
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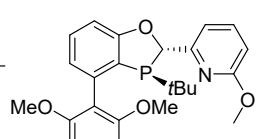
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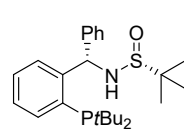
L10



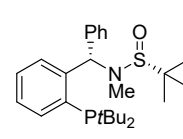
L11



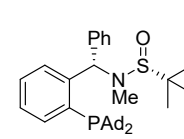
L12



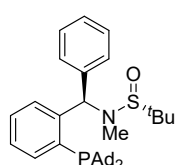
L13



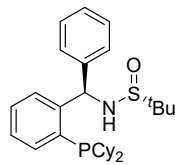
L14



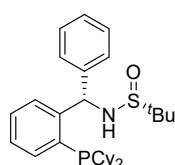
L15



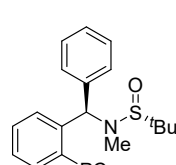
L16



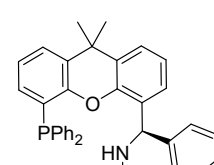
L17



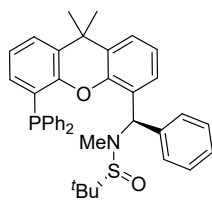
L18



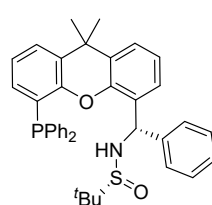
L19



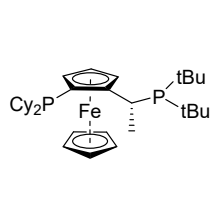
L20



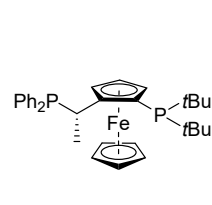
L21



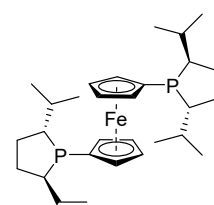
L22



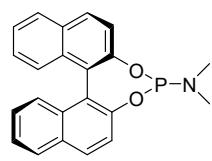
L23



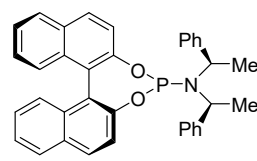
L24



L25

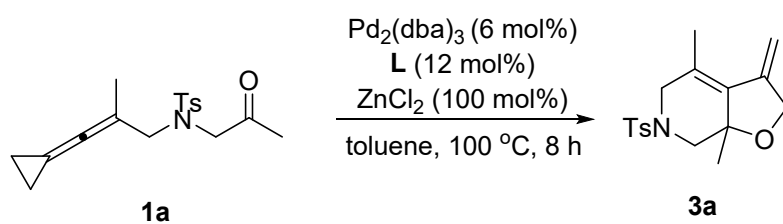


L26

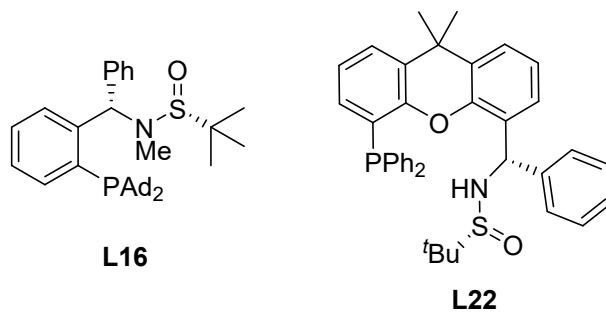
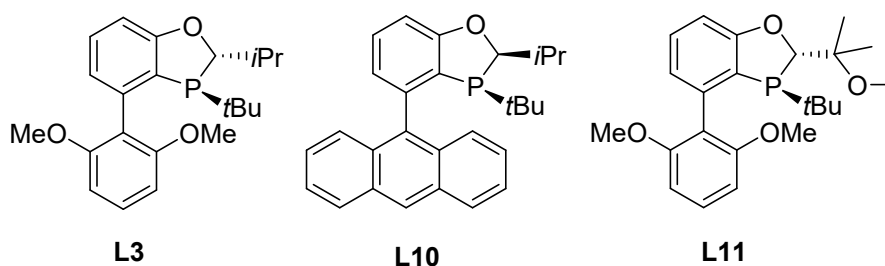


L27

**Table S3.** Studies of the enantioselective [3+2] cycloaddition reactions



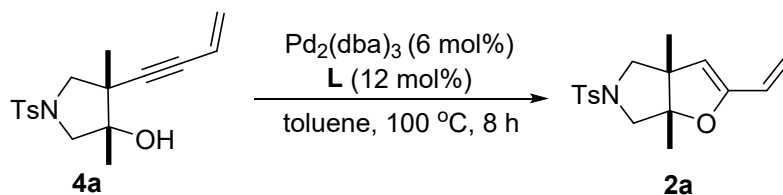
Entry	L	Yield (%)	ee <sup>c</sup> (%)
1	<b>L3</b>	36	0
2	<b>L18</b>	20	0
3	<b>L19</b>	26	0
4	<b>L14</b>	NR	0
5	<b>L26</b>	NR	0



## 6. Control experiment and the other proposed reaction mechanisms

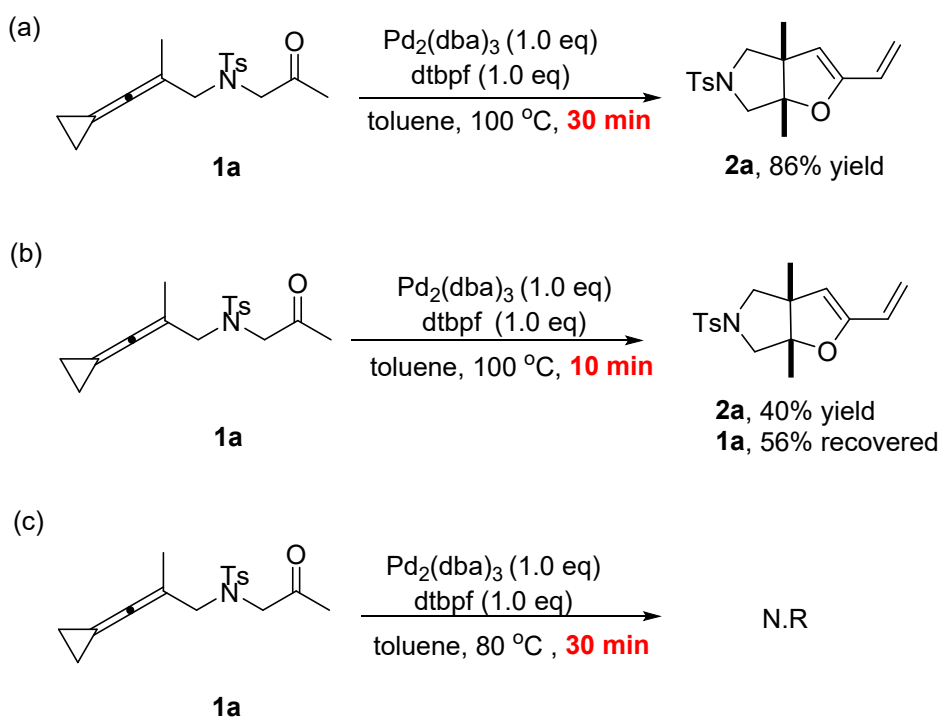
### 6.1 Control experiment

#### 6.1.1 Transformation experiment of 4a to 2a



To a 10 mL dried tube was charged with **4a** (0.1 mmol, 1.0 equiv), Pd<sub>2</sub>(dba)<sub>3</sub> (6 mol%) and **L** (12 mol%). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (1.0 mL) was added into the tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **2a**.

#### 6.1.2 Equivalent catalyst and ligand reactions



To a 10 mL dried tube was charged with **1a** (0.1 mmol, 1.0 equiv), Pd<sub>2</sub>(dba)<sub>3</sub> (1.0 equiv) and **L** (1.0 equiv). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (1.0 mL) was added into the tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding product **2a**.

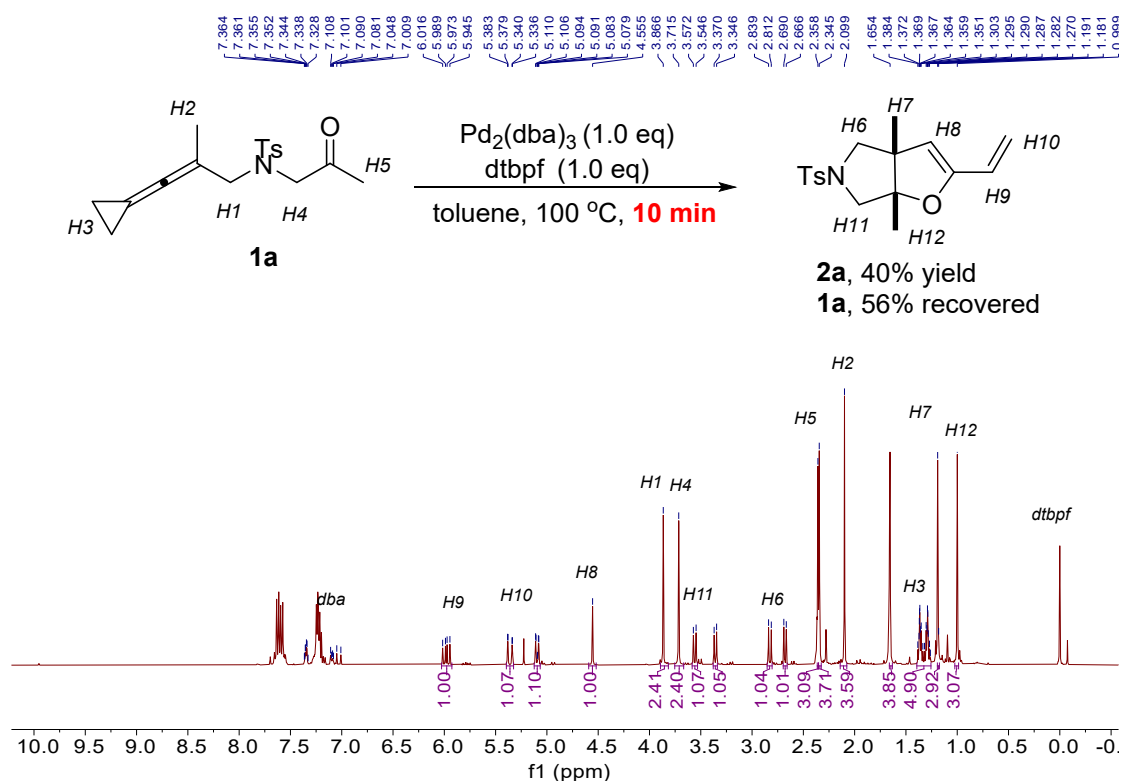
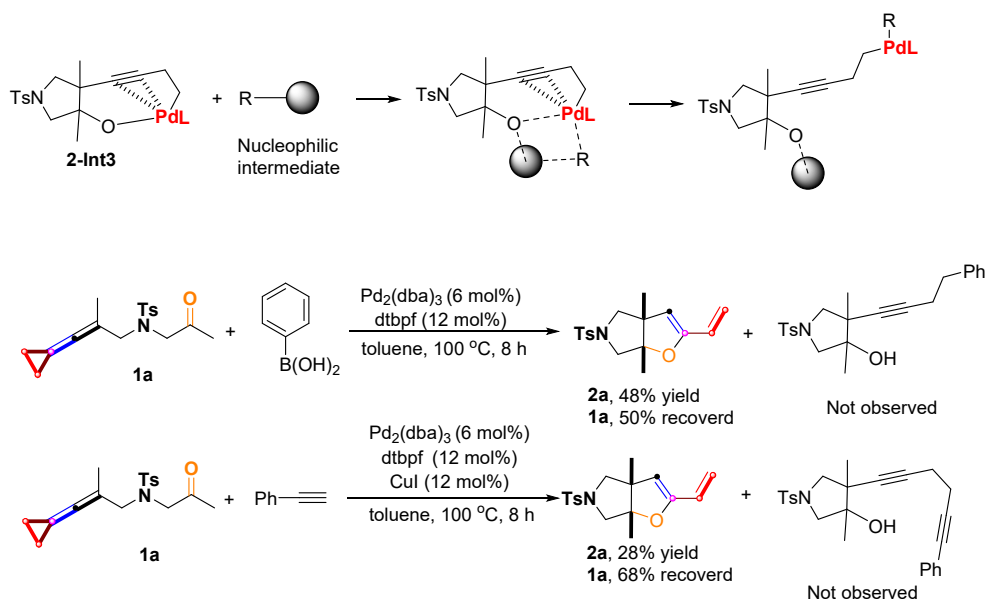


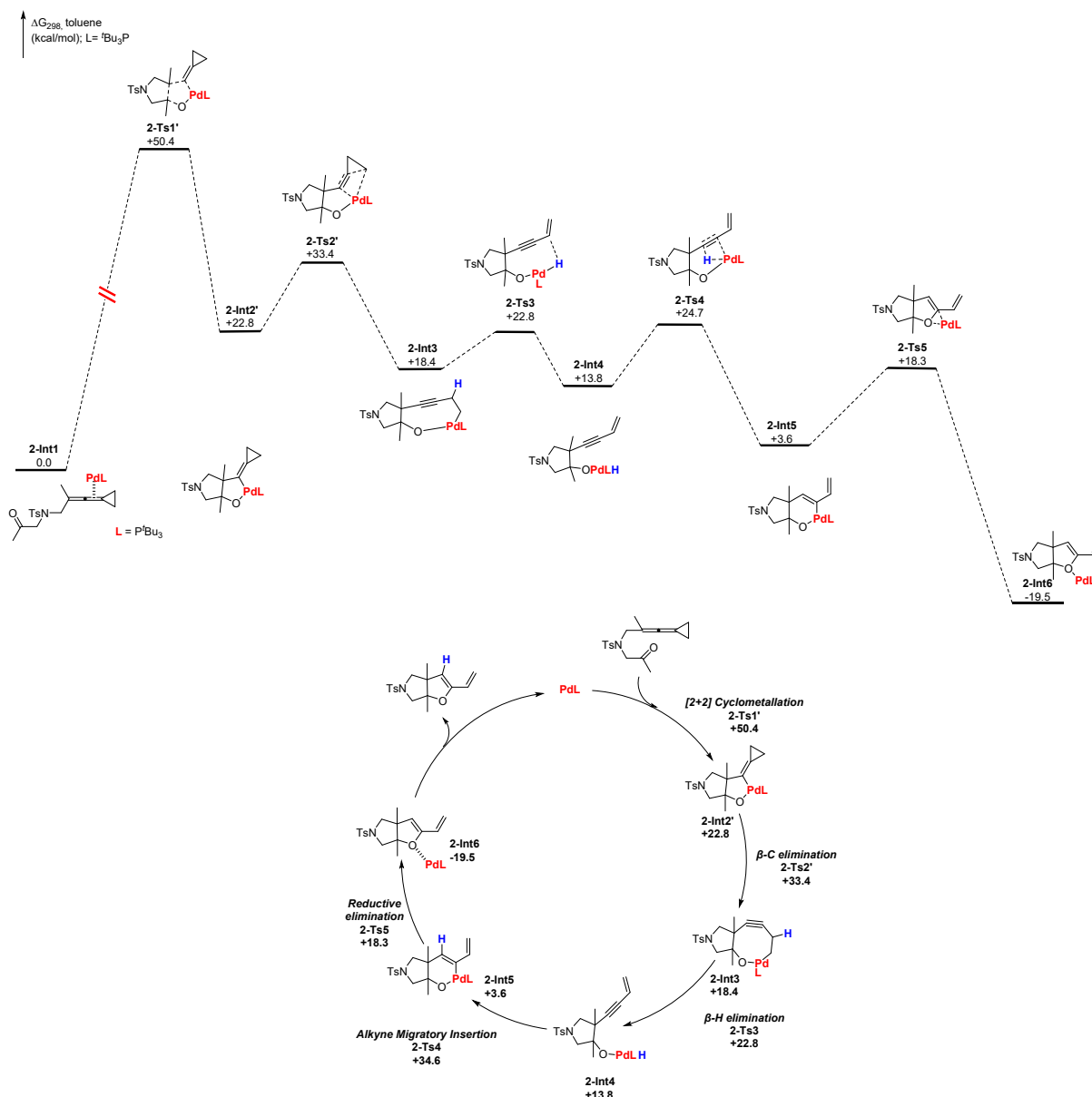
Figure S1.  $^1\text{H}$  NMR spectra of equivalent catalysts and ligands reaction after 10 min

### 6.1.3 Cross-coupling reactions involving nucleophilic reagents



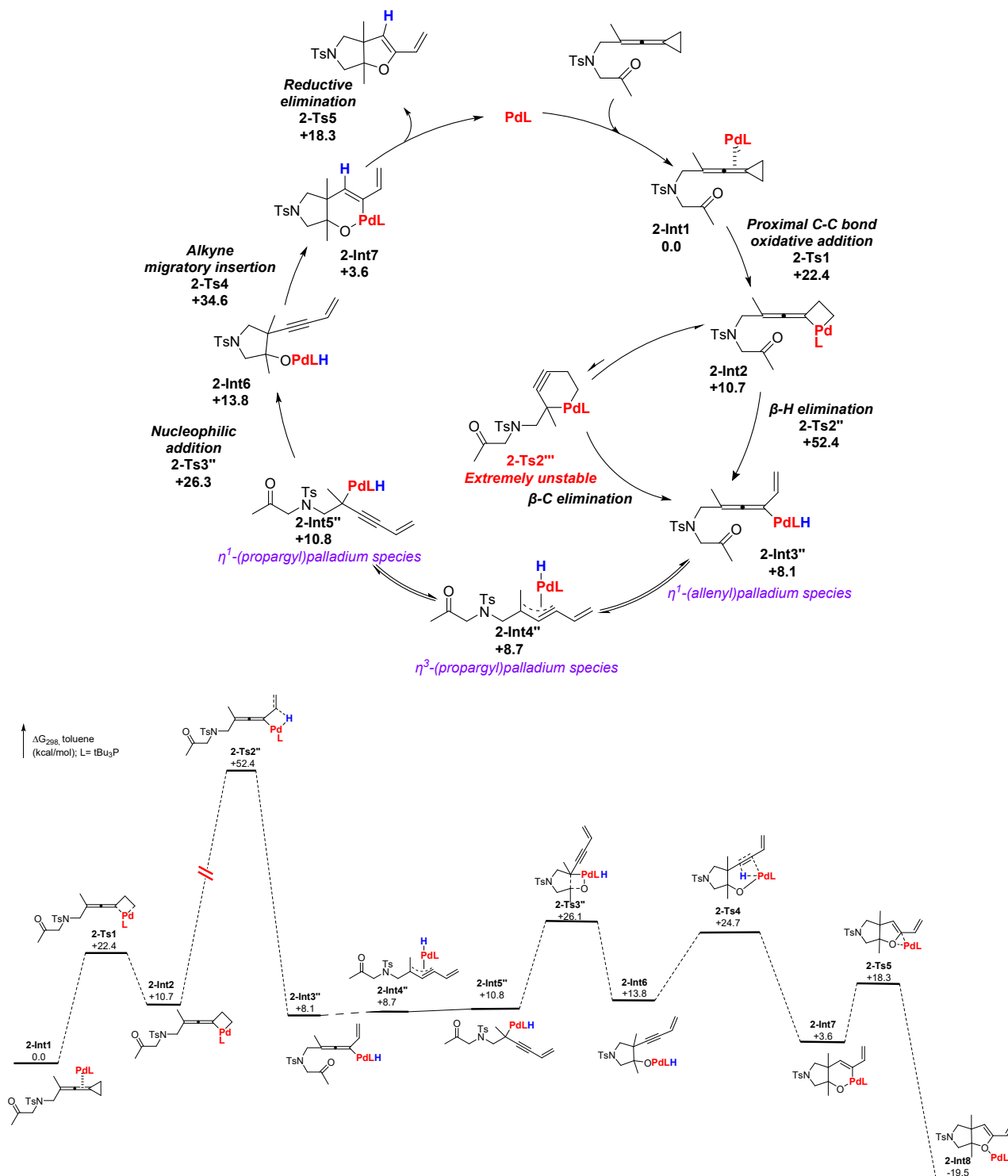
To a 10 mL dried tube was charged with **1a** (0.1 mmol, 1.0 equiv), phenylboronic acid (0.12 mmol, 1.2 equiv) or phenylacetylene (0.12 mmol, 1.2 equiv) and CuI (12 mol%), Pd<sub>2</sub>(dba)<sub>3</sub> (6 mol%) and L (12 mol%). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (1.0 mL) was added into the tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO<sub>2</sub>) to give the corresponding products.

## 6.2 The other proposed reaction mechanisms



**Scheme S1.** Proposed mechanism involving [2+2] cyclometallation process.

We also investigated another possible pathway to form the intermediate **2-Int3**. We propose that the reaction initiates through a cyclometallation process via **2-Ts1'** to give an intermediate **2-Int2'**, but it requires an extremely high energy barrier (50.4 kcal/mol) to implement the process. **2-Int2'** can occur β-carbon elimination to generate **2-Int3** via **2-Ts2'** with an energy barrier of 10.6 kcal/mol.



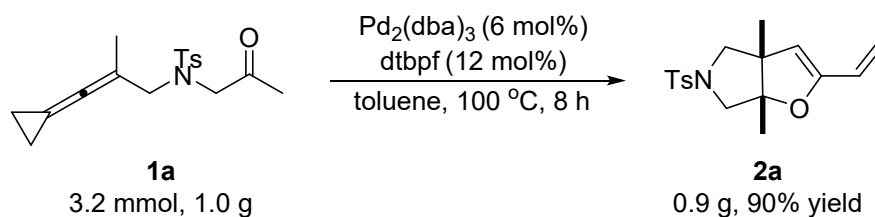
**Scheme S2.** Proposed catalytic cycle

We investigated an alternative reaction pathway starting from a stable palladium complex **2-Int1** (shown in Scheme S2), in which the allene units of **1a** is coordinated to palladium catalyst. The **2-Int1** can undergo an oxidative cyclometallation to give a palladacyclic **2-Int2** through **2-Ts1** with an energy barrier of 22.4 kcal/mol. The intermediate **2-Int2** subsequently undergoes  $\beta$ -hydrogen

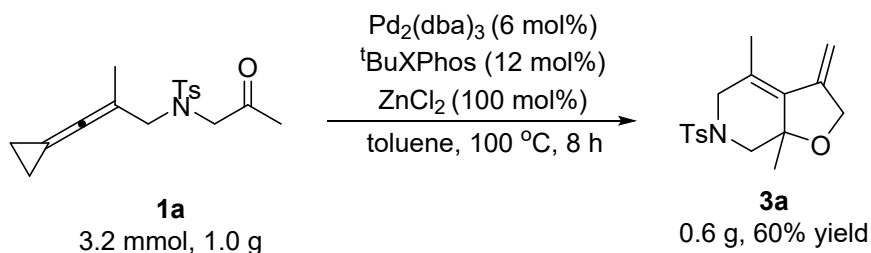


elimination to generate an intermediate **2-Int3**'' via transition state **2-TS2**'' with an extremely high energy barrier of 41.7 kcal/mol. We envisaged the formation of **2-Int2**''' through the isomerization of **2-Int2**, but the optimization process of **2-Int2**''' indicates that this type of intermediate is unstable and still goes back to **2-Int2** intermediate. Then, the  $\eta^1$ -(allenyl)palladium-H **2-Int3**'' could be transformed to  $\eta^3$ -(propargyl)palladium-H species **2-Int4**'' ( $\Delta G = 0.6$  kcal/mol) and  $\eta^1$ -(propargyl)palladium-H species **2-Int5**'' ( $\Delta G = 2.1$  kcal/mol). Subsequently, intramolecular C=O bond insertion occurs via **2-Ts3**'' to give **2-Int6** with an activation free energy of 15.3 kcal/ mol. Then **2-Int6** undergo migratory insertion via **2-Ts4** to generate **2-Int7** with a free energy of 20.8 kcal/ mol. Subsequently, reductive elimination of **2-Int7** is followed to afford **2-Int8** with an energy barrier of 14.7 kcal/ mol. This reaction pathway also involves the step having extremely high energy barrier, thus, we exclude this pathway.

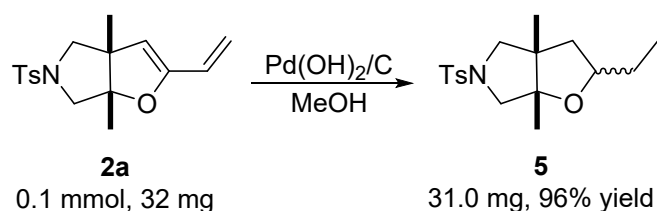
## 7. Gram scale reaction and synthetic transformation of the products



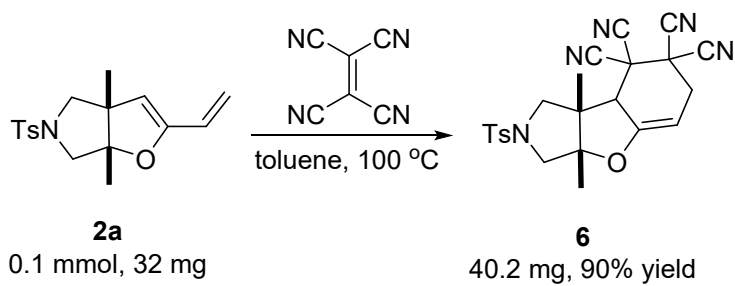
To a 10 mL dried tube was charged with **1a** (1.0 g, 3.2 mmol),  $\text{Pd}_2\text{dba}_3$  (175.7 mg, 0.19 mmol) and dtbpf (182.2 mg, 0.38 mmol). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (40.0 mL) was added into the reaction tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography ( $\text{SiO}_2$ ) to give the corresponding product **2a** (0.9 g, 90% yield).



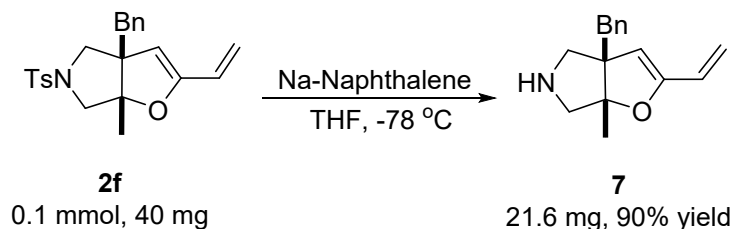
To a 10 mL dried tube was charged with **1a** (1.0 g, 3.2 mmol),  $\text{Pd}_2\text{dba}_3$  (175.7 mg, 0.19 mmol) and  $^t\text{BuXPhos}$  (162.8 mg, 0.38 mmol) and  $\text{ZnCl}_2$  (435.2 mg, 3.2 mmol). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (40.0 mL) was added into the reaction tube. The reaction mixture was stirred at 100 °C for 8 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography ( $\text{SiO}_2$ ) to give the corresponding product **3a** (0.6 g, 60% yield).



To a solution of **2a** (32.0 mg, 0.1 mmol) in MeOH (5 mL) was added Pd(OH)<sub>2</sub>/C (7.6 mg, 20% w/w). The reaction system was charged with H<sub>2</sub> balloon and the reaction mixture was stirred at rt for 12 h. The reaction mixture was filtered and the volatiles were removed on a rotary evaporator. The residues were passed through a short silica chromatography (PE/EA = 1/1) to afford the desired product **5** (31 mg, 96% yield).



To a 10 mL dried tube was charged with **2a** (32 mg, 0.1 mmol), 1,1,2,2-tetracyanoethene (2.0 equiv, 0.2 mmol) and 1.0 mL toluene and the resulting mixture was stirred at 100 °C for 3 h. The reaction mixture was filtered and the volatiles were removed on a rotary evaporator. The residues were passed through a short silica chromatography (PE/EA = 4/1) to afford the desired product **6** (40.2 mg, 90% yield).

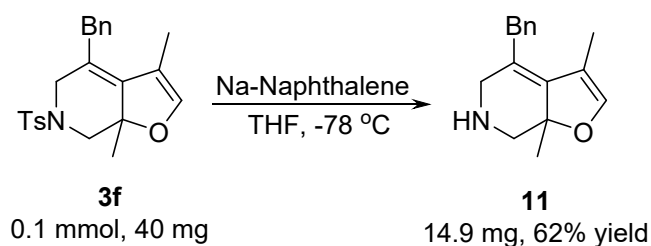


A solution 1.0 M of sodium naphthalenide in THF was prepared as follows: to a stirred solution of naphthalene (5.0 g, 39 mmol) in 39 mL of THF, sodium metal (1.1 g, 47 mmol) was added under



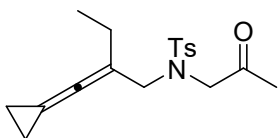
The reaction mixture was stirred for 3 h. After quenched by adding aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution and extracted by EA, the combined organic phase was washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/EA = 4:1) to give the desired product **9** (28.9 mg, 58% yield).

The 2,5-dimethylpyrazole (113 mg, 1.2 mmol) and CrO<sub>3</sub> (2.2 mg, 0.006 mmol, 0.06 eq.) was added in dry DCM (1.0 mL) at -20 °C. After stirring for 15 min at this temperature, a solution of **3a** (32 mg, 0.10 mmol) in DCM (0.5 mL) was added dropwise, and the resulting mixture was stirred for an additional hour. Then, NaOH (5M, 1.0 mL) was added and the reaction mixture was further stirred at 0 °C for 30 min. The reaction was quenched by 1.0 M HCl solution, extracted with EtOAc (3 x 10 mL) and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The organic phase was then concentrated under reduced pressure and the residue was purified by a flash chromatography (PE/EA = 4:1) to afford the corresponding product **10** (11.9 mg, 36%).



A solution 1.0 M of sodium naphthalenide in THF was prepared as follows: to a stirred solution of naphthalene (5.0 g, 39 mmol) in 39 mL of THF, sodium metal (1.1 g, 47 mmol) was added under nitrogen atmosphere, and the resulting solution was stirred for 1 h. A solution of **3f** (40 mg, 0.1 mmol) in anhydrous THF (2.0 mL) was cooled to -78 °C under nitrogen atmosphere and 1.0 mL (1.0 mmol) of 1.0 M sodium naphthalenide in THF was added dropwise. The reaction mixture was stirred for 40 min at this temperature. After being stirred for 30 min, the reaction was quenched with saturated NH<sub>4</sub>Cl aqueous solution, extracted with ethyl acetate, dried over anhydrous MgSO<sub>4</sub>, filtered, and evaporated. The residue was chromatographed through a silica gel column (DCM/MeOH = 6/1) to afford product **11** (14.9 mg, 62% yield).

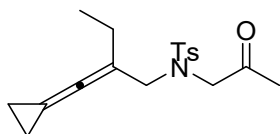
## 8. Spectroscopic data of substrates 1.



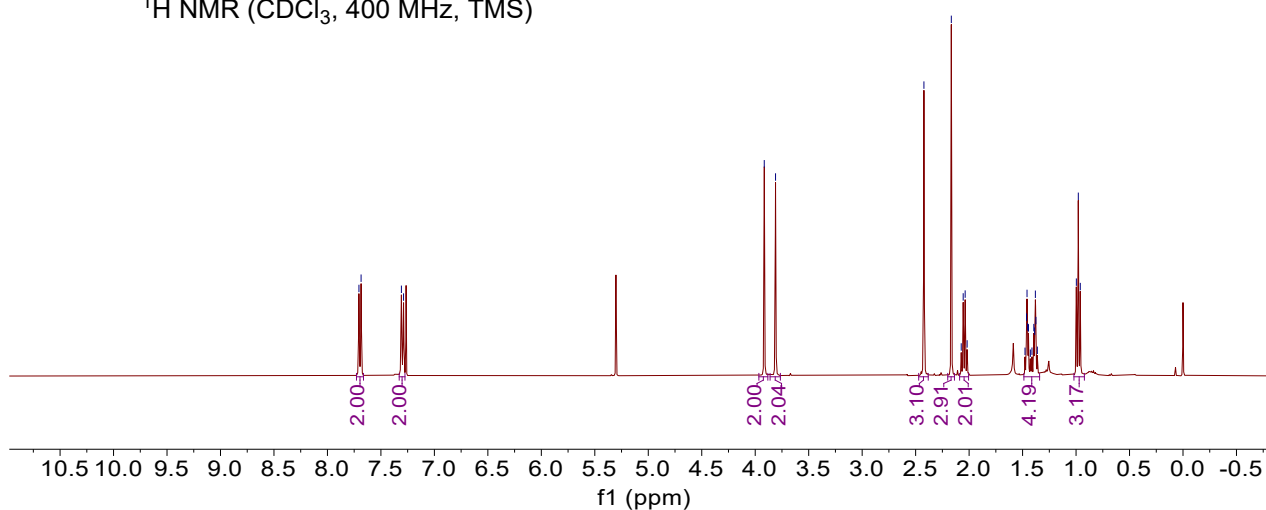
### *N*-(2-(cyclopropylidene- $\lambda^5$ -methylene)butyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide

#### (1b)

A colorless oil, 90% yield, 299.7 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 3.90 (s, 2H), 3.85 (s, 2H), 2.42 (s, 3H), 2.28 (p,  $J = 6.8$  Hz, 1H), 2.17 (s, 3H), 1.48 – 1.32 (m, 4H), 1.01 (t,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  204.1, 187.9, 143.5, 136.0, 129.6, 127.5, 108.0, 79.7, 55.7, 50.7, 28.6, 27.0, 21.6, 21.5, 7.4. IR (neat)  $\nu$  815, 987, 1157, 1216, 1346, 1447, 2018, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 356.1291, Found: 356.1293.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



— 204.056

— 187.935

— 143.497

— 135.991

— 129.575

— 127.498

— 108.041

— 79.738

— 77.389

— 77.071

— 76.753

— 55.707

— 50.688

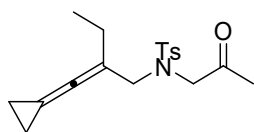
— 28.558

— 26.971

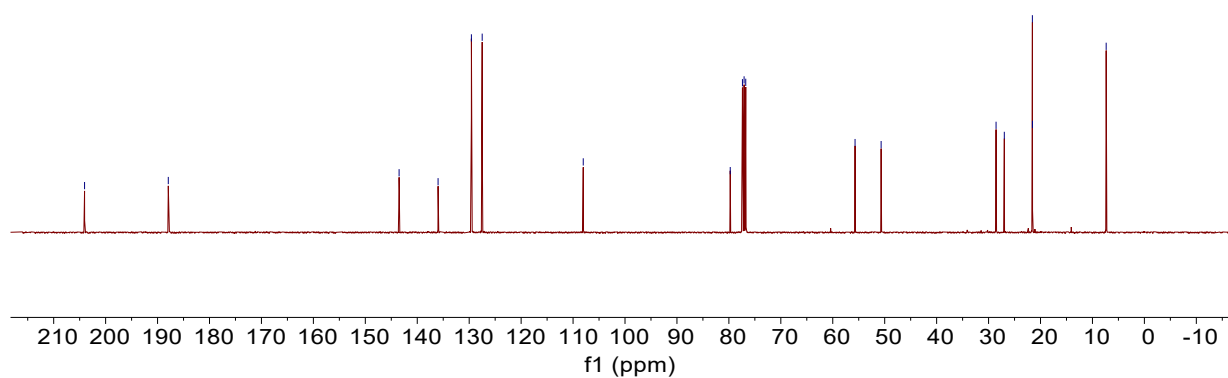
— 21.566

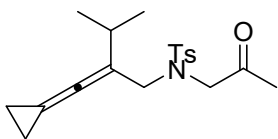
— 21.547

— 7.357



$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, TMS)





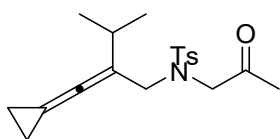
***N*-(2-(cyclopropylidene- $\lambda^5$ -methylene)-3-methylbutyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1c)**

A colorless oil, 88% yield, 305.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 3.90 (s, 2H), 3.85 (s, 2H), 2.42 (s, 3H), 2.28 (p,  $J = 6.8$  Hz, 1H), 2.17 (s, 3H), 1.48 – 1.32 (m, 4H), 1.01 (d,  $J = 6.8$  Hz, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  204.0, 188.6, 143.5, 136.1, 129.6, 127.5, 103.3, 79.3, 55.8, 52.1, 26.9, 23.5, 21.6, 12.1, 7.3. IR (neat)  $\nu$  815, 987, 1157, 1216, 1346, 1447, 2018, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 370.1447, Found: 370.1440.

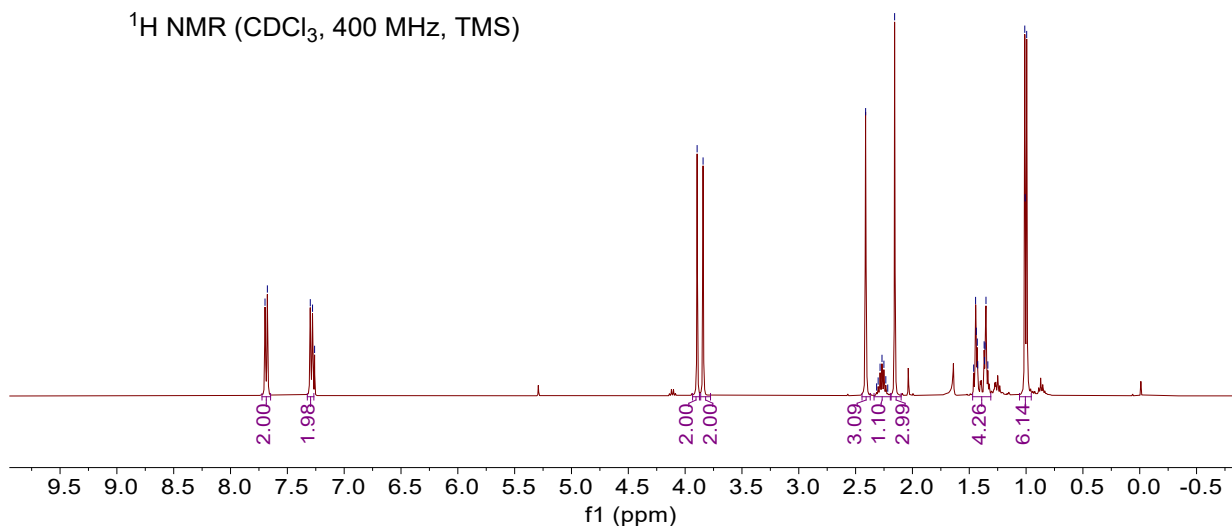
7.697  
7.676  
7.298  
7.278  
7.260

3.895  
3.842

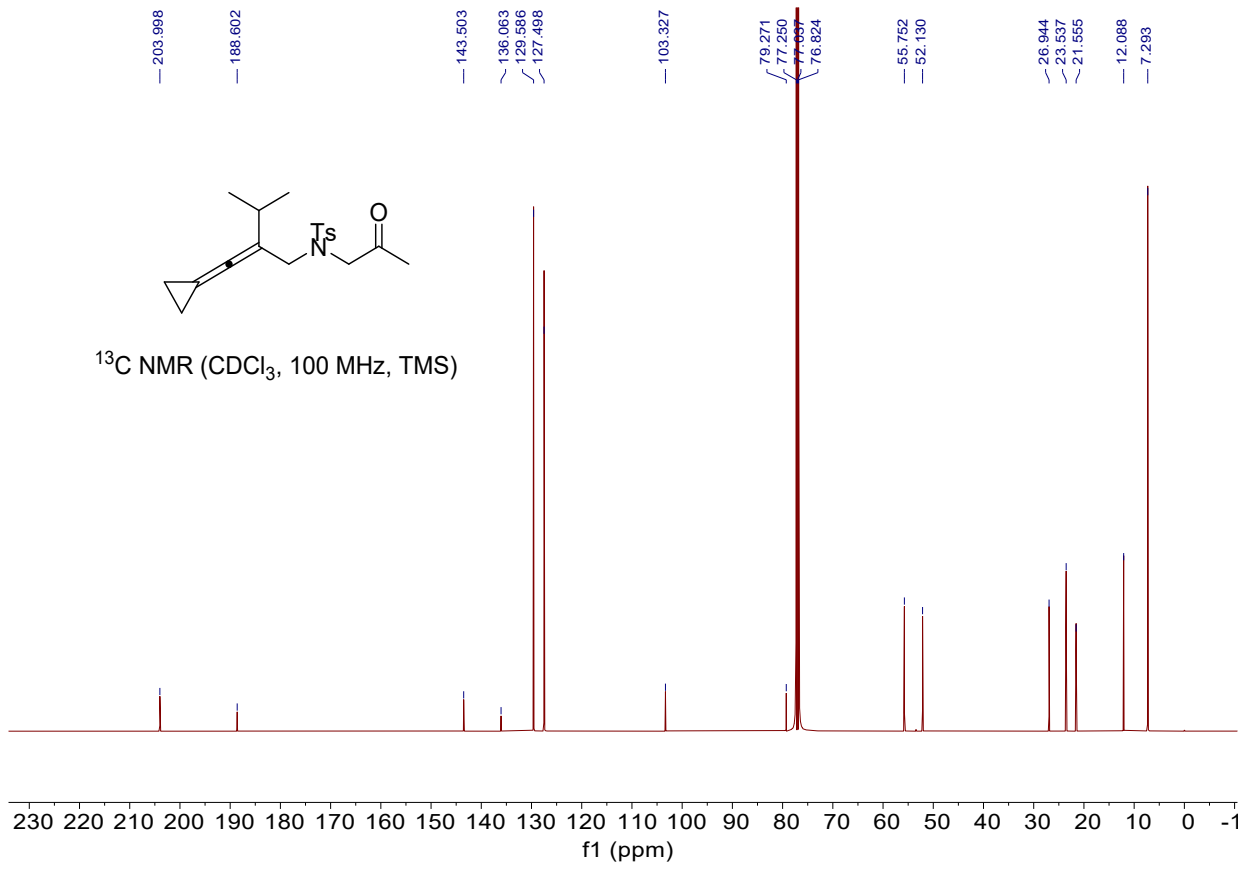
2.412  
2.315  
2.302  
2.285  
2.268  
2.251  
2.234  
2.217  
2.157  
1.461  
1.444  
1.438  
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1.361  
1.353  
1.337  
1.012  
1.008  
0.995

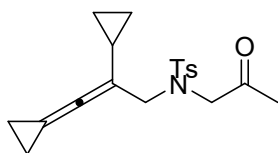


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





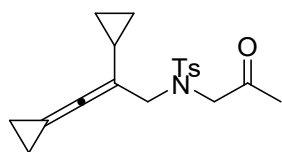




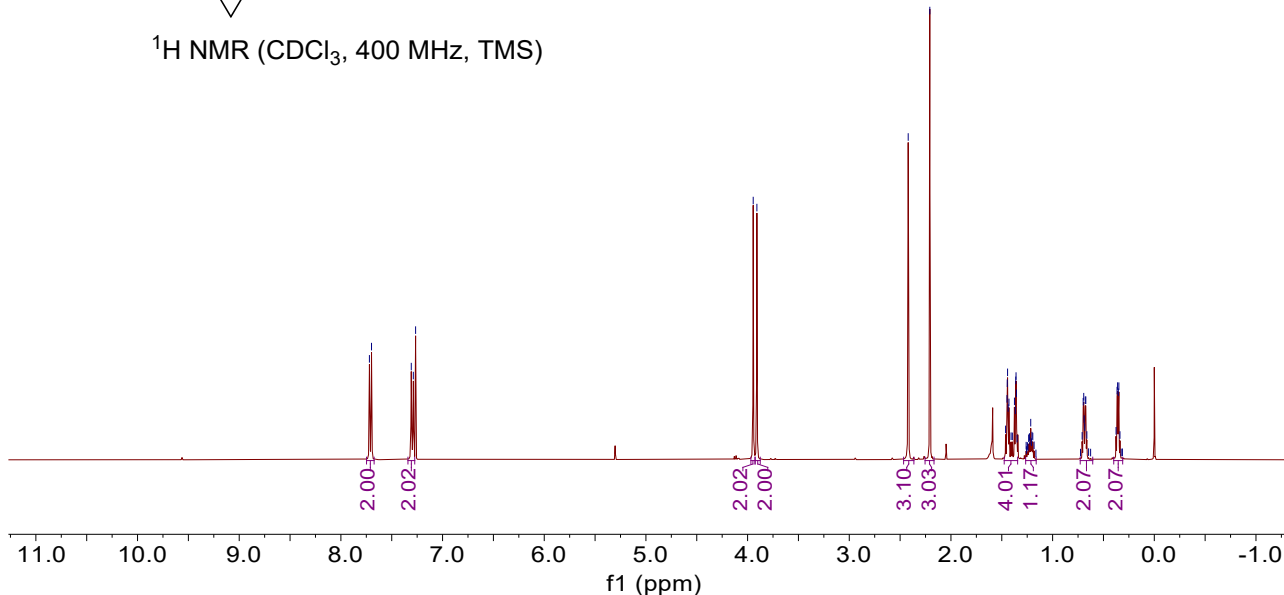
***N*-(2-cyclopropyl-3-cyclopropylidene- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide**

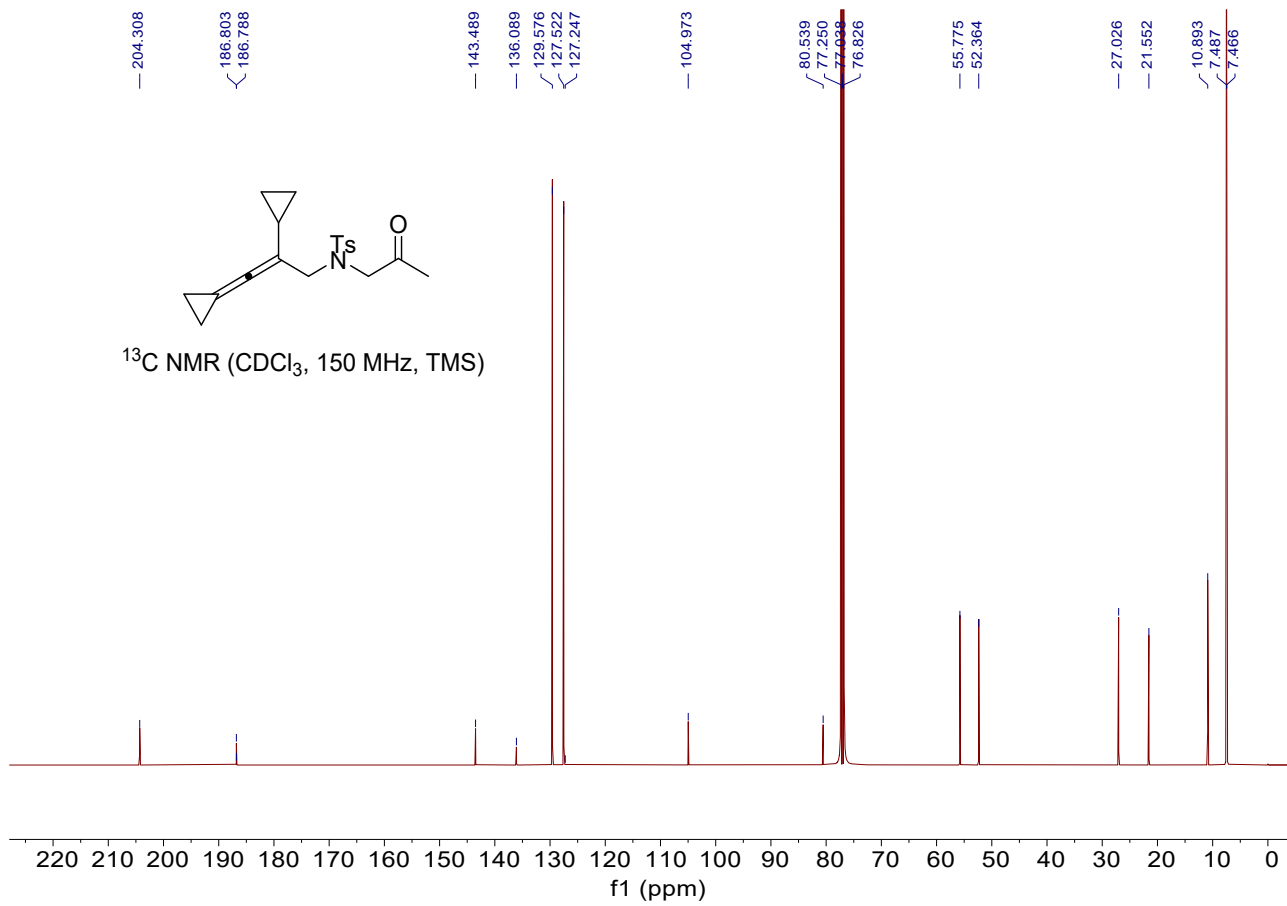
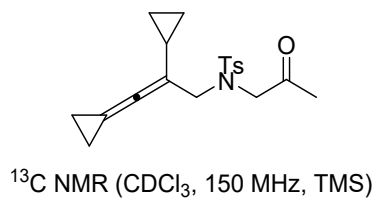
**(1d)**

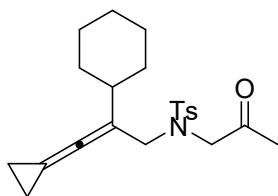
A colorless oil, 90% yield, 310.5 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.71 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 3.94 (s, 2H), 3.91 (s, 2H), 2.42 (s, 3H), 2.21 (s, 3H), 1.48 – 1.34 (m, 4H), 1.27 – 1.16 (m, 1H), 0.73 – 0.61 (m, 2H), 0.40 – 0.31 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  204.3, 186.80, 186.78, 143.5, 136.1, 129.6, 127.5, 127.2, 105.0, 80.5, 55.8, 52.4, 27.0, 21.6, 10.9, 7.48, 7.46. IR (neat)  $\nu$  815, 987, 1157, 1216, 1346, 1447, 2018, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 368.1290, Found: 368.1293.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

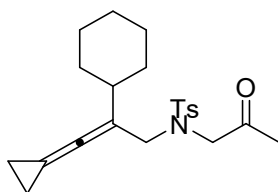




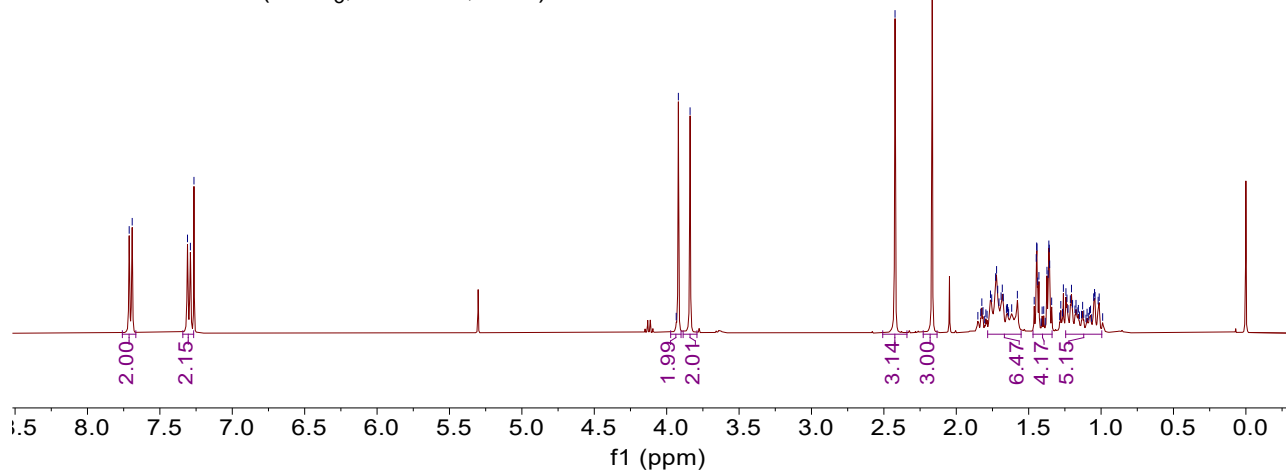


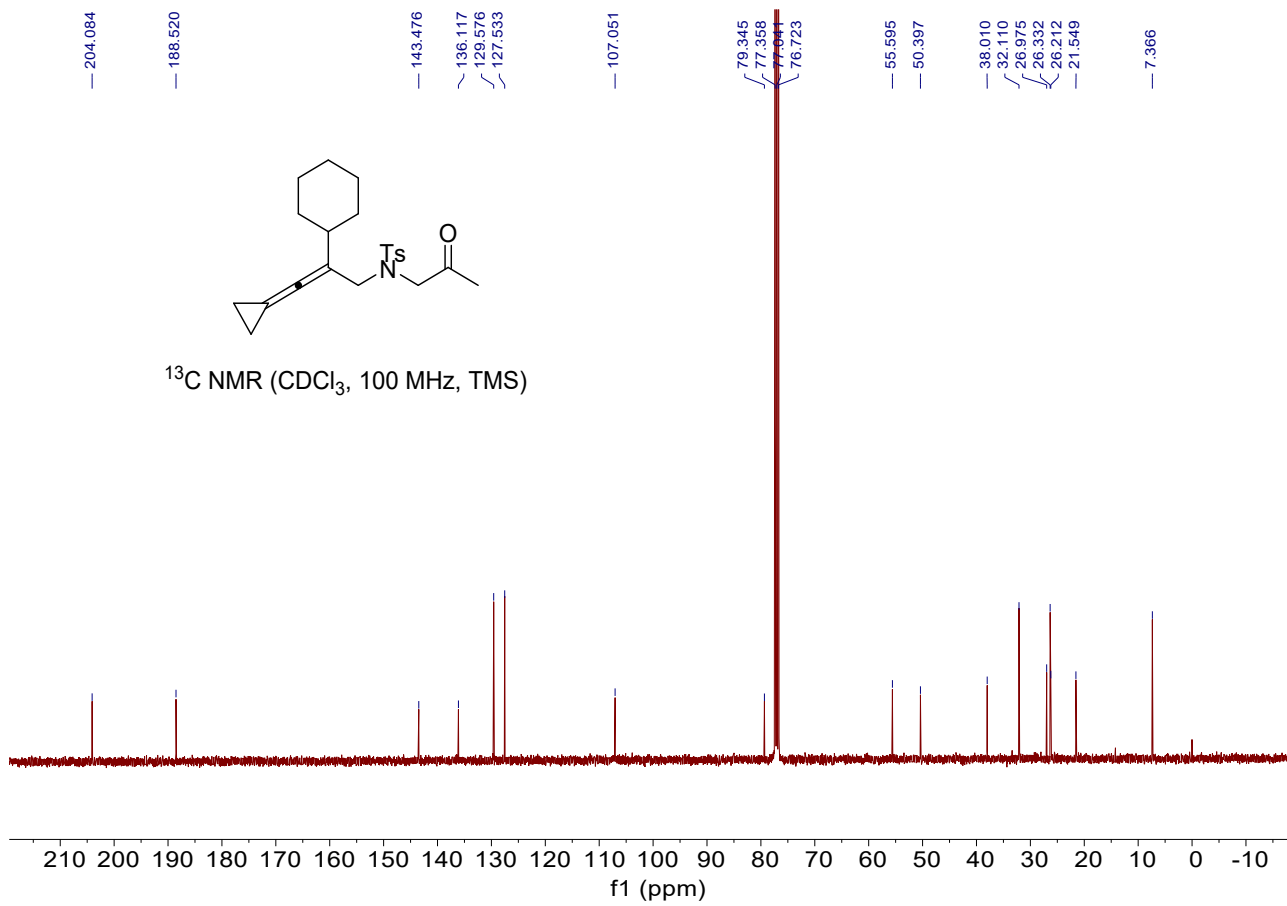
***N*-(2-cyclohexyl-3-cyclopropylidene- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide  
(1e)**

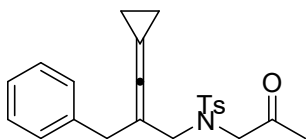
A yellow oil, 90% yield, 348.3 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 3.92 (s, 2H), 3.84 (s, 2H), 2.42 (s, 3H), 2.17 (s, 3H), 1.78 – 1.55 (m, 6H), 1.47 – 1.34 (m, 4H), 1.24 – 1.00 (m, 5H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  204.1, 188.5, 143.5, 136.1, 129.6, 127.5, 107.1, 79.3, 55.6, 50.4, 38.0, 32.1, 27.0, 26.3, 26.2, 21.5, 7.4. IR (neat)  $\nu$  815, 987, 1157, 1216, 1346, 1447, 2018, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{29}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 410.1760, Found: 410.1757.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

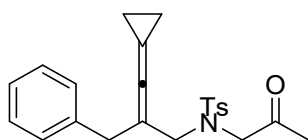




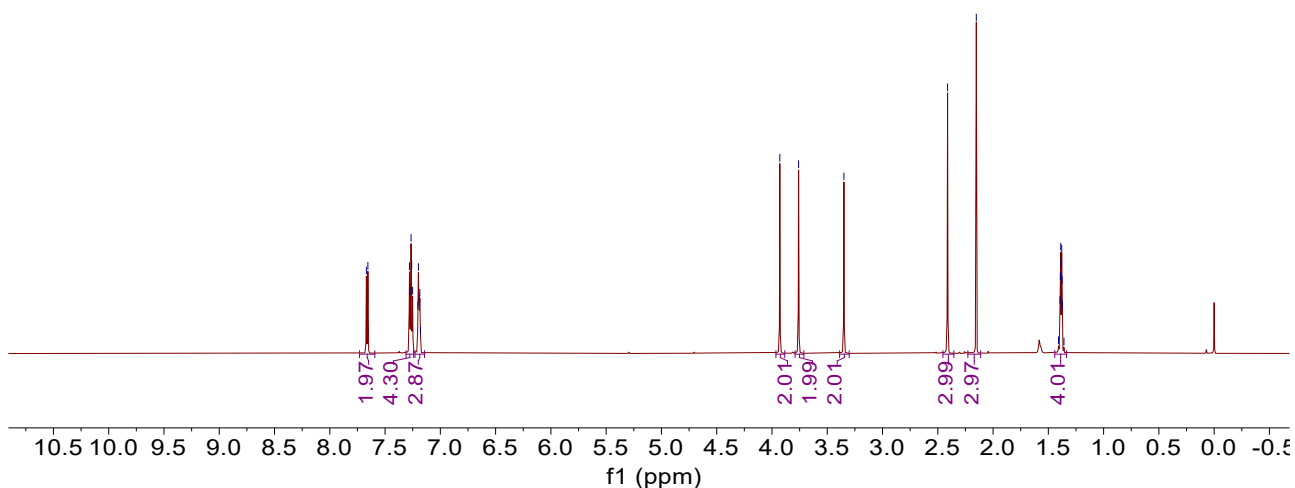


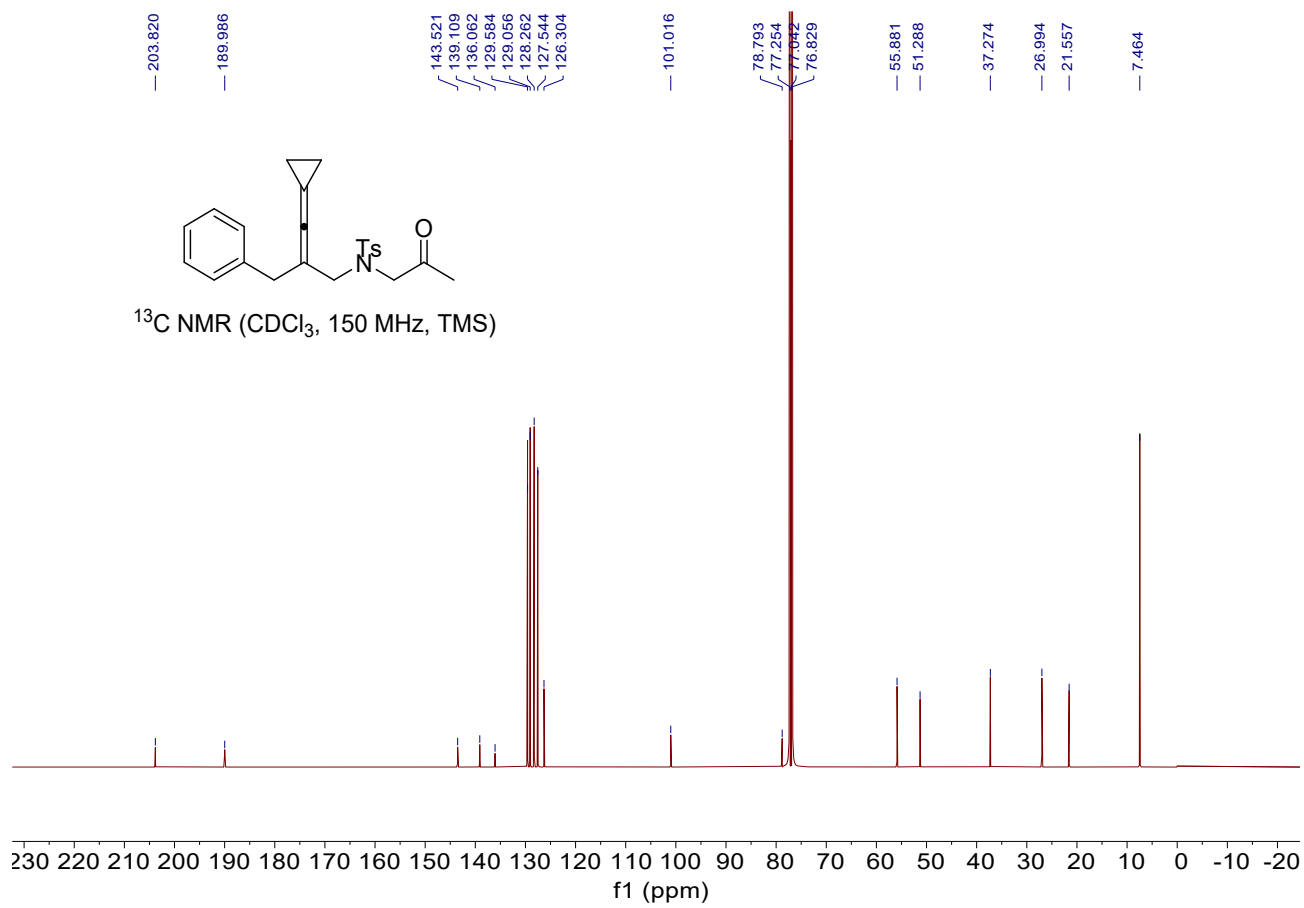
***N*-(2-benzyl-3-cyclopropylidene- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1f)**

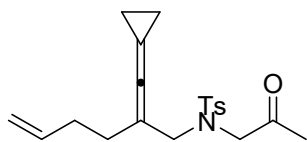
A yellow oil, 90% yield, 355.5 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.66 (d,  $J = 8.0$  Hz, 2H), 7.31 – 7.24 (m, 4H), 7.23 – 7.14 (m, 3H), 3.93 (s, 2H), 3.76 (s, 2H), 3.35 (s, 2H), 2.41 (s, 3H), 2.15 (s, 3H), 1.44 – 1.34 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  203.8, 190.0, 143.5, 139.1, 136.1, 129.6, 129.1, 128.3, 127.5, 126.3, 101.0, 78.8, 55.9, 51.3, 37.3, 27.0, 21.6, 7.5. IR (neat)  $\nu$  768, 1157, 1346, 1497, 1736, 2021, 2937, 3034, 3055  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1446.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

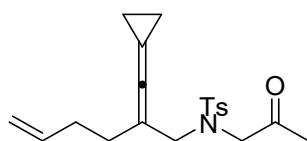




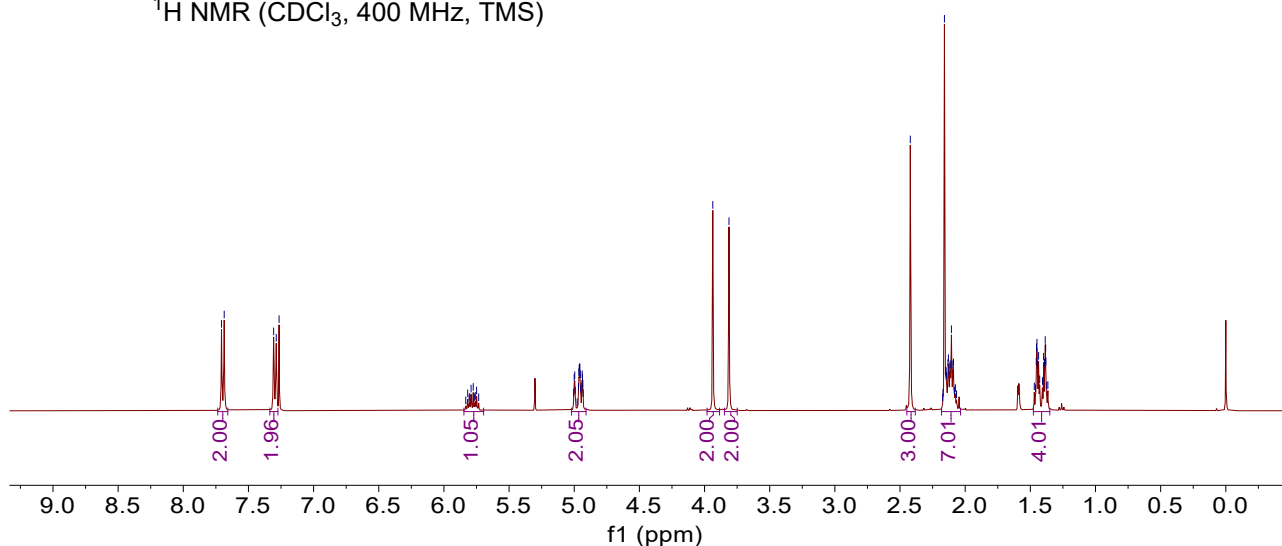


***N*-(2-(cyclopropylidene- $\lambda^5$ -methylene)hex-5-en-1-yl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1g)**

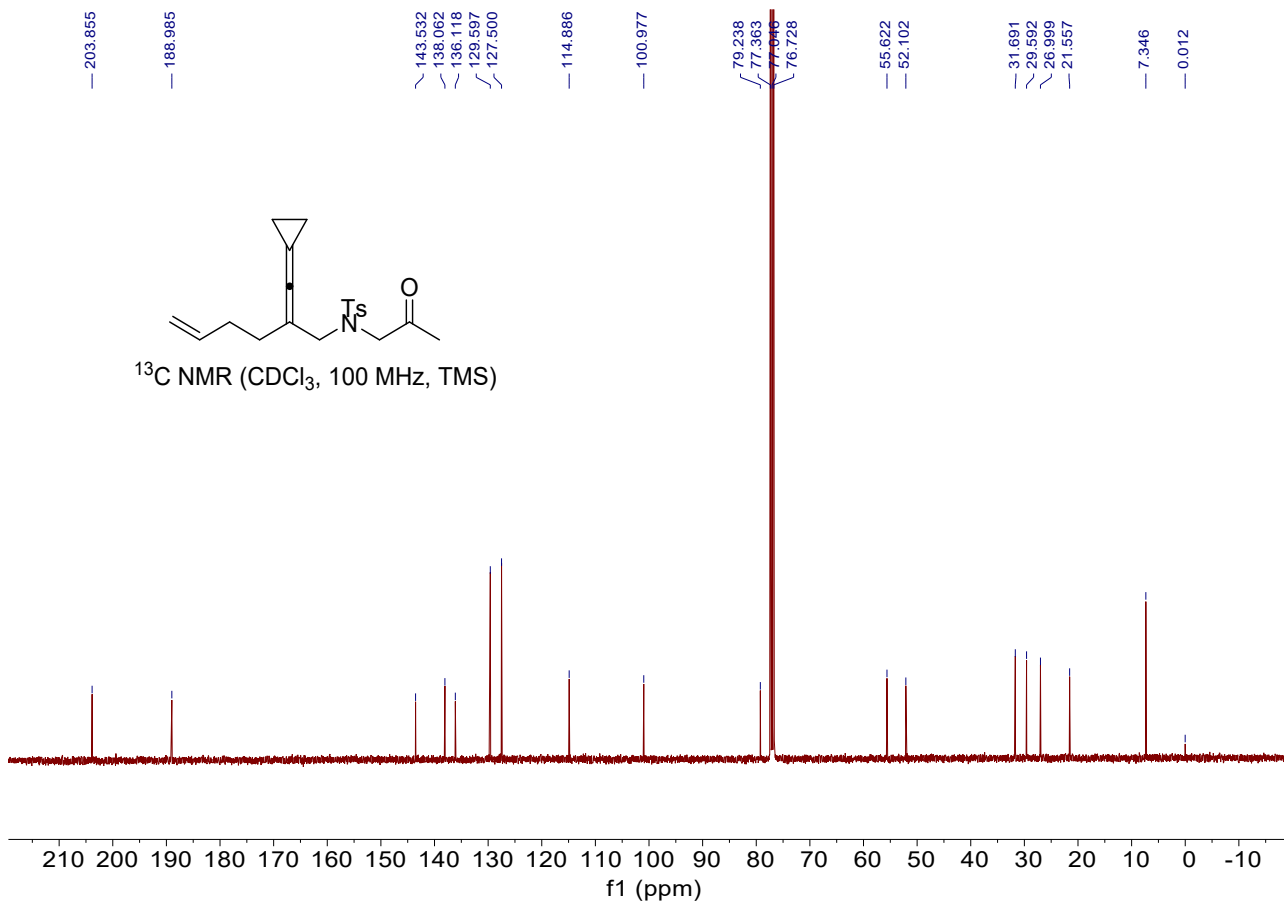
A colorless oil, 88% yield, 315.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 5.85 – 5.70 (m, 1H), 5.02 – 4.91 (m, 2H), 3.94 (s, 2H), 3.81 (s, 2H), 2.42 (s, 3H), 2.18 – 2.04 (m, 7H), 1.48 – 1.35 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  203.9, 189.0, 143.5, 138.1, 136.1, 129.6, 127.5, 114.9, 101.0, 79.2, 55.6, 52.1, 31.7, 29.6, 27.0, 21.6, 7.3. IR (neat)  $\nu$  668, 1157, 1348, 1737, 2020, 2926, 2970, 2989  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{20}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 382.1447, Found: 382.1449.

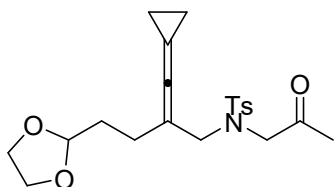


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



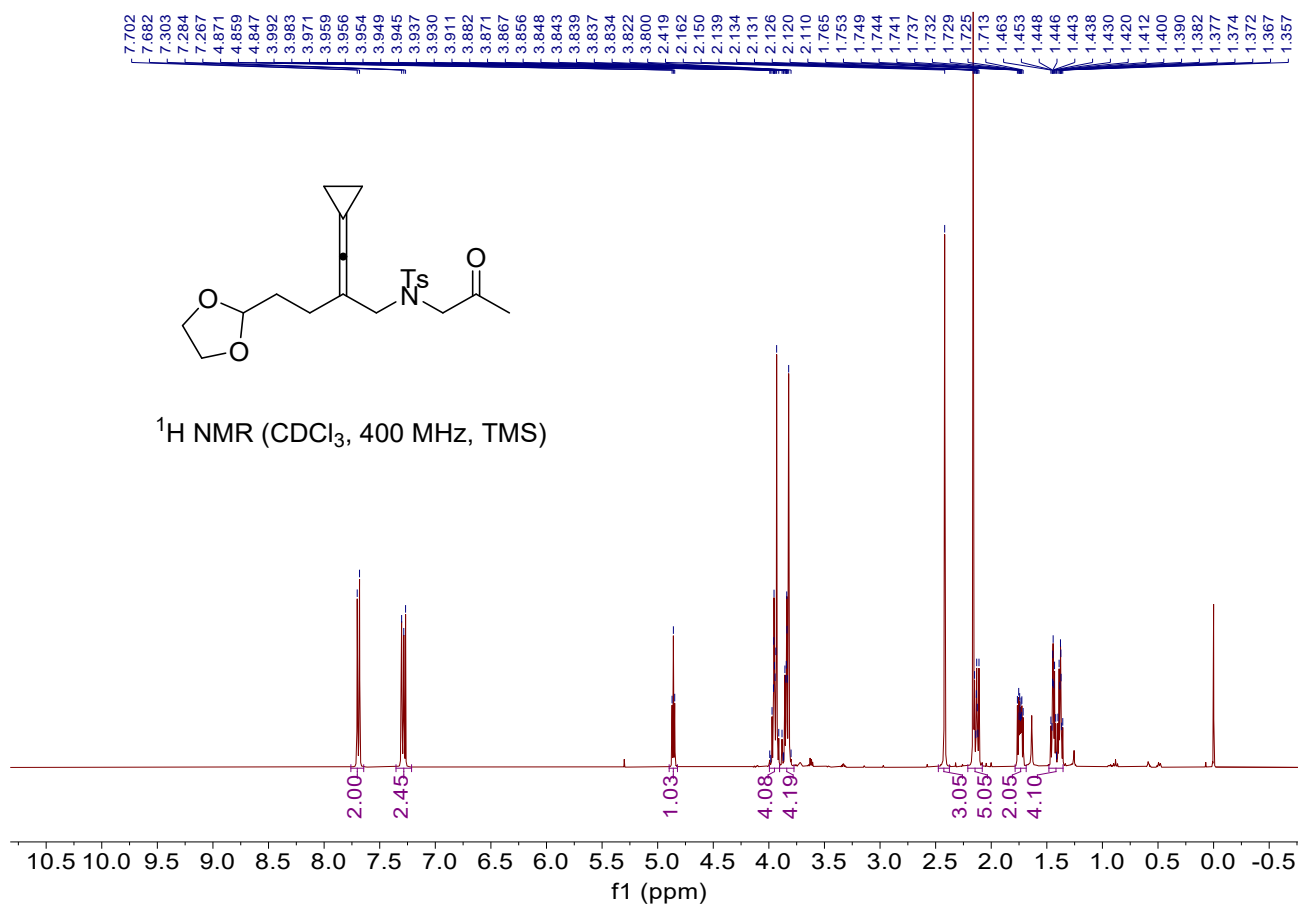


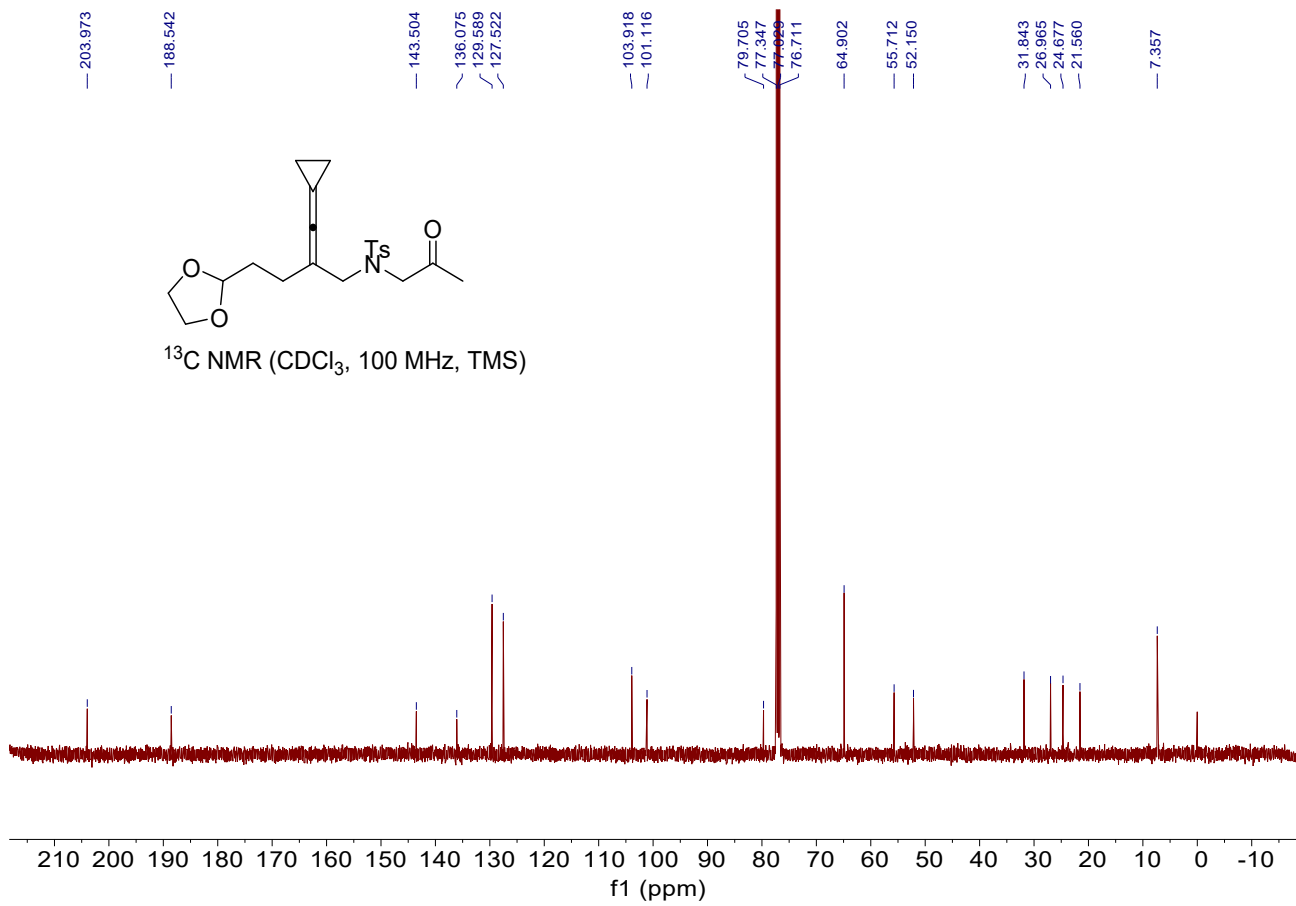


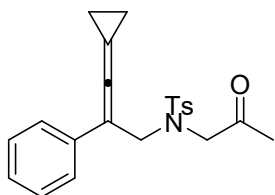


***N*-(2-(cyclopropylidene- $\lambda^5$ -methylene)-4-(1,3-dioxolan-2-yl)butyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1h)**

A yellow oil, 80% yield, 324.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 4.86 (t,  $J = 4.8$  Hz, 1H), 4.00 – 3.90 (m, 4H), 3.90 – 3.77 (m, 4H), 2.42 (s, 3H), 2.21 – 2.08 (m, 5H), 1.79 – 1.69 (m, 2H), 1.48 – 1.35 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  204.0, 188.5, 143.5, 136.1, 129.6, 127.5, 103.9, 101.1, 79.7, 64.9, 55.7, 52.1, 31.8, 27.0, 24.7, 21.6, 7.4. IR (neat)  $\nu$  668, 987, 1157, 1346, 1736, 2019, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{27}\text{NO}_5\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 428.1502, Found: 428.1506.

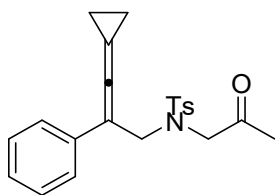




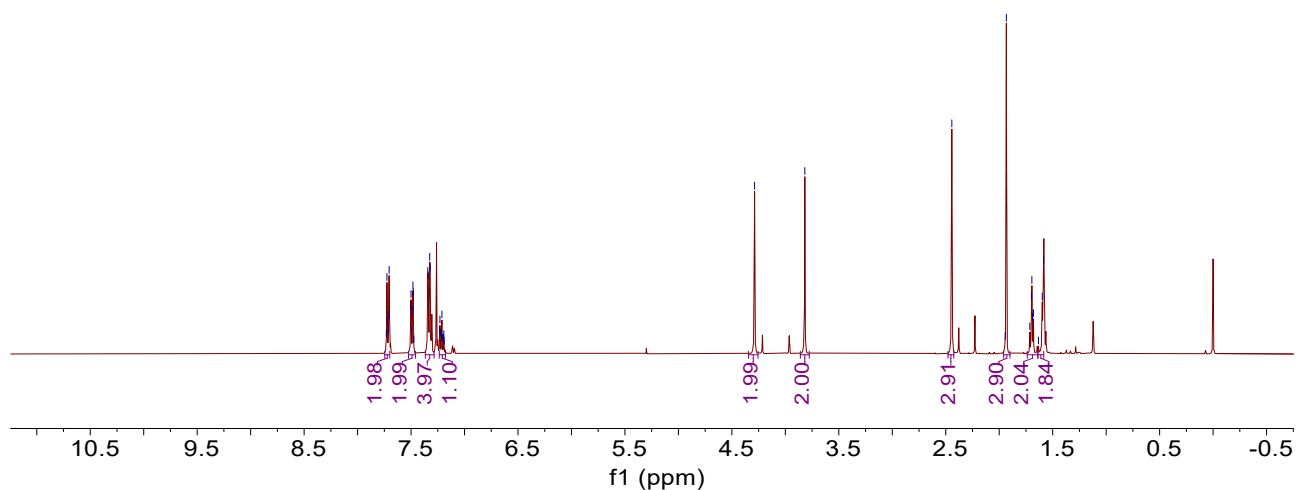


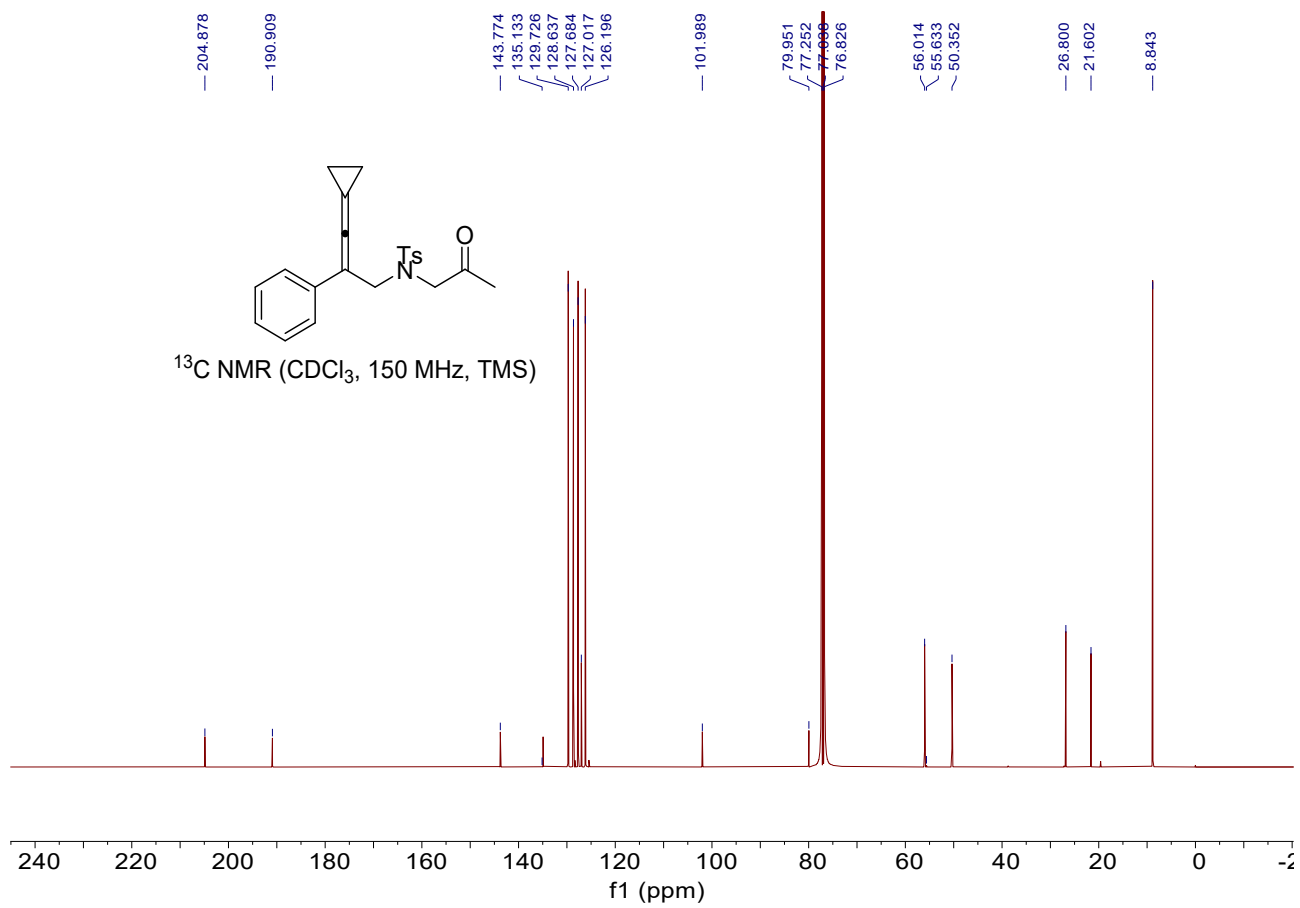
***N*-(3-cyclopropylidene-2-phenyl- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (**1i**)**

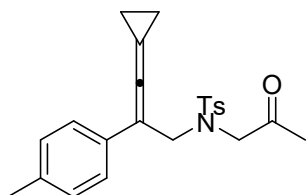
A yellow oil, 90% yield, 342.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.75 – 7.70 (m, 2H), 7.52 – 7.46 (m, 2H), 7.37 – 7.28 (m, 4H), 7.24 – 7.18 (m, 1H), 4.29 (s, 2H), 3.82 (s, 2H), 2.44 (s, 3H), 1.93 (s, 3H), 1.74 – 1.64 (m, 2H), 1.64 – 1.58 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  204.9, 190.9, 143.8, 135.1, 129.7, 128.6, 127.7, 127.0, 126.2, 102.0, 80.0, 56.0, 55.6, 50.4, 26.8, 21.6, 8.8. IR (neat)  $\nu$  668, 987, 1228, 1216, 1346, 1737, 2013, 2869, 2916, 2979  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 404.1291, Found: 404.1298.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

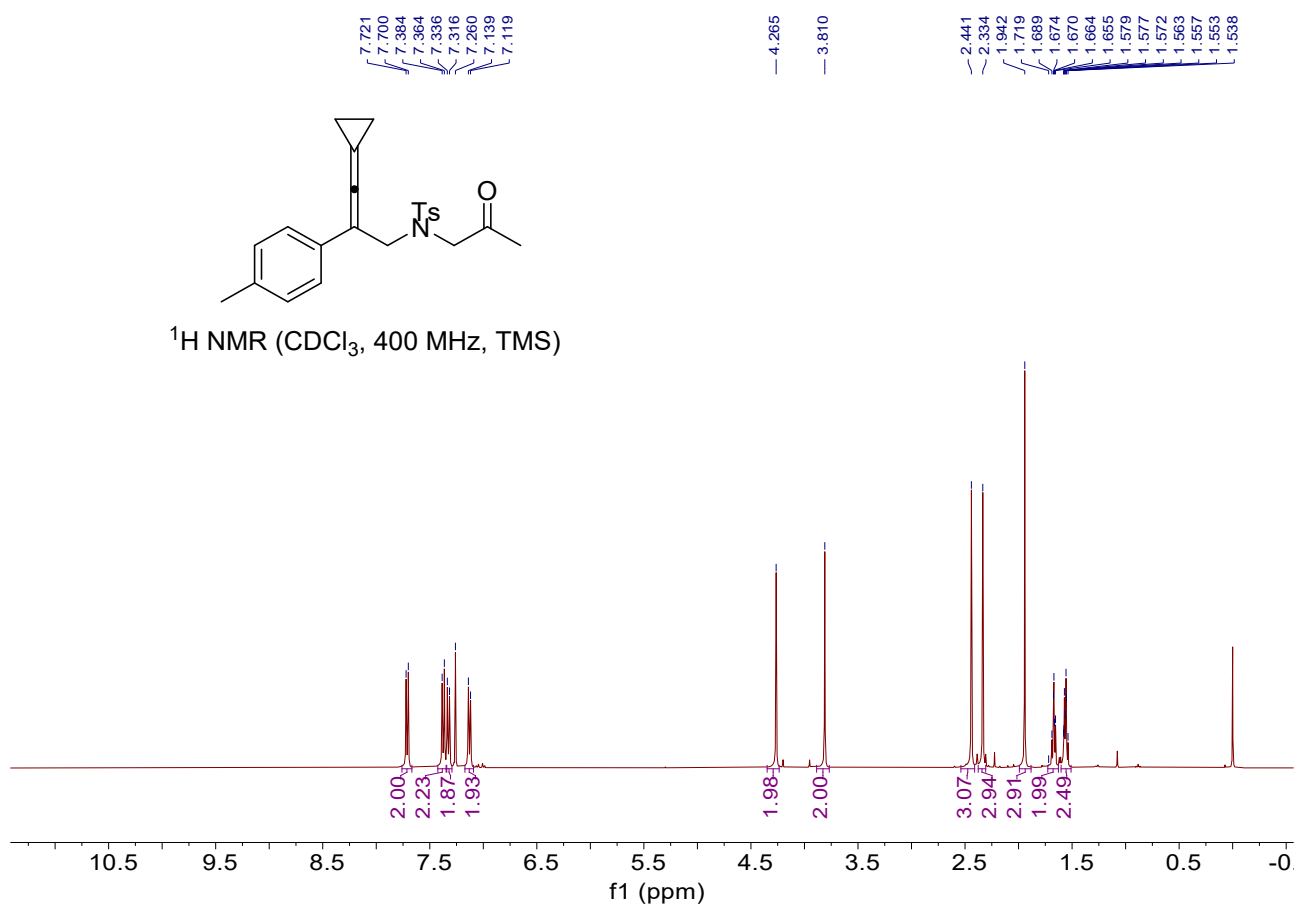


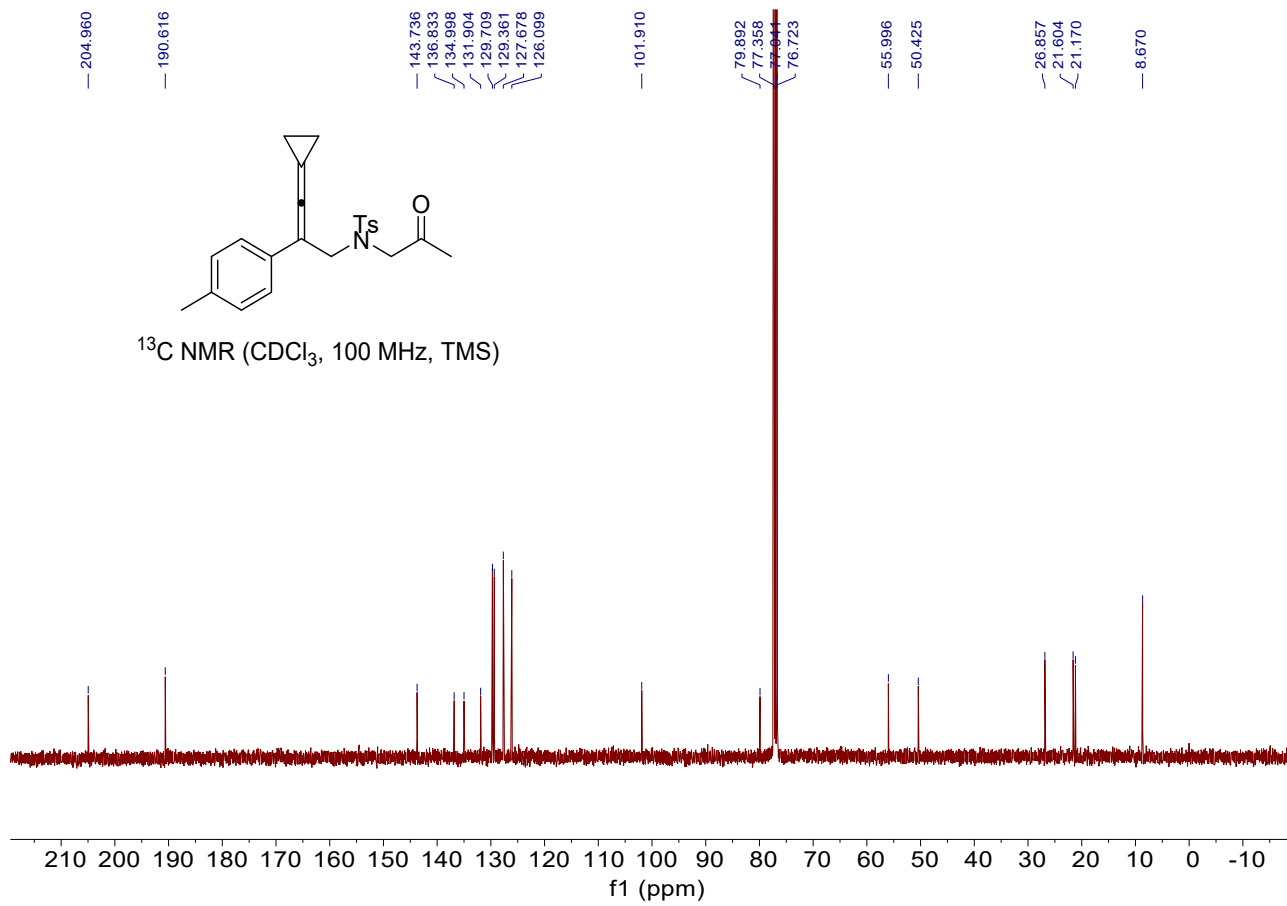


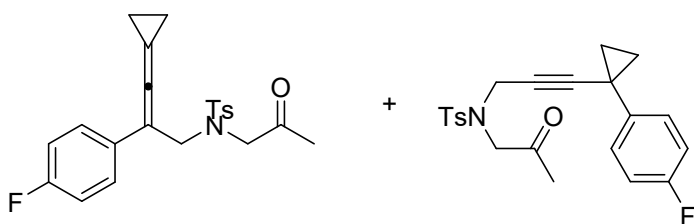


***N*-(3-cyclopropylidene-2-(*p*-tolyl)- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1j)**

A yellow oil, 88% yield, 355.5 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.71 (d,  $J = 8.4$  Hz, 2H), 7.37 (d,  $J = 8.4$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 7.13 (d,  $J = 8.0$  Hz, 2H), 4.26 (s, 2H), 3.81 (s, 2H), 2.44 (s, 3H), 2.33 (s, 3H), 1.94 (s, 3H), 1.71 – 1.62 (m, 2H), 1.60 – 1.51 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  205.0, 190.6, 143.7, 136.8, 135.0, 131.9, 129.7, 129.4, 127.7, 126.1, 101.9, 79.9, 56.0, 50.4, 26.9, 21.6, 21.2, 8.7. IR (neat)  $\nu$  655, 987, 1159, 1350, 1737, 2008, 2869, 2932, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1455.

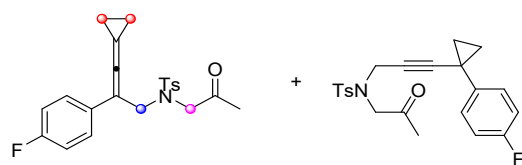




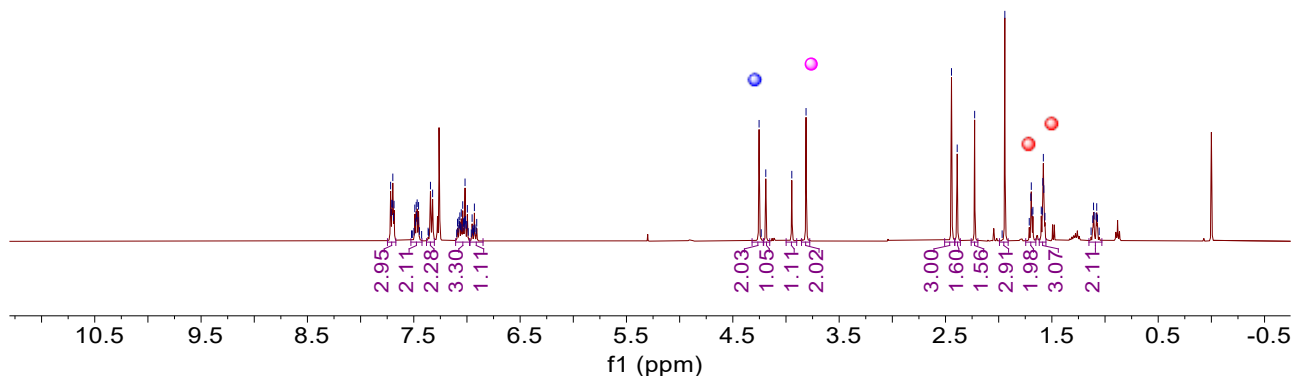


***N*-(3-cyclopropylidene-2-(4-fluorophenyl)- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1k+1k' = 1.5: 1)**

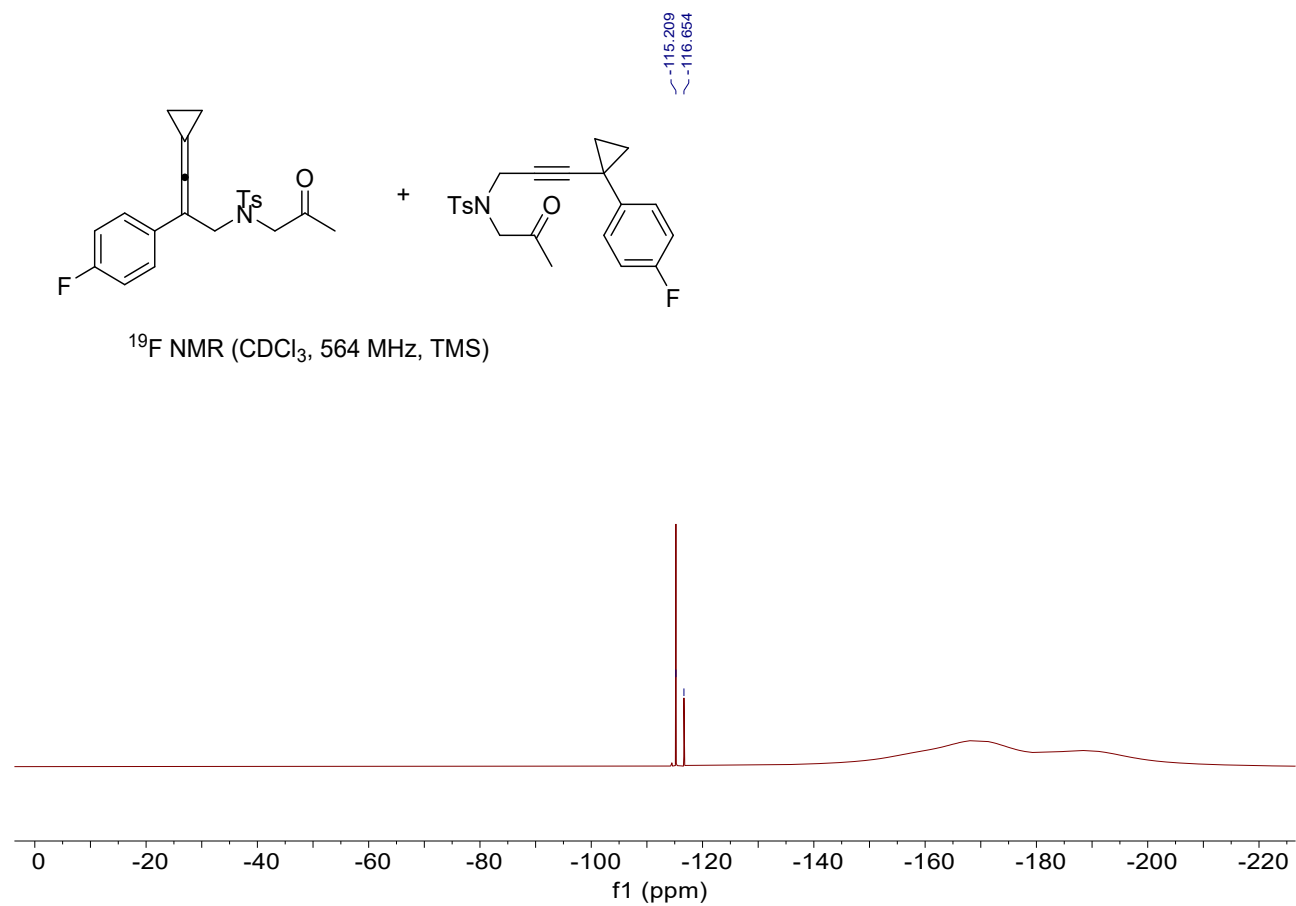
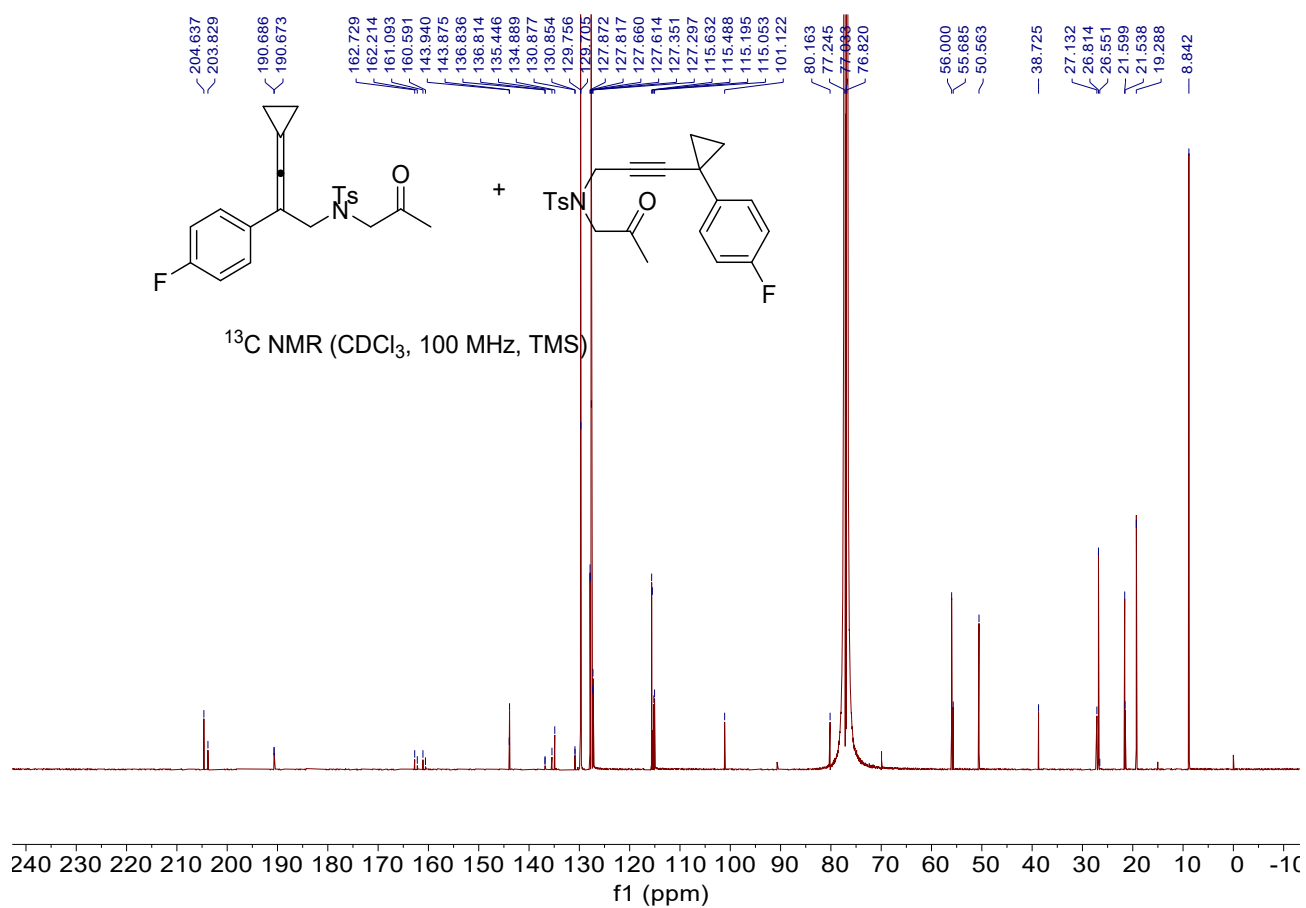
A colorless oil, 60% yield, 240.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.75 – 7.67 (m, 3H), 7.53 – 7.42 (m, 2H), 7.38 – 7.31 (m, 2H), 7.11 – 6.97 (m, 3H), 6.98 – 6.85 (m, 1H), 4.25 (s, 2H), 4.19 (s, 1H), 3.95 (s, 1H), 3.81 (s, 2H), 2.44 (s, 3H), 2.39 (s, 2H), 2.23 (s, 2H), 1.94 (s, 3H), 1.75 – 1.65 (m, 2H), 1.62 – 1.56 (m, 2H), 1.15 – 1.03 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  204.6, 203.8, 190.7, 190.7, 162.7, 162.2, 161.1, 160.6, 143.9, 143.9, 136.8, 136.8, 135.4, 134.9, 130.9, 130.9, 129.8, 129.7, 127.9, 127.8, 127.7, 127.6, 127.4, 127.3, 115.6, 115.5, 115.2, 115.1, 101.1, 80.2, 56.0, 55.7, 50.6, 38.7, 27.1, 26.8, 26.6, 21.6, 21.5, 19.3, 8.8.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.2, -116.5. IR (neat)  $\nu$  668, 987, 1157, 1216, 1346, 1734, 2008, 2829, 2926, 2950  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{FSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1193.

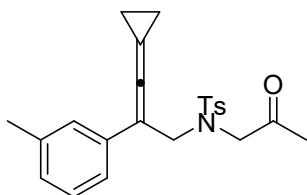


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



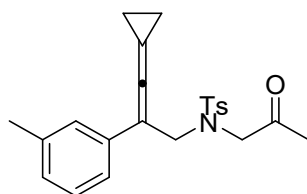




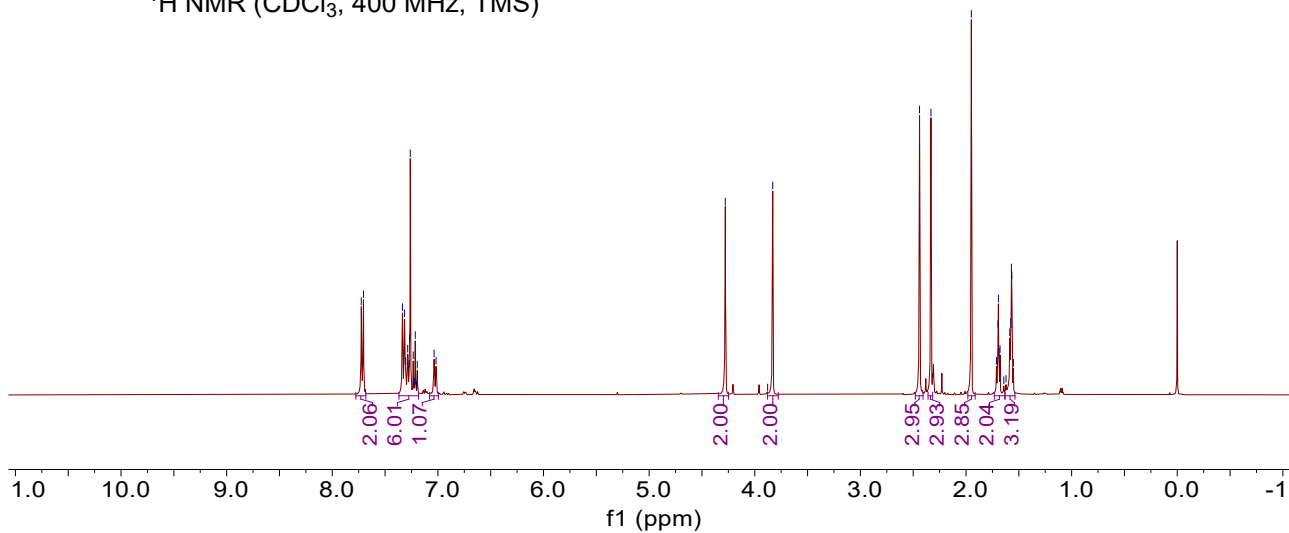


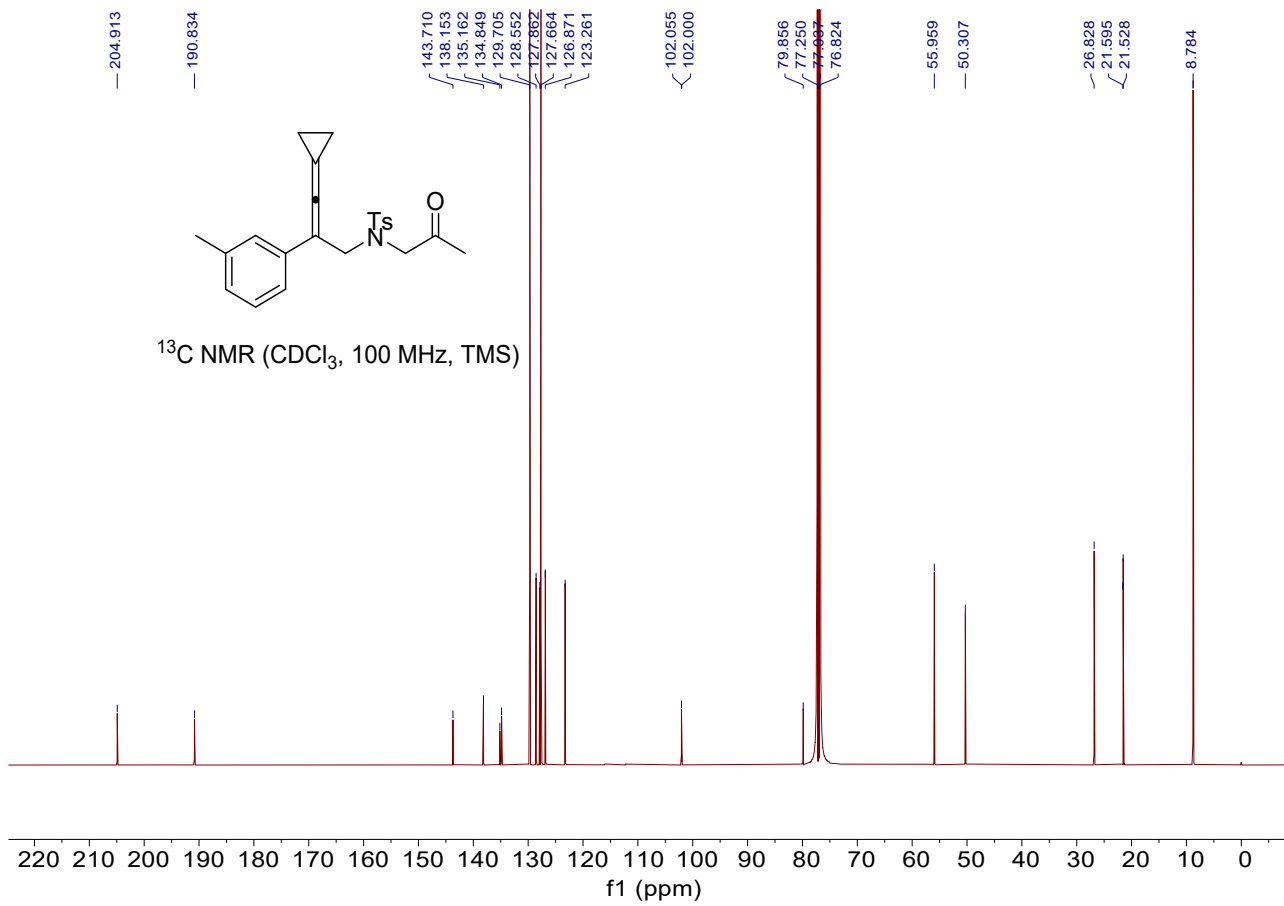
**N-(3-cyclopropylidene-2-(m-tolyl)-λ<sup>5</sup>-allyl)-4-methyl-N-(2-oxopropyl)benzenesulfonamide (11)**

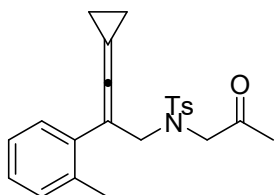
A yellow oil, 90% yield, 355.4 mg. <sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.18 (m, 6H), 7.08 – 6.99 (m, 1H), 4.28 (s, 2H), 3.83 (s, 2H), 2.44 (s, 3H), 2.33 (s, 3H), 1.95 (s, 3H), 1.73 – 1.63 (m, 2H), 1.63 – 1.54 (m, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100 MHz) δ 204.9, 190.8, 143.7, 138.2, 135.2, 134.8, 129.7, 128.6, 127.9, 127.7, 126.9, 123.3, 102.0, 79.9, 56.0, 50.3, 26.8, 21.6, 21.5, 8.8. IR (neat) ν 655, 987, 1157, 1350, 1737, 2008, 2929, 2966 cm<sup>-1</sup>. HRMS (ESI) calcd. for C<sub>23</sub>H<sub>25</sub>NO<sub>3</sub>SNa (M+Na)<sup>+</sup>: 418.1447, Found: 418.1445.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, TMS)

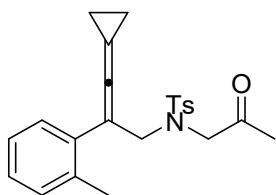
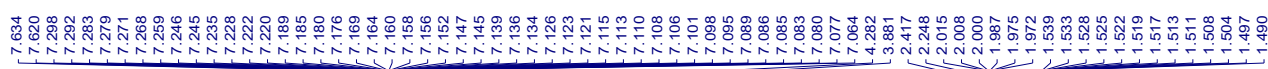




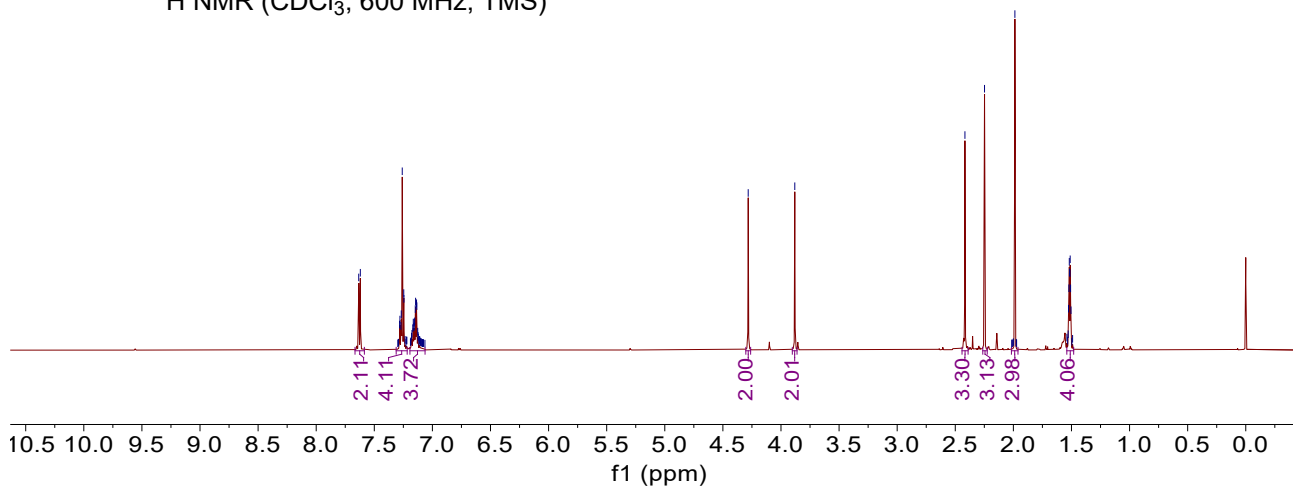


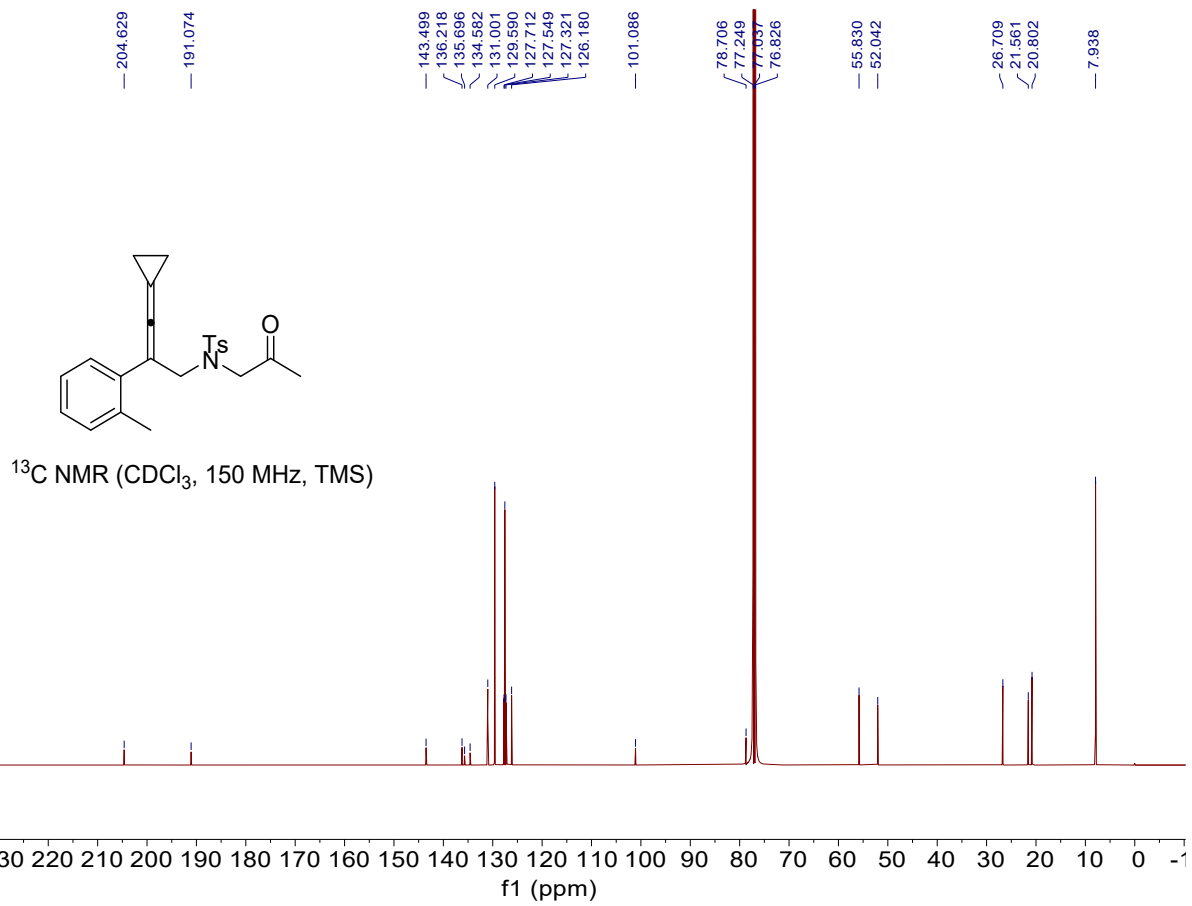
***N*-(3-cyclopropylidene-2-(*o*-tolyl)- $\lambda^5$ -allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1m)**

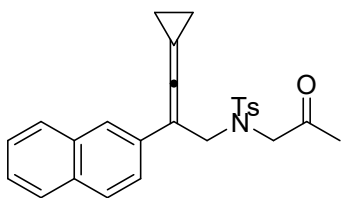
A red oil, 89% yield, 355.0 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz) 7.63 (d,  $J = 8.4$  Hz, 2H), 7.31 – 7.22 (m, 2H), 7.19 – 7.06 (m, 4H), 4.28 (s, 2H), 3.88 (s, 2H), 2.42 (s, 3H), 2.25 (s, 3H), 1.99 (s, 3H), 1.54 – 1.48 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  204.6, 191.07, 191.06, 143.5, 136.2, 135.7, 134.6, 131.0, 129.6, 127.7, 127.5, 127.3, 126.2, 101.1, 78.9, 55.8, 52.0, 26.7, 21.6, 20.8, 7.9. IR (neat)  $\nu$  668, 987, 1157, 1348, 1737, 2017, 2969, 3026  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1442.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

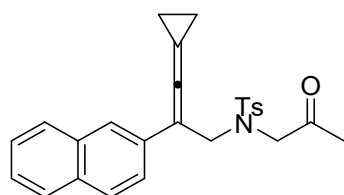




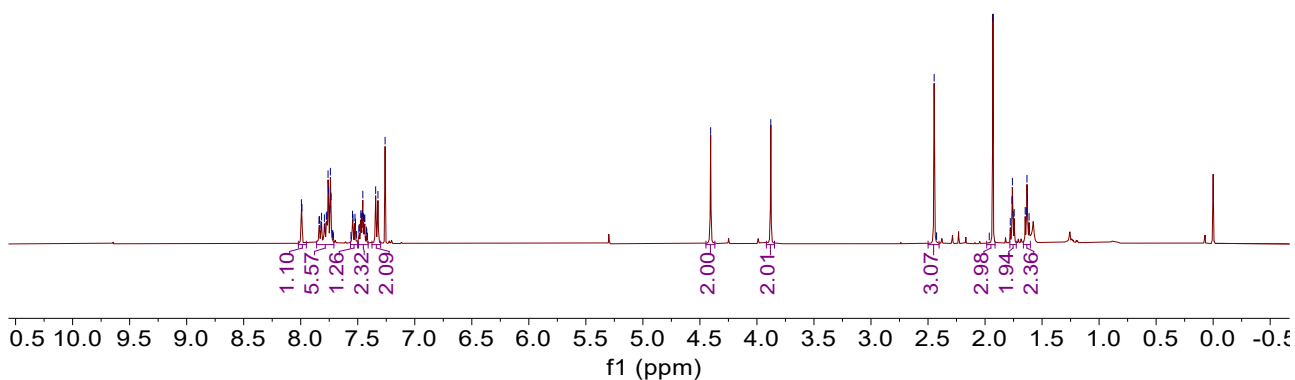


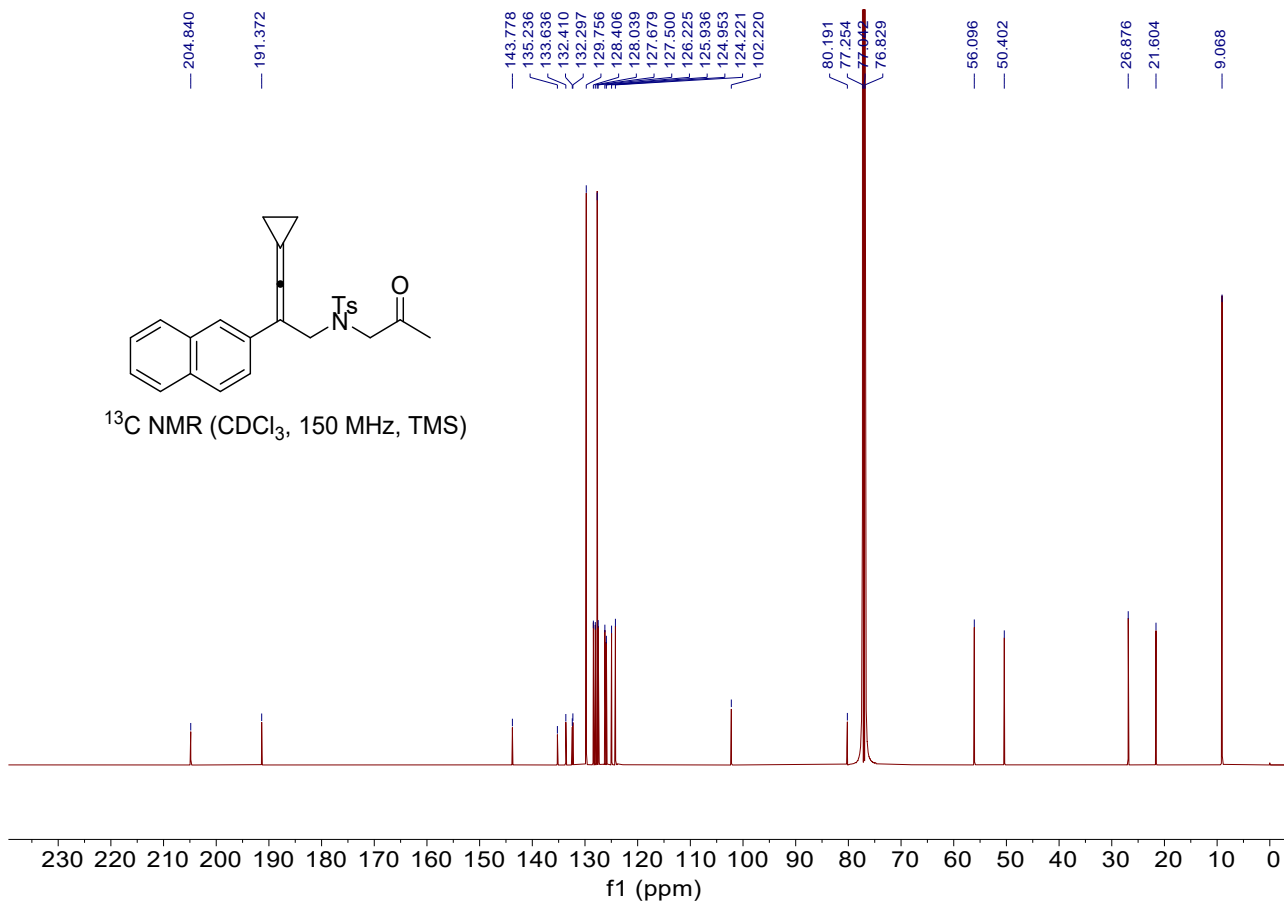
***N*-(3-cyclopropylidene-2-(naphthalen-2-yl)-λ<sup>5</sup>-allyl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1n)**

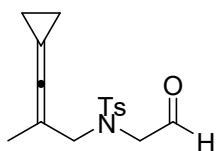
A red oil, 91% yield, 388.4 mg. <sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz) δ 7.99 (s, 1H), 7.86 – 7.71 (m, 5H), 7.56 – 7.50 (m, 1H), 7.49 – 7.41 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 4.41 (s, 2H), 3.88 (s, 2H), 2.45 (s, 3H), 1.93 (s, 3H), 1.78 – 1.73 (m, 2H), 1.66 – 1.60 (m, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100 MHz) δ 204.8, 191.4, 143.8, 135.2, 133.6, 132.4, 132.3, 129.8, 128.4, 128.0, 127.7, 127.5, 126.2, 125.9, 125.0, 124.2, 102.2, 80.2, 56.1, 50.4, 26.9, 21.6, 9.1. IR (neat) ν 668, 987, 1219, 1359, 1757, 2003, 2926, 2959 cm<sup>-1</sup>. HRMS (ESI) calcd. for C<sub>26</sub>H<sub>25</sub>NO<sub>3</sub>SNa (M+Na)<sup>+</sup>: 454.1447, Found: 454.1455.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, TMS)

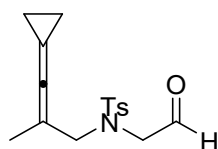




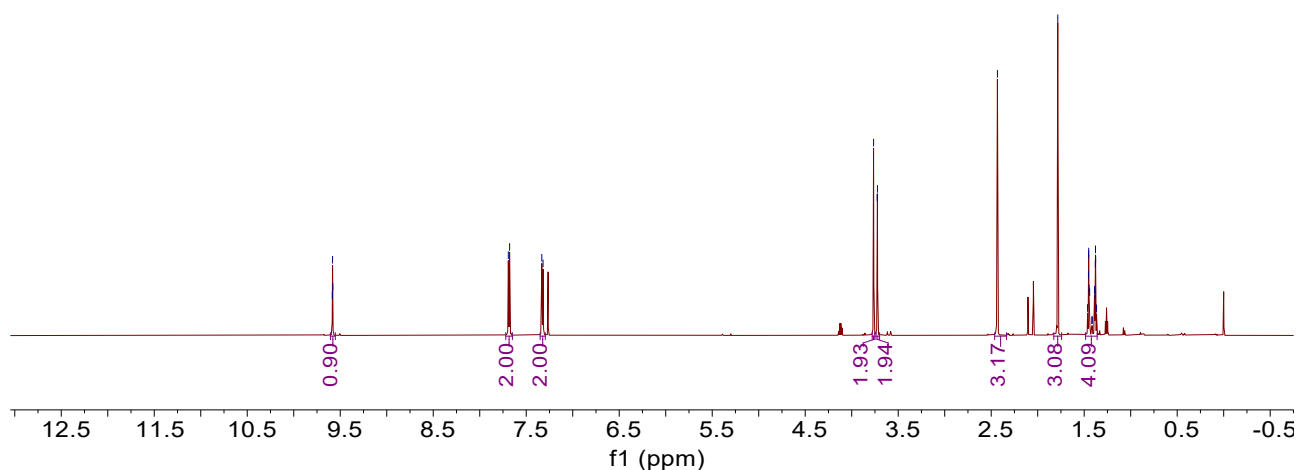


***N*-(3-cyclopropylidene-2-methyl-λ<sup>5</sup>-allyl)-4-methyl-*N*-(2-oxoethyl)benzenesulfonamide (1o)**

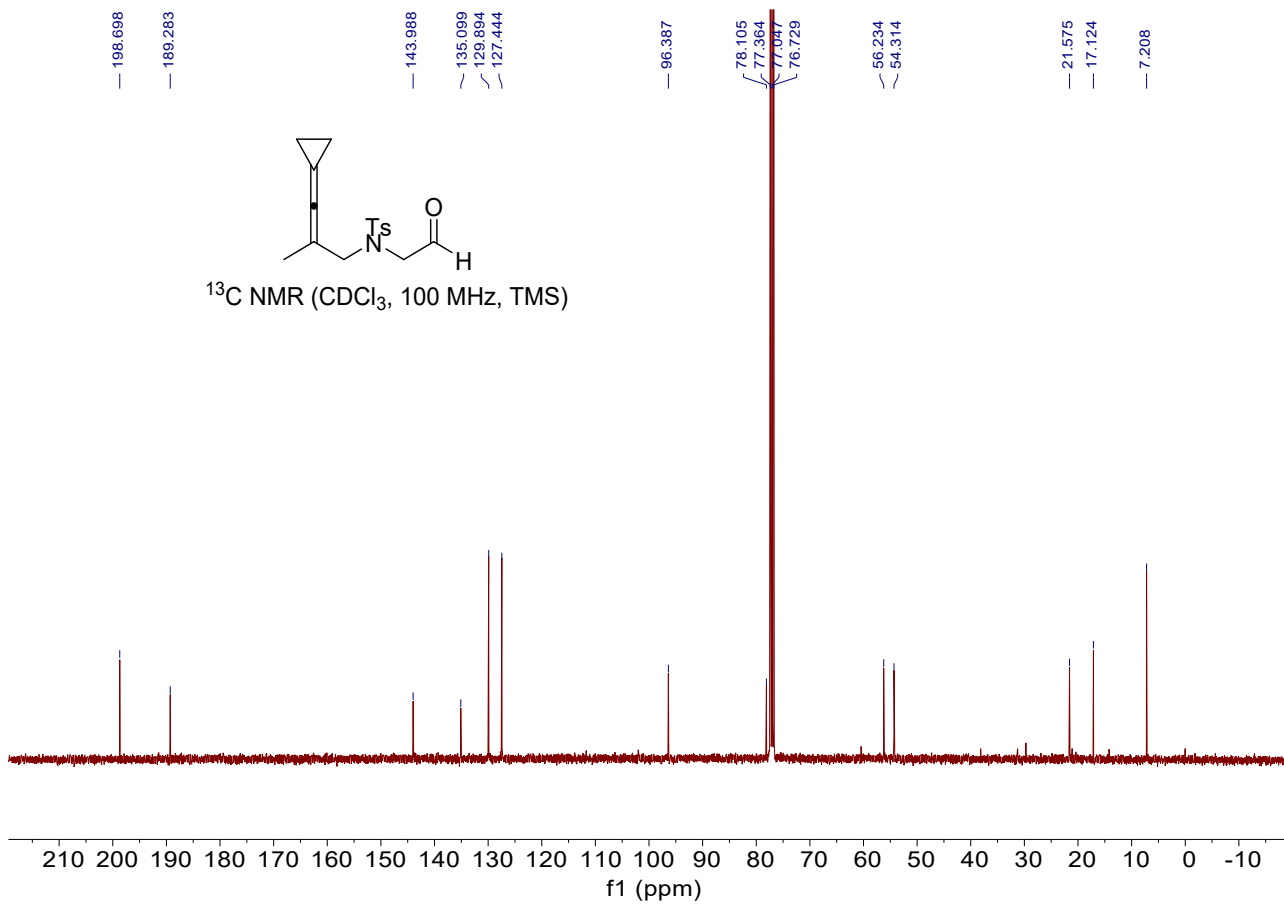
A colorless oil, 60% yield, 183.4 mg. <sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 600 MHz) δ 9.58 (t, *J* = 1.6 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 3.76 (s, 2H), 3.72 (d, *J* = 1.6 Hz, 2H), 2.43 (s, 3H), 1.78 (s, 3H), 1.48 – 1.36 (m, 4H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100 MHz) δ 202.8, 187.6, 139.8, 128.9, 128.2, 126.1, 105.6, 78.7, 43.4, 40.5, 31.4, 20.1, 6.8. IR (neat) ν 668, 987, 1157, 1346, 1737, 2021, 2839, 2926, 2989 cm<sup>-1</sup>. HRMS (ESI) calcd. for C<sub>16</sub>H<sub>19</sub>NO<sub>3</sub>SNa (M+Na)<sup>+</sup>: 328.0978, Found: 328.0979.

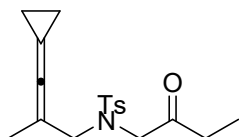


<sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz, TMS)









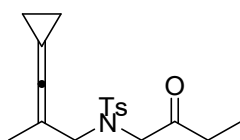
***N*-(3-cyclopropylidene-2-methyl-λ<sup>5</sup>-allyl)-4-methyl-*N*-(2-oxobutyl)benzenesulfonamide (1p)**

A colorless oil, 92% yield, 300.0 mg. <sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 3.97 (s, 2H), 3.79 (s, 2H), 2.49 (q, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 1.72 (s, 3H), 1.45 – 1.40 (m, 2H), 1.39 – 1.33 (m, 2H), 1.04 (t, *J* = 7.2 Hz, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 150 MHz) δ 206.4, 189.2, 143.4, 136.3, 129.6, 127.5, 96.7, 77.7, 54.6, 53.1, 32.7, 21.6, 17.1, 7.5, 7.1. IR (neat) ν 667, 987, 1157, 1339, 1732, 2022, 2906, 2979 cm<sup>-1</sup>. HRMS (ESI) calcd. for C<sub>18</sub>H<sub>23</sub>NO<sub>3</sub>SNa (M+Na)<sup>+</sup>: 356.1291, Found: 356.1285.

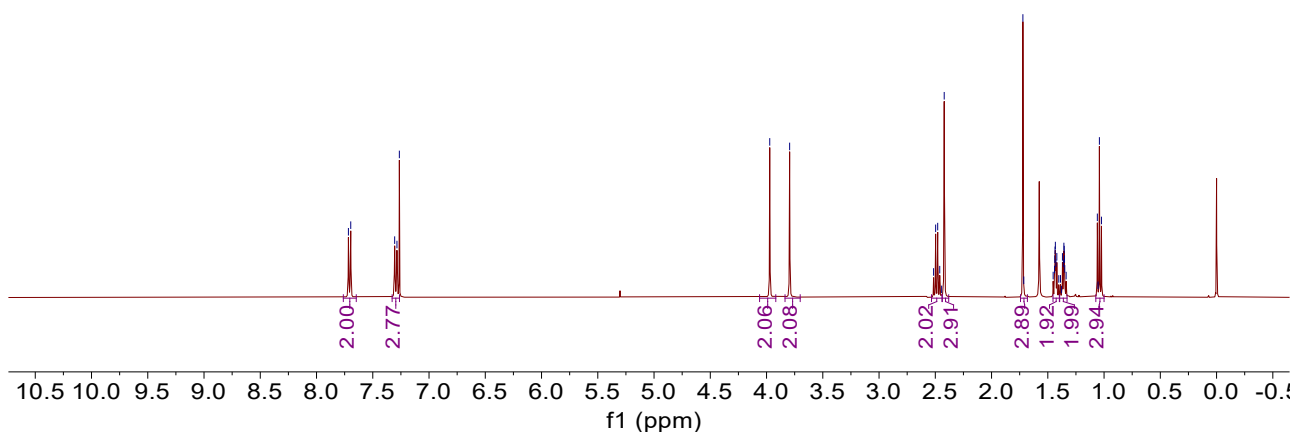
7.717  
7.696  
7.305  
7.285  
7.264

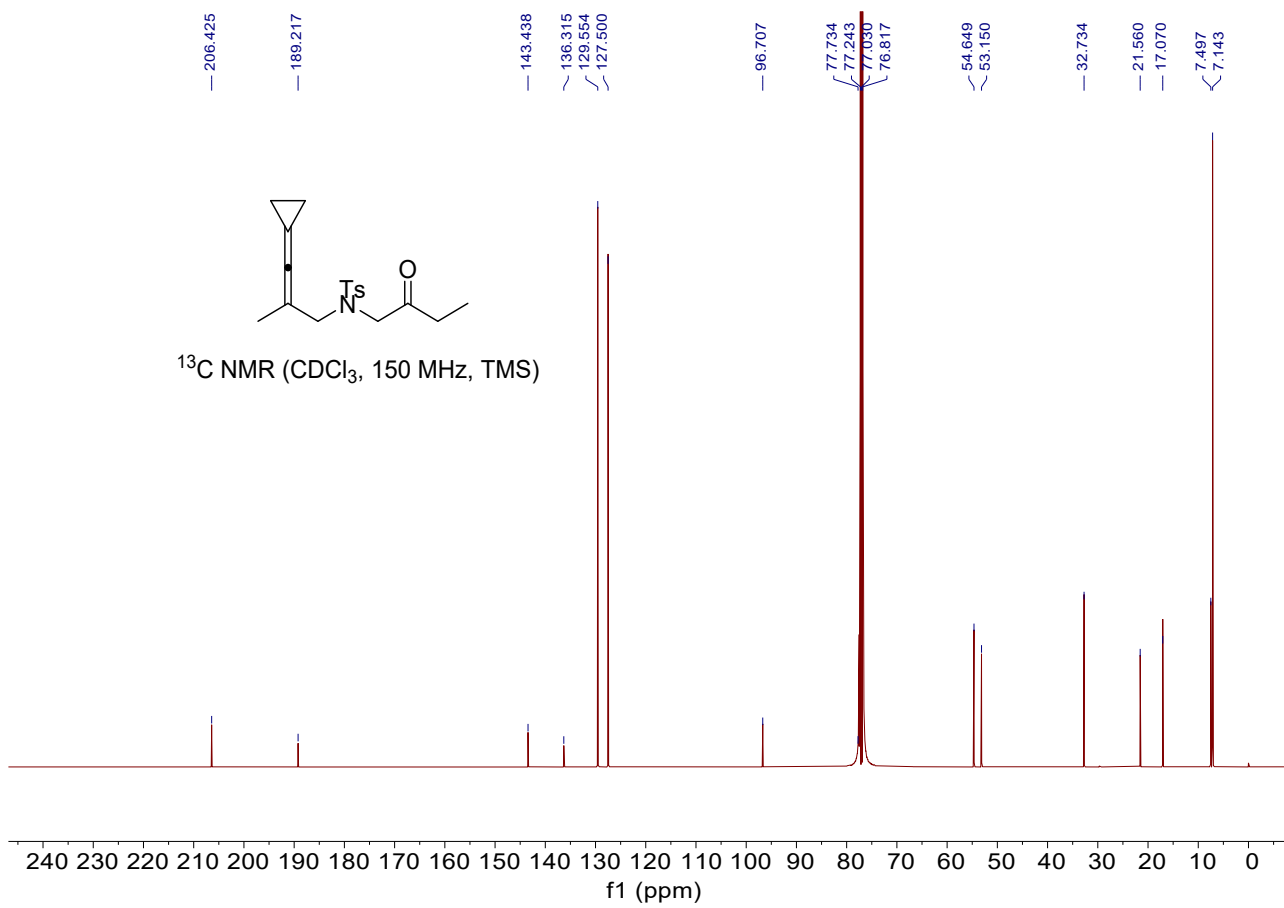
3.972  
3.795

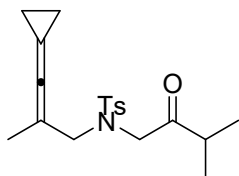
2.515  
2.497  
2.479  
2.461  
2.444  
2.421  
1.721  
1.453  
1.440  
1.438  
1.436  
1.433  
1.428  
1.420  
1.370  
1.362  
1.357  
1.354  
1.351  
1.349  
1.060  
1.041  
1.023



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, TMS)

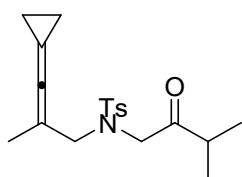




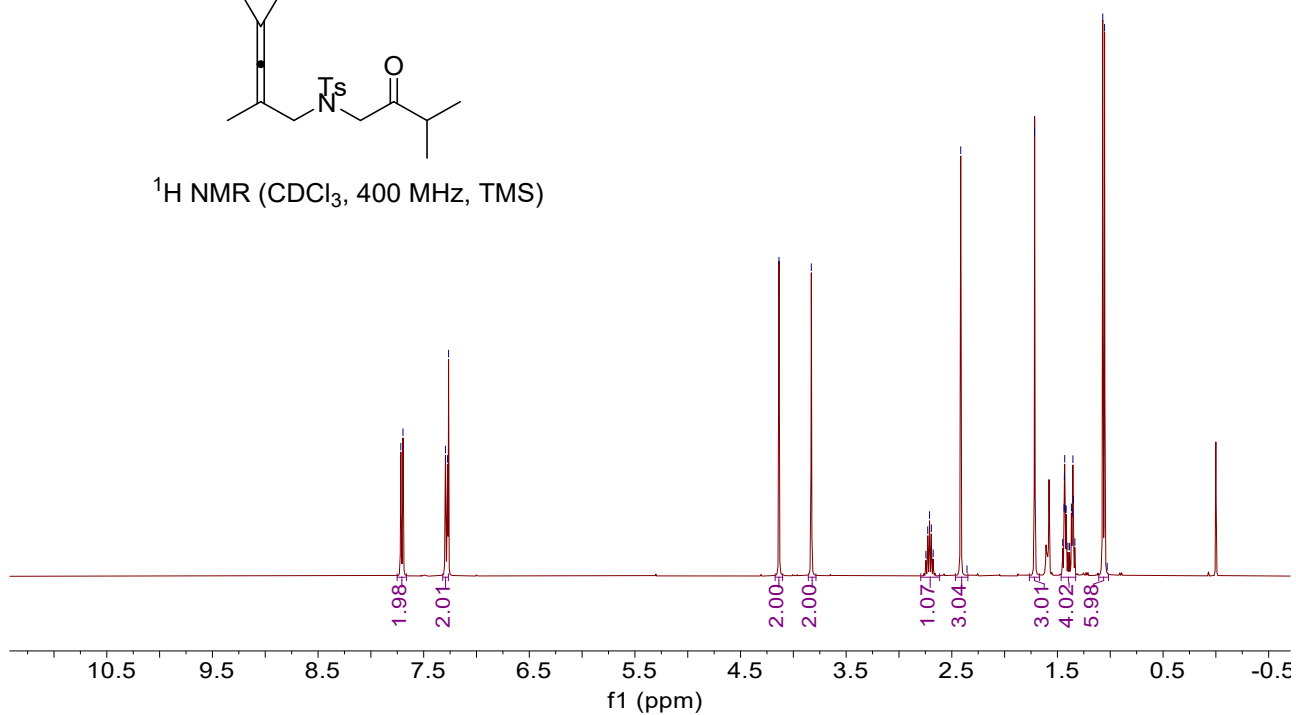


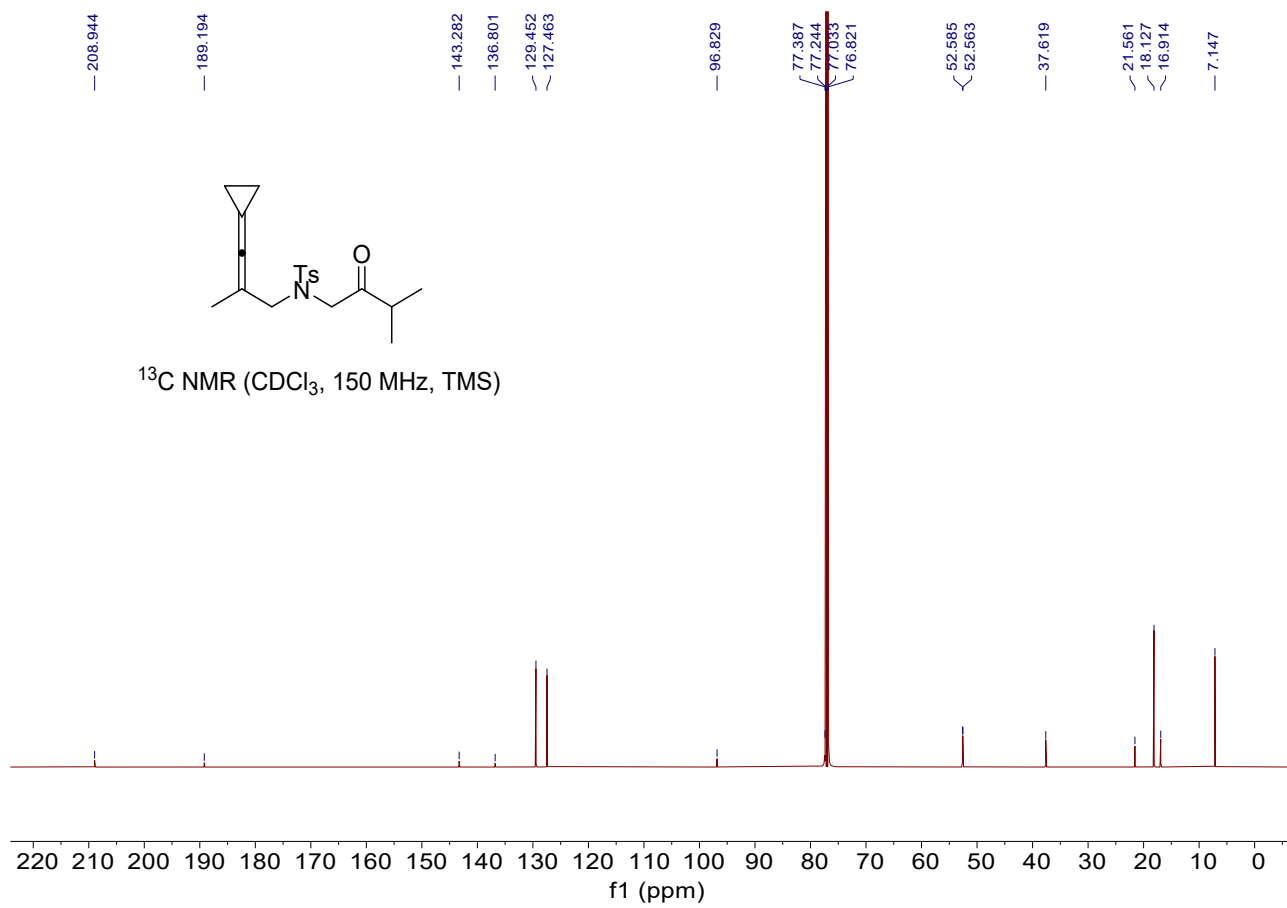
***N*-(3-cyclopropylidene-2-methyl-λ<sup>5</sup>-allyl)-4-methyl-*N*-(3-methyl-2-oxobutyl)benzenesulfonamide (1q)**

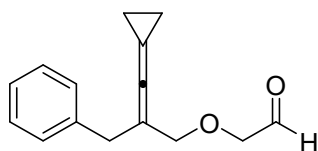
A colorless oil, 80% yield, 277.6 mg. <sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 4.14 (s, 2H), 3.83 (s, 2H), 2.71 (hept, *J* = 7.0 Hz, 1H), 2.42 (s, 3H), 1.72 (s, 3H), 1.46 – 1.33 (m, 4H), 1.06 (d, *J* = 7.0 Hz, 6H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100 MHz) δ 208.9, 189.2, 143.3, 136.8, 129.5, 127.5, 96.8, 77.4, 52.58, 52.56, 37.6, 21.6, 18.1, 16.9, 7.1. IR (neat) ν 660, 987, 1157, 1346, 1730, 2024, 2869, 2934, 2970 cm<sup>-1</sup>. HRMS (ESI) calcd. for C<sub>19</sub>H<sub>25</sub>NO<sub>3</sub>SNa (M+Na)<sup>+</sup>: 370.1447, Found: 370.1441.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, TMS)

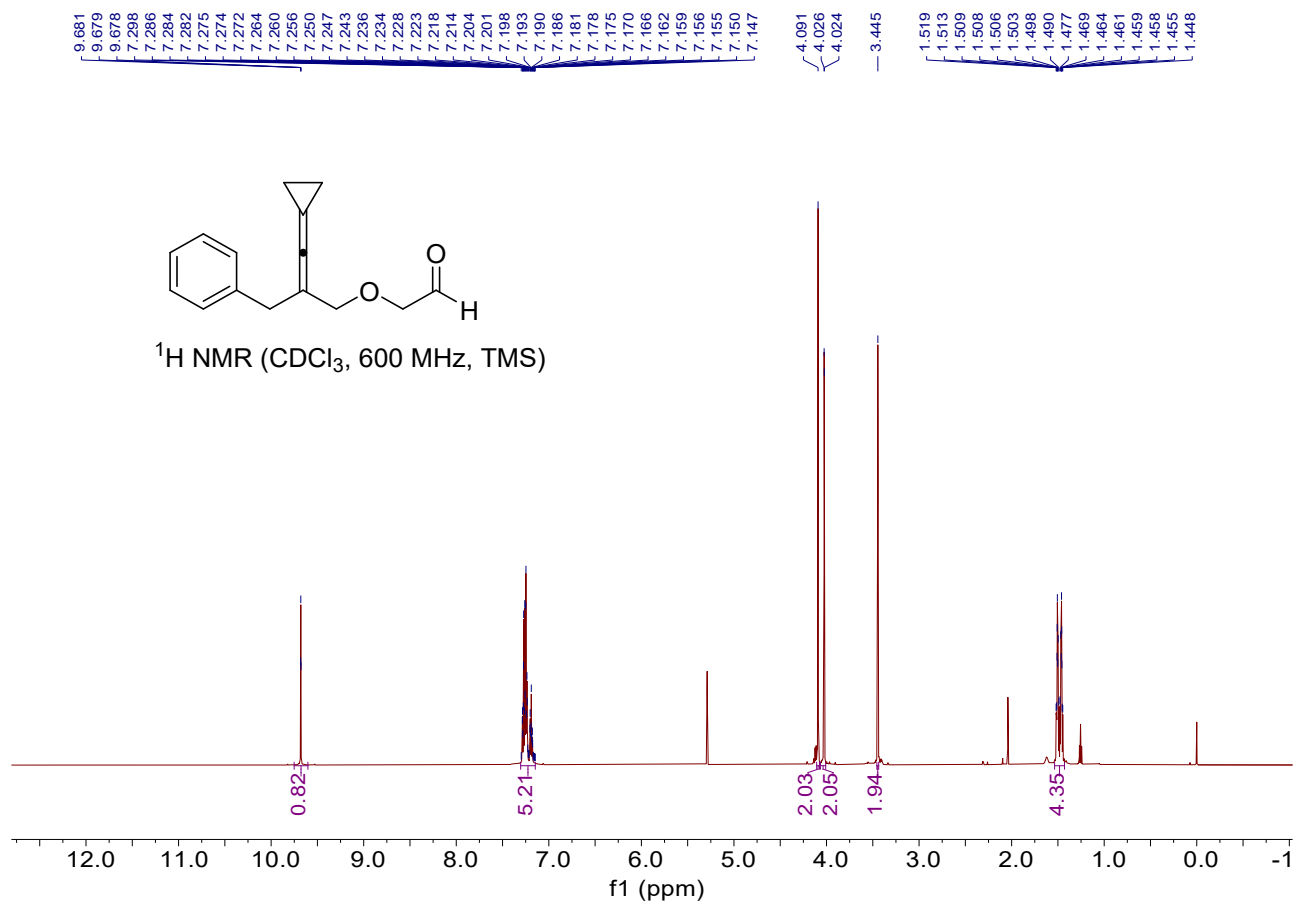






### 2-((2-benzyl-3-cyclopropylidene- $\lambda^5$ -allyl)oxy)acetaldehyde (**1ad**)

A colorless oil, 60% yield, 136.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  9.68 (t,  $J = 1.0$  Hz, 1H), 7.30 – 7.15 (m, 5H), 4.09 (s, 2H), 4.02 (d,  $J = 1.0$  Hz, 2H), 3.45 (s, 2H), 1.54 – 1.43 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  201.1, 189.4, 139.3, 129.0, 128.3, 126.3, 102.0, 78.2, 74.8, 72.4, 37.1, 7.7. IR (neat)  $\nu$  668, 987, 1228, 1737, 2022, 2924, 2976, 3026  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{15}\text{H}_{16}\text{O}_2\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 251.1042, Found: 251.1035.



— 201.105

— 189.369

— 139.330

129.001

128.272

126.260

— 102.031

78.203

77.397

77.078

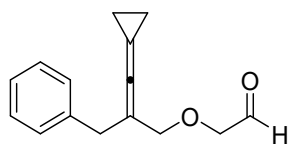
76.760

74.771

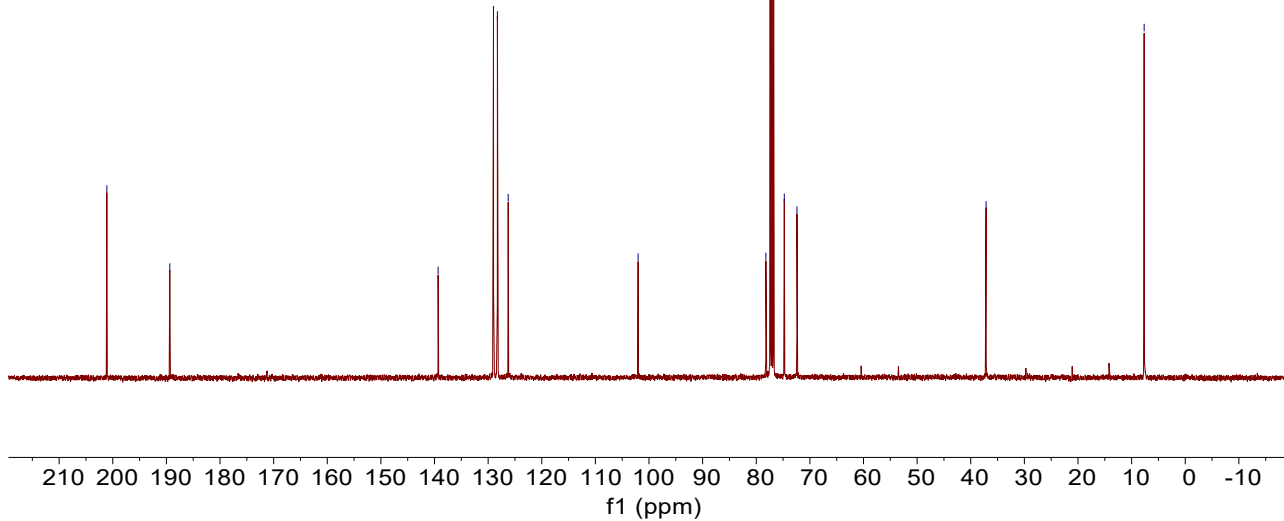
72.410

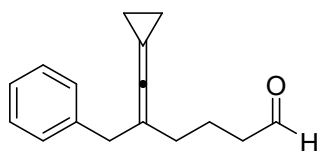
— 37.141

— 7.663



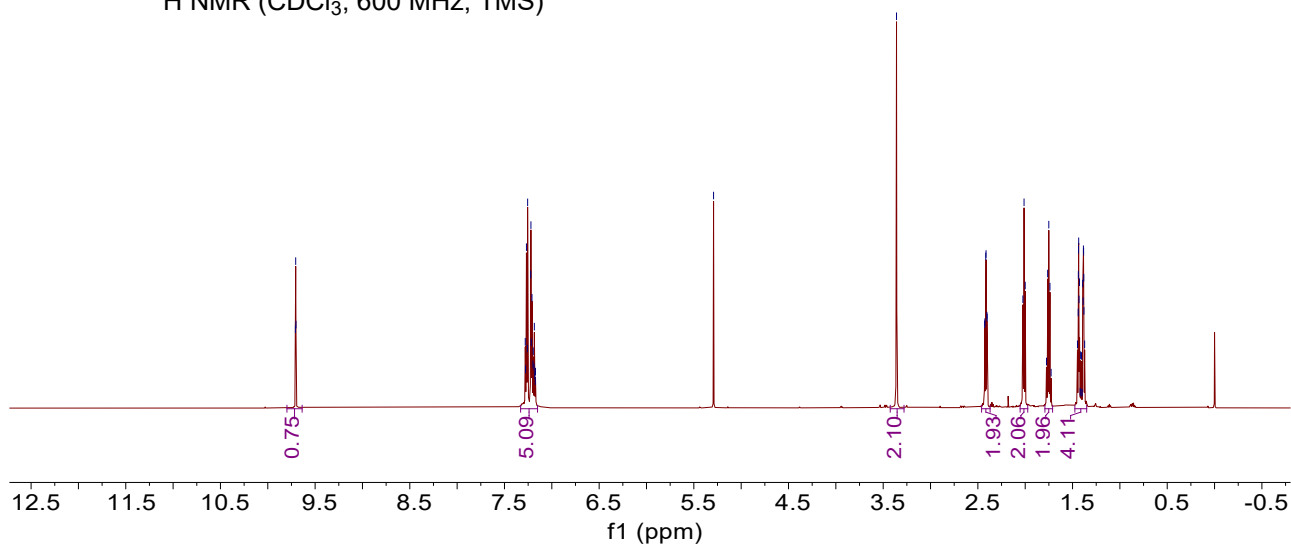
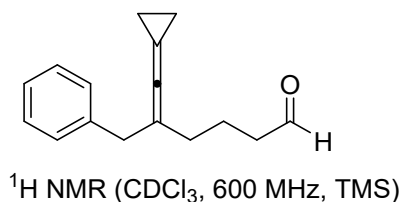
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



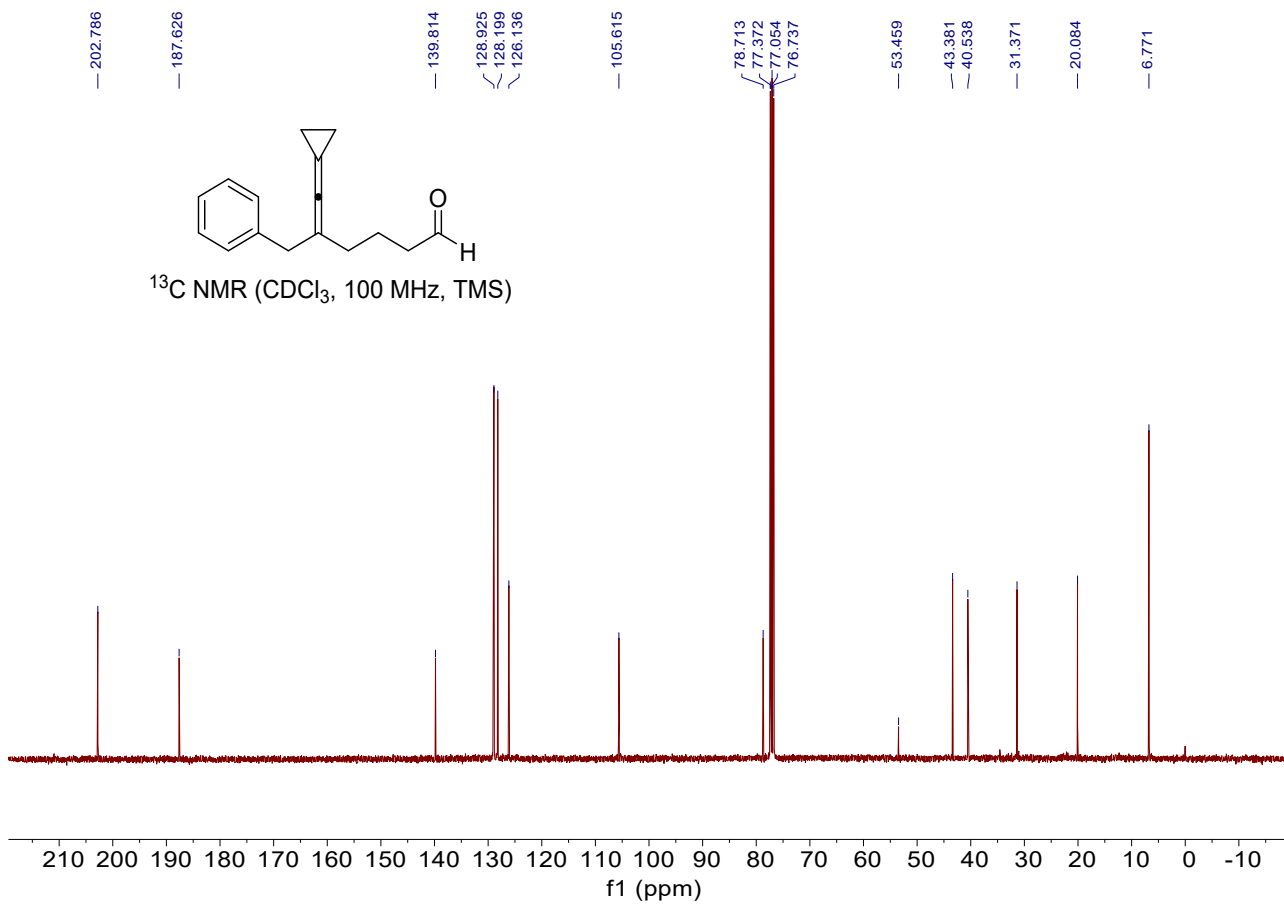


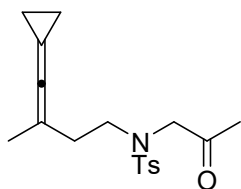
### 5-benzyl-6-cyclopropylidene- $\lambda^5$ -hex-5-enal (1ae)

A colorless oil, 60% yield, 136.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  9.71 (t,  $J = 1.8$  Hz, 1H), 7.33 – 7.15 (m, 5H), 3.36 (s, 2H), 2.42 (td,  $J = 7.6, 1.8$  Hz, 2H), 2.01 (t,  $J = 7.6$  Hz, 2H), 1.75 (p,  $J = 7.6$  Hz, 2H), 1.48 – 1.35 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  202.8, 187.6, 139.8, 128.9, 128.2, 126.1, 105.6, 78.7, 53.5, 43.4, 40.5, 31.4, 20.1, 6.8. IR (neat)  $\nu$  668, 987, 1228, 1737, 2022, 2924, 2976, 3026  $\text{cm}^{-1}$ . HRMS (EI) calcd. for  $\text{C}_{16}\text{H}_{18}\text{O}$ : 226.1352, Found: 226.1355.



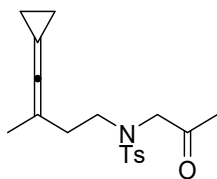




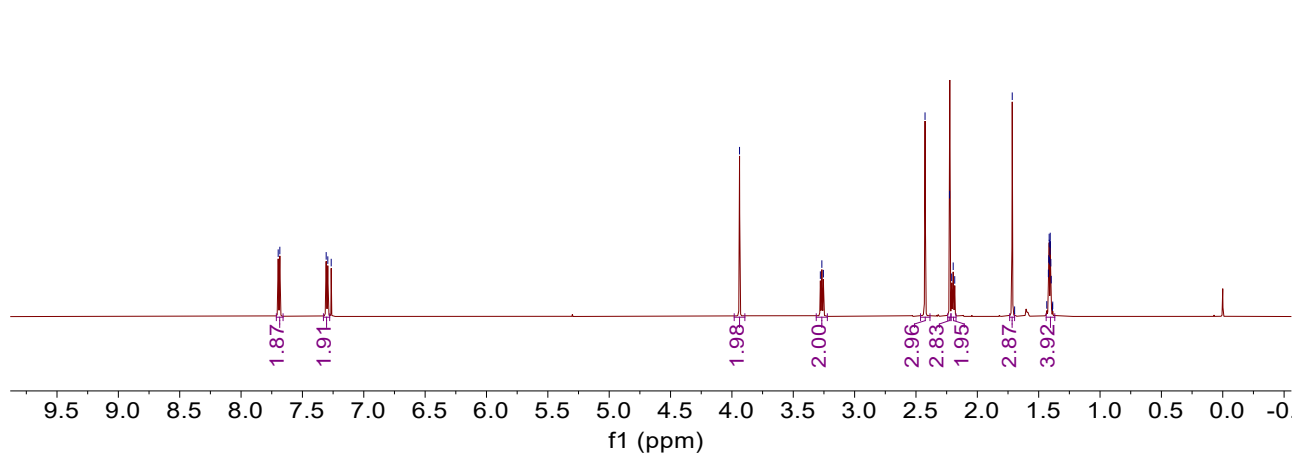


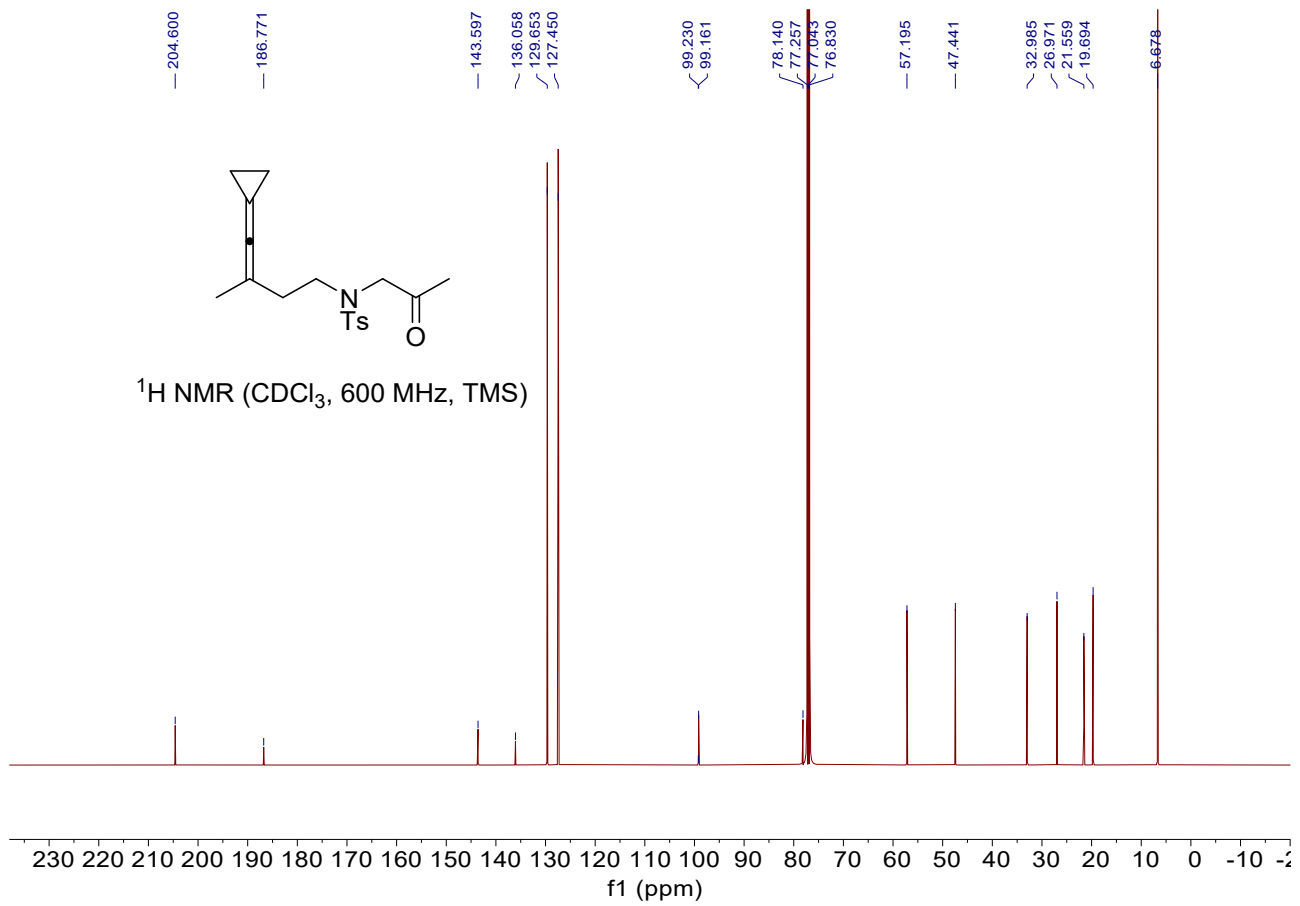
***N*-(4-cyclopropylidene-3-methyl-λ<sup>5</sup>-but-3-en-1-yl)-4-methyl-*N*-(2-oxopropyl)benzenesulfonamide (1af)**

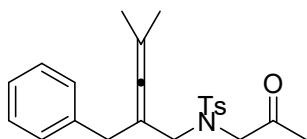
A colorless oil, 90% yield, 299.7 mg. <sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 600 MHz) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.94 (s, 2H), 3.27 (t, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 2.23 (s, 3H), 2.20 (t, *J* = 7.2 Hz, 2H), 1.72 (s, 3H), 1.44 – 1.37 (m, 4H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 150 MHz) δ 204.6, 186.8, 143.6, 136.1, 129.7, 127.5, 99.23, 99.16, 78.1, 57.2, 47.4, 33.0, 27.0, 21.6, 19.7, 6.7. IR (neat) ν 668, 988, 1219, 1711, 2010, 2932, 2976, 3031 cm<sup>-1</sup>. HRMS (ESI) calcd. for C<sub>18</sub>H<sub>23</sub>NO<sub>3</sub>NaS (M+Na)<sup>+</sup>: 356.1290, Found: 356.1289.



<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, TMS)

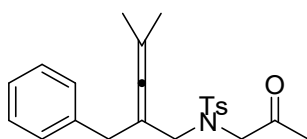




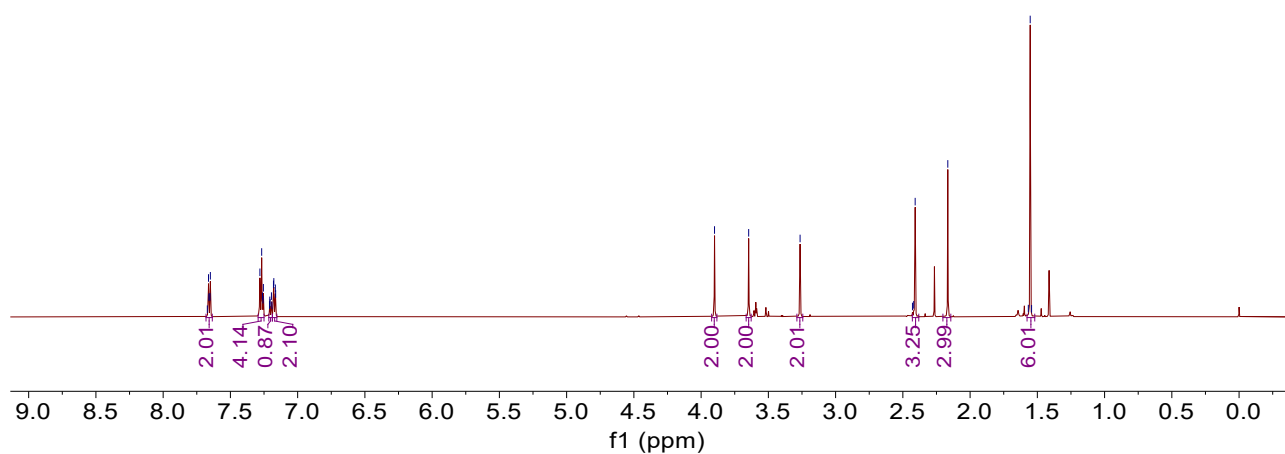


**N-(2-benzyl-4-methyl- $\lambda^5$ -penta-2,3-dien-1-yl)-4-methyl-N-(2-oxopropyl)benzenesulfonamide (1f)**

A yellow oil, 90% yield, 355.5 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.68 – 7.63 (m, 2H), 7.29 – 7.25 (m, 4H), 7.21 – 7.19 (m, 1H), 7.19 – 7.15 (m, 2H), 3.90 (s, 2H), 3.65 (s, 2H), 3.26 (s, 2H), 2.41 (s, 3H), 2.17 (s, 3H), 1.55 (s, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  204.0, 202.4, 143.5, 139.5, 136.0, 129.6, 129.0, 128.2, 127.5, 126.2, 97.3, 96.8, 63.9, 55.9, 51.3, 37.1, 26.9, 21.5, 20.3. IR (neat)  $\nu$  701, 1157, 1344, 1497, 1735, 2020, 2907, 3034  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{28}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 398.1785, Found: 398.1800.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)



203.973  
202.420

143.548  
139.453  
135.975  
129.615  
129.005  
128.225  
127.514  
126.194

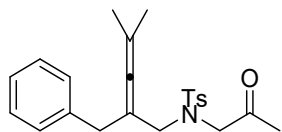
97.271  
96.799

77.384  
77.066  
76.749

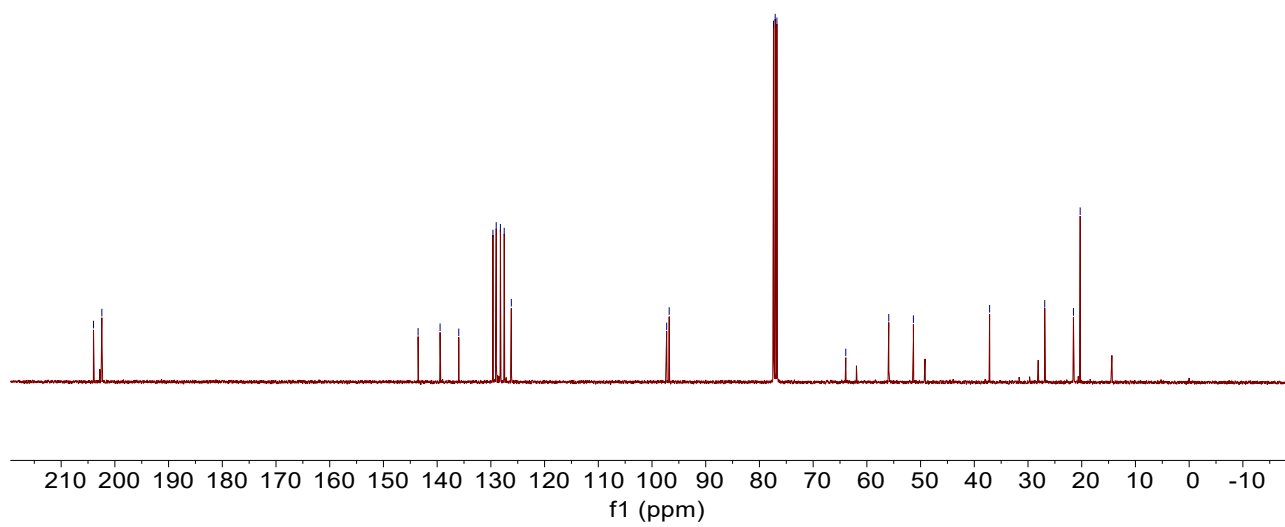
63.926  
55.922  
51.336

37.148

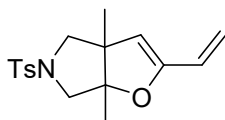
26.886  
21.541  
20.288



<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)

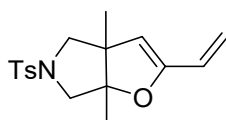


## 9. Spectroscopic data of products 2-14

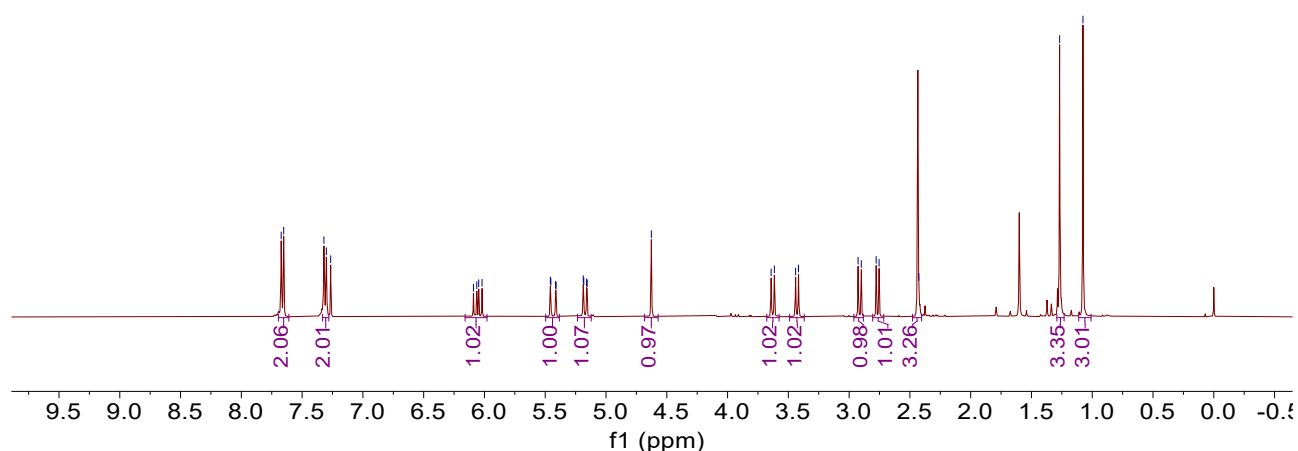


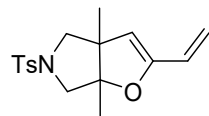
### 3a,6a-dimethyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2a)

A colorless oil, 96% yield, 30.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.66 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.06 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.43 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.17 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.63 (s, 1H), 3.63 (d,  $J = 10.4$  Hz, 1H), 3.43 (d,  $J = 9.6$  Hz, 1H), 2.91 (d,  $J = 10.4$  Hz, 1H), 2.77 (d,  $J = 9.6$  Hz, 1H), 2.43 (s, 3H), 1.27 (s, 3H), 1.08 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.6, 143.7, 132.4, 129.6, 128.0, 125.7, 116.5, 107.8, 92.4, 60.8, 60.7, 55.1, 21.6, 20.5, 19.8. IR (neat)  $\nu$  664, 760, 1029, 1092, 1162, 1346, 1596, 2853, 2924, 2956  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{21}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 342.1134, Found: 342.1133. Enantiomeric excess was determined by HPLC with a Chiralpak AD column [ $\lambda = 254\text{nm}$ ; eluent: Hexane/Isopropanol = 90/10; Flow rate: 0.8 mL/min;  $t_{\text{major}} = 25.95$  min,  $t_{\text{minor}} = 28.54$  min.; ee% = 20%.  $[\alpha]_{\text{D}}^{20} = +11.6$  (c 0.1, DCM).

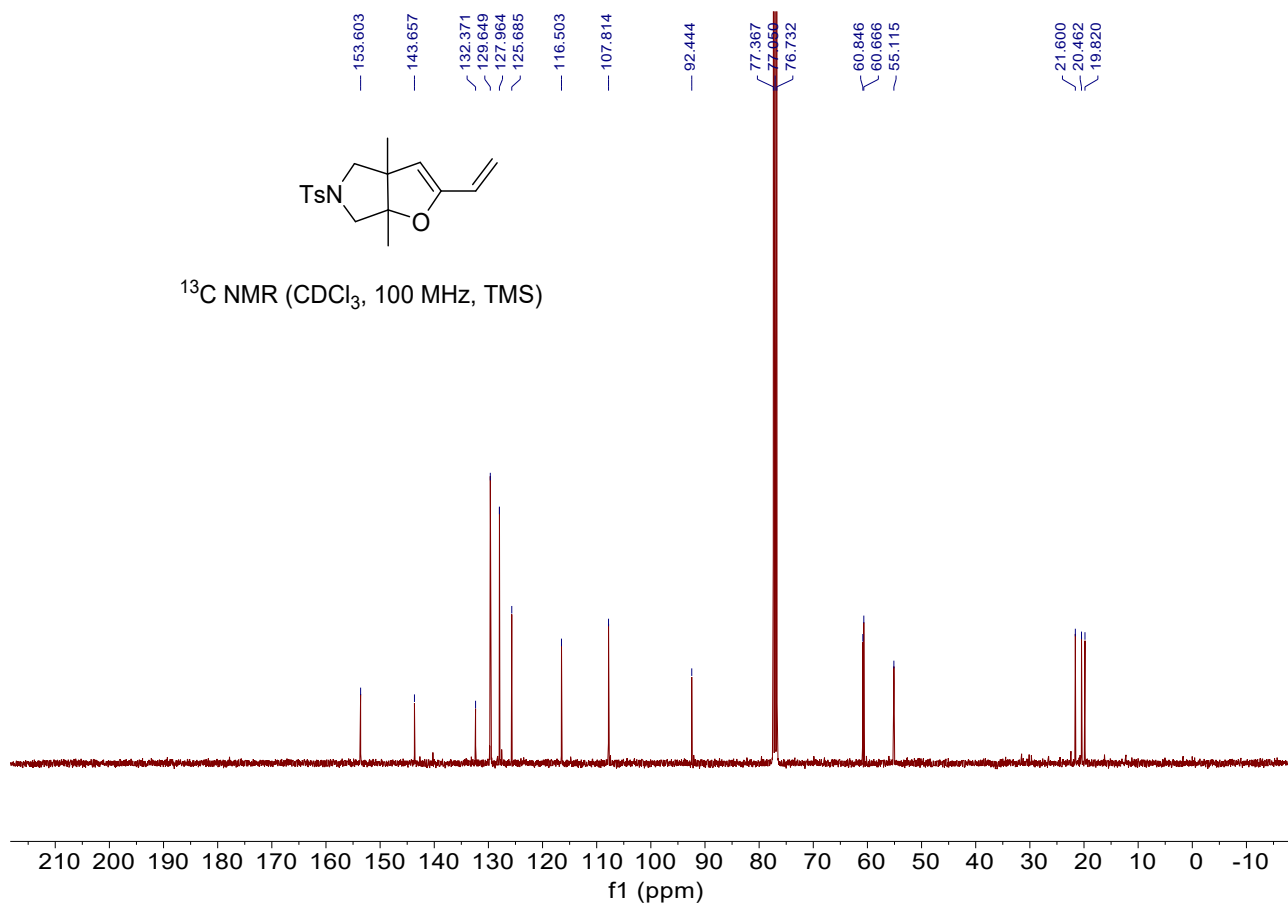


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

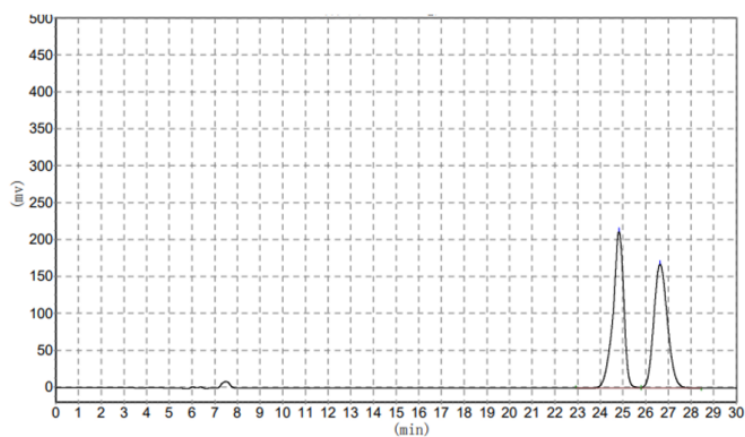




$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)

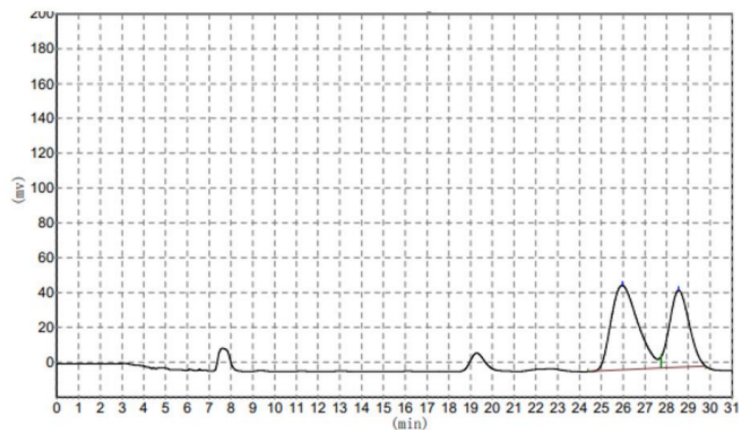


### Racemic



	Retention time	Height	Area	Area %
1	24.823	212025.063	6981464.500	49.9043
2	26.638	167807.008	7008242.000	50.0957
Total		379833.000	13989706.500	100.0000

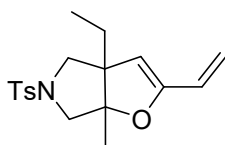
### Chiral



	Retention time	Height	Area	Area %
1	25.958	48700.676	4212416.500	60.5686
2	28.548	44283.008	2742368.000	39.4314
Total		92983.684	6954784.500	100.0000

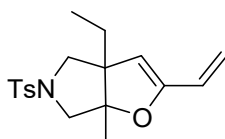
Translation: Enantiomeric excess was determined by HPLC with a Chiralpak AD column [ $\lambda = 254$  nm; eluent: Hexane/Isopropanol = 90/10; Flow rate: 0.8 mL/min;  $t_{\text{major}} = 25.95$  min,  $t_{\text{minor}} = 28.54$  min.; ee% = 20%].



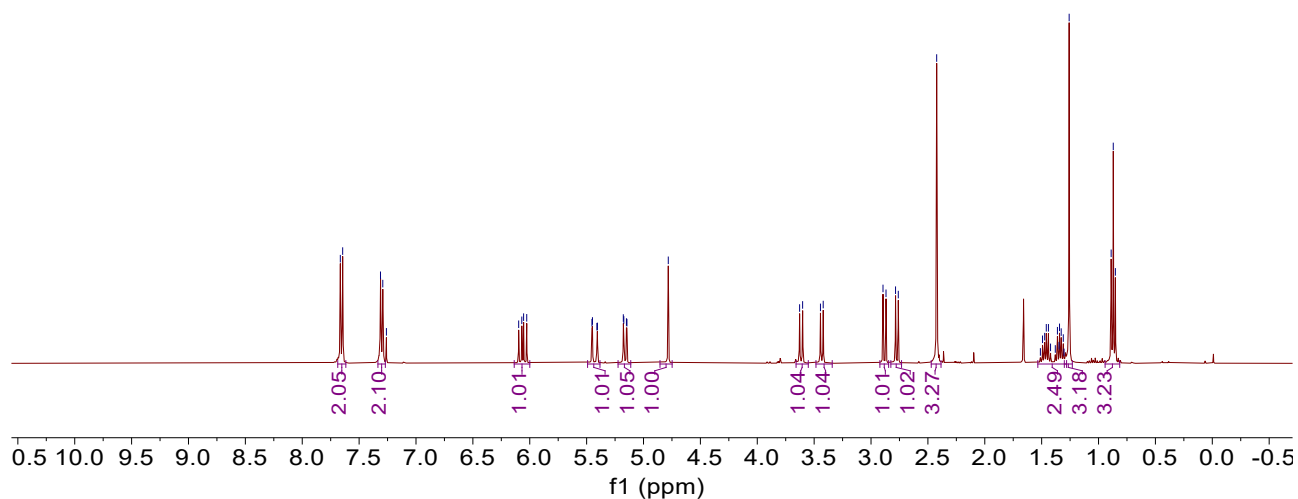


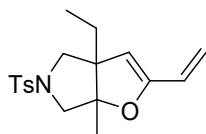
### 3a-ethyl-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2b)

A colorless oil, 92% yield, 30.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.65 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 6.06 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.43 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.16 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.78 (s, 1H), 3.61 (d,  $J = 10.4$  Hz, 1H), 3.43 (d,  $J = 9.6$  Hz, 1H), 2.88 (d,  $J = 10.4$  Hz, 1H), 2.77 (d,  $J = 9.6$  Hz, 1H), 2.42 (s, 3H), 1.53 – 1.28 (m, 2H), 1.26 (s, 3H), 0.87 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  154.2, 143.6, 132.6, 129.6, 127.9, 125.8, 116.5, 105.0, 92.7, 61.0, 59.1, 58.9, 29.7, 27.7, 21.6, 19.4, 9.8. IR (neat)  $\nu$  664, 830, 1092, 1163, 1346, 1592, 2848, 2869, 2916, 2969  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 356.1291, Found: 356.1292.

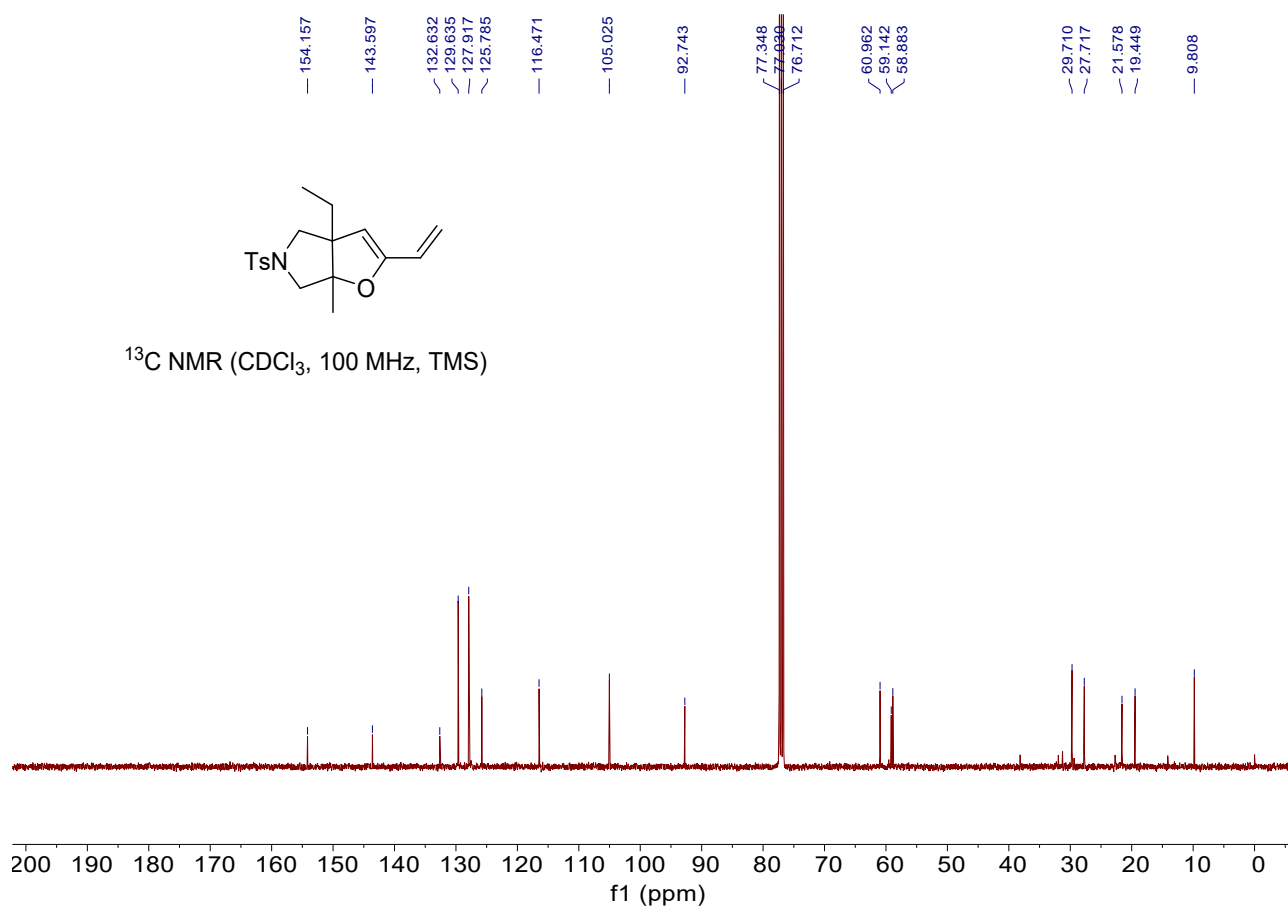


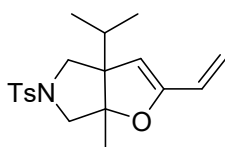
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





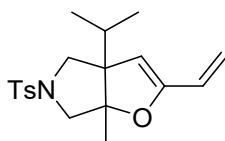
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



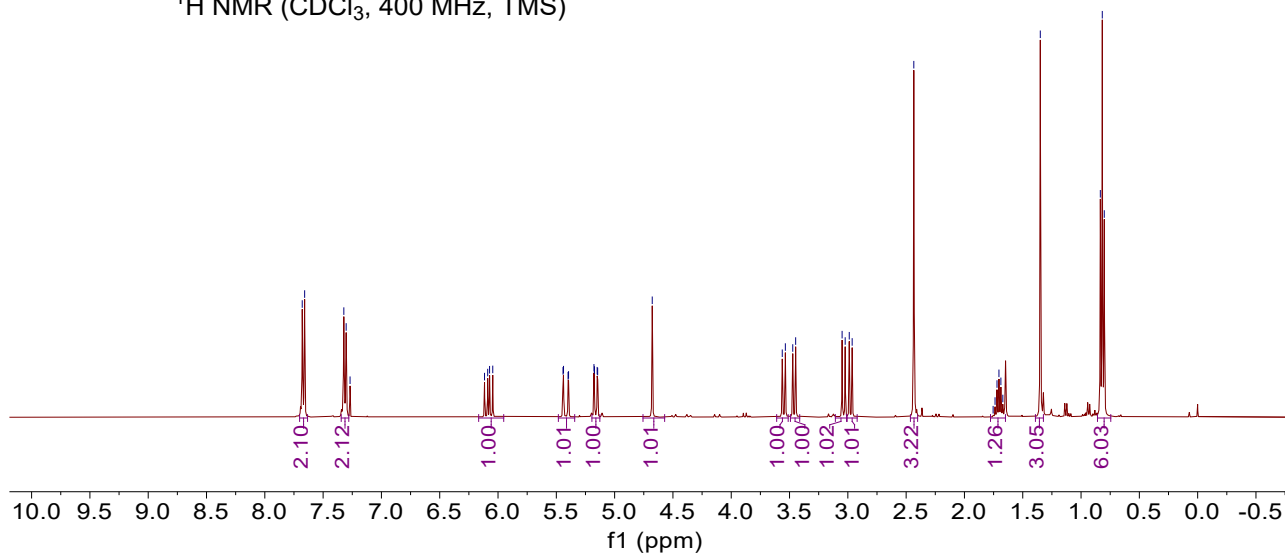


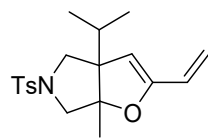
### 3a-isopropyl-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2c)

A colorless oil, 90% yield, 31.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.67 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.08 (dd,  $J = 17.4, 10.8$  Hz, 1H), 5.42 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.16 (dd,  $J = 11.2, 1.6$  Hz, 1H), 4.68 (s, 1H), 3.55 (d,  $J = 10.4$  Hz, 1H), 3.46 (d,  $J = 10.0$  Hz, 1H), 3.04 (d,  $J = 10.4$  Hz, 1H), 2.98 (d,  $J = 10.0$  Hz, 1H), 2.43 (s, 3H), 1.70 (hept,  $J = 6.8$  Hz, 1H), 1.35 (s, 3H), 0.82 (d,  $J = 6.8$  Hz, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  154.5, 143.6, 132.9, 129.6, 127.8, 125.8, 116.3, 104.3, 92.5, 62.1, 61.9, 57.4, 31.1, 21.6, 19.5, 19.2, 19.1. IR (neat)  $\nu$  663, 815, 1092, 1161, 1341, 1597, 2848, 2867, 2932, 2968  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{26}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 348.1628, Found: 348.1619.

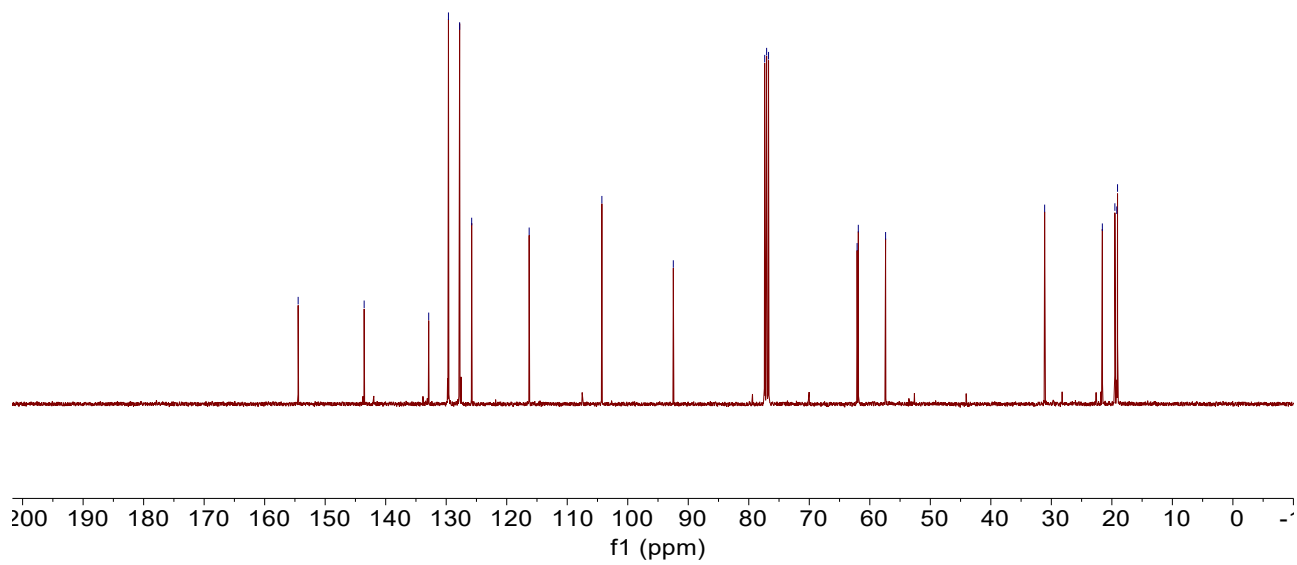


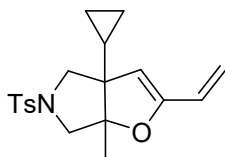
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





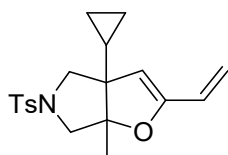
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



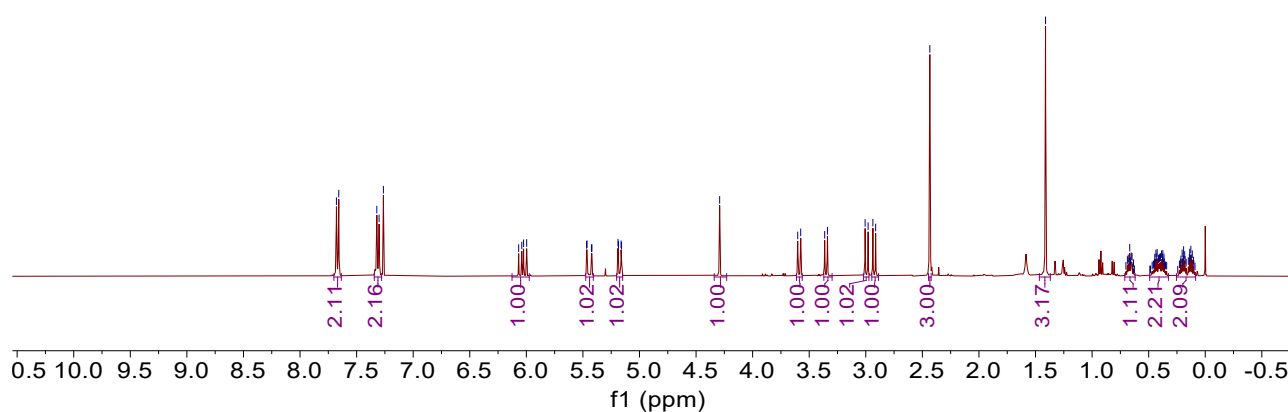


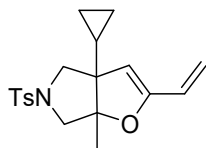
### 3a-cyclopropyl-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2d)

A colorless oil, 80% yield, 27.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.67 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.03 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.44 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.17 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.29 (s, 1H), 3.59 (d,  $J = 10.8$  Hz, 1H), 3.35 (d,  $J = 9.6$  Hz, 1H), 2.99 (d,  $J = 10.8$  Hz, 1H), 2.93 (d,  $J = 9.6$  Hz, 1H), 2.43 (s, 3H), 1.41 (s, 3H), 0.71 – 0.62 (m, 1H), 0.49 – 0.33 (m, 2H), 0.25 – 0.09 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  155.4, 143.6, 132.5, 129.6, 128.0, 125.6, 116.7, 101.7, 93.4, 61.2, 59.9, 59.7, 21.6, 20.3, 13.9, 1.6, 0.2. IR (neat)  $\nu$  664, 815, 1092, 1163, 1347, 1593, 2849, 2869, 2928, 2998  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 368.1291, Found: 368.1288.

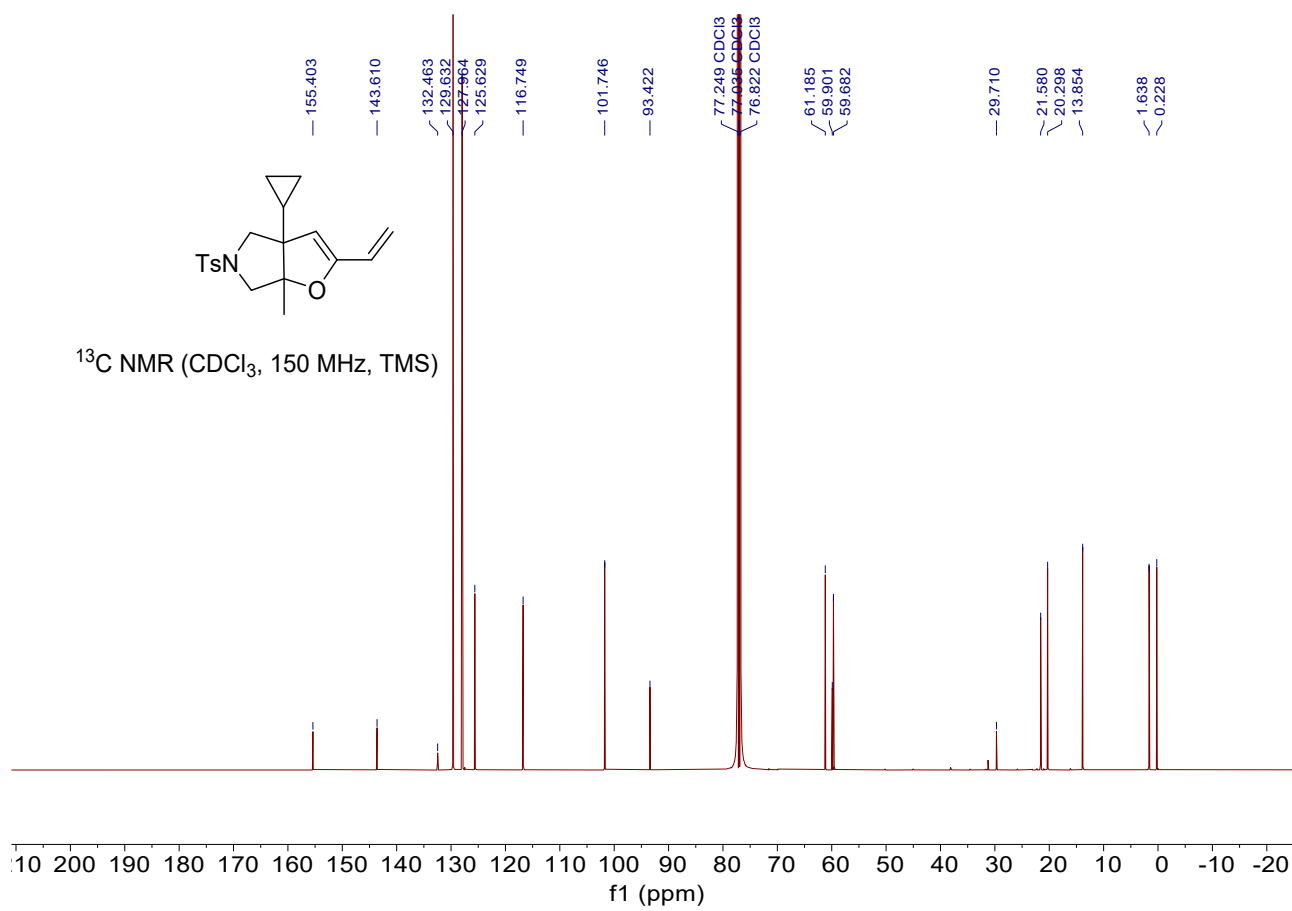


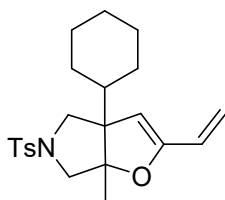
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





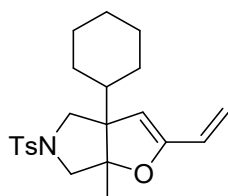
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, TMS)



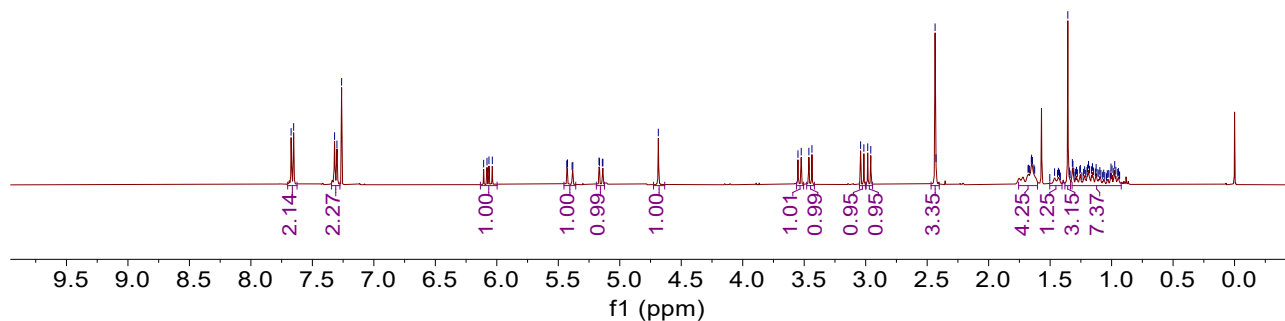


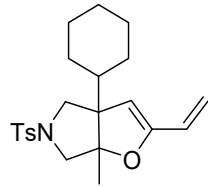
**3a-cyclohexyl-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2e)**

A colorless oil, 72% yield, 27.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.66 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.07 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.41 (dd,  $J = 17.4, 2.4$  Hz, 1H), 5.15 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.69 (s, 1H), 3.54 (d,  $J = 10.6$  Hz, 1H), 3.45 (d,  $J = 10.0$  Hz, 1H), 3.03 (d,  $J = 10.6$  Hz, 1H), 2.97 (d,  $J = 10.0$  Hz, 1H), 2.44 (s, 3H), 1.76 – 1.60 (m, 4H), 1.50 – 1.40 (m, 1H), 1.36 (s, 3H), 1.32 – 0.92 (m, 7H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  154.1, 143.5, 133.0, 129.6, 127.8, 125.8, 116.2, 105.4, 92.6, 61.9, 61.6, 57.3, 42.0, 29.3, 29.0, 26.7, 26.3, 26.1, 26.0, 21.6, 19.5. IR (neat)  $\nu$  666, 815, 1092, 1163, 1347, 1592, 2852, 2929  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{15}\text{H}_{19}\text{NO}_2\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 410.1760, Found: 410.1761.

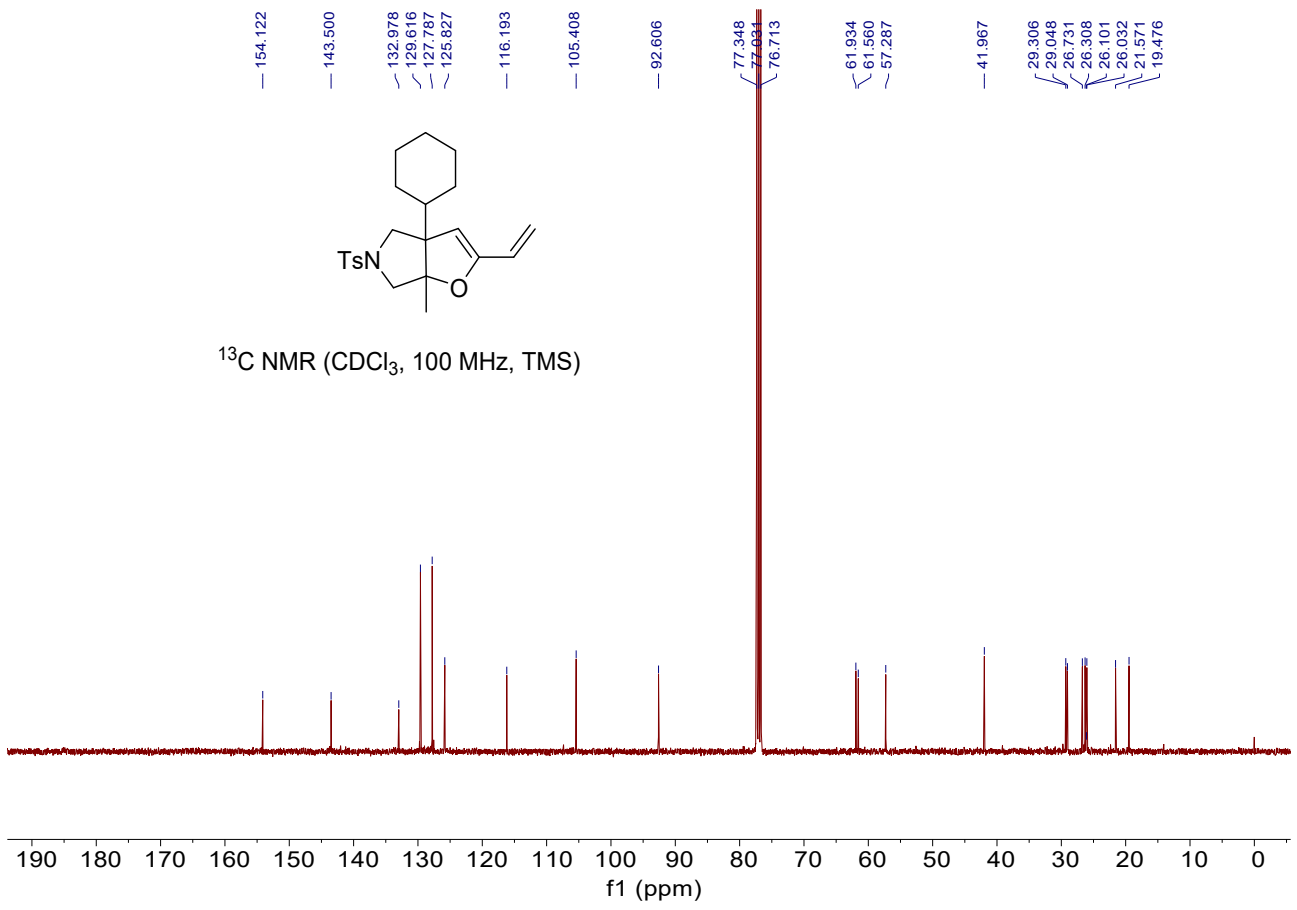


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

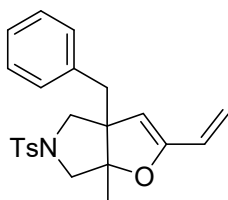




$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)

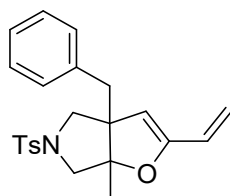




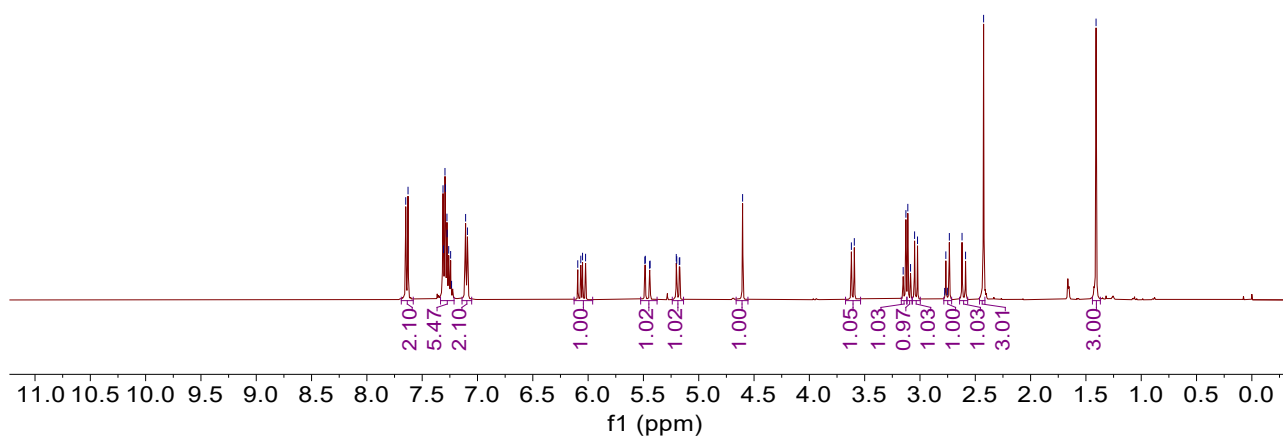


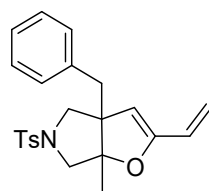
**3a-benzyl-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2f)**

A yellow oil, 94% yield, 36.3 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.64 (d,  $J = 8.4$  Hz, 2H), 7.33 – 7.21 (m, 5H), 7.10 (d,  $J = 6.6$  Hz, 2H), 6.06 (dd,  $J = 17.2$ , 11.0 Hz, 1H), 5.46 (dd,  $J = 17.2$ , 1.6 Hz, 1H), 5.19 (dd,  $J = 10.8$ , 1.6 Hz, 1H), 4.60 (s, 1H), 3.61 (d,  $J = 10.8$  Hz, 1H), 3.14 (d,  $J = 10.0$  Hz, 1H), 3.10 (d,  $J = 10.0$  Hz, 1H), 3.04 (d,  $J = 10.4$  Hz, 1H), 2.75 (d,  $J = 12.8$  Hz, 1H), 2.60 (d,  $J = 12.8$  Hz, 1H), 2.42 (s, 3H), 1.41 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  157.2, 145.3, 137.5, 132.7, 129.1, 128.5, 127.9, 126.7, 125.8, 117.2, 107.3, 94.4, 62.1, 59.3, 58.0, 42.9, 29.2, 21.6, 19.8. IR (neat)  $\nu$  665, 987, 1220, 1355, 1592, 2849, 2917  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1447.

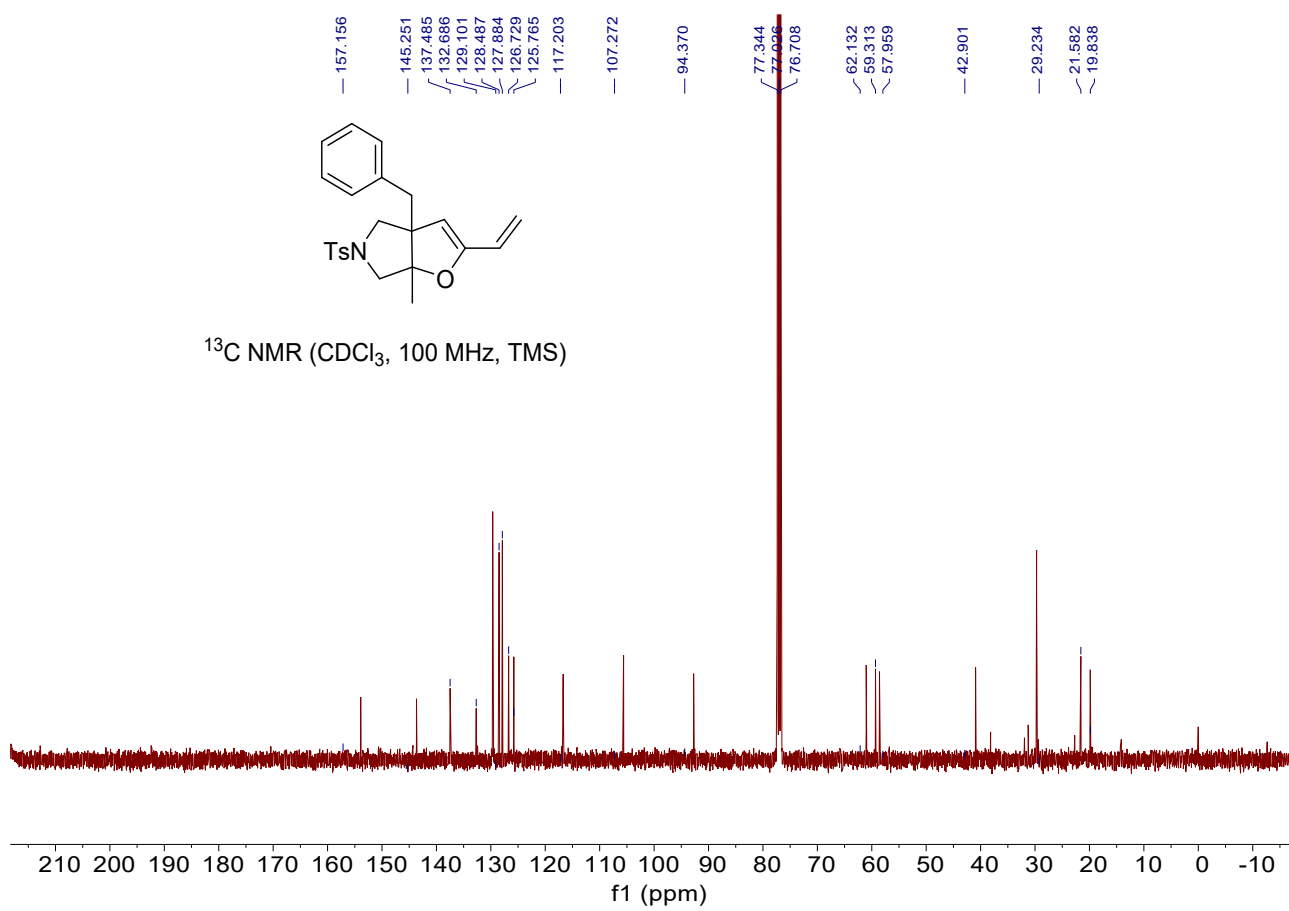


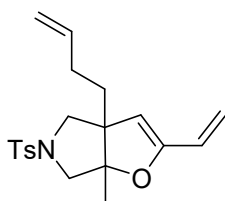
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





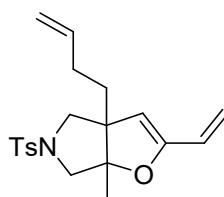
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



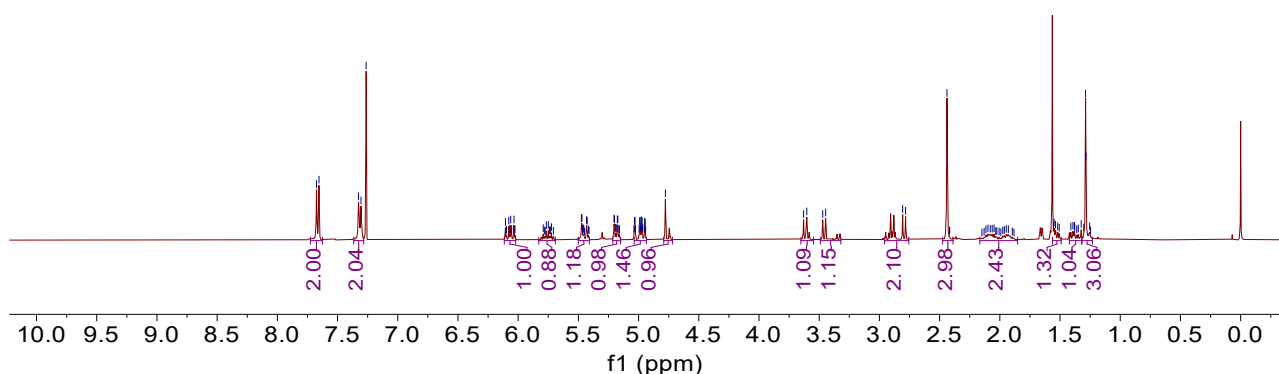


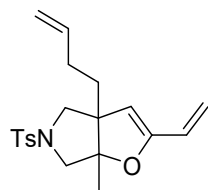
**3a-(but-3-en-1-yl)-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2g)**

A yellow oil, 82% yield, 29.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.66 (d,  $J = 8.0$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 6.07 (ddd,  $J = 17.2, 11.2, 3.2$  Hz, 1H), 5.83 – 5.69 (m, 1H), 5.44 (ddd,  $J = 17.2, 6.0, 1.6$  Hz, 1H), 5.18 (ddd,  $J = 11.2, 5.6, 1.6$  Hz, 1H), 5.04 – 4.94 (m, 1H), 4.78 (s, 1H), 3.62 (d,  $J = 10.6$  Hz, 1H), 3.46 (d,  $J = 9.6$  Hz, 1H), 2.79 (d,  $J = 9.6$  Hz, 2H), 2.44 (s, 3H), 2.17 – 1.85 (m, 2H), 1.56 – 1.49 (m, 1H), 1.42 – 1.32 (m, 1H), 1.30 – 1.24 (m, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  155.7, 142.7, 138.0, 129.7, 127.9, 125.7, 116.7, 115.1, 105.1, 92.9, 60.8, 59.0, 58.4, 34.4, 29.8, 21.6, 19.6. IR (neat)  $\nu$  665, 987, 1347, 1640, 2851, 2869, 2926, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{20}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 382.1447, Found: 382.1444.

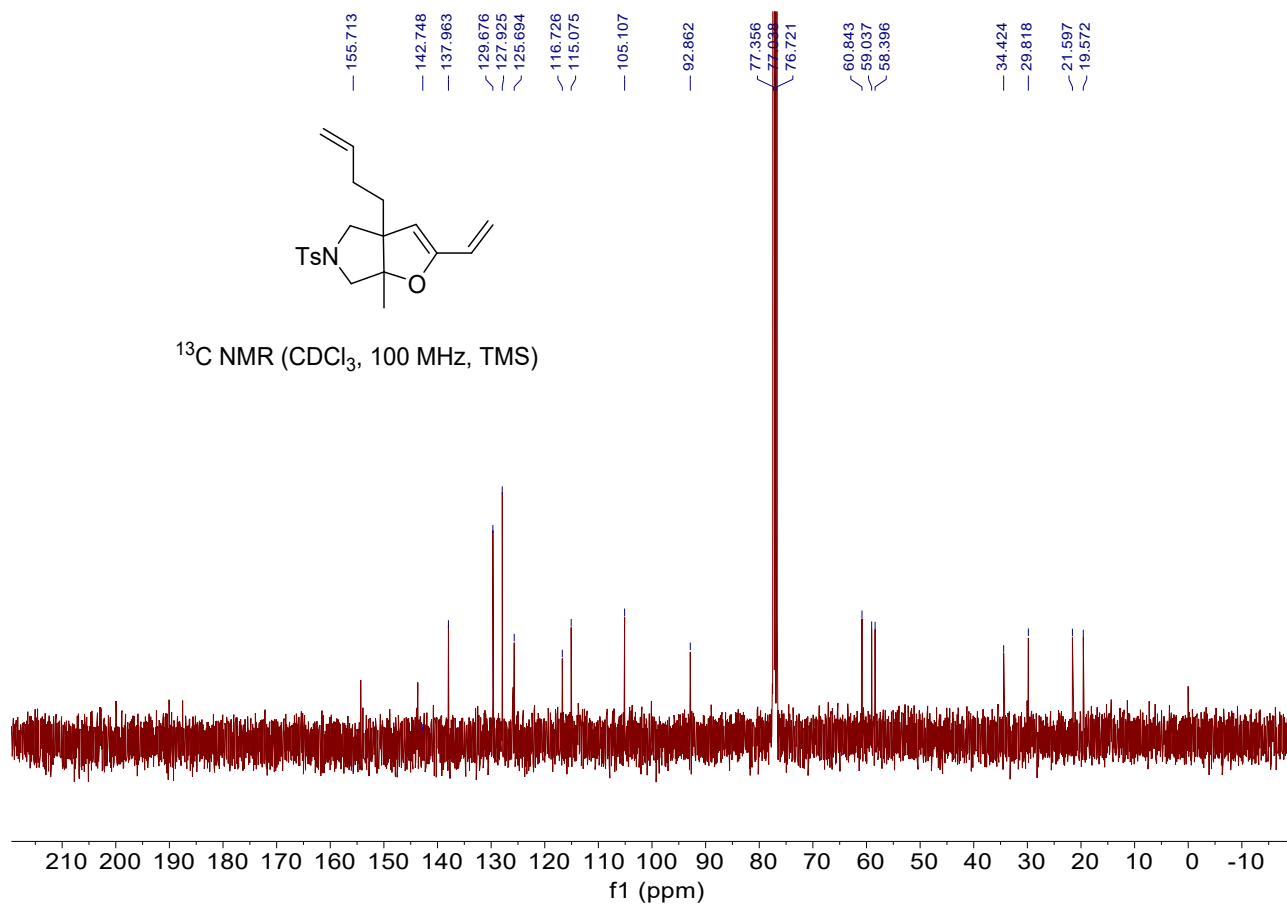


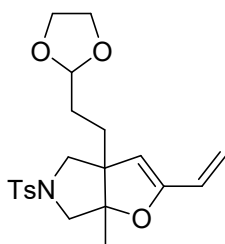
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





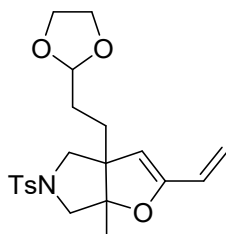
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



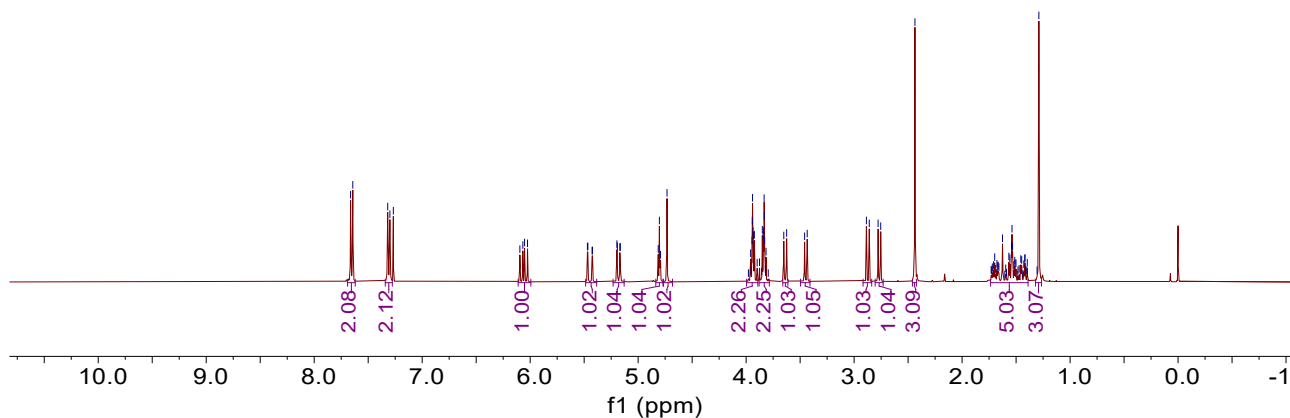


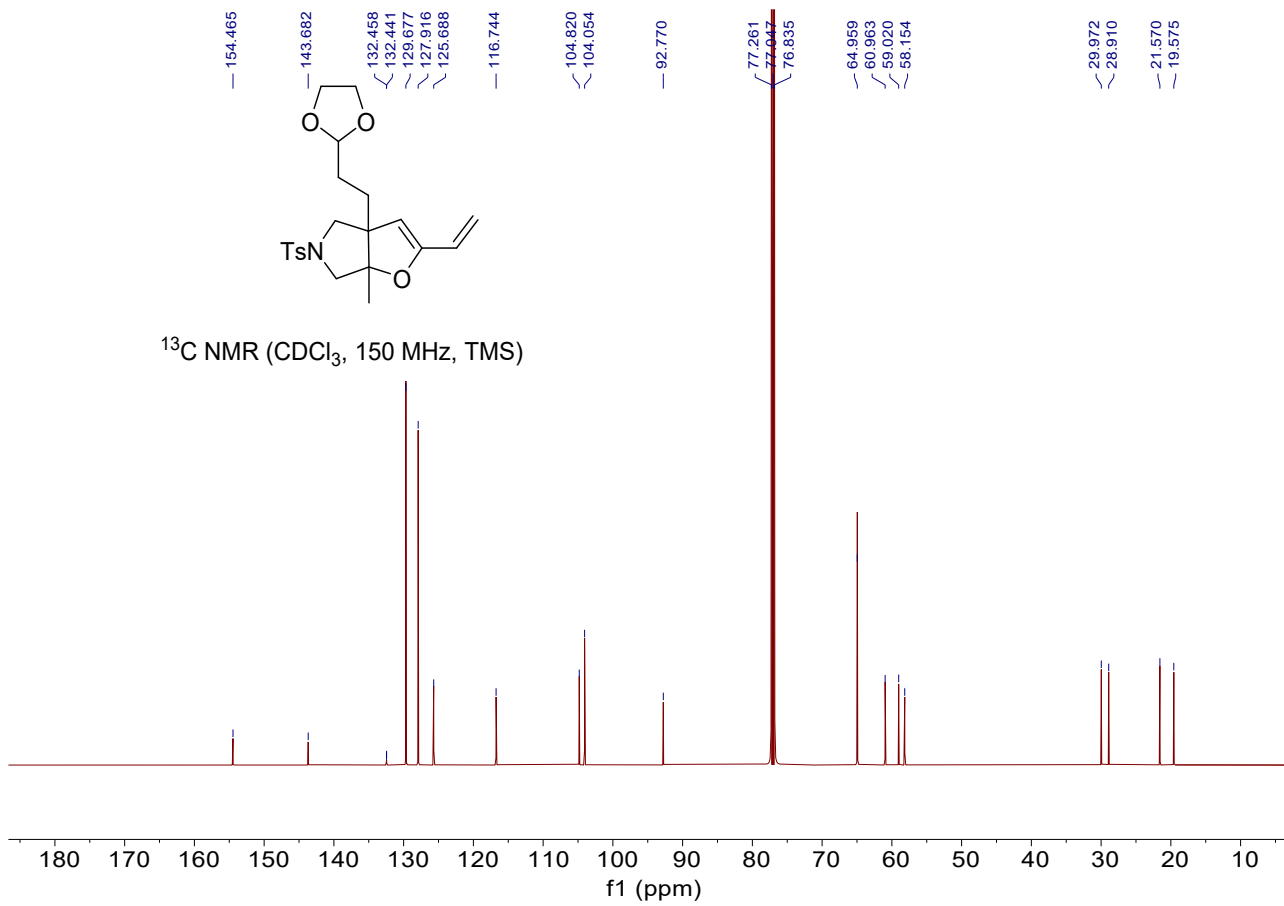
**3a-(2-(1,3-dioxolan-2-yl)ethyl)-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2h)**

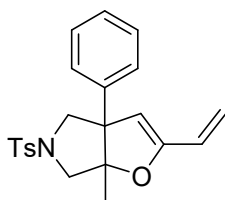
A brown oil, 93% yield, 35.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.65 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.06 (dd,  $J = 17.2, 11.2$  Hz, 1H), 5.45 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.18 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.80 (t,  $J = 4.4$  Hz, 1H), 4.73 (s, 1H), 4.00 – 3.89 (m, 2H), 3.88 – 3.79 (m, 2H), 3.64 (d,  $J = 10.4$  Hz, 1H), 3.45 (d,  $J = 9.6$  Hz, 1H), 2.87 (d,  $J = 10.6$  Hz, 1H), 2.77 (d,  $J = 9.6$  Hz, 1H), 2.44 (s, 3H), 1.74 – 1.39 (m, 5H), 1.29 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  154.5, 143.7, 132.5, 132.4, 129.7, 127.9, 125.7, 116.7, 104.8, 104.1, 92.8, 65.0, 61.0, 59.0, 58.2, 30.0, 28.9, 21.6, 19.6. IR (neat)  $\nu$  664, 815, 1220, 1356, 1709, 2018, 2880, 2919, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{28}\text{NO}_5\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 406.1683, Found: 406.1688.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

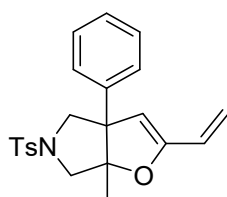
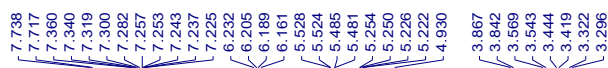




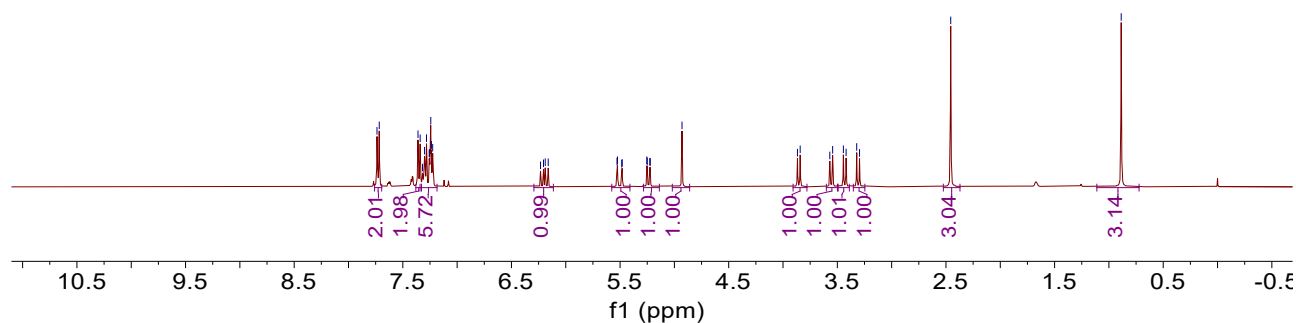


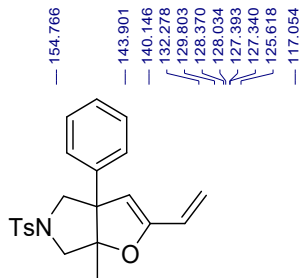
### 6a-methyl-3a-phenyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2i)

A yellow oil, 94% yield, 35.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.35 (d,  $J = 8.0$  Hz, 2H), 7.34 – 7.19 (m, 5H), 6.20 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.50 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.24 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.93 (s, 1H), 3.85 (d,  $J = 10.0$  Hz, 1H), 3.56 (d,  $J = 10.4$  Hz, 1H), 3.43 (d,  $J = 10.0$  Hz, 1H), 3.31 (d,  $J = 10.4$  Hz, 1H), 2.46 (s, 3H), 0.89 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  154.8, 143.9, 140.1, 132.3, 129.8, 128.4, 128.0, 127.4, 127.3, 125.6, 117.1, 106.4, 94.9, 63.4, 61.0, 60.8, 22.3, 21.6. IR (neat)  $\nu$  660, 815, 987, 1157, 1216, 1346, 1447, 2018, 2899, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 404.1291, Found: 404.1296.

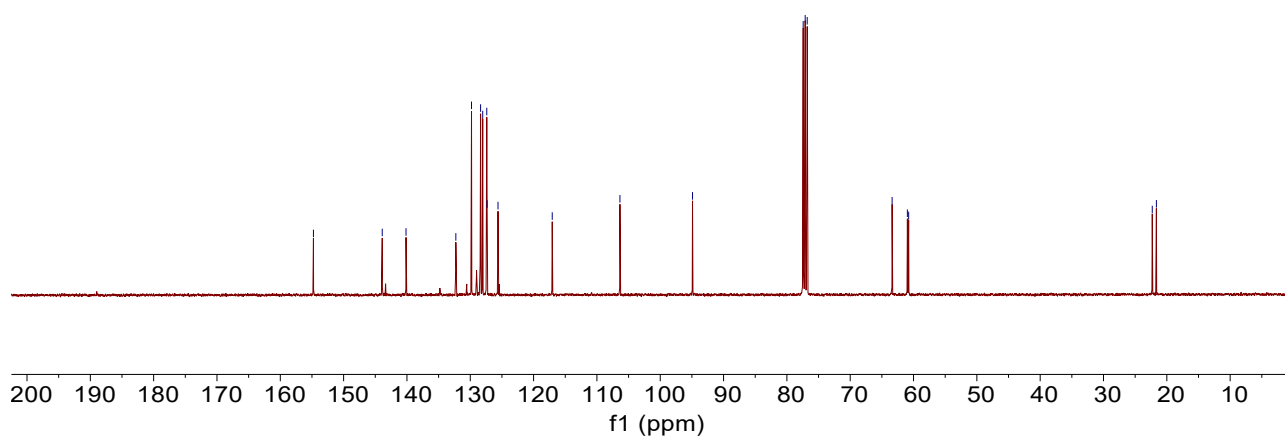


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

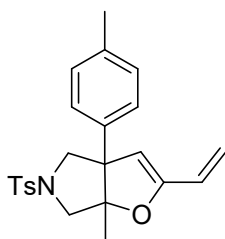




<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)

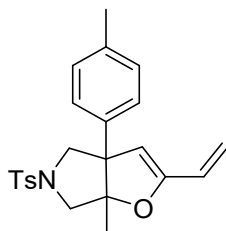




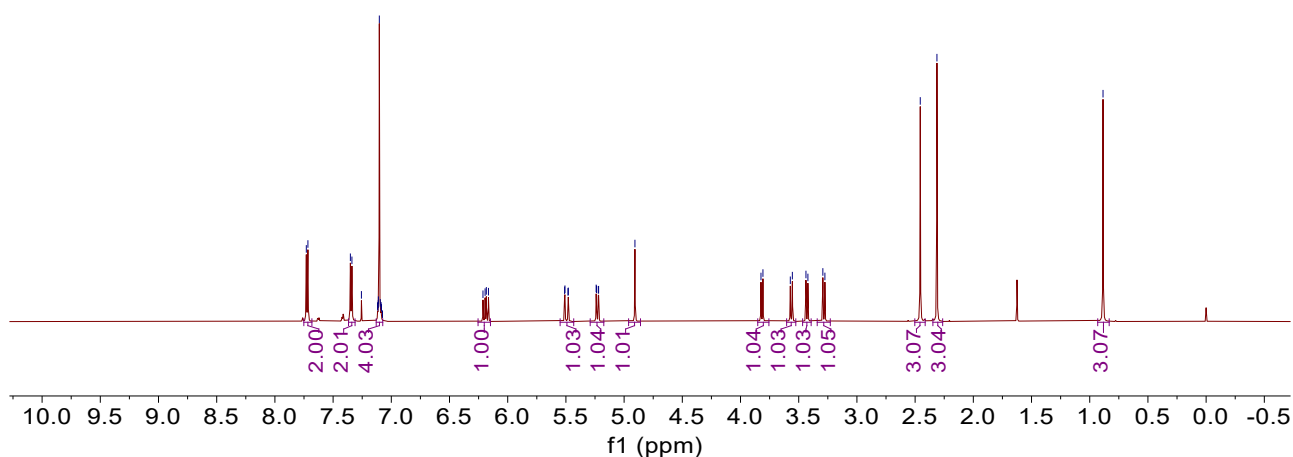


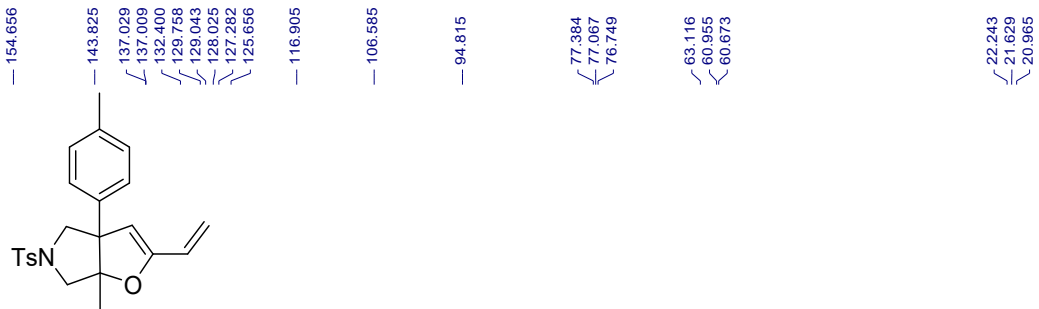
**6a-methyl-3a-(p-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2j)**

A yellow oil, 90% yield, 35.5 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.34 (d,  $J = 8.0$  Hz, 2H), 7.13 – 7.07 (m, 4H), 6.19 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.50 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.23 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.91 (s, 1H), 3.82 (d,  $J = 10.0$  Hz, 1H), 3.56 (d,  $J = 10.5$  Hz, 1H), 3.43 (d,  $J = 10.0$  Hz, 1H), 3.28 (d,  $J = 10.5$  Hz, 1H), 2.46 (s, 3H), 2.31 (s, 3H), 0.89 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  154.7, 143.8, 137.02, 137.00, 132.4, 129.8, 129.0, 128.0, 127.3, 125.7, 116.9, 106.6, 94.8, 63.1, 61.0, 60.7, 22.2, 21.6, 21.0. IR (neat)  $\nu$  665, 1163, 1348, 1596, 2846, 2929, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1447.

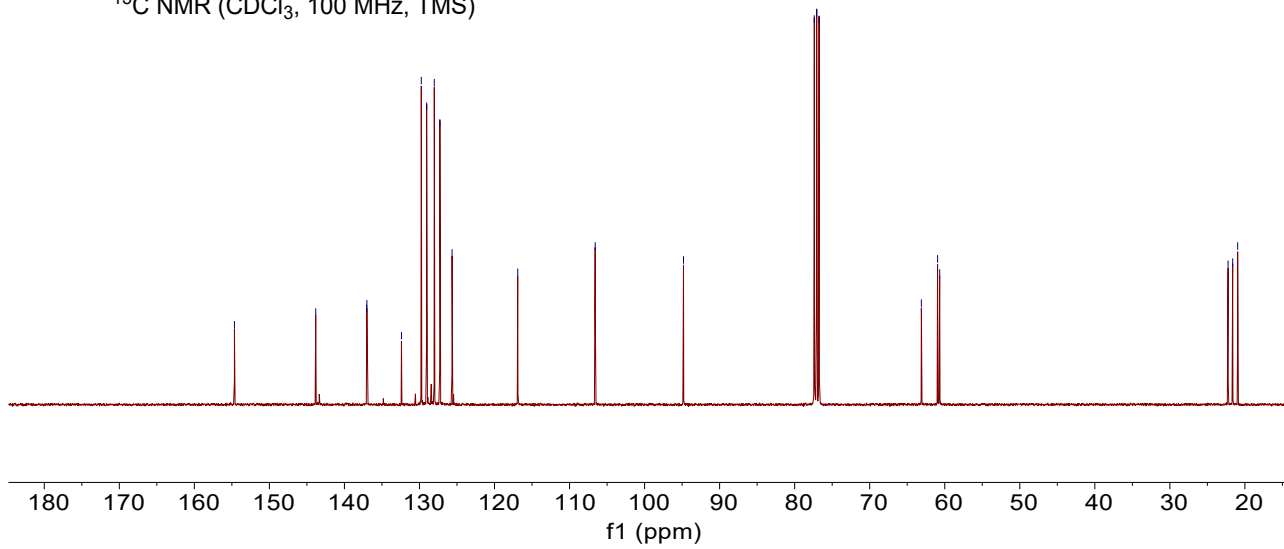


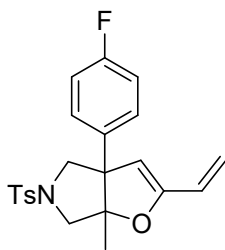
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





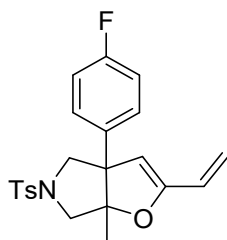
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



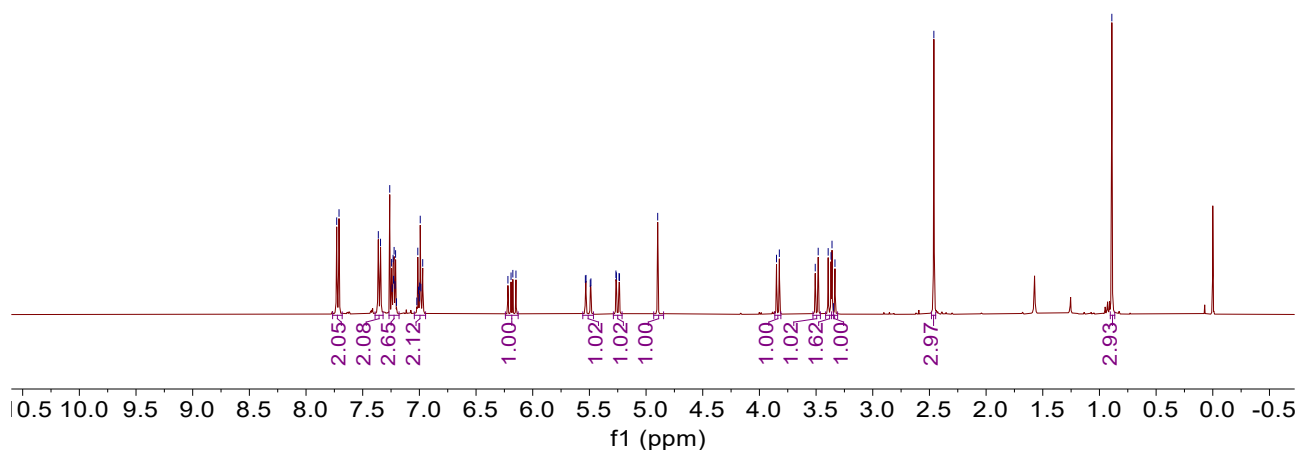


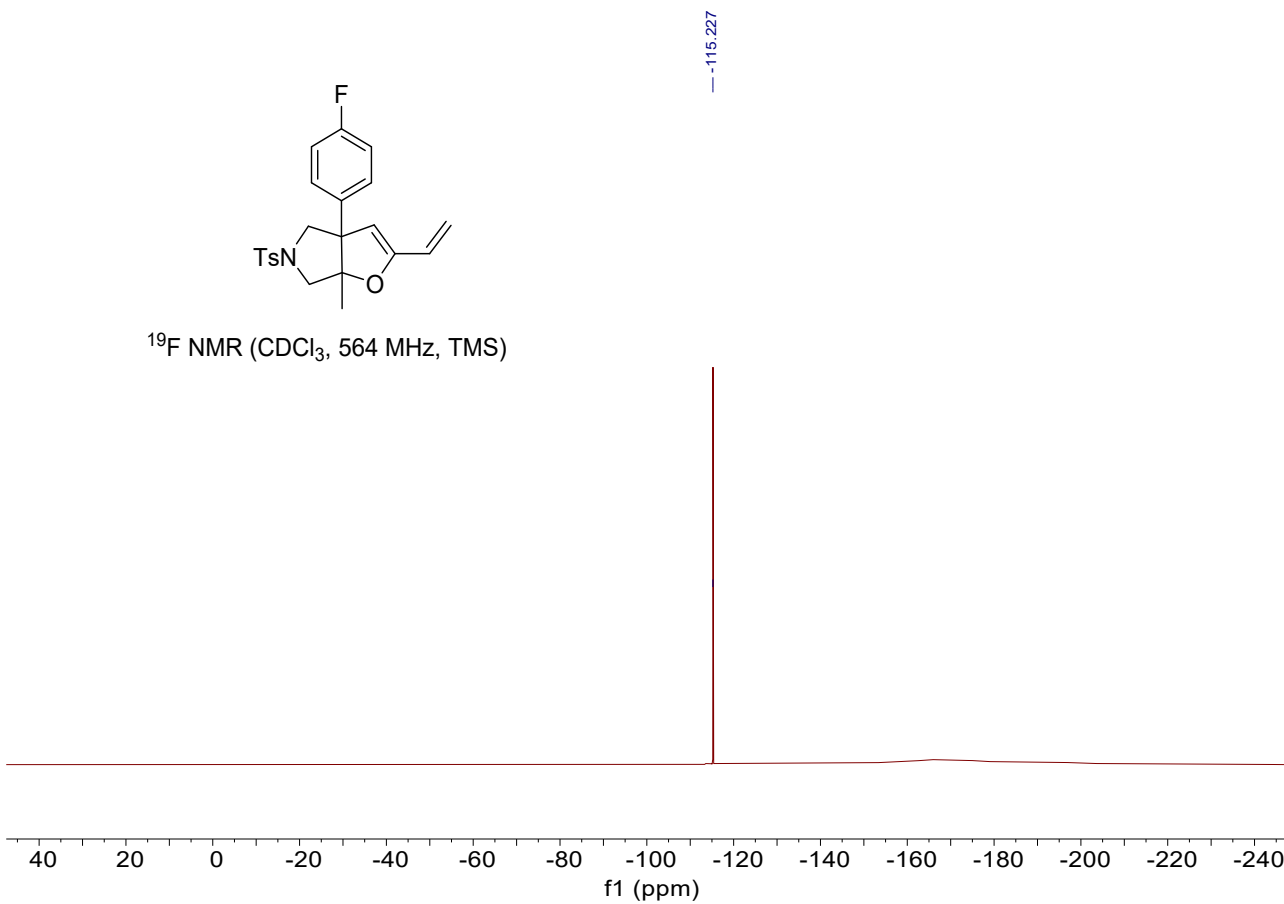
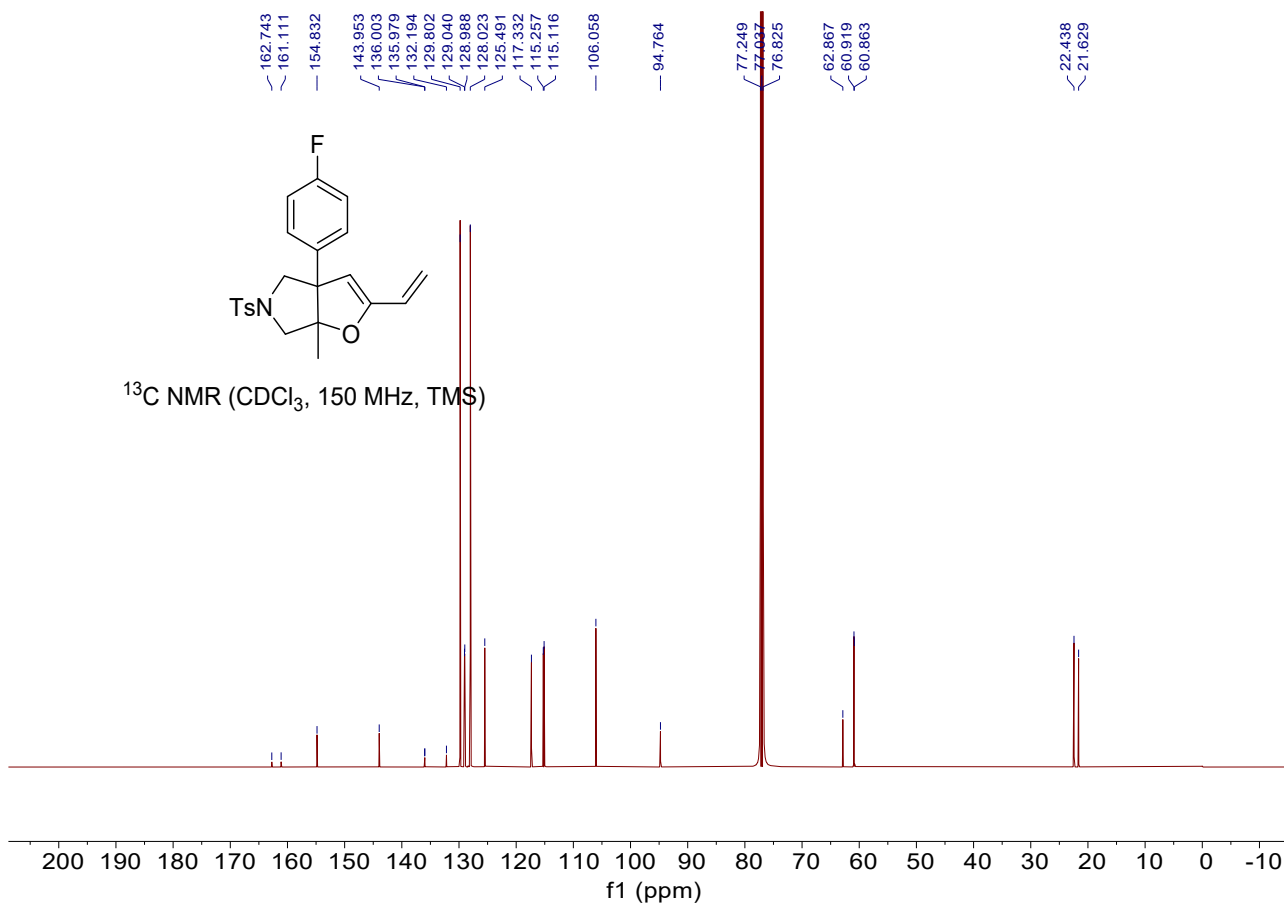
**3a-(4-fluorophenyl)-6a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2k)**

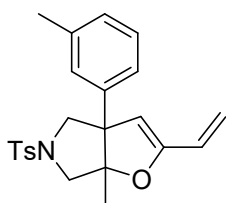
A red oil, 90% yield, 35.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.35 (d,  $J = 8.0$  Hz, 2H), 7.27 – 7.18 (m, 2H), 7.04 – 6.95 (m, 2H), 6.18 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.51 (dd,  $J = 17.2, 2.4$  Hz, 1H), 5.25 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.90 (s, 1H), 3.84 (d,  $J = 10.0$  Hz, 1H), 3.49 (d,  $J = 10.4$  Hz, 1H), 3.38 (d,  $J = 10.0$  Hz, 2H), 3.35 (d,  $J = 10.4$  Hz, 1H), 2.46 (s, 3H), 0.89 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  161.9 (d,  $J_{\text{C-F}} = 244.8$  Hz), 154.8, 144.0, 136.00, 135.97, 132.2, 129.8, 129.0 (d,  $J_{\text{C-F}} = 7.8$  Hz), 128.0, 125.5, 117.3, 115.2 (d,  $J_{\text{C-F}} = 21.1$  Hz), 106.1, 94.8, 62.9, 60.91, 60.86, 22.4, 21.6.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.3. IR (neat)  $\nu$  663, 1163, 1349, 1598, 2857, 2928  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{SFNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1195.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

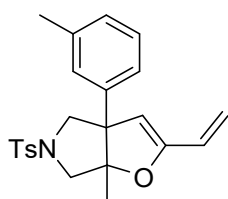




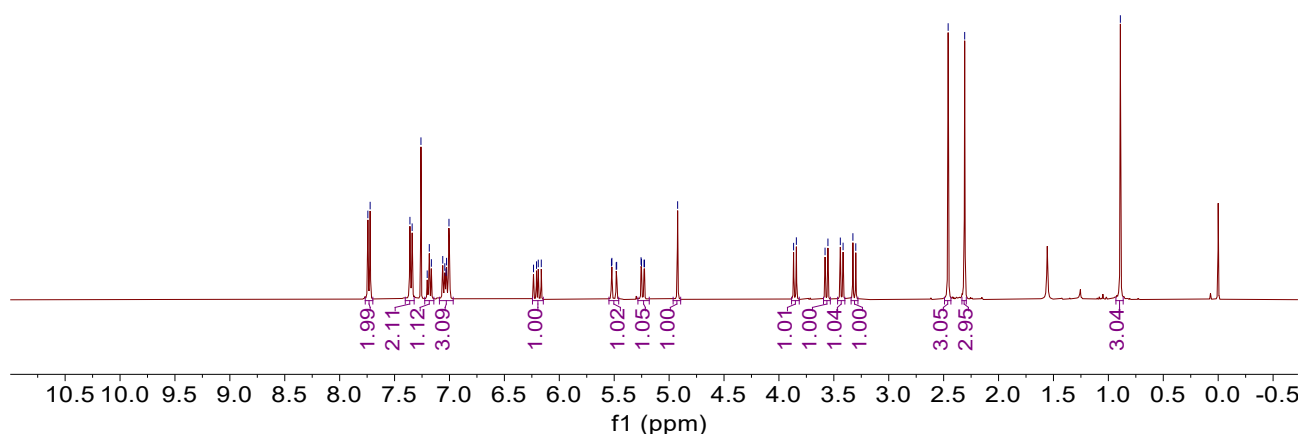


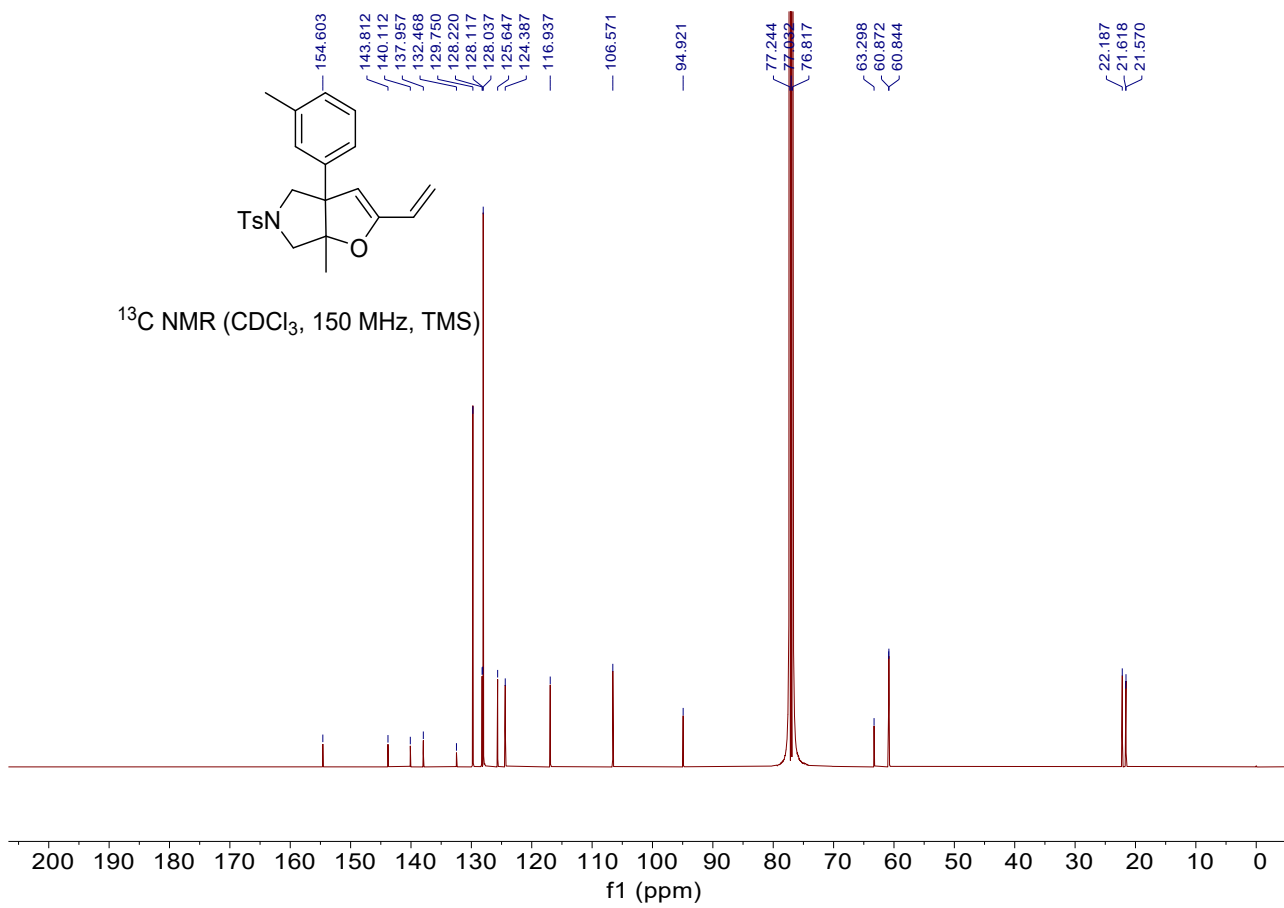
**6a-methyl-3a-(m-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (21)**

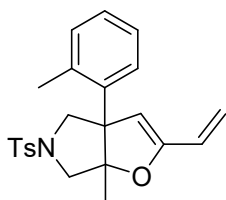
A yellow oil, 90% yield, 35.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.35 (d,  $J = 8.0$  Hz, 2H), 7.18 (t,  $J = 7.6$  Hz, 1H), 7.09 – 6.97 (m, 3H), 6.20 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.50 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.24 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.92 (s, 1H), 3.85 (d,  $J = 10.0$  Hz, 1H), 3.57 (d,  $J = 10.4$  Hz, 1H), 3.43 (d,  $J = 10.0$  Hz, 1H), 3.31 (d,  $J = 10.4$  Hz, 1H), 2.46 (s, 3H), 2.31 (s, 3H), 0.89 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  154.6, 143.8, 140.1, 138.0, 132.5, 129.8, 128.2, 128.1, 128.0, 125.6, 124.4, 116.9, 106.6, 94.9, 63.3, 60.9, 60.8, 22.2, 21.61, 21.57. IR (neat)  $\nu$  665, 836, 1163, 1348, 1954, 2856, 2929  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1449.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

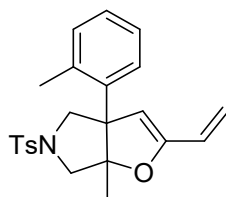




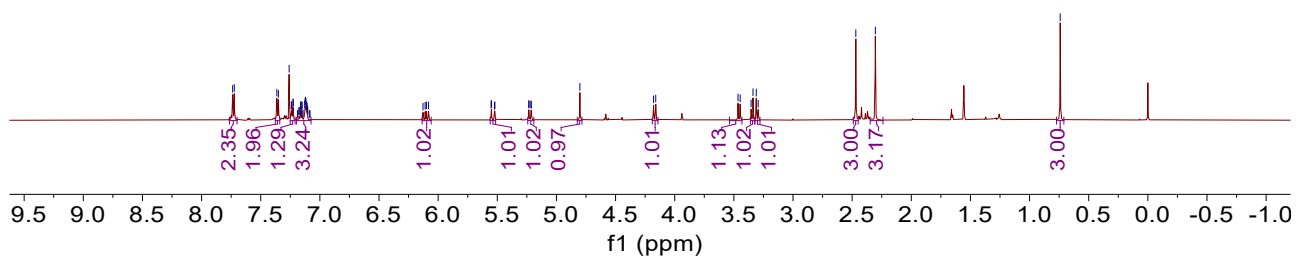


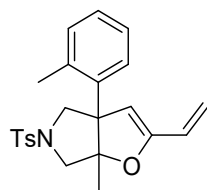
**6a-methyl-3a-(o-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2m)**

A yellow oil, 78% yield, 30.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.07 (m, 3H), 6.10 (dd,  $J = 17.4$ , 11.0 Hz, 1H), 5.54 (dd,  $J = 17.4$ , 1.6 Hz, 1H), 5.22 (dd,  $J = 11.0$ , 1.6 Hz, 1H), 4.80 (s, 1H), 4.17 (d,  $J = 11.0$  Hz, 1H), 3.46 (d,  $J = 11.0$  Hz, 1H), 3.35 (d,  $J = 9.6$  Hz, 1H), 3.30 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 2.30 (s, 3H), 0.74 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  152.3, 143.8, 136.9, 136.6, 132.7, 132.4, 129.8, 128.0, 127.7, 127.5, 126.6, 125.9, 125.7, 117.0, 109.5, 97.1, 63.2, 61.1, 58.4, 22.4, 22.1, 21.6. IR (neat)  $\nu$  664, 1220, 1356, 1596, 2857, 2926, 3002  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1443.

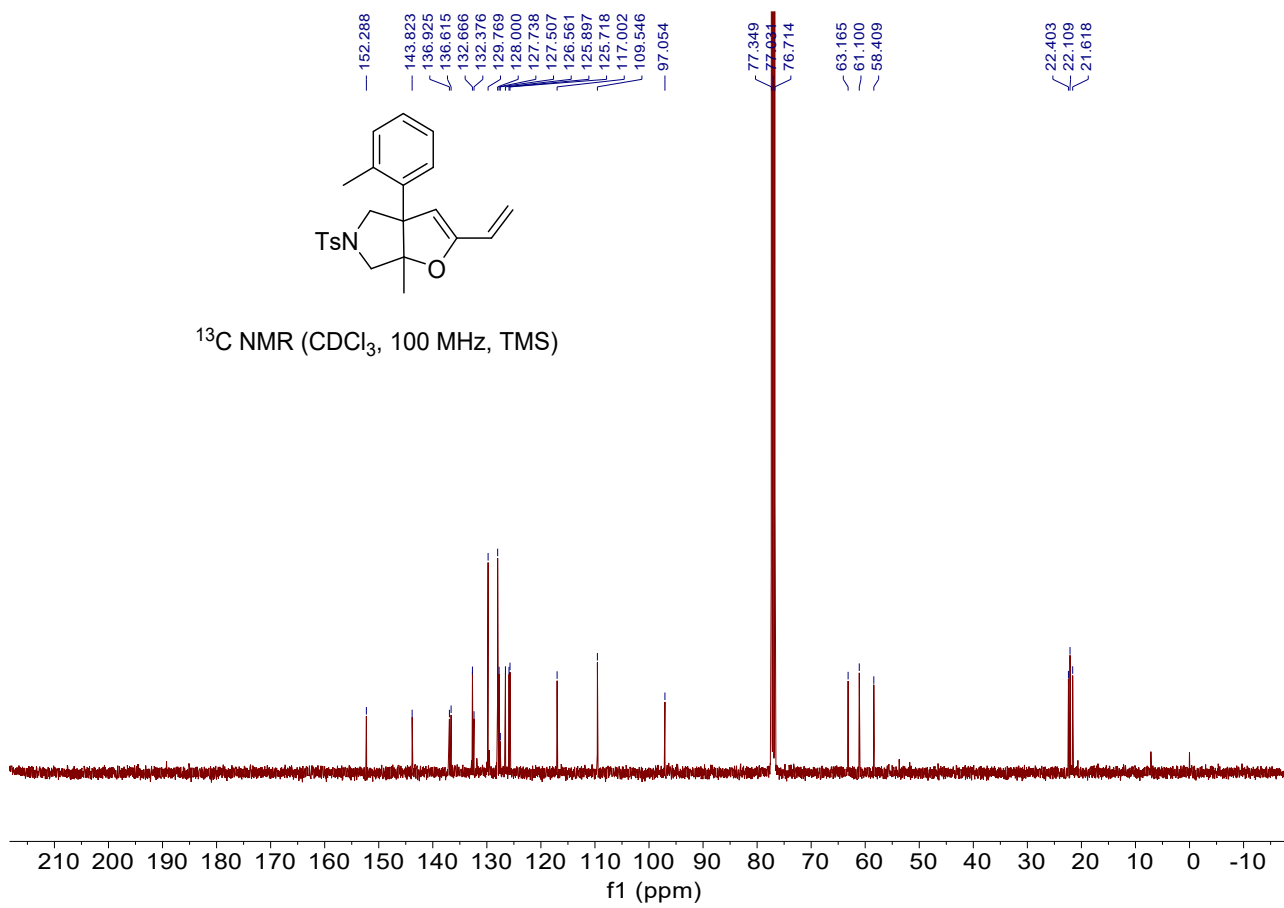


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

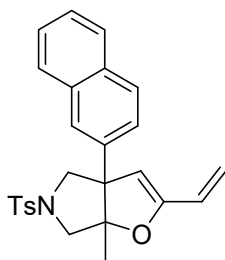




$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)

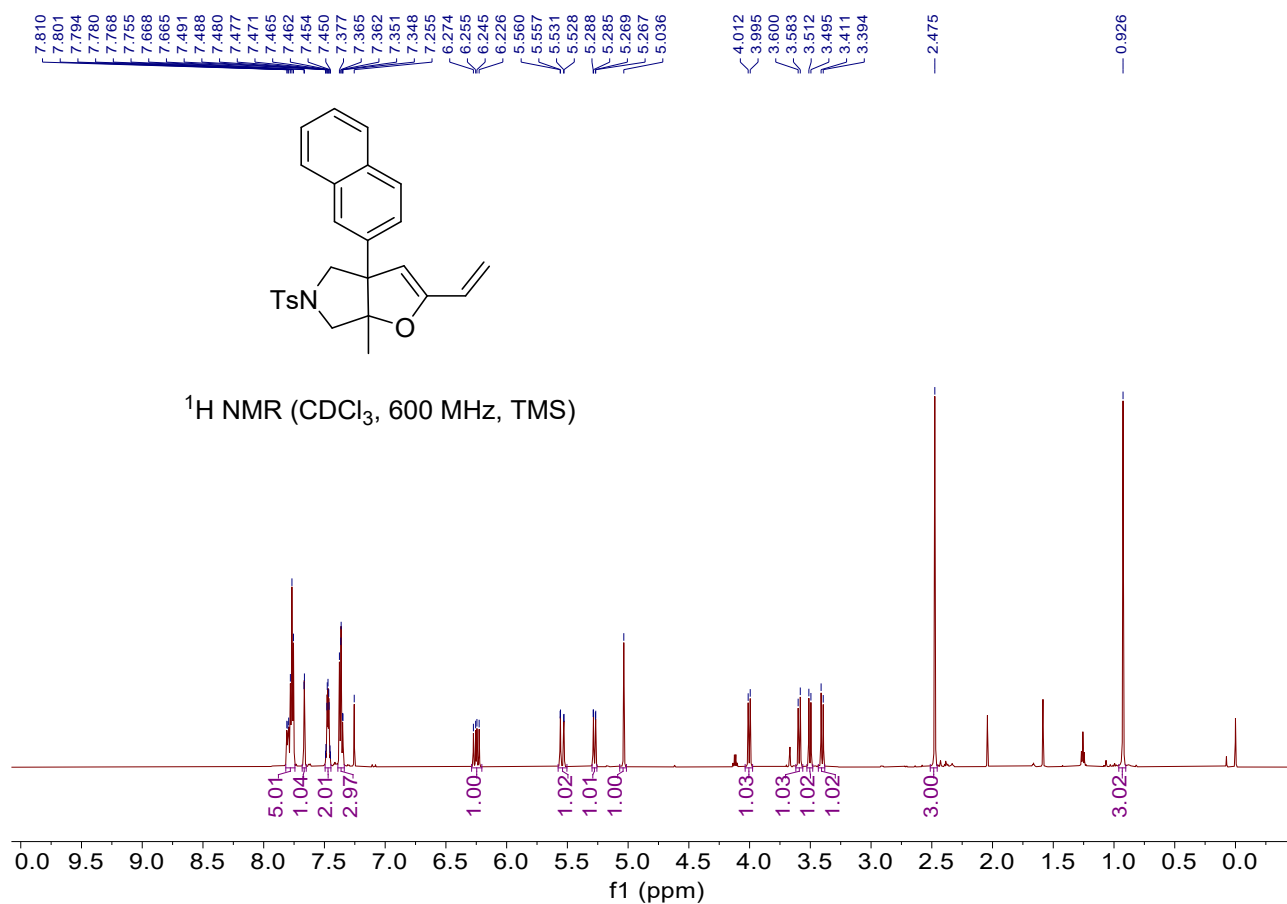






**6a-methyl-3a-(naphthalen-2-yl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2n)**

A red oil, 82% yield, 34.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.82 – 7.74 (m, 5H), 7.67 (d,  $J$  = 2.0 Hz, 1H), 7.47 (td,  $J$  = 6.0, 3.2 Hz, 2H), 7.39 – 7.34 (m, 3H), 6.25 (dd,  $J$  = 17.4, 11.0 Hz, 1H), 5.54 (dd,  $J$  = 17.4, 1.6 Hz, 1H), 5.28 (dd,  $J$  = 11.0, 1.6 Hz, 1H), 5.04 (s, 1H), 4.00 (d,  $J$  = 10.0 Hz, 1H), 3.59 (d,  $J$  = 10.4 Hz, 1H), 3.50 (d,  $J$  = 10.0 Hz, 1H), 3.40 (d,  $J$  = 10.4 Hz, 1H), 2.48 (s, 3H), 0.93 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  154.8, 143.9, 137.6, 133.0, 132.5, 132.4, 129.8, 128.09, 128.06, 128.05, 127.5, 126.4, 126.22, 126.20, 125.7, 125.4, 117.2, 106.4, 95.0, 63.5, 61.0, 60.8, 22.3, 21.7. IR (neat)  $\nu$  663, 818, 1162, 1347, 1595, 2866, 2927, 3047  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{26}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 454.1447, Found: 454.1446.



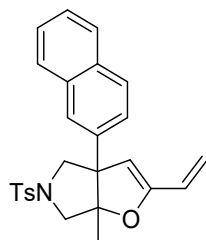
154.831  
143.911  
137.644  
132.979  
132.453  
132.434  
129.817  
128.094  
128.069  
128.053  
127.490  
126.364  
126.223  
126.203  
125.656  
125.429  
117.201  
106.420

94.973

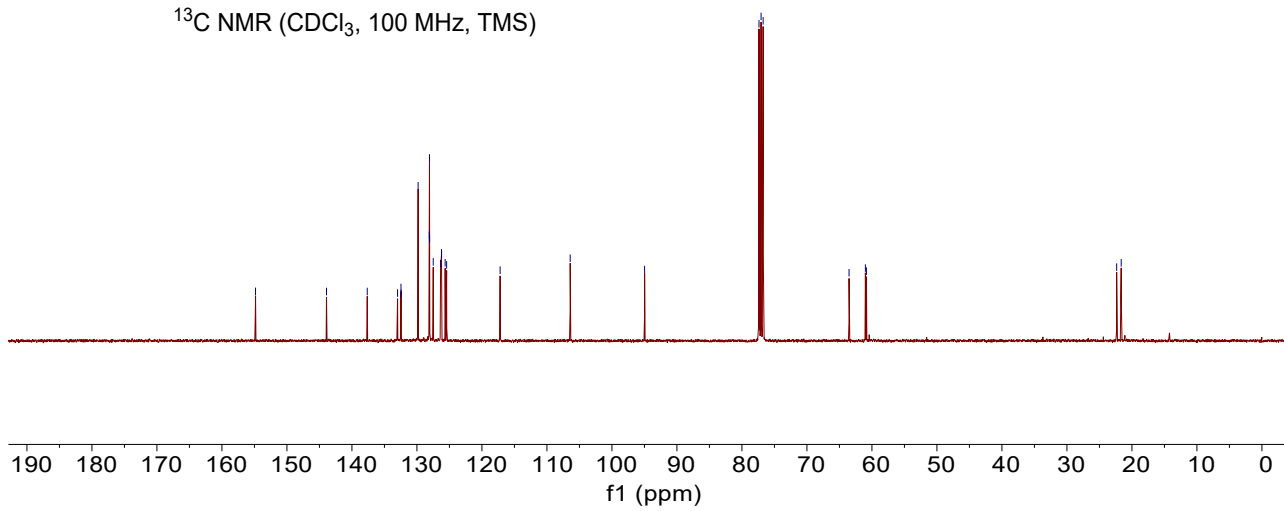
77.372  
77.055  
76.737

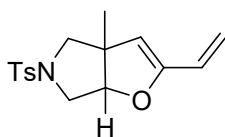
63.519  
61.006  
60.847

22.347  
21.650



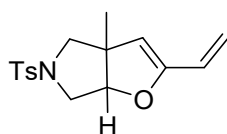
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



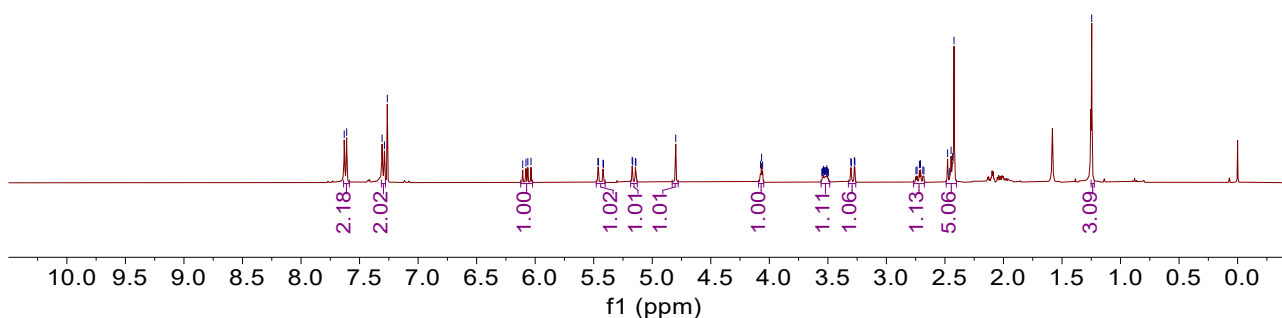


### 3a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2o)

A colorless oil, 80% yield, 22.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.62 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 6.07 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.44 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.16 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.80 (s, 1H), 4.07 (t,  $J = 3.6$  Hz, 1H), 3.56 – 3.48 (m, 1H), 3.29 (dd,  $J = 11.9, 1.6$  Hz, 1H), 2.77 – 2.68 (m, 1H), 2.49 – 2.40 (m, 5H), 1.25 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  155.4, 143.4, 134.0, 129.7, 127.5, 125.9, 116.2, 110.3, 83.6, 52.8, 45.1, 41.5, 25.5, 22.0, 21.5. IR (neat)  $\nu$  815, 987, 1157, 1216, 1346, 1447, 2018, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{19}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 328.0978, Found: 328.0979.



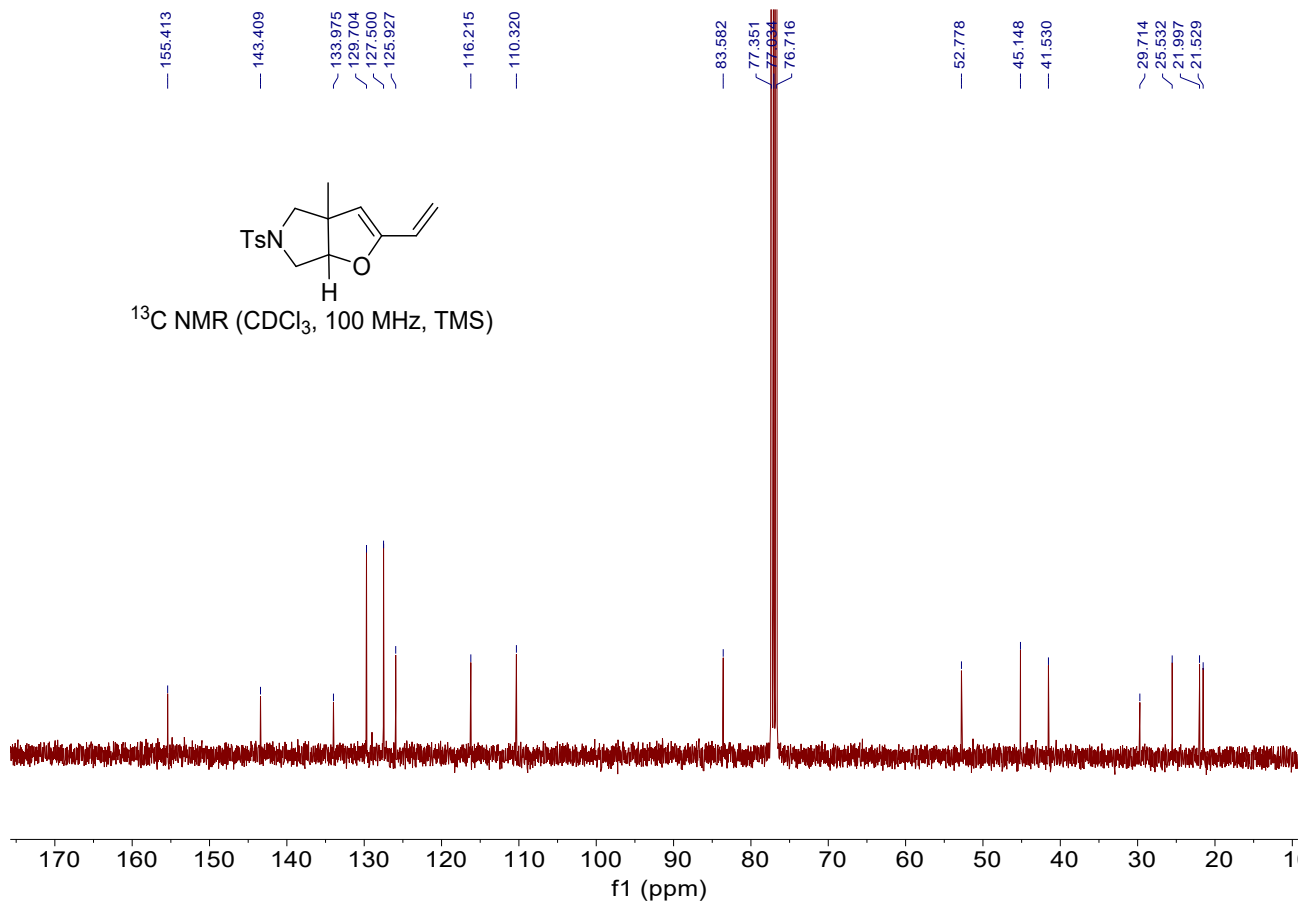
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

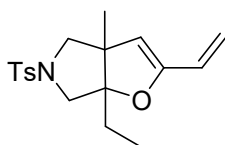


— 155.413  
— 143.409  
~ 133.975  
~ 129.704  
~ 127.500  
~ 125.927  
— 116.215  
— 110.320

C=C1C(=O)N(C1)C(C)C

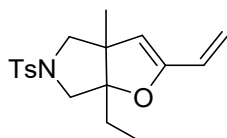
H  
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



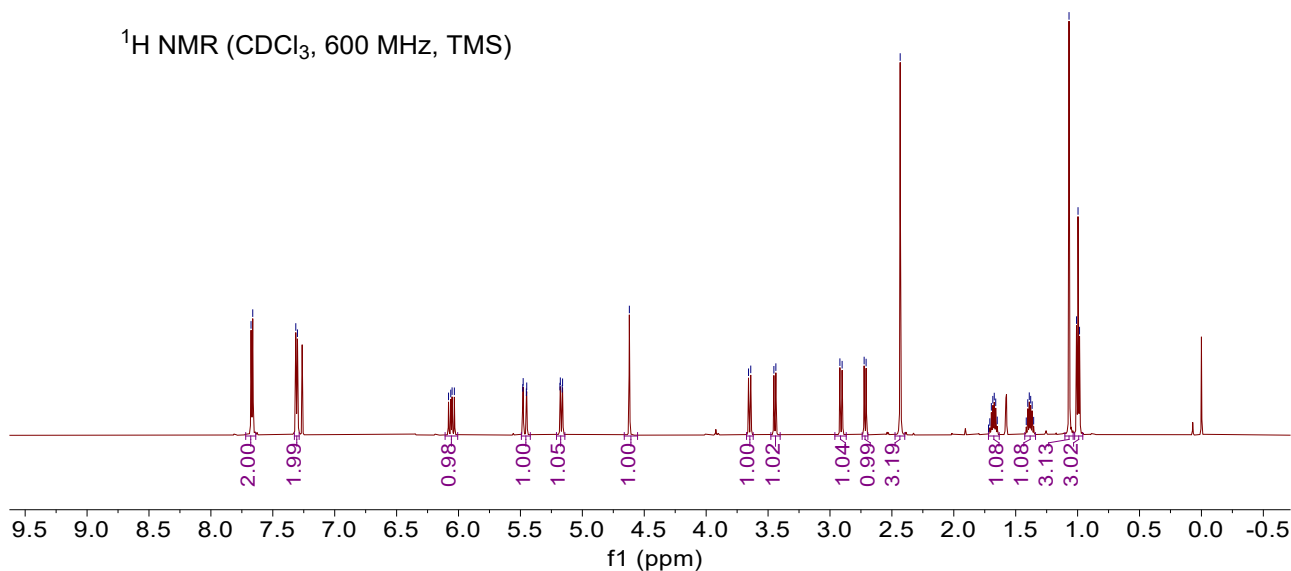


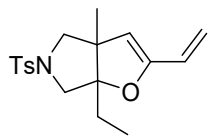
### 6a-ethyl-3a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2p)

A colorless oil, 86% yield, 28.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.67 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.06 (dd,  $J = 17.4, 10.8$  Hz, 1H), 5.47 (dd,  $J = 17.4, 1.8$  Hz, 1H), 5.17 (dd,  $J = 10.8, 1.8$  Hz, 1H), 4.62 (s, 1H), 3.65 (d,  $J = 10.8$  Hz, 1H), 3.45 (d,  $J = 9.6$  Hz, 1H), 2.91 (d,  $J = 10.8$  Hz, 1H), 2.72 (d,  $J = 9.6$  Hz, 1H), 2.43 (s, 3H), 1.68 (dq,  $J = 14.4, 7.2$  Hz, 1H), 1.38 (dq,  $J = 14.4, 7.2$  Hz, 1H), 1.07 (s, 3H), 1.00 (t,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.7, 143.6, 132.6, 129.6, 127.9, 125.7, 116.4, 107.9, 94.9, 60.9, 58.7, 55.5, 26.7, 21.6, 19.9, 8.4. IR (neat)  $\nu$  664, 1162, 1346, 1579, 2883, 2953, 2975  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{24}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 334.1471, Found: 334.1464.

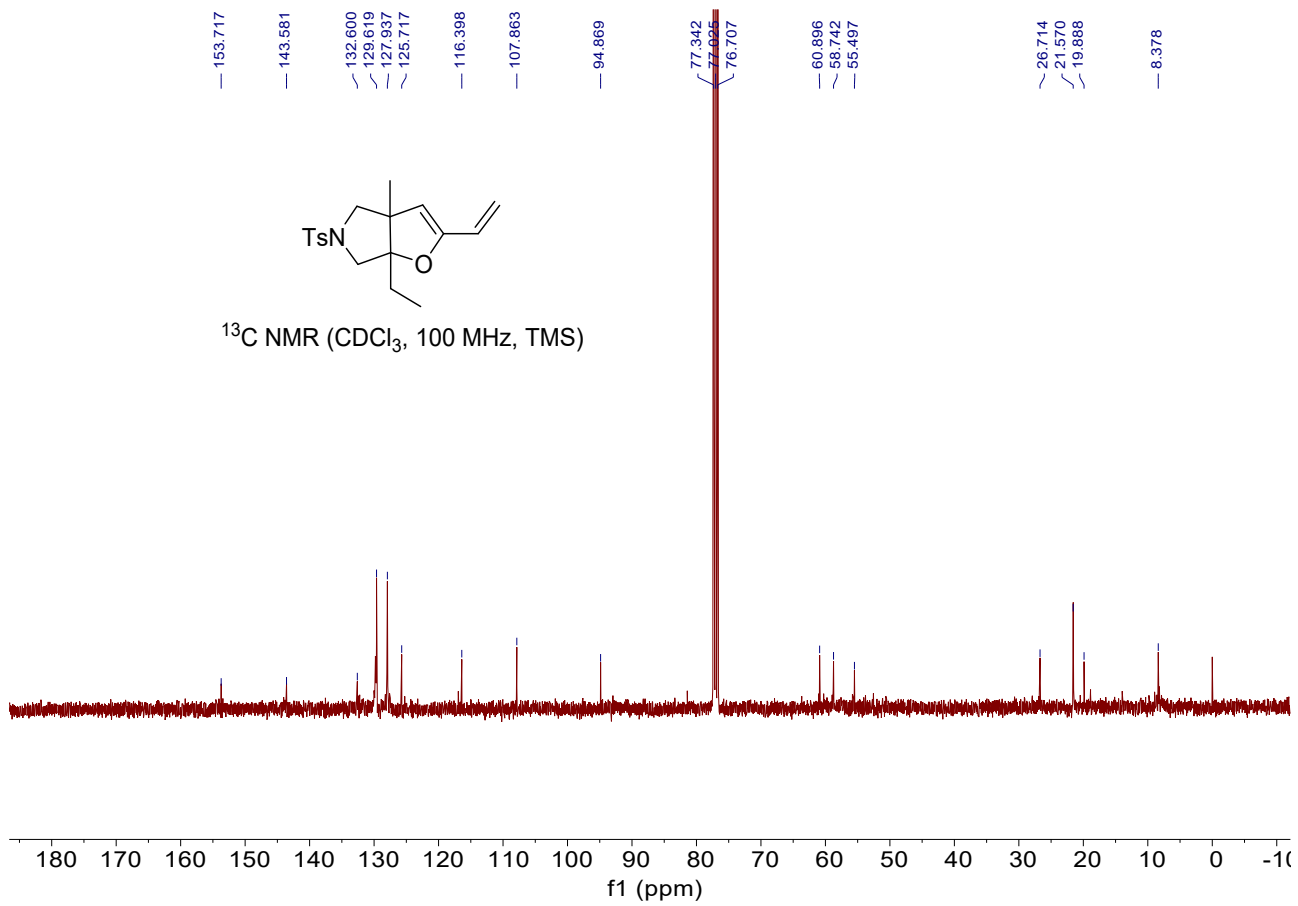


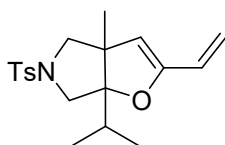
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)





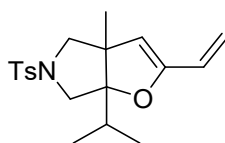
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



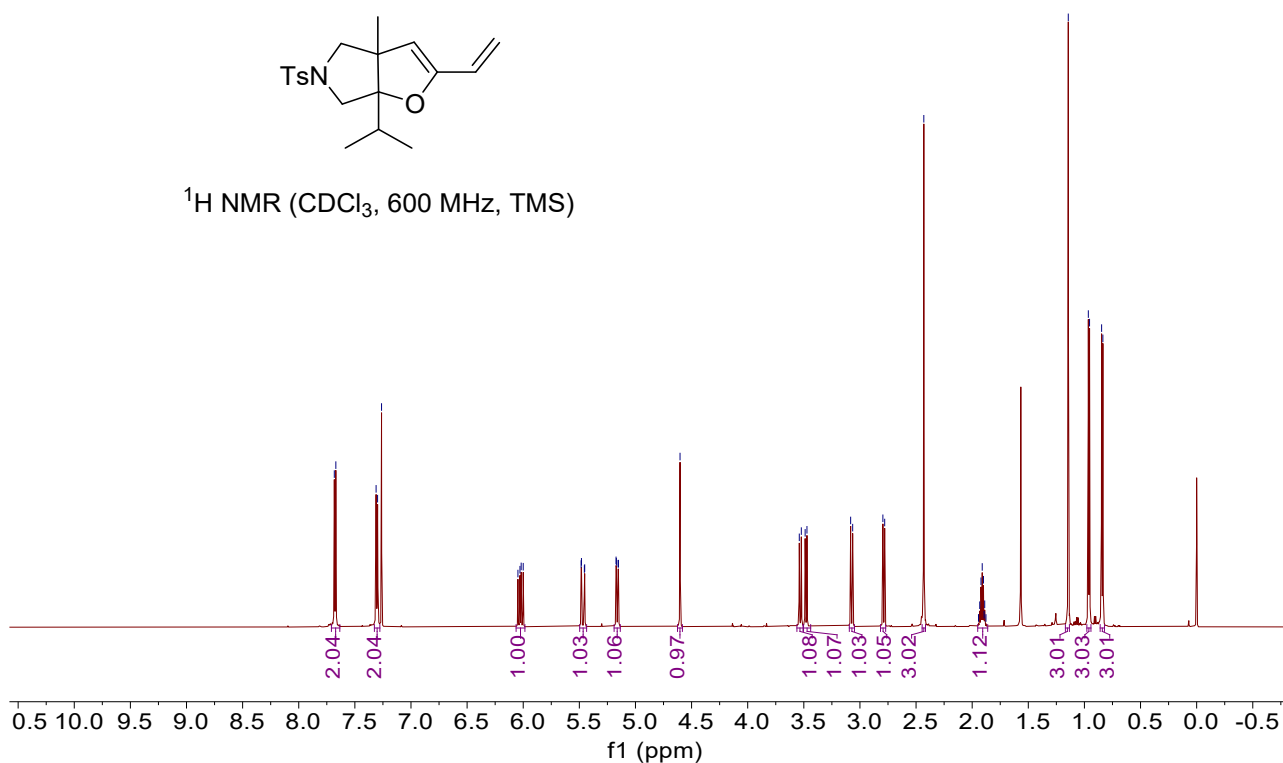


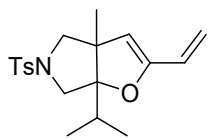
**6a-isopropyl-3a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2q)**

A colorless oil, 80% yield, 27.7 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.68 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 6.02 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.47 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.16 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.60 (s, 1H), 3.53 (d,  $J = 10.8$  Hz, 1H), 3.48 (d,  $J = 9.6$  Hz, 1H), 3.07 (d,  $J = 10.8$  Hz, 1H), 2.79 (d,  $J = 9.6$  Hz, 1H), 2.43 (s, 3H), 1.91 (hept,  $J = 6.8$  Hz, 1H), 1.14 (s, 3H), 0.96 (d,  $J = 6.8$  Hz, 3H), 0.84 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  153.8, 143.5, 132.9, 129.6, 127.9, 125.6, 116.3, 109.1, 96.7, 61.2, 56.9, 55.5, 31.4, 21.6, 19.5, 18.0, 17.4. IR (neat)  $\nu$  667, 829, 1164, 1347, 1592, 2866, 2934, 2969  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 370.1447, Found: 370.1440.

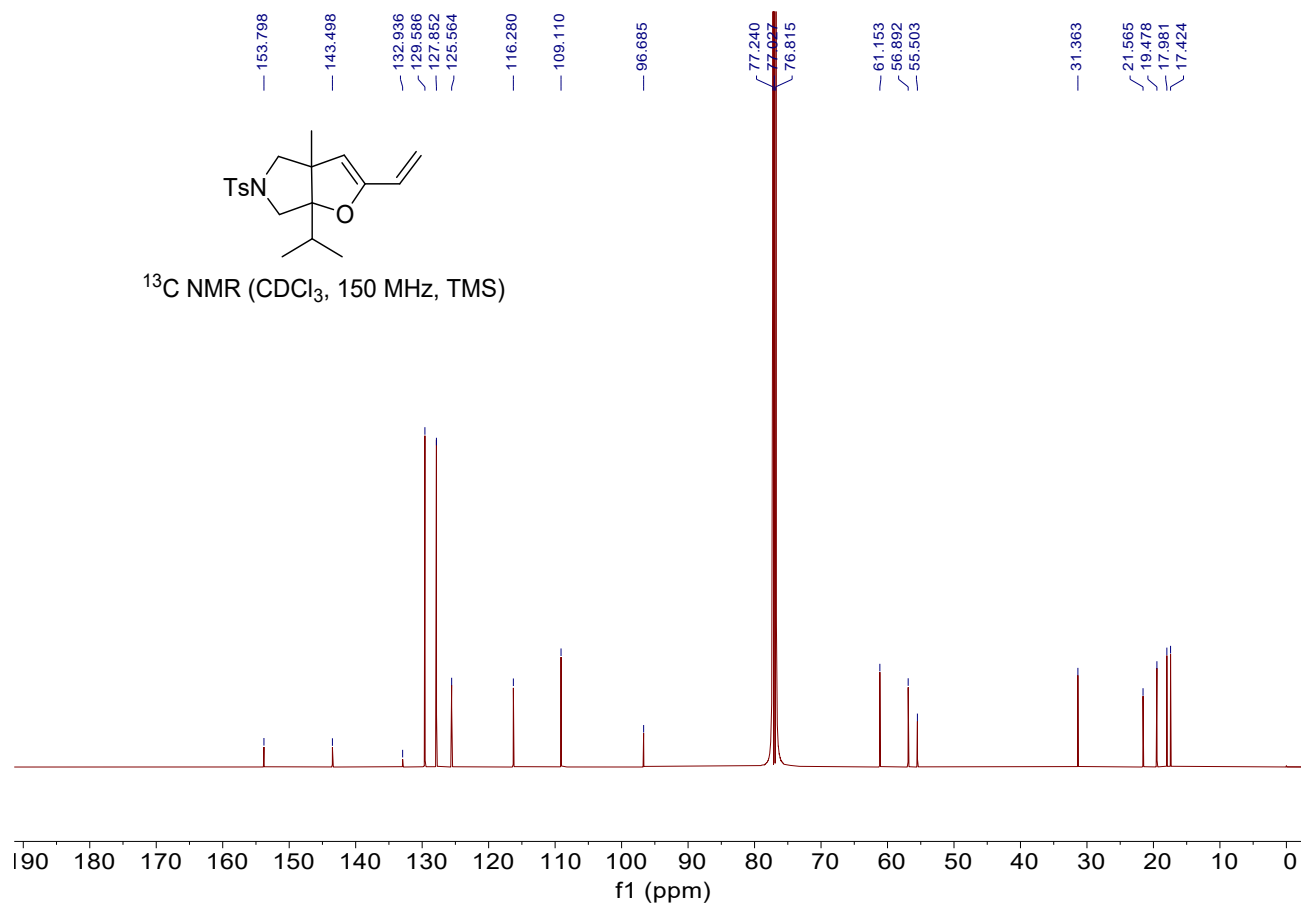


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

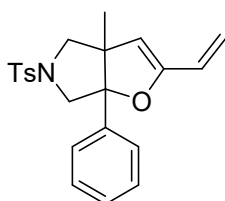




$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, TMS)

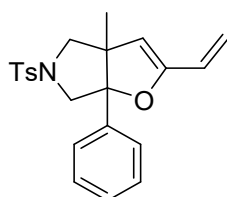




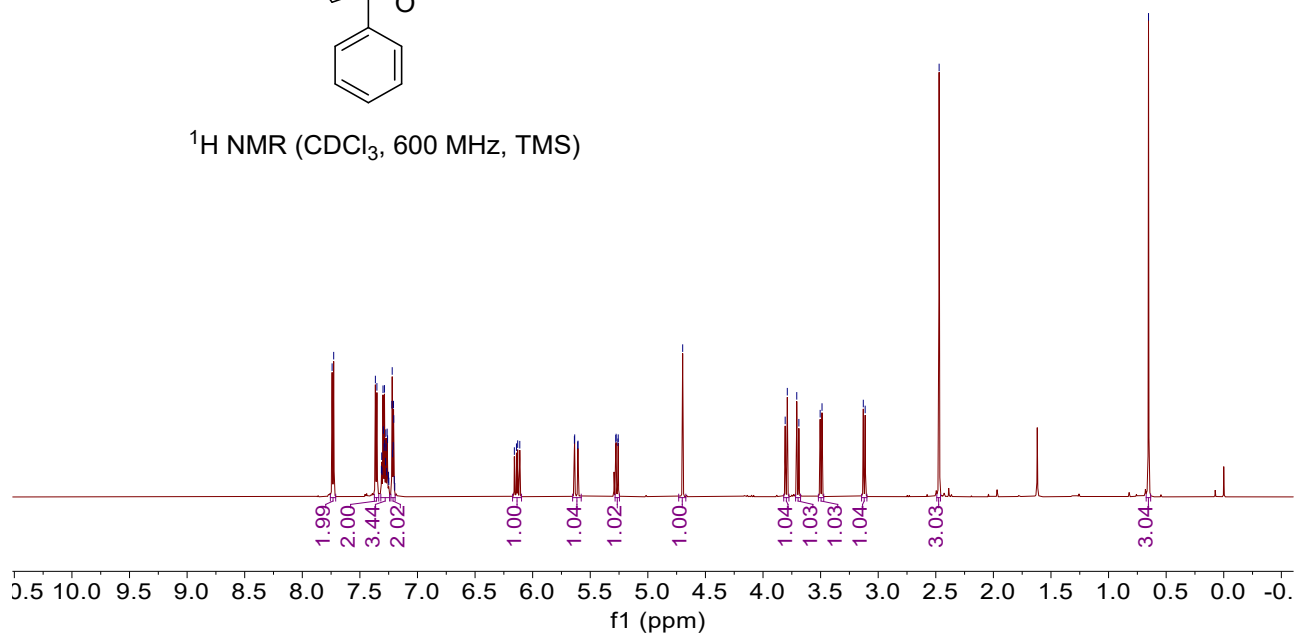


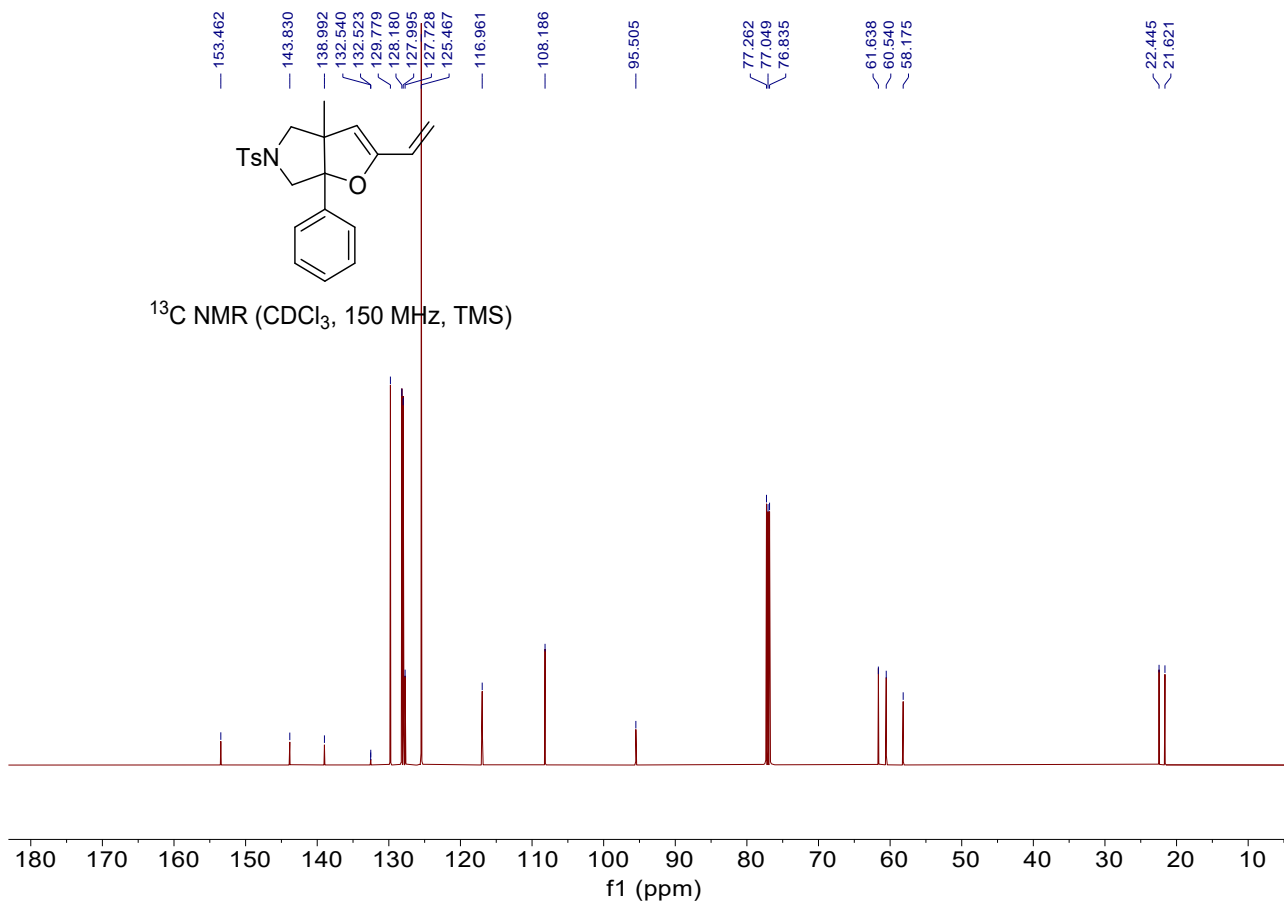
### 3a-methyl-6a-phenyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2r)

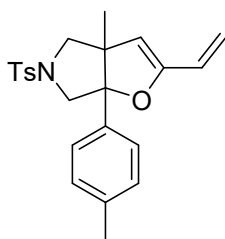
A yellow oil, 82% yield, 31.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.32 – 7.24 (m, 3H), 7.23 – 7.19 (m, 2H), 6.14 (dd,  $J = 17.4$ , 11.0 Hz, 1H), 5.62 (dd,  $J = 17.4$ , 1.6 Hz, 1H), 5.27 (dd,  $J = 11.0$ , 1.6 Hz, 1H), 4.70 (s, 1H), 3.80 (d,  $J = 11.0$  Hz, 1H), 3.70 (d,  $J = 11.0$  Hz, 1H), 3.50 (d,  $J = 9.6$  Hz, 1H), 3.12 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 0.65 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  153.5, 143.8, 139.0, 132.54, 132.52, 129.8, 128.2, 128.0, 127.7, 125.5, 117.0, 108.2, 95.5, 61.6, 60.5, 58.2, 22.4, 21.6. IR (neat)  $\nu$  665, 765, 1285, 1347, 1596, 2956, 2971  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 404.1291, Found: 404.1285.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)





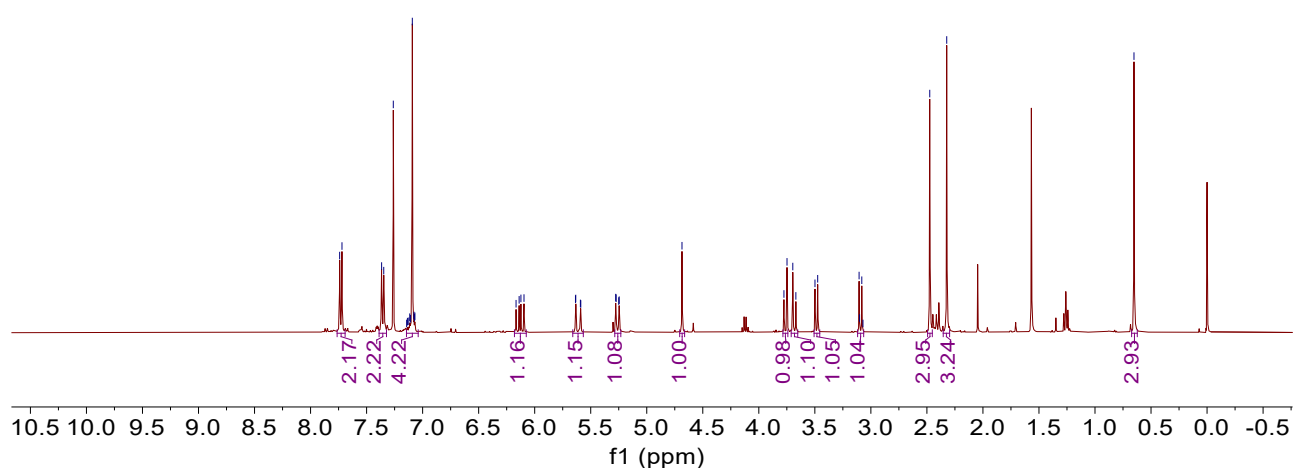


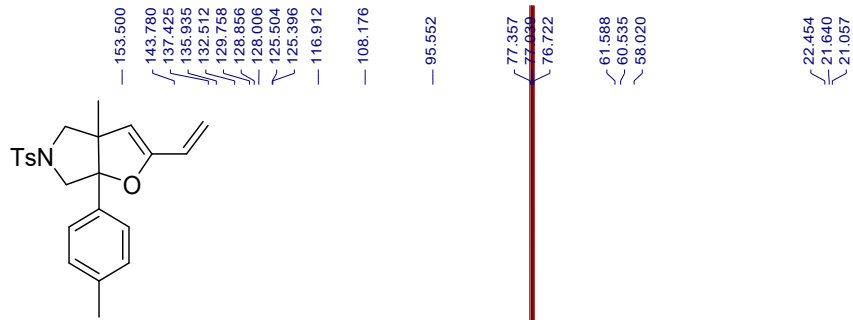
**3a-methyl-6a-(p-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2s)**

A yellow oil, 80% yield, 31.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.02 – 7.14 (m, 4H), 6.13 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.61 (dd,  $J = 17.4, 1.2$  Hz, 1H), 5.26 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.69 (s, 1H), 3.76 (d,  $J = 11.0$  Hz, 1H), 3.68 (d,  $J = 11.0$  Hz, 1H), 3.49 (d,  $J = 9.6$  Hz, 1H), 3.09 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 2.32 (s, 3H), 0.65 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.5, 143.8, 137.4, 135.9, 132.5, 129.8, 128.9, 128.0, 125.5, 125.4, 116.9, 108.2, 95.6, 61.6, 60.5, 58.0, 22.5, 21.6, 21.1. IR (neat)  $\nu$  666, 815, 1164, 1326, 1596, 2841, 2929, 2981  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1442.

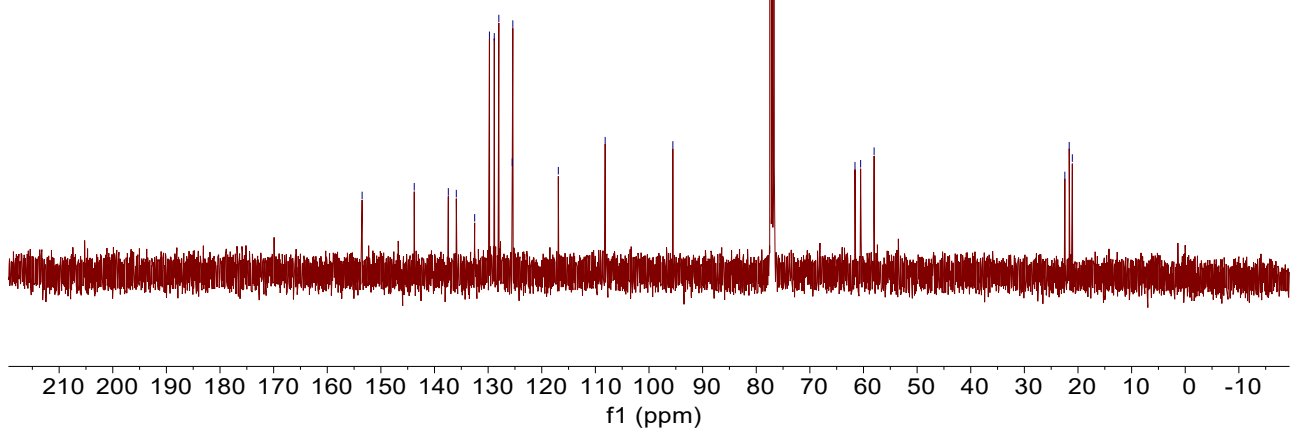


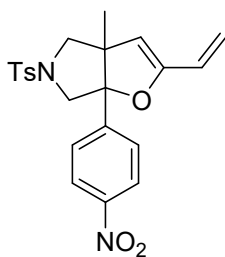
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





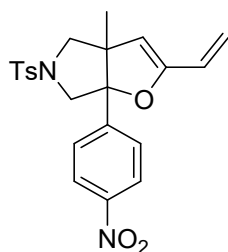
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



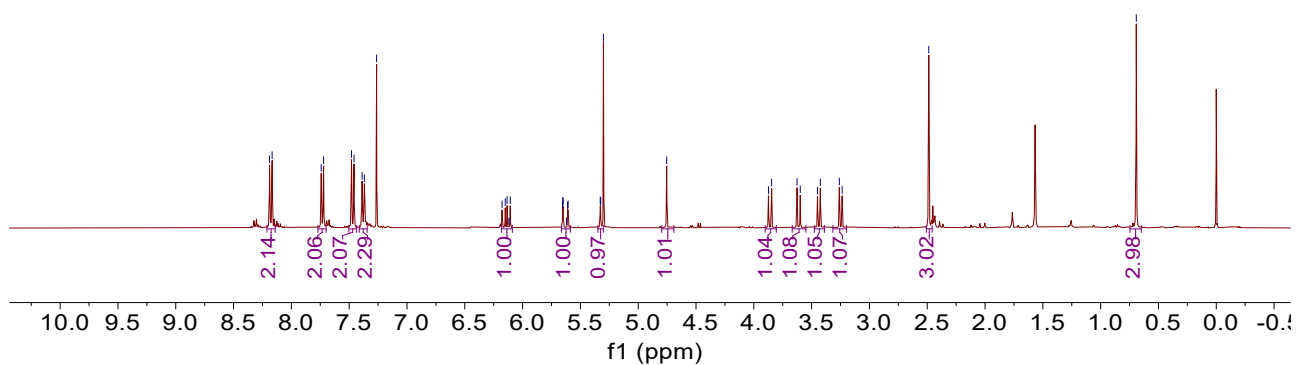


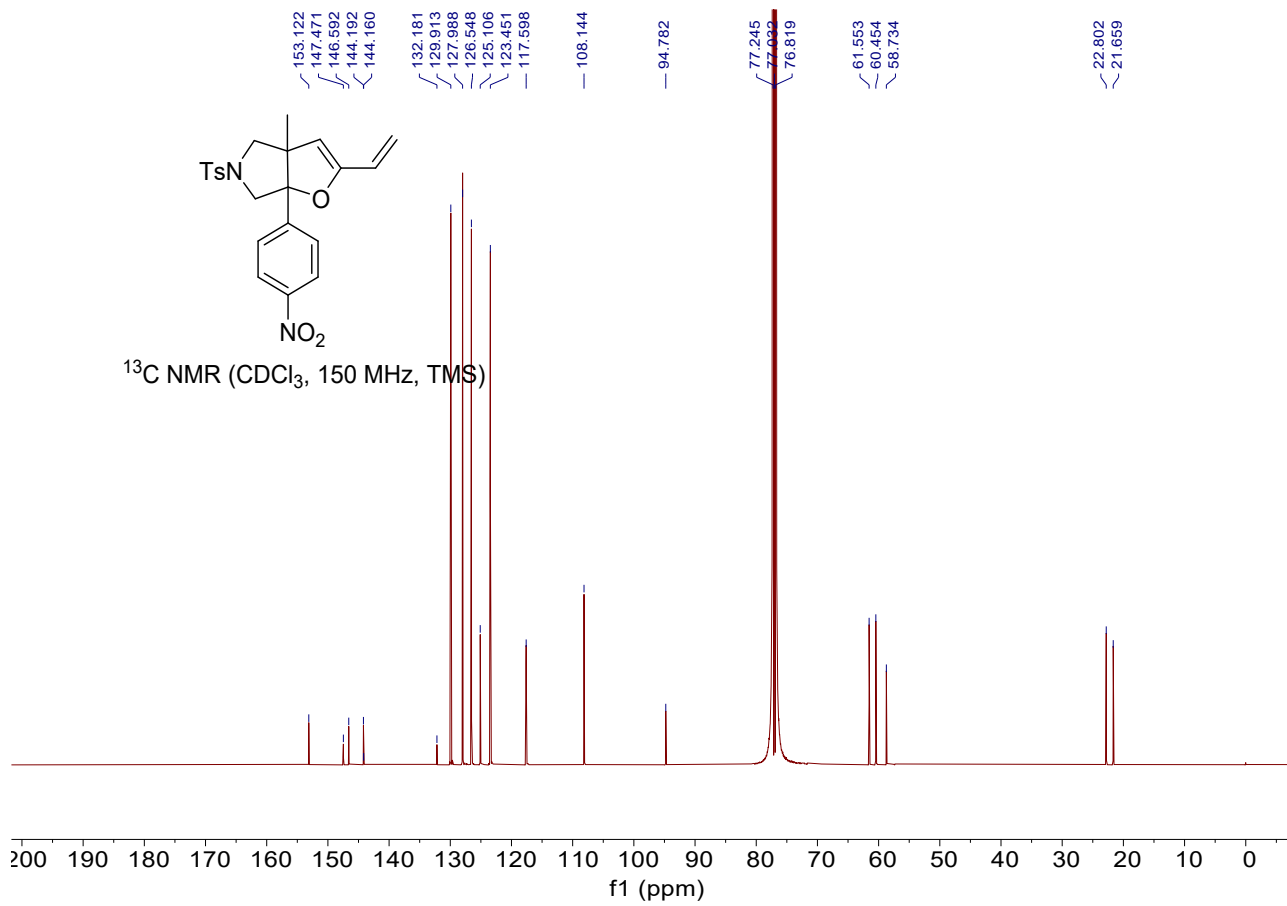
**3a-methyl-6a-(4-nitrophenyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2t)**

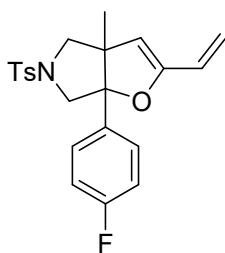
A red oil, 62% yield, 26.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  8.18 (d,  $J = 9.0$  Hz, 2H), 7.73 (d,  $J = 8.0$  Hz, 2H), 7.47 (d,  $J = 9.0$  Hz, 2H), 7.38 (d,  $J = 8.0$  Hz, 2H), 6.14 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.66 – 5.59 (m, 1H), 5.33 (d,  $J = 1.6$  Hz, 1H), 4.75 (s, 1H), 3.86 (d,  $J = 10.8$  Hz, 1H), 3.61 (d,  $J = 10.8$  Hz, 1H), 3.44 (d,  $J = 9.8$  Hz, 1H), 3.25 (d,  $J = 9.8$  Hz, 1H), 2.49 (s, 3H), 0.69 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  153.1, 147.5, 146.6, 144.19, 144.16, 132.2, 129.9, 128.0, 126.5, 125.1, 123.5, 117.6, 108.1, 94.8, 61.6, 60.5, 58.7, 22.8, 21.7. IR (neat)  $\nu$  662, 853, 1163, 1231, 1597, 2848, 2942, 2964  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{N}_2\text{O}_5\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 449.1141, Found: 449.1147.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

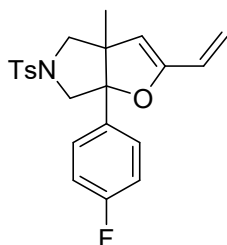




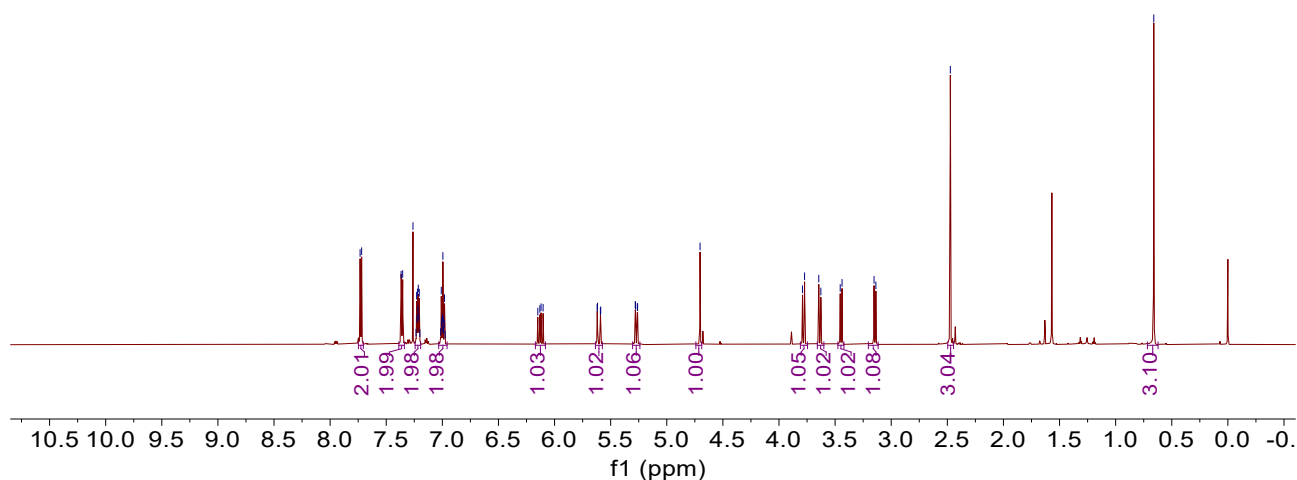


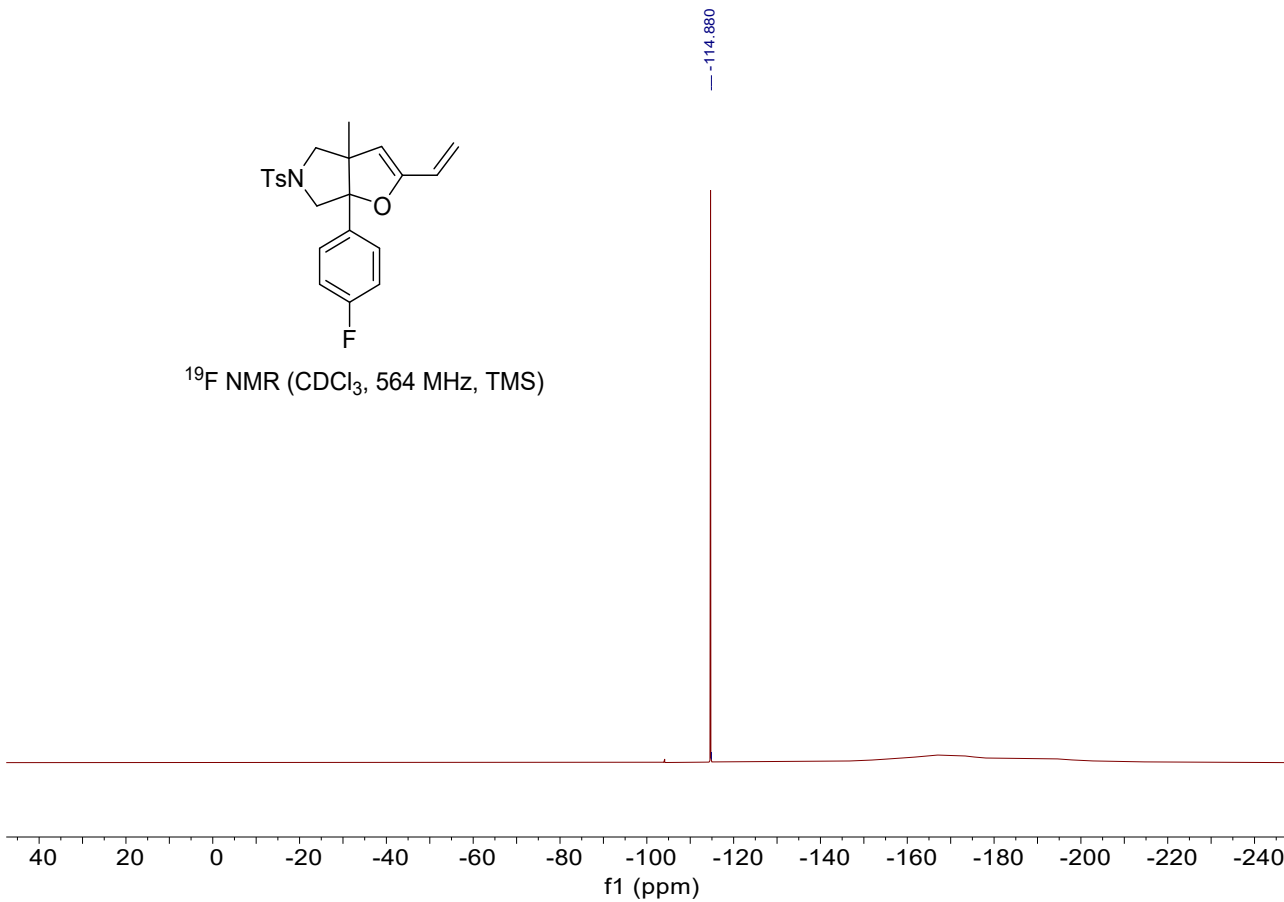
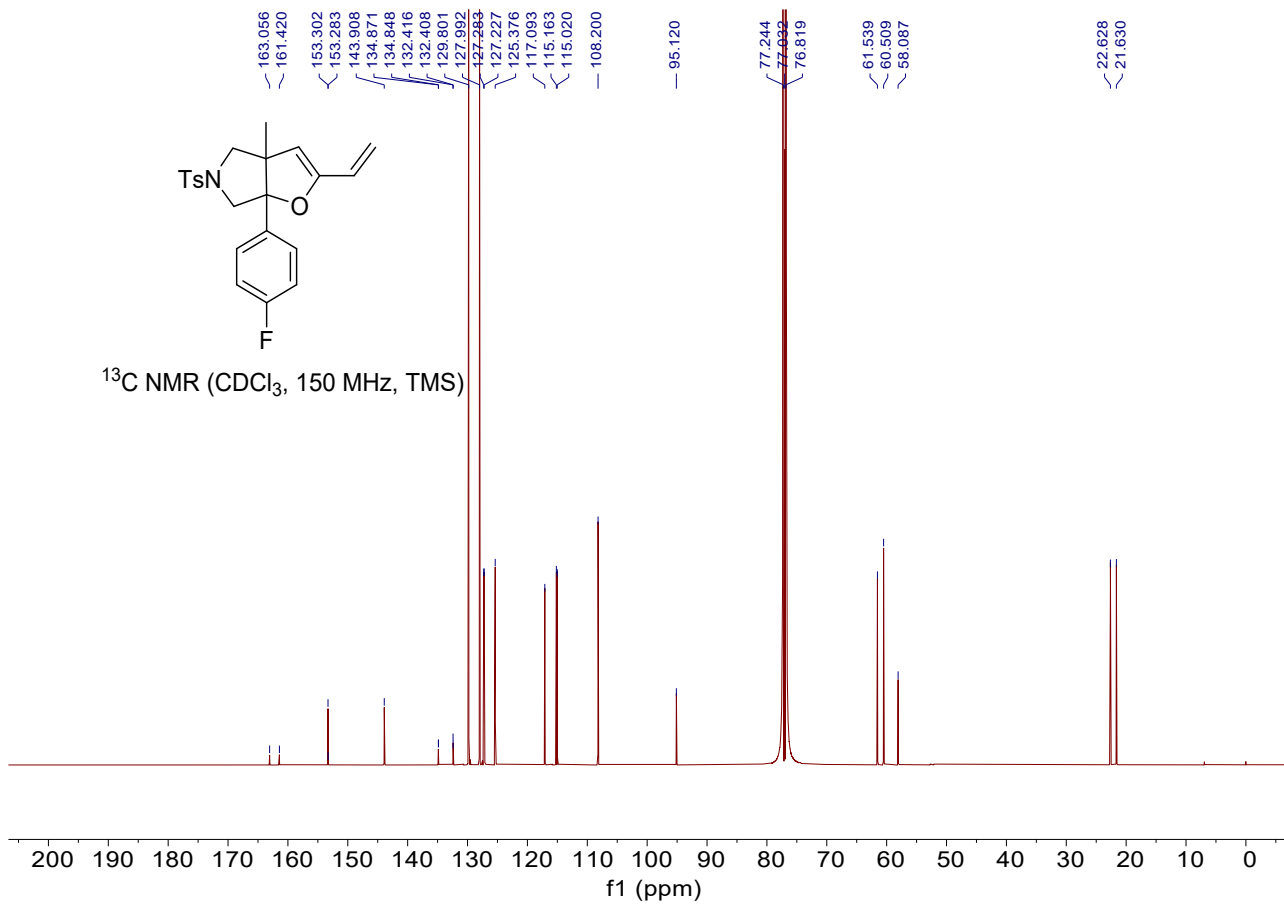
**6a-(4-fluorophenyl)-3a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2u)**

A brown oil, 80% yield, 32.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.73 (d,  $J = 8.4$ , 2H), 7.36 (d,  $J = 8.4$  Hz, 2H), 7.24 – 7.19 (m, 2H), 7.03 – 6.96 (m, 2H), 6.13 (dd,  $J = 17.4$ , 11.0 Hz, 1H), 5.60 (dd,  $J = 17.4$ , 1.6 Hz, 1H), 5.27 (dd,  $J = 11.0$ , 1.6 Hz, 1H), 4.70 (s, 1H), 3.78 (d,  $J = 11.0$  Hz, 1H), 3.64 (d,  $J = 11.0$  Hz, 1H), 3.45 (d,  $J = 9.6$  Hz, 1H), 3.14 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 0.66 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  163.2 (d,  $J_{\text{C-F}} = 245.4$  Hz), 153.30, 153.28, 143.9, 134.9, 134.8, 132.41, 132.40, 129.8, 128.0, 127.3 (d,  $J_{\text{C-F}} = 8.4$  Hz), 125.4, 117.1, 115.1 (d,  $J_{\text{C-F}} = 21.5$  Hz), 108.2, 95.1, 61.5, 60.5, 58.1, 22.6, 21.6.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -114.9. IR (neat)  $\nu$  661, 815, 1157, 1216, 1346, 1447, 2869, 2926, 2959  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{FSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1196.

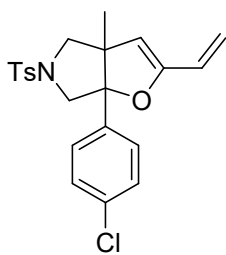


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)



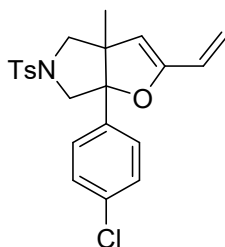




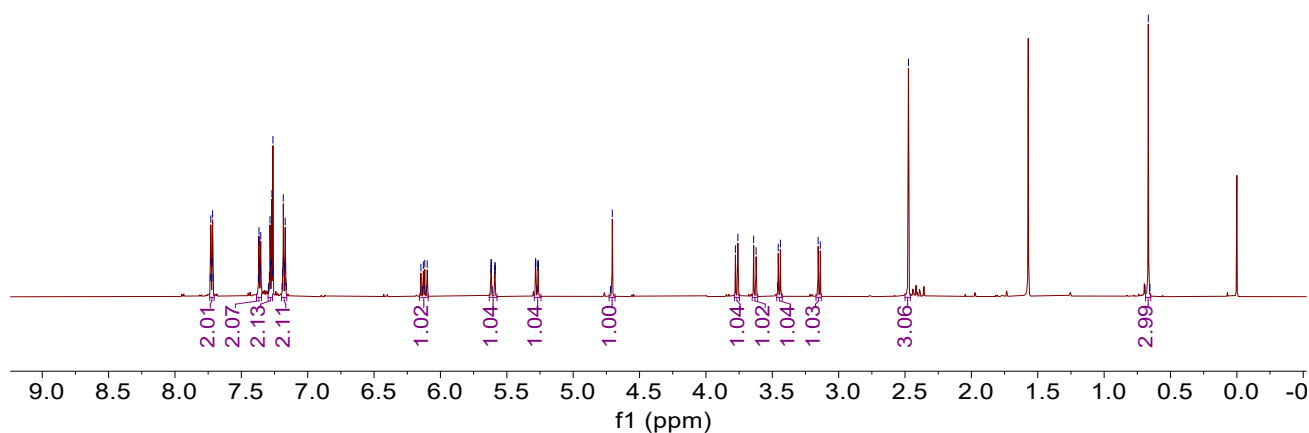


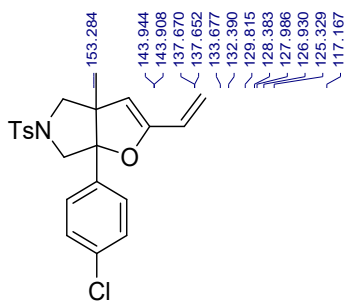
**6a-(4-chlorophenyl)-3a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2v)**

A yellow oil, 82% yield, 35.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.30 – 7.26 (m, 2H), 7.20 – 7.16 (m, 2H), 6.12 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.60 (dd,  $J = 17.4, 1.6$ , Hz, 1H), 5.29 – 5.24 (m, 1H), 4.71 (s, 1H), 3.77 (d,  $J = 11.0$  Hz, 1H), 3.63 (d,  $J = 11.0$  Hz, 1H), 3.45 (d,  $J = 9.8$  Hz, 1H), 3.15 (d,  $J = 9.8$  Hz, 1H), 2.47 (s, 3H), 0.67 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  153.3, 143.94, 143.90, 137.67, 137.65, 133.7, 132.4, 129.8, 128.4, 128.0, 126.9, 125.3, 117.2, 108.2, 95.03, 95.01, 61.5, 60.5, 58.2, 22.6, 21.6. IR (neat)  $\nu$  660, 825, 997, 116, 1347, 2869, 2956  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{SNaCl}$  ( $\text{M}+\text{Na}$ ) $^+$ : 438.0901, Found: 438.0907.

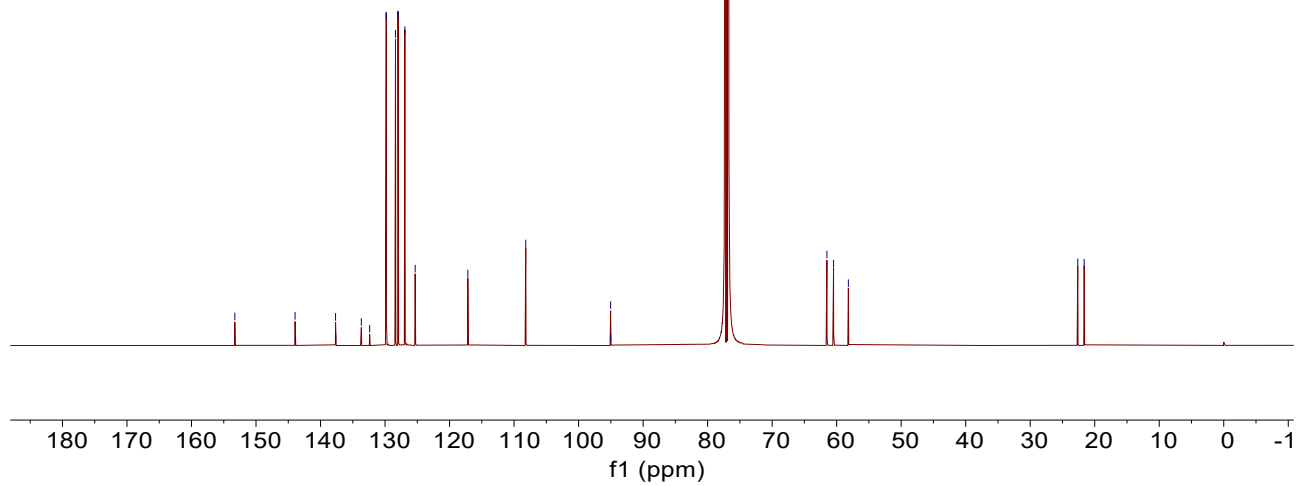


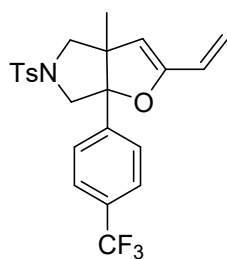
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)





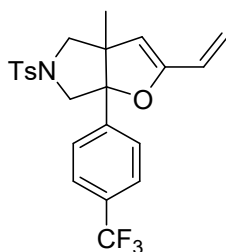
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, TMS)



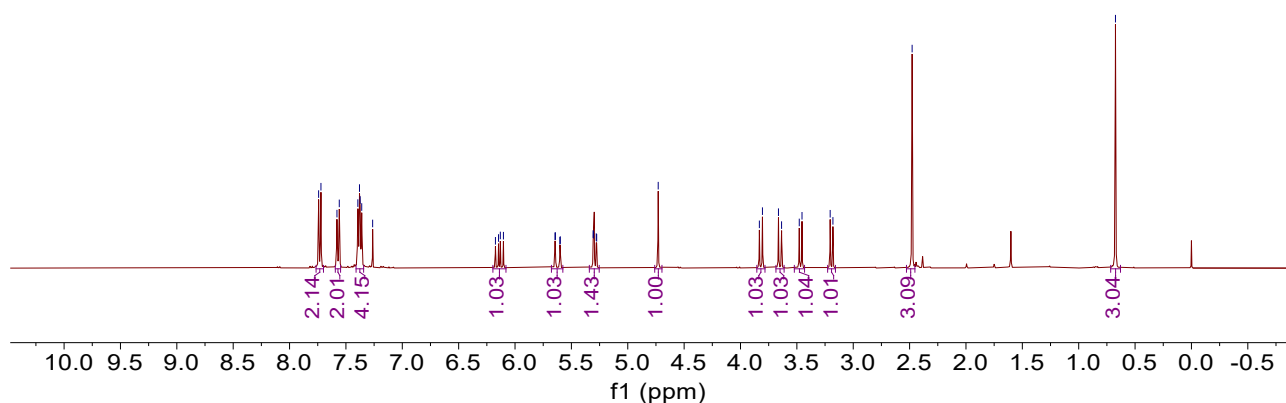


**3a-methyl-5-tosyl-6a-(4-(trifluoromethyl)phenyl)-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2w)**

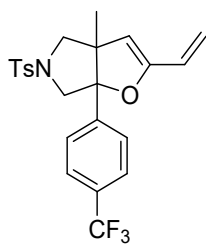
A colorless oil, 82% yield, 36.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.57 (d,  $J = 8.0$  Hz, 2H), 7.41 – 7.34 (m, 4H), 6.14 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.62 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.29 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.73 (s, 1H), 3.82 (d,  $J = 10.8$  Hz, 1H), 3.65 (d,  $J = 11.0$  Hz, 1H), 3.47 (d,  $J = 9.6$  Hz, 1H), 3.19 (d,  $J = 9.6$  Hz, 1H), 2.48 (s, 3H), 0.67 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.3, 144.0, 143.2, 130.3 (q,  $J_{\text{C-F}} = 32.4$  Hz), 129.9, 129.6, 128.0, 125.9, 125.8 (q,  $J_{\text{C-F}} = 3.8$  Hz), 124.0 (q,  $J_{\text{C-F}} = 270.3$  Hz), 117.3, 108.2, 95.0, 61.6, 60.5, 58.4, 22.7, 21.6.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.6. IR (neat)  $\nu$  666, 841, 1164, 1326, 1596, 2841, 2929, 2984  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{22}\text{NO}_3\text{F}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 472.1165, Found: 472.1166.



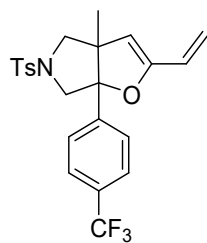
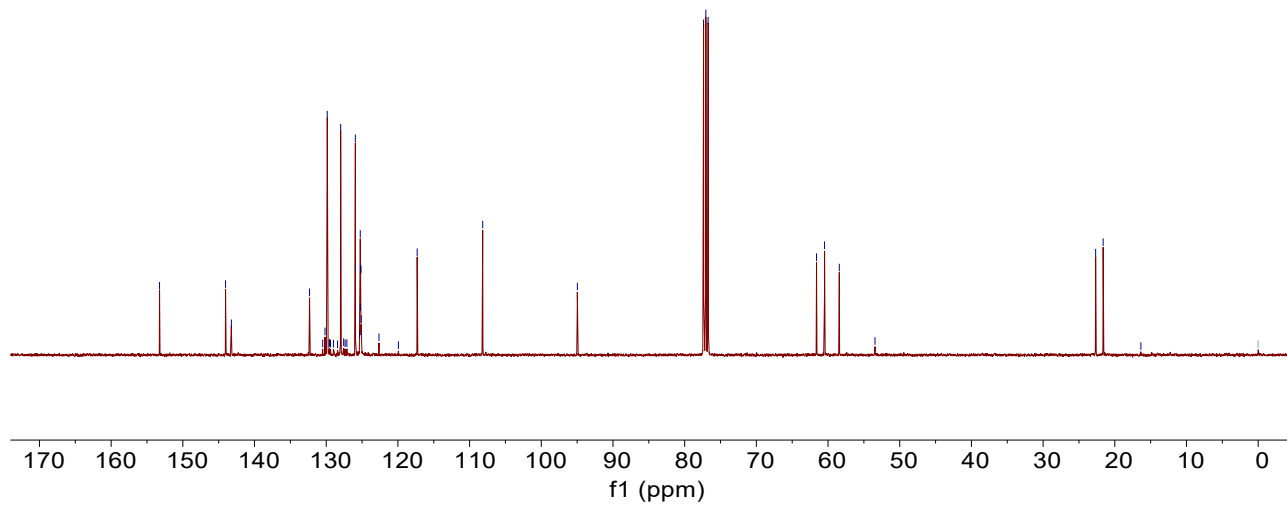
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



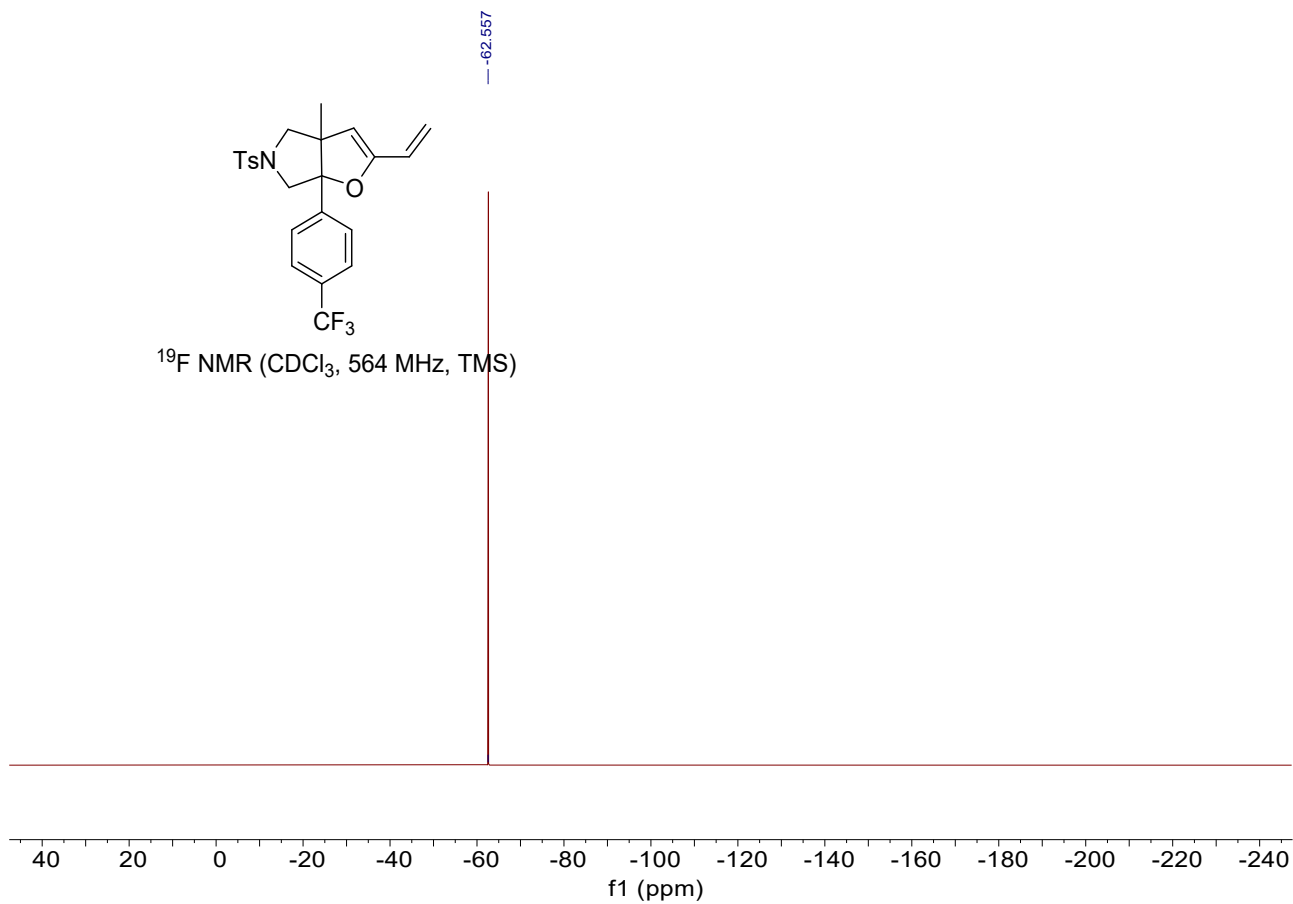
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 143.229  
 132.325  
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 130.168  
 129.857  
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 127.364  
 127.115  
 125.937  
 125.341  
 125.251  
 125.231  
 125.194  
 125.156  
 125.119  
 122.637  
 119.934  
 117.312  
 108.171  
 94.973  
 77.364  
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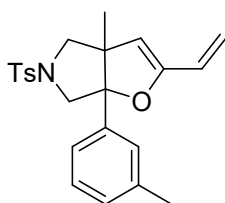


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



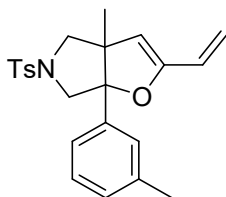
$^{19}\text{F}$  NMR ( $\text{CDCl}_3$ , 564 MHz, TMS)



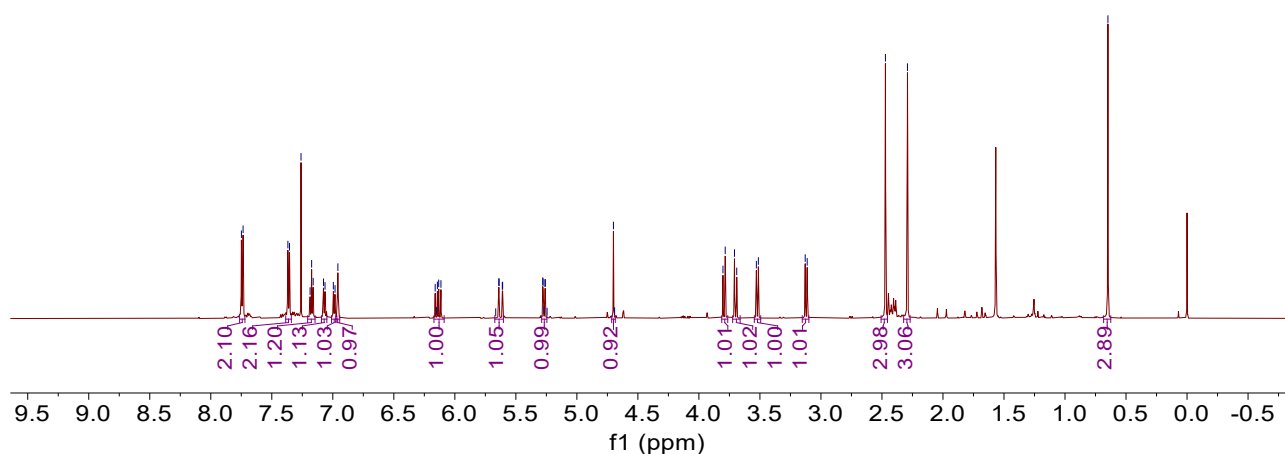


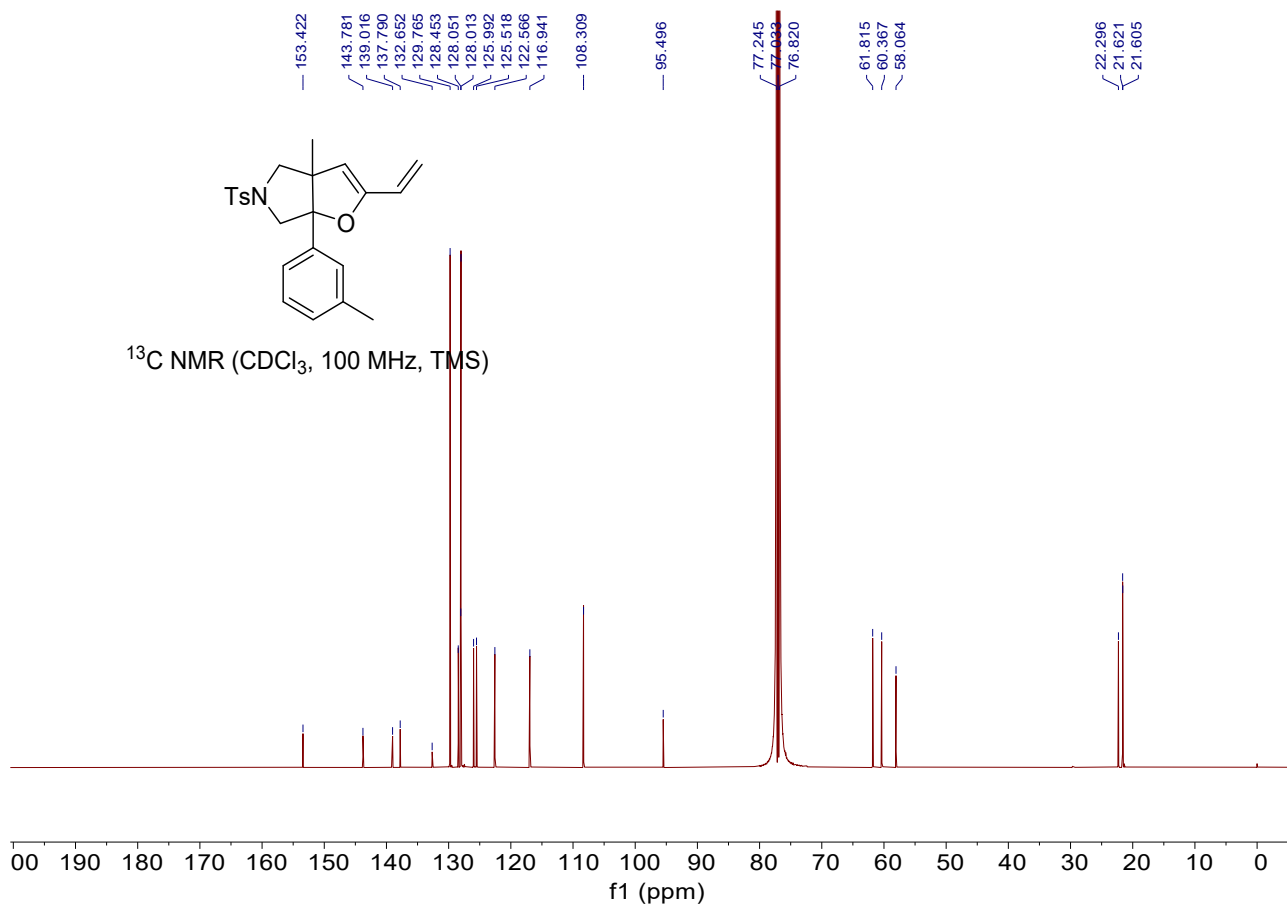
**3a-methyl-6a-(m-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2x)**

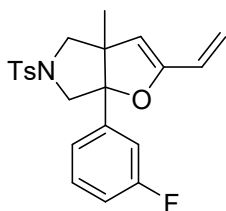
A yellow oil, 80% yield, 31.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.74 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.17 (t,  $J = 7.6$  Hz, 1H), 7.07 (d,  $J = 7.6$  Hz, 1H), 6.99 (d,  $J = 8.4$  Hz, 1H), 6.96 (s, 1H), 6.14 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.62 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.27 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.70 (s, 1H), 3.79 (d,  $J = 11.2$  Hz, 1H), 3.70 (d,  $J = 11.2$  Hz, 1H), 3.52 (d,  $J = 9.6$  Hz, 1H), 3.12 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 2.29 (s, 3H), 0.65 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.4, 143.8, 139.0, 137.8, 132.7, 129.8, 128.5, 128.1, 128.0, 126.0, 125.5, 122.6, 116.9, 108.3, 95.5, 61.8, 60.4, 58.1, 22.3, 21.62, 21.60. IR (neat)  $\nu$  668, 813, 1163, 1349, 1594, 2851, 2927, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1443.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

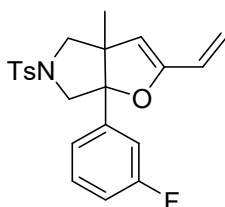




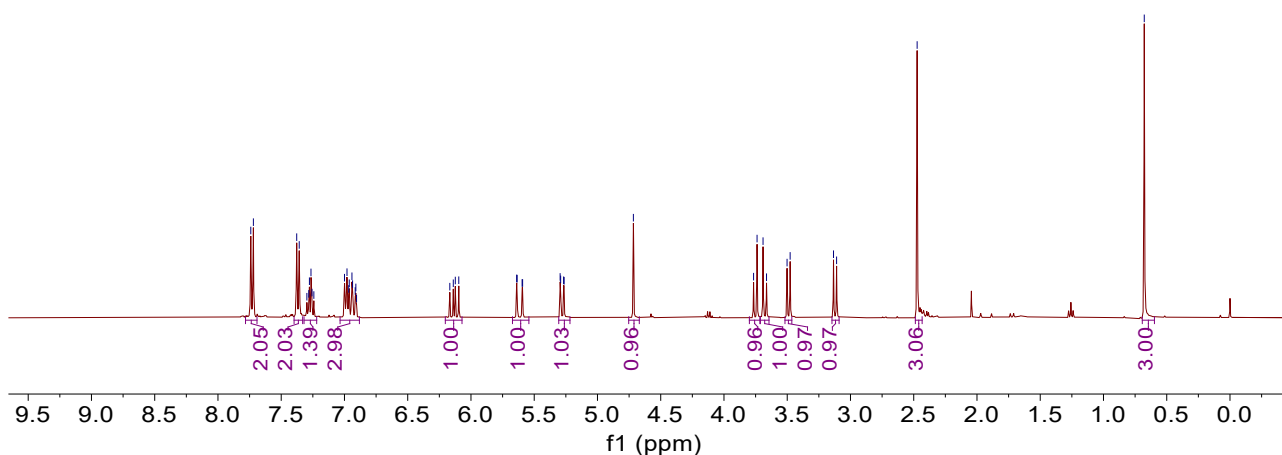


**6a-(3-fluorophenyl)-3a-methyl-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2y)**

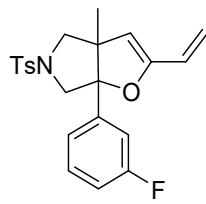
A colorless oil, 70% yield, 28.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.37 (d,  $J = 8.0$  Hz, 2H), 7.32 – 7.22 (m, 1H), 7.03 – 6.88 (m, 3H), 6.13 (dd,  $J = 17.2$ , 11.0 Hz, 1H), 5.62 (dd,  $J = 17.2$ , 1.6 Hz, 1H), 5.28 (dd,  $J = 11.0$ , 1.6 Hz, 1H), 4.72 (s, 1H), 3.75 (d,  $J = 11.0$  Hz, 1H), 3.68 (d,  $J = 11.0$  Hz, 1H), 3.49 (d,  $J = 9.6$  Hz, 1H), 3.12 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 0.68 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  162.7 (d,  $J_{\text{C-F}} = 244.3$  Hz), 153.3, 144.0, 141.8 (d,  $J_{\text{C-F}} = 7.2$  Hz), 132.3, 129.8, 129.7 (d,  $J_{\text{C-F}} = 8.6$  Hz), 128.0, 125.3, 121.1 (d,  $J_{\text{C-F}} = 3.0$  Hz), 117.2, 114.6 (d,  $J_{\text{C-F}} = 21.0$  Hz), 112.8 (d,  $J_{\text{C-F}} = 23.1$  Hz), 108.2, 94.99, 94.97, 61.6, 60.4, 58.3, 22.4, 21.6.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.4. IR (neat)  $\nu$  678, 1157, 1216, 1351, 1596, 2921, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{FSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1190.



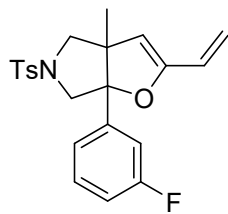
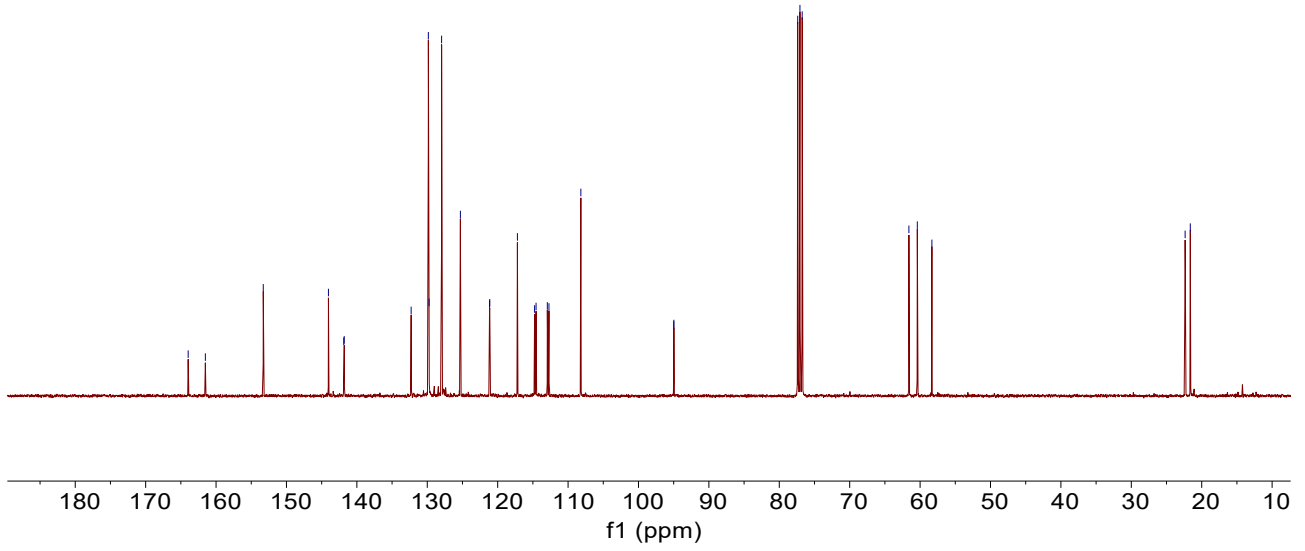
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



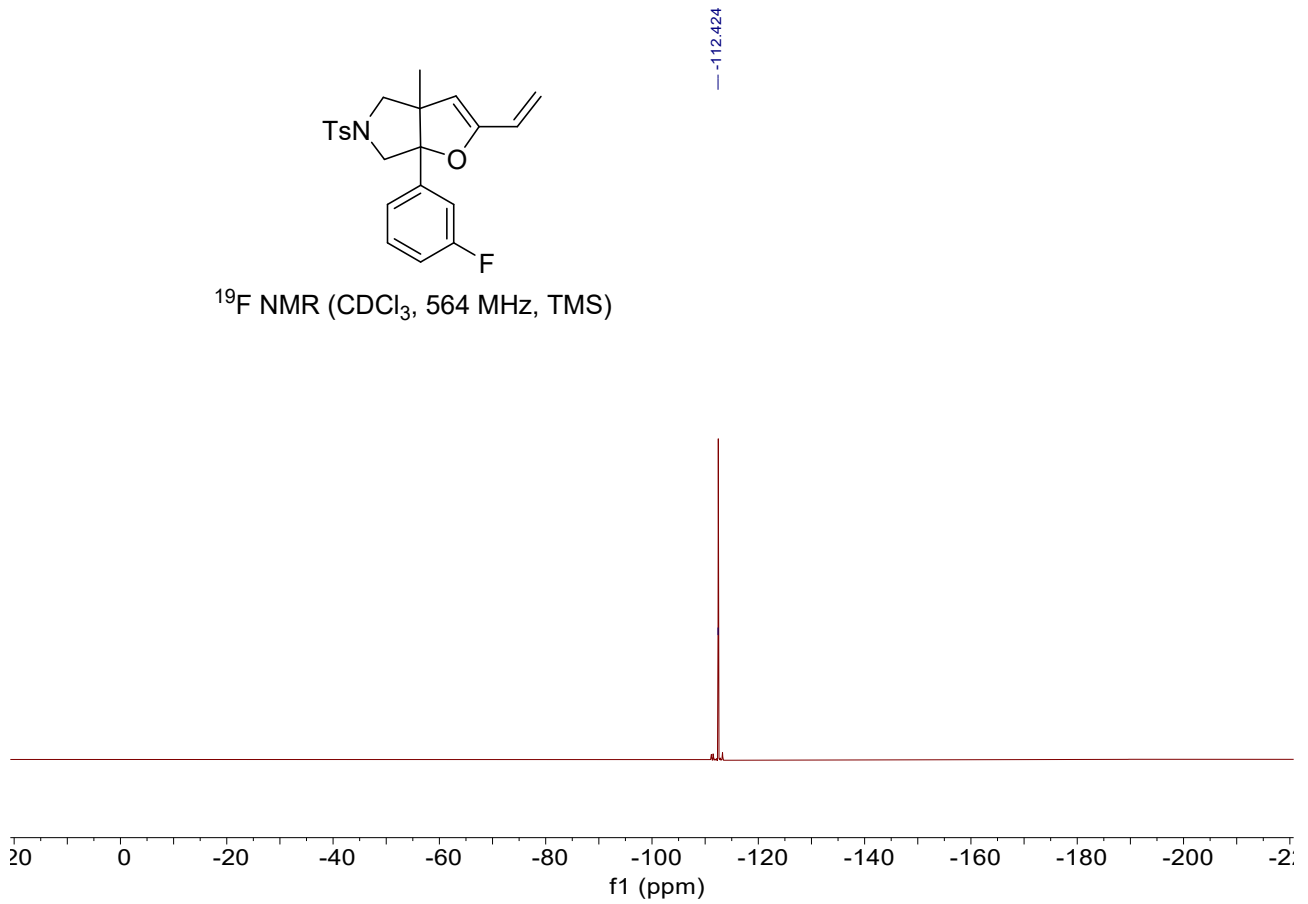
163.962  
 161.519  
 153.296  
 144.038  
 141.864  
 141.792  
 132.290  
 129.847  
 129.743  
 127.965  
 125.295  
 121.153  
 121.123  
 117.197  
 114.757  
 114.547  
 112.946  
 112.715  
 108.185  
 94.991  
 94.972  
 77.384  
 77.066  
 76.749  
 61.591  
 60.396  
 58.324  
 22.355  
 21.623



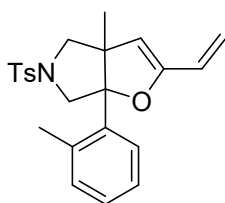
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



<sup>19</sup>F NMR (CDCl<sub>3</sub>, 564 MHz, TMS)

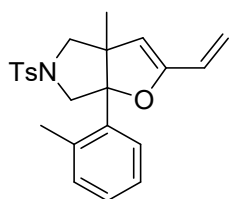




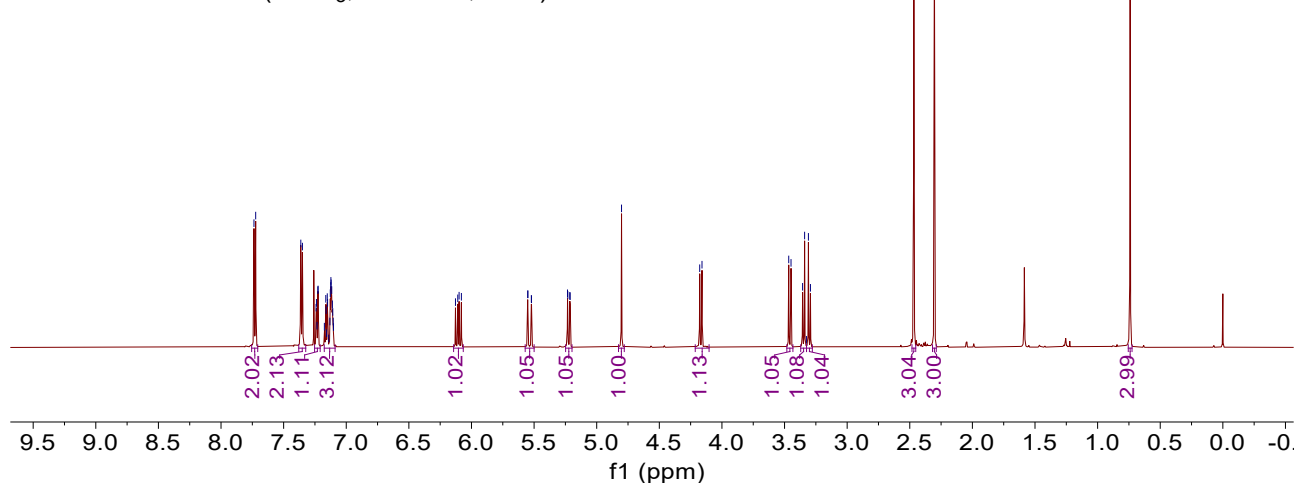


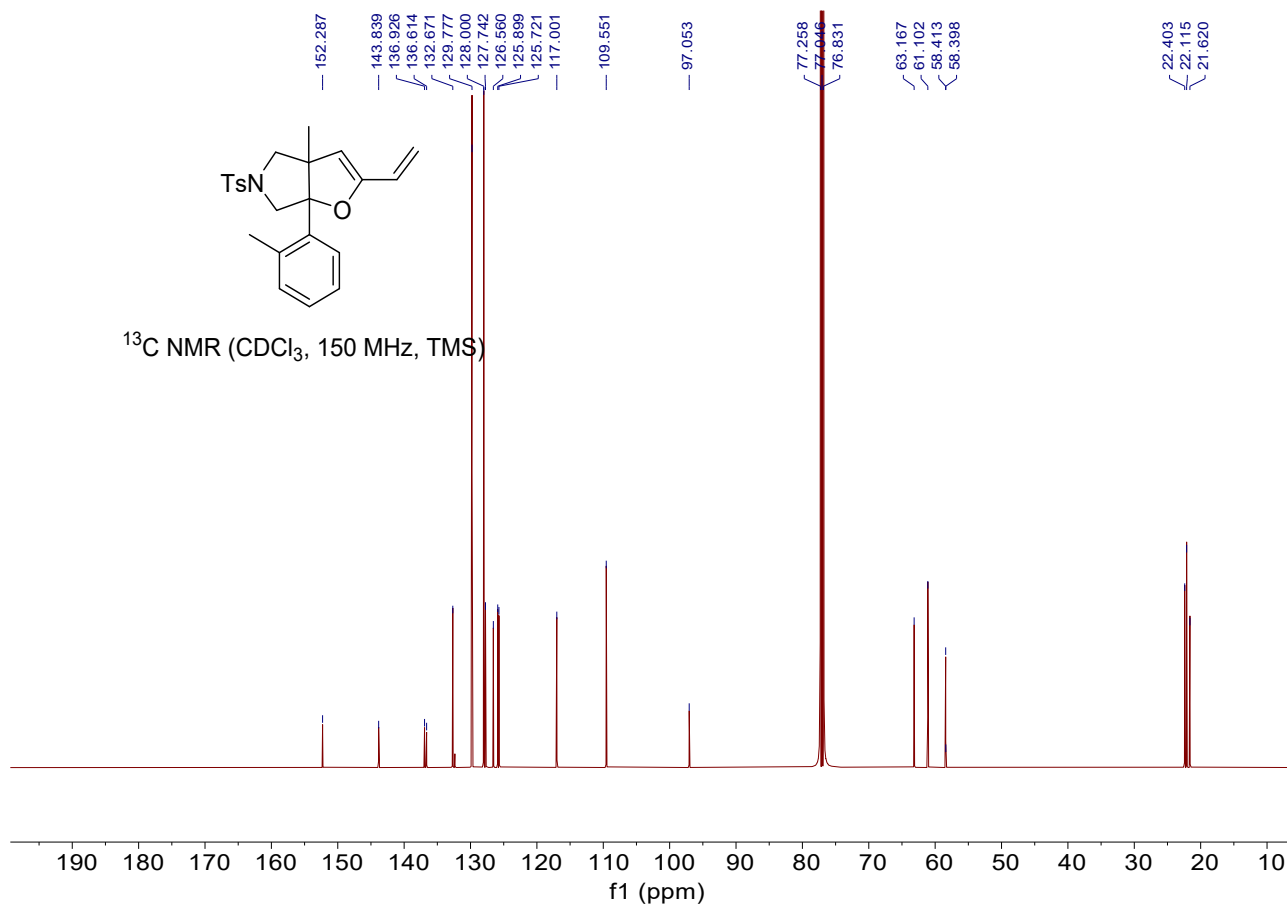
### 3a-methyl-6a-(o-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2z)

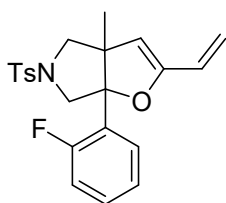
A yellow oil, 78% yield, 30.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.23 (dd,  $J = 8.0, 1.6$  Hz, 1H), 7.18 – 7.09 (m, 3H), 6.10 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.54 (dd,  $J = 17.2, 0.8$  Hz, 1H), 5.22 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.80 (s, 1H), 4.17 (d,  $J = 11.0$  Hz, 1H), 3.46 (d,  $J = 11.0$  Hz, 1H), 3.35 (d,  $J = 9.6$  Hz, 1H), 3.30 (d,  $J = 9.6$  Hz, 1H), 2.47 (s, 3H), 2.30 (s, 3H), 0.74 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  152.3, 143.8, 136.9, 136.6, 132.7, 129.8, 128.0, 127.7, 126.6, 125.9, 125.7, 117.0, 109.6, 97.1, 63.2, 61.1, 58.41, 58.40, 22.4, 22.1, 21.6. IR (neat)  $\nu$  667, 815, 1092, 1183, 1348, 1595, 2858, 2932, 2970  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1446.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

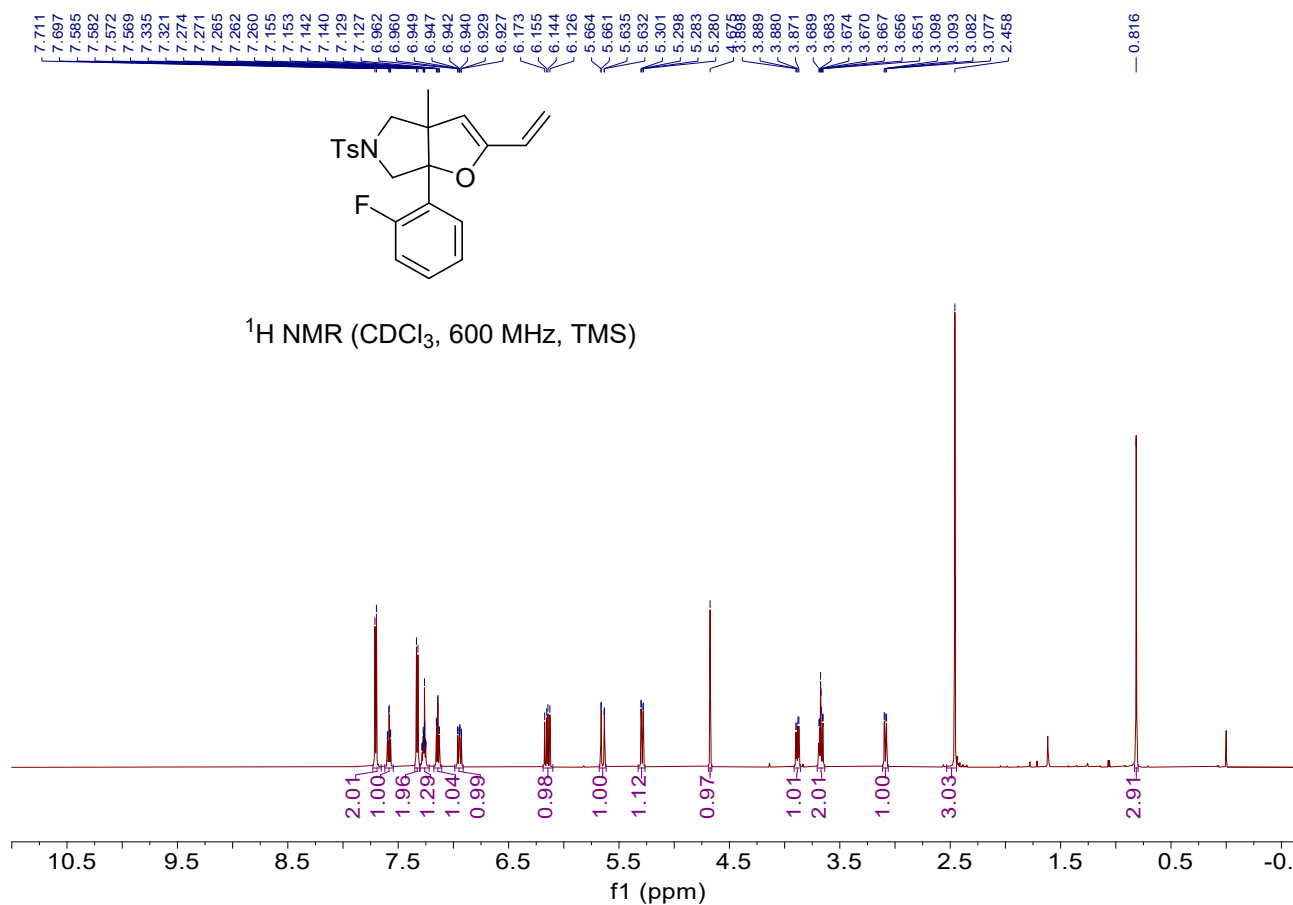


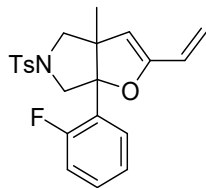




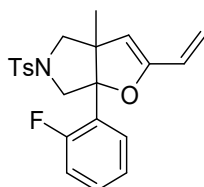
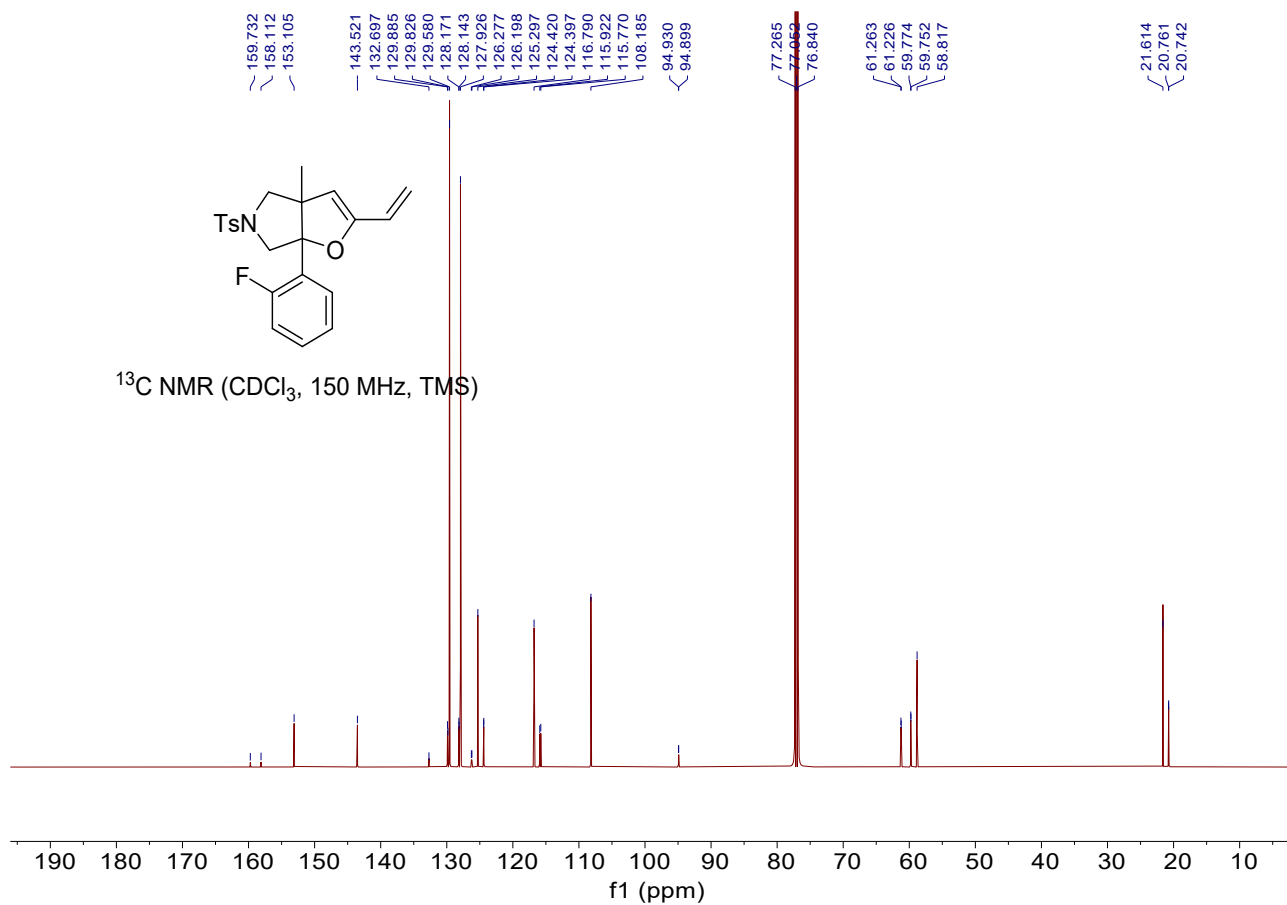
### 3a-methyl-6a-(o-tolyl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2aa)

A red oil, 78% yield, 31.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.58 (d,  $J = 8.0$  Hz, 1H), 7.33 (d,  $J = 8.0$  Hz, 2H), 7.30 – 7.22 (m, 1H), 7.14 (td,  $J = 7.6, 1.2$  Hz, 1H), 6.94 (dd,  $J = 12.0, 8.0$ , Hz, 1H), 6.15 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.65 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.29 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.68 (s, 1H), 3.88 (dd,  $J = 11.2, 5.2$  Hz, 1H), 3.70 – 3.64 (m, 2H), 3.09 (dd,  $J = 9.6, 3.2$  Hz, 1H), 2.46 (s, 3H), 0.82 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  158.9 (d,  $J_{\text{C-F}} = 243.0$  Hz), 153.1, 143.5, 132.7, 129.8 (d,  $J_{\text{C-F}} = 8.9$  Hz), 129.6, 128.1 (d,  $J_{\text{C-F}} = 4.2$  Hz), 127.9, 126.2 (d,  $J_{\text{C-F}} = 10.9$  Hz), 125.3, 124.4 (d,  $J_{\text{C-F}} = 3.5$  Hz), 116.8, 115.8 (d,  $J_{\text{C-F}} = 22.8$  Hz), 108.2, 94.93, 94.89, 61.2 (d,  $J_{\text{C-F}} = 5.6$  Hz), 59.7 (d,  $J_{\text{C-F}} = 3.3$  Hz), 58.8, 21.6, 20.7 (d,  $J_{\text{C-F}} = 2.9$  Hz).  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -108.5. IR (neat)  $\nu$  678, 1218, 1353, 1596, 2921, 2966, 3023  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{FSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1205.

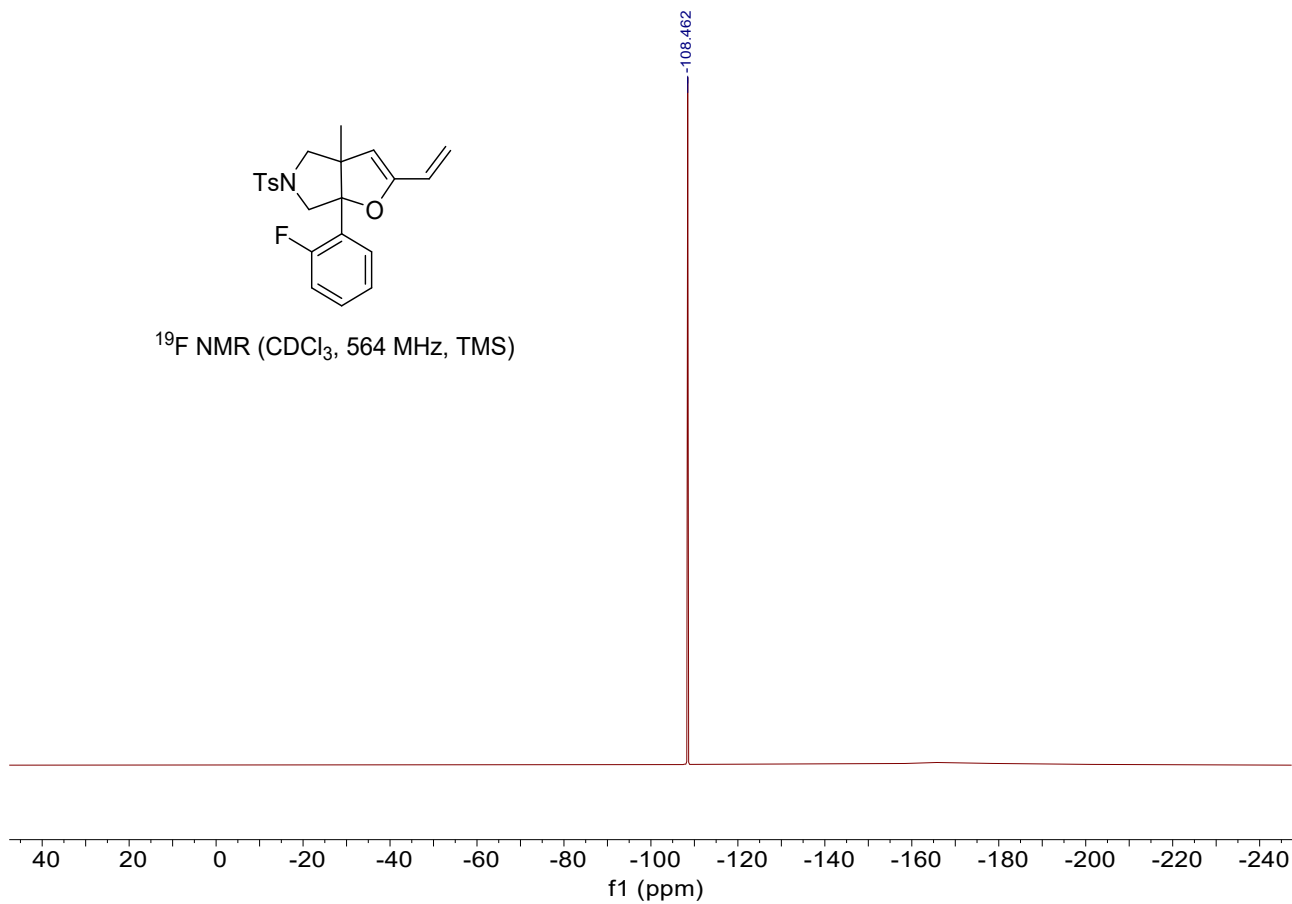


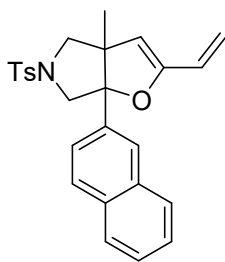


<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, TMS)



<sup>19</sup>F NMR (CDCl<sub>3</sub>, 564 MHz, TMS)

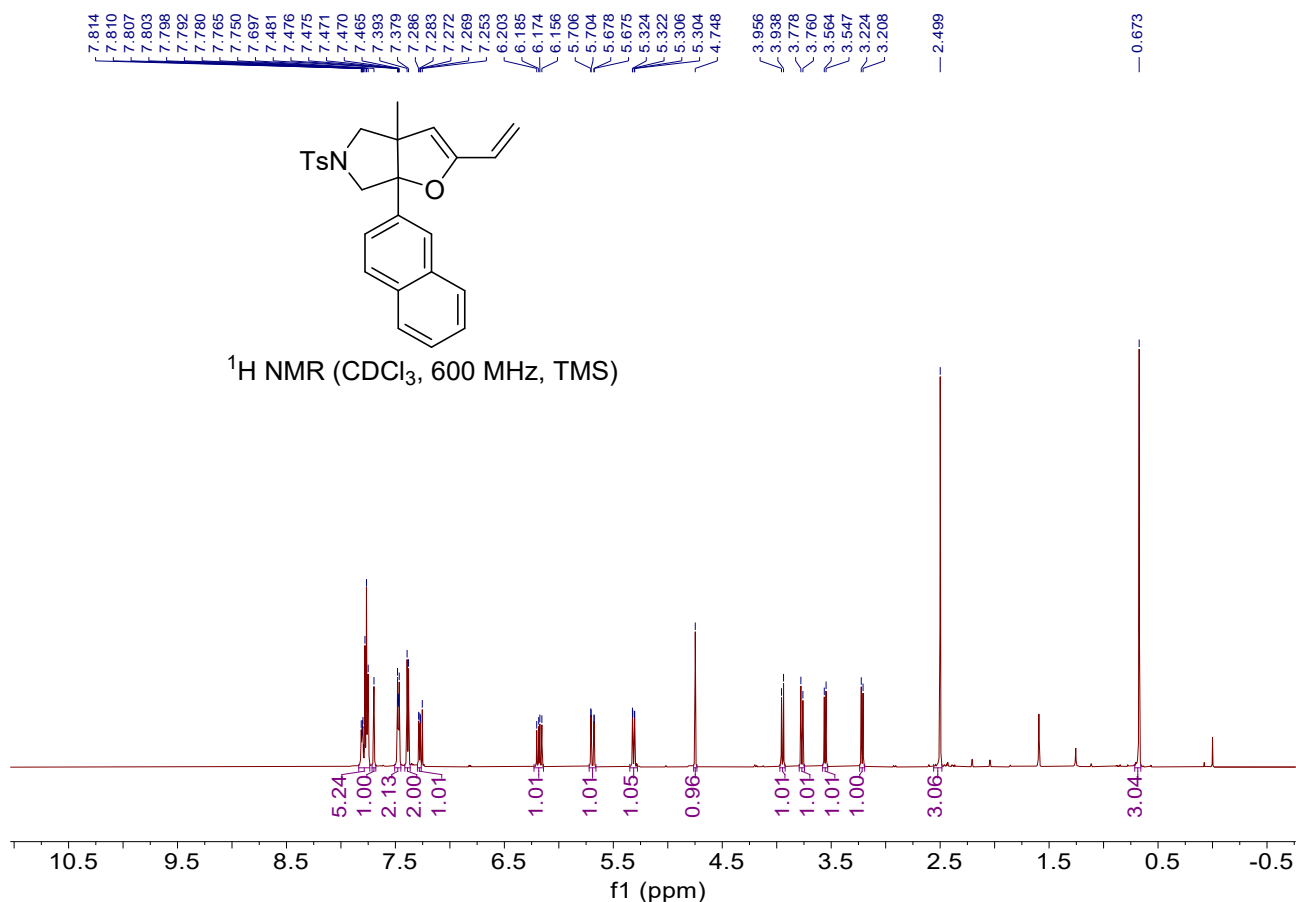


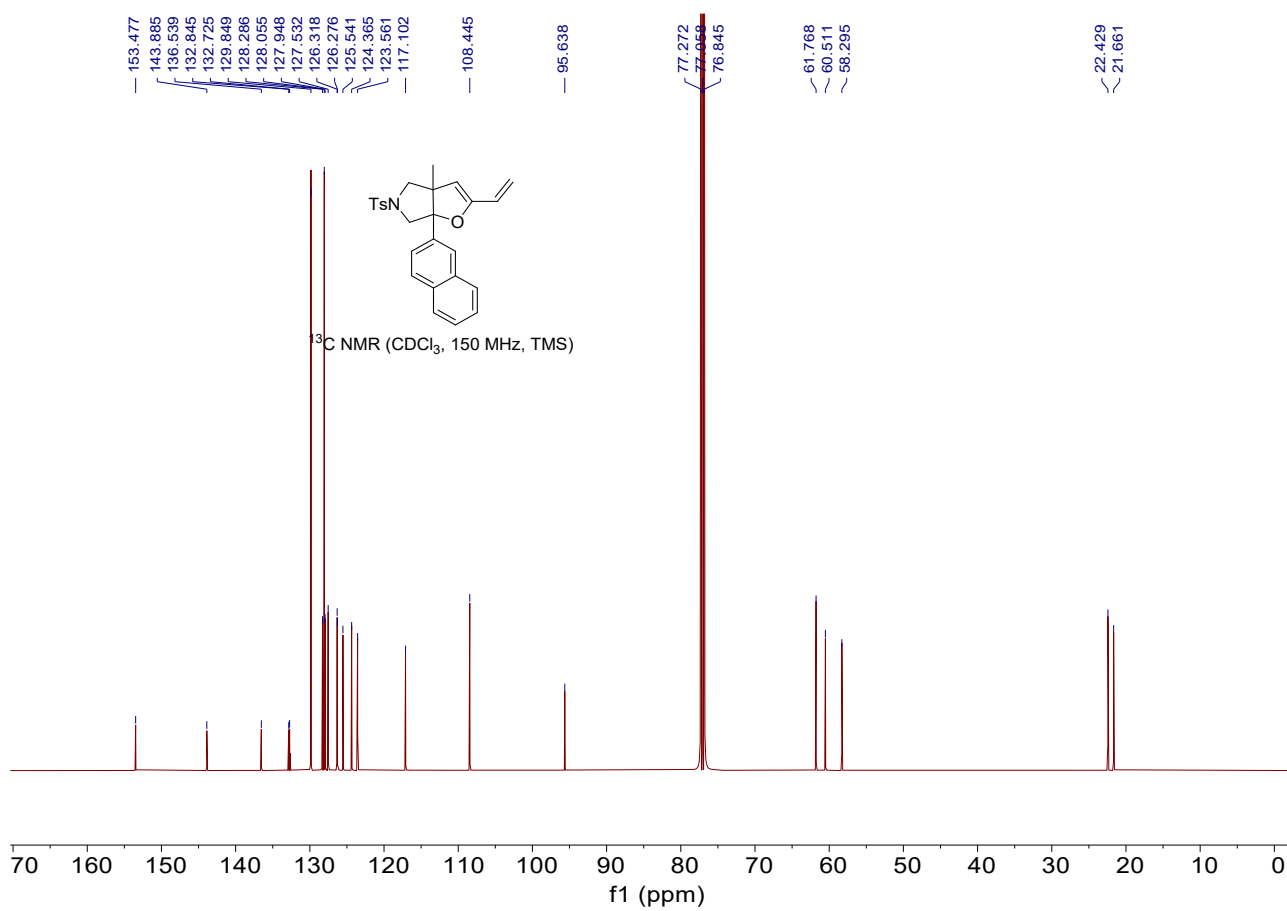


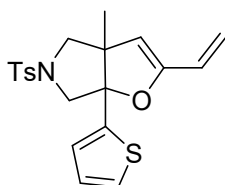
**3a-methyl-6a-(naphthalen-2-yl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole**

**(2ab)**

A colorless oil, 80% yield, 34.5 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.84 – 7.74 (m, 5H), 7.70 (s, 1H), 7.51 – 7.45 (m, 2H), 7.39 (d,  $J = 8.0$  Hz, 2H), 7.28 (dd,  $J = 8.4, 2.0$  Hz, 1H), 6.18 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.69 (dd,  $J = 17.2, 1.6$  Hz, 1H), 5.31 (dd,  $J = 11.2, 1.6$  Hz, 1H), 4.75 (s, 1H), 3.95 (d,  $J = 11.2$  Hz, 1H), 3.77 (d,  $J = 11.2$  Hz, 1H), 3.56 (d,  $J = 10.0$  Hz, 1H), 3.22 (d,  $J = 10.0$  Hz, 1H), 2.50 (s, 3H), 0.67 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  153.5, 143.9, 136.5, 132.8, 132.7, 129.8, 128.3, 128.1, 127.9, 127.5, 126.31, 126.27, 125.5, 124.4, 123.6, 117.1, 108.4, 95.6, 61.8, 60.5, 58.3, 22.4, 21.7. IR (neat)  $\nu$  678, 1157, 1228, 1351, 1596, 2921, 2966, 3031  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{26}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 454.1447, Found: 454.1447.

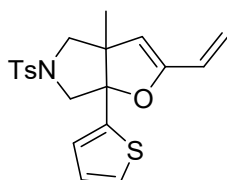




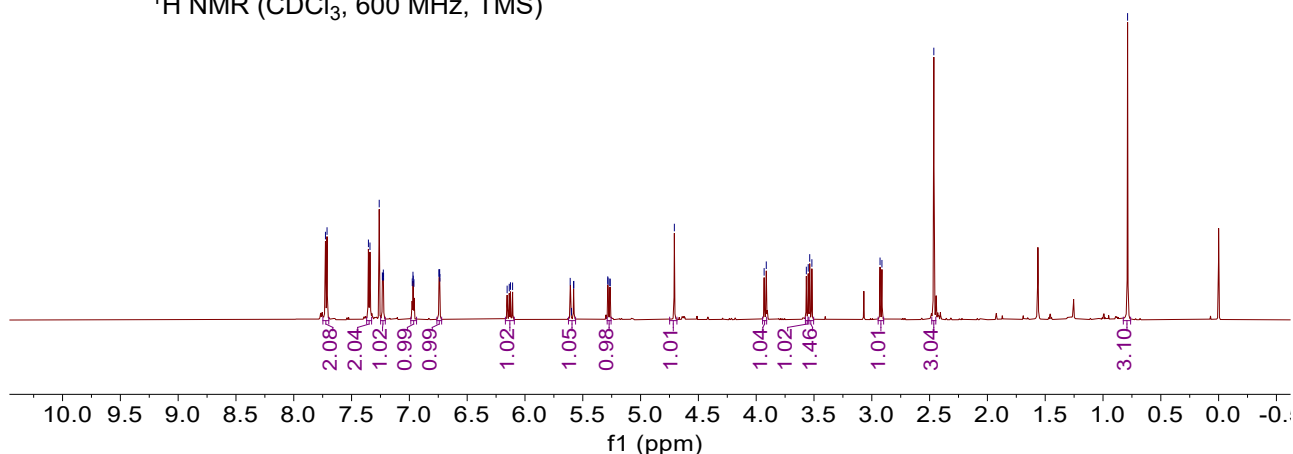


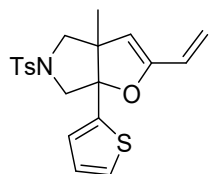
**3a-methyl-6a-(thiophen-2-yl)-5-tosyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (2ac)**

A brown oil, 36% yield, 13.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.35 (d,  $J = 8.0$  Hz, 2H), 7.23 (dd,  $J = 5.2, 1.2$  Hz, 1H), 6.97 (dd,  $J = 5.2, 3.6$  Hz, 1H), 6.74 (dd,  $J = 3.6, 1.2$  Hz, 1H), 6.13 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.62 – 5.56 (m, 1H), 5.27 (dd,  $J = 11.2, 1.6$  Hz, 1H), 4.71 (s, 1H), 3.92 (d,  $J = 11.2$  Hz, 1H), 3.56 (d,  $J = 9.6$  Hz, 1H), 3.53 (d,  $J = 11.2$  Hz, 1H), 2.92 (d,  $J = 9.6$  Hz, 1H), 2.46 (s, 3H), 0.79 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.9, 143.9, 142.6, 132.5, 129.8, 128.0, 127.1, 125.2, 125.1, 124.0, 117.3, 107.3, 95.0, 61.4, 60.4, 58.4, 21.64, 21.62. IR (neat)  $\nu$  664, 813, 1024, 1164, 1347, 1595, 2849, 2922  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{20}\text{H}_{21}\text{NO}_3\text{S}_2\text{Na}$  ( $\text{M}+\text{Na}$ ) $^+$ : 410.0855, Found: 410.0853.

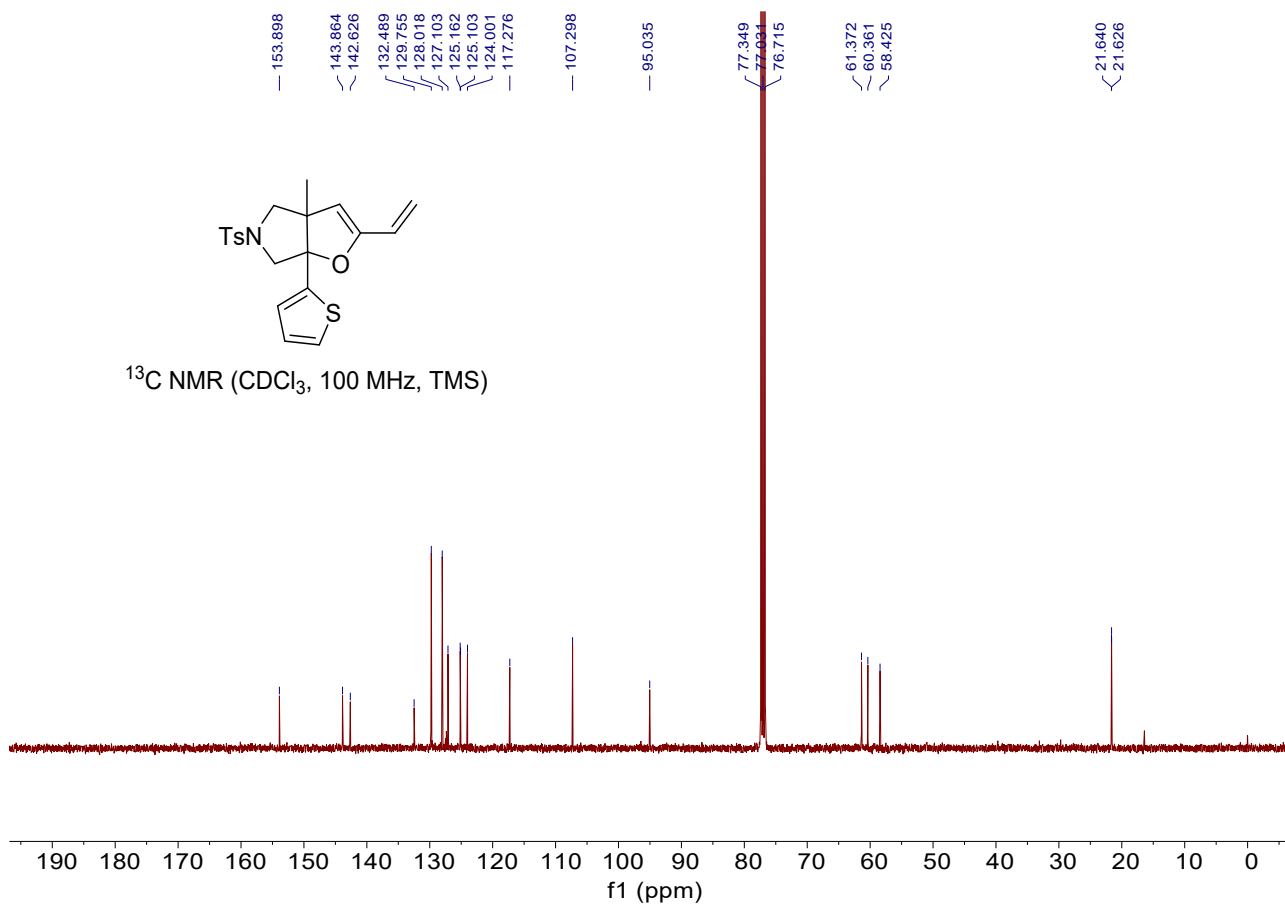


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

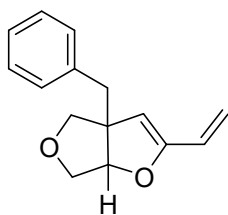




$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)

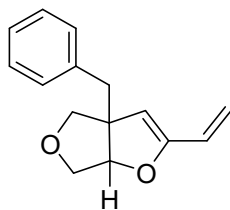




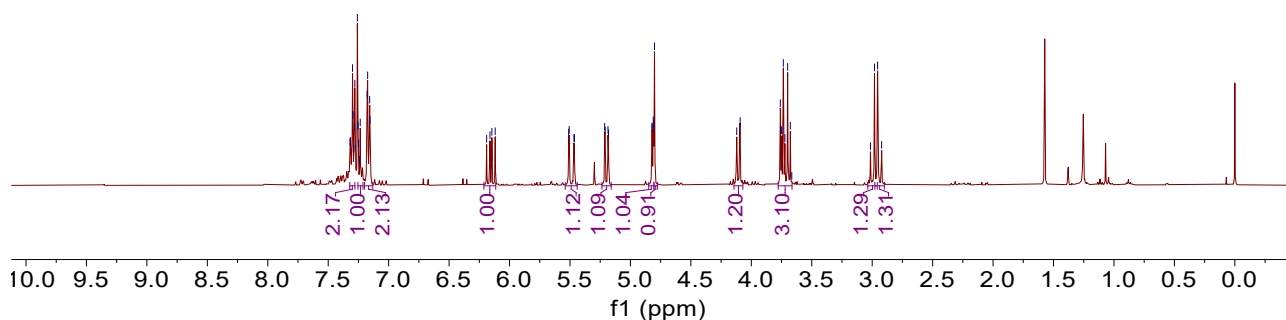


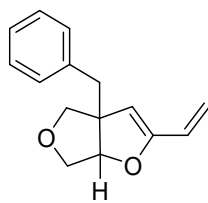
### 3a-benzyl-2-vinyl-3a,4,6,6a-tetrahydrofuro[3,4-b]furan (2ad)

A colorless oil, 86% yield, 19.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.32 – 7.28 (m, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.13 (m, 2H), 6.15 (dd,  $J = 17.4, 11.0$  Hz, 1H), 5.49 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.20 (dd,  $J = 11.0, 1.6$  Hz, 1H), 4.82 (dd,  $J = 4.5, 1.2$  Hz, 1H), 4.80 (s, 1H), 4.11 (d,  $J = 11.3$  Hz, 1H), 3.78 – 3.66 (m, 3H), 3.00 (d,  $J = 13.2$  Hz, 1H), 2.94 (d,  $J = 13.2$  Hz, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  155.6, 137.7, 129.7, 128.4, 126.6, 125.7, 116.4, 105.6, 89.7, 78.5, 75.8, 61.3, 42.9. IR (neat)  $\nu$  668, 1227, 1365, 1566, 2927, 2968  $\text{cm}^{-1}$ . HRMS (EI) calcd. for  $\text{C}_{15}\text{H}_{16}\text{O}_2$ : 228.1147, Found: 228.1145.

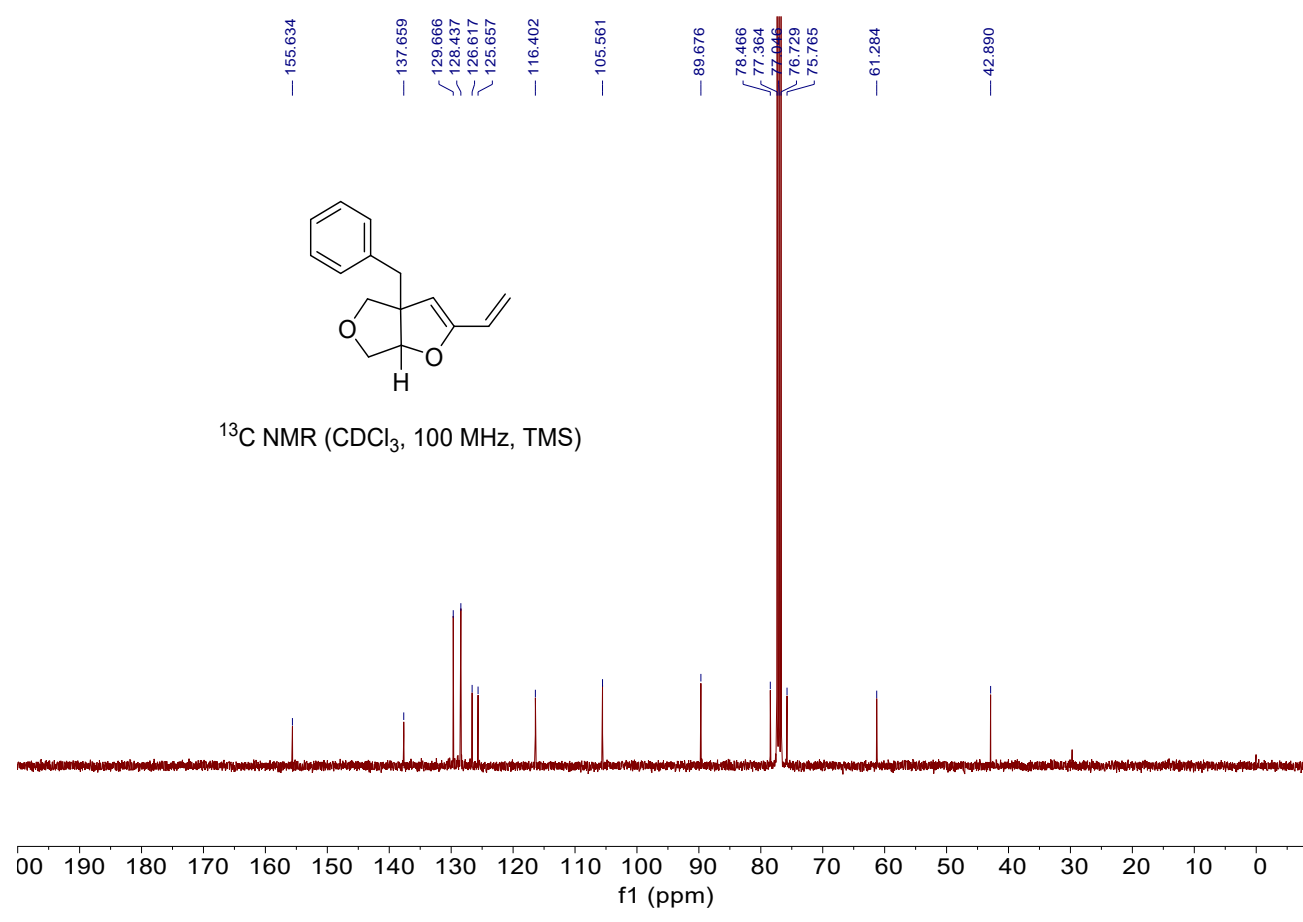


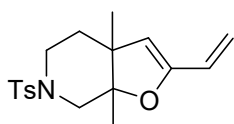
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





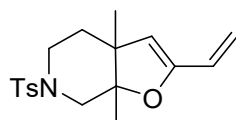
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



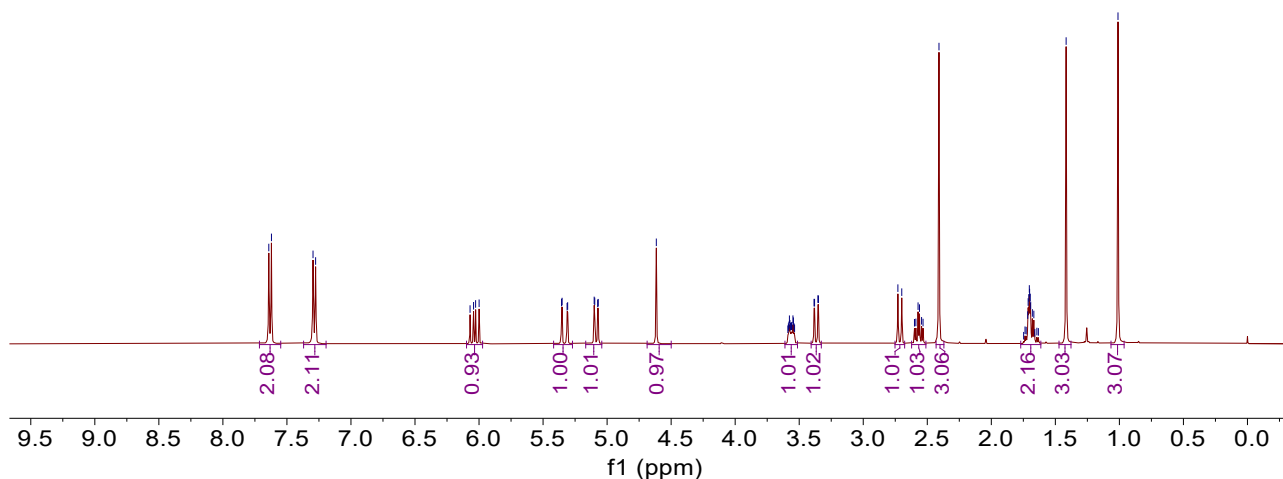


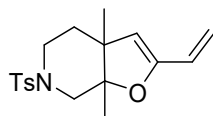
### 3a,7a-dimethyl-6-tosyl-2-vinyl-3a,4,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (2ae)

A colorless oil, 80% yield, 26.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.63 (d,  $J = 8.4$  Hz, 2H), 7.29 (d,  $J = 8.4$  Hz, 2H), 6.03 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.33 (dd,  $J = 17.2, 1.2$  Hz, 1H), 5.09 (dd,  $J = 10.8, 1.8$  Hz, 1H), 4.62 (s, 1H), 3.61 – 3.51 (m, 1H), 3.37 (dd,  $J = 12.0, 1.6$  Hz, 1H), 2.71 (d,  $J = 12.0$  Hz, 1H), 2.57 (td,  $J = 11.2, 4.4$  Hz, 1H), 2.41 (s, 3H), 1.77 – 1.61 (m, 2H), 1.42 (s, 3H), 1.01 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  153.1, 143.3, 134.1, 129.7, 127.5, 126.0, 115.7, 110.5, 85.4, 51.7, 46.6, 43.3, 33.5, 24.3, 21.5, 19.2. IR (neat)  $\nu$  668, 1162, 1227, 1505, 1566, 2925, 2968, 3034  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{23}\text{NO}_3\text{NaS}$  (M) $^+$ : 356.1291, Found: 356.1283.

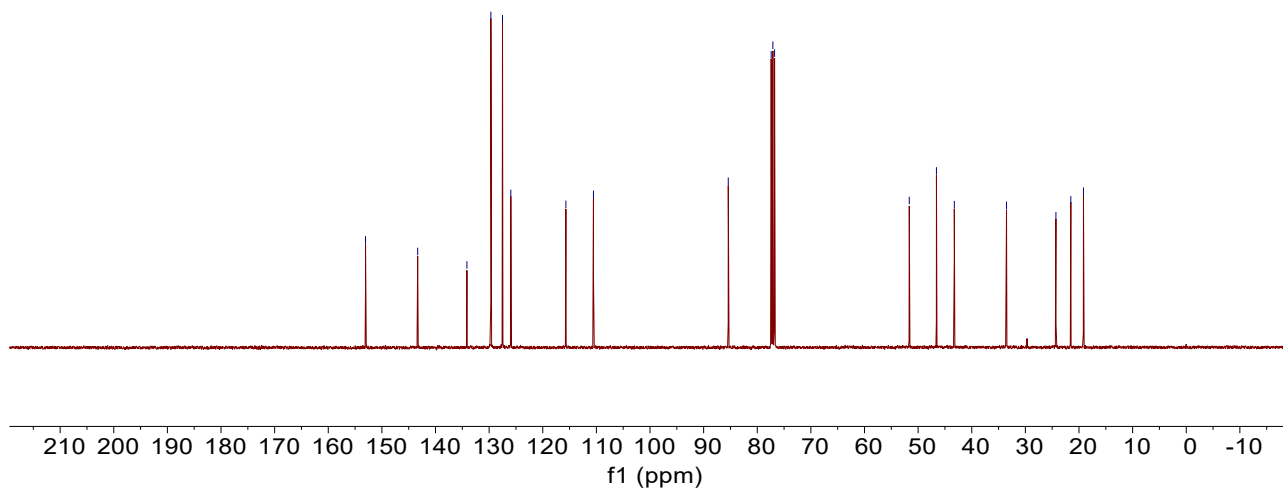


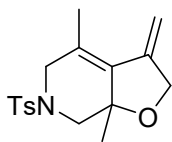
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





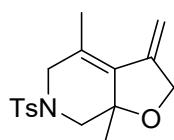
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



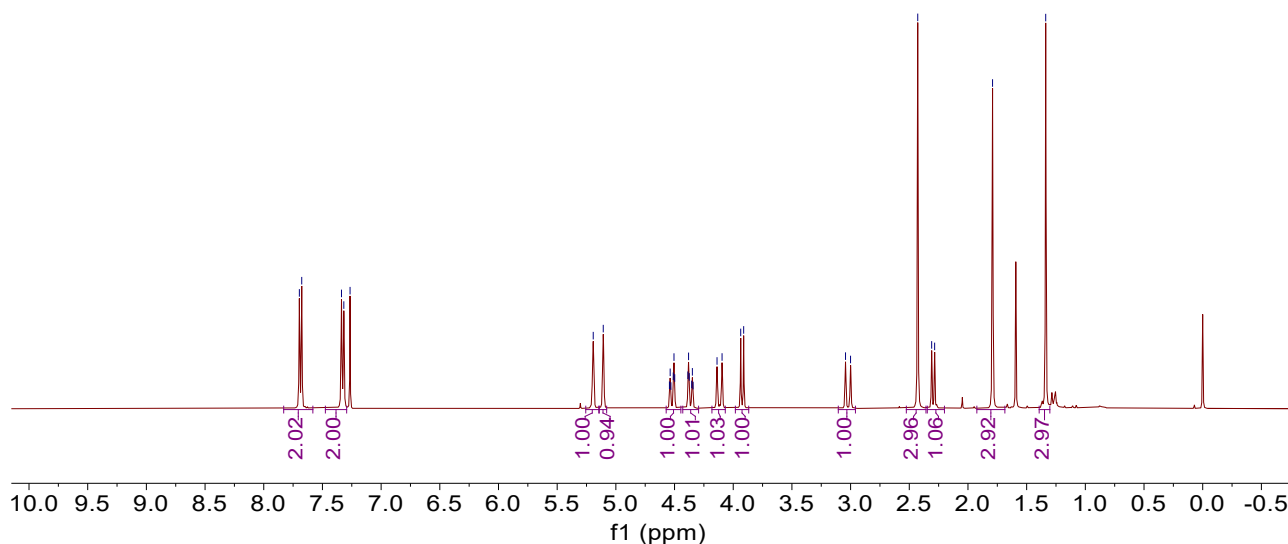


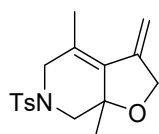
### 4,7a-dimethyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3a)

A colorless oil, 92% yield, 29.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 5.19 (s, 1H), 5.11 (s, 1H), 4.52 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.36 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.12 (d,  $J = 17.2$  Hz, 1H), 3.92 (d,  $J = 10.0$  Hz, 1H), 3.02 (d,  $J = 17.2$  Hz, 1H), 2.43 (s, 3H), 2.30 (d,  $J = 10.0$  Hz, 1H), 1.79 (s, 3H), 1.34 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.7, 142.7, 134.6, 133.4, 129.8, 127.5, 124.0, 107.4, 79.6, 69.9, 52.6, 49.6, 22.4, 21.5, 16.2. IR (neat)  $\nu$  667, 813, 1163, 1326, 1598, 2861, 2925, 2976  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{21}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 342.1134, Found: 342.1133.

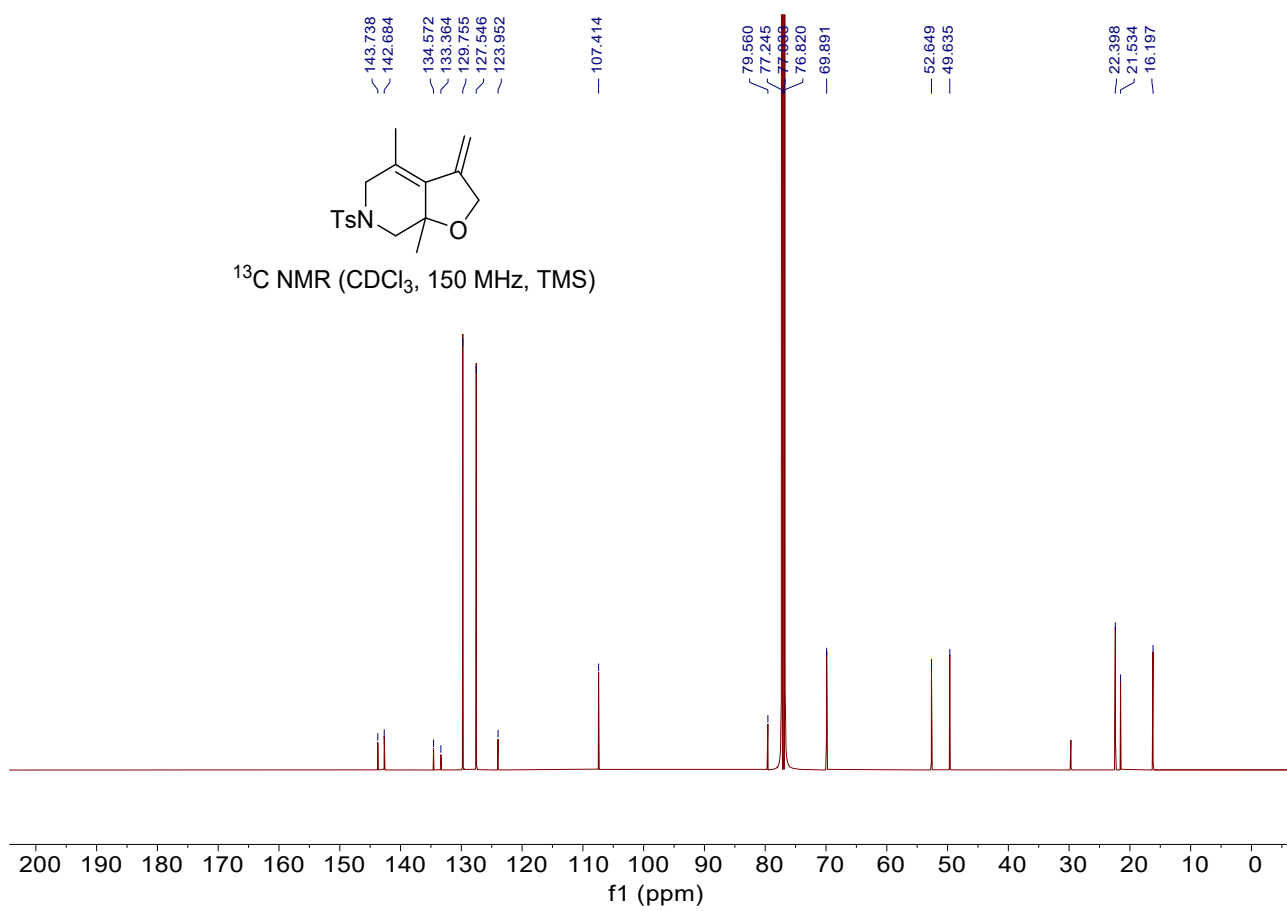


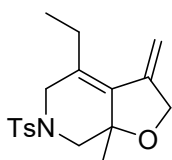
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





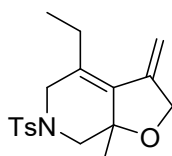
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, TMS)



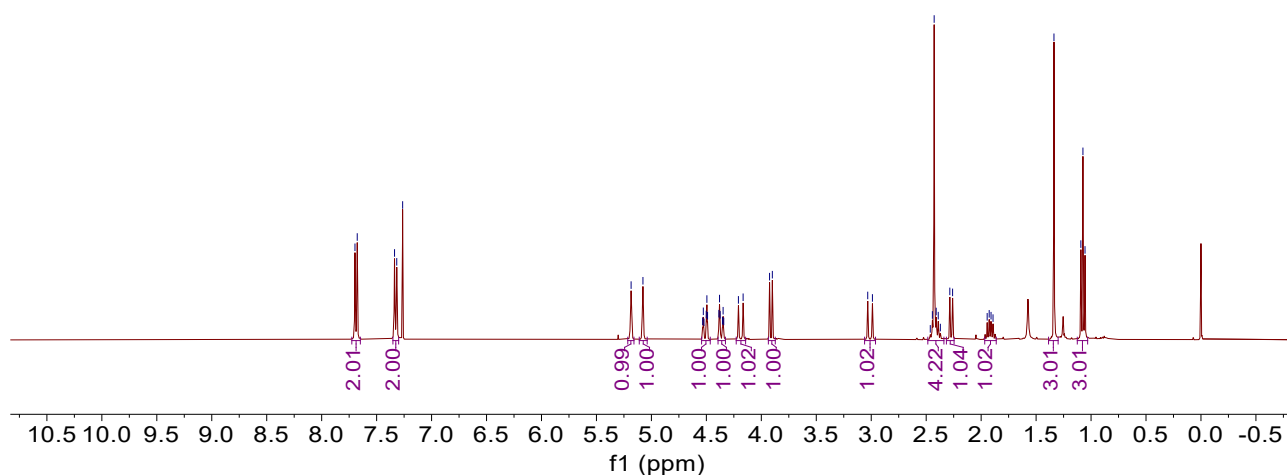


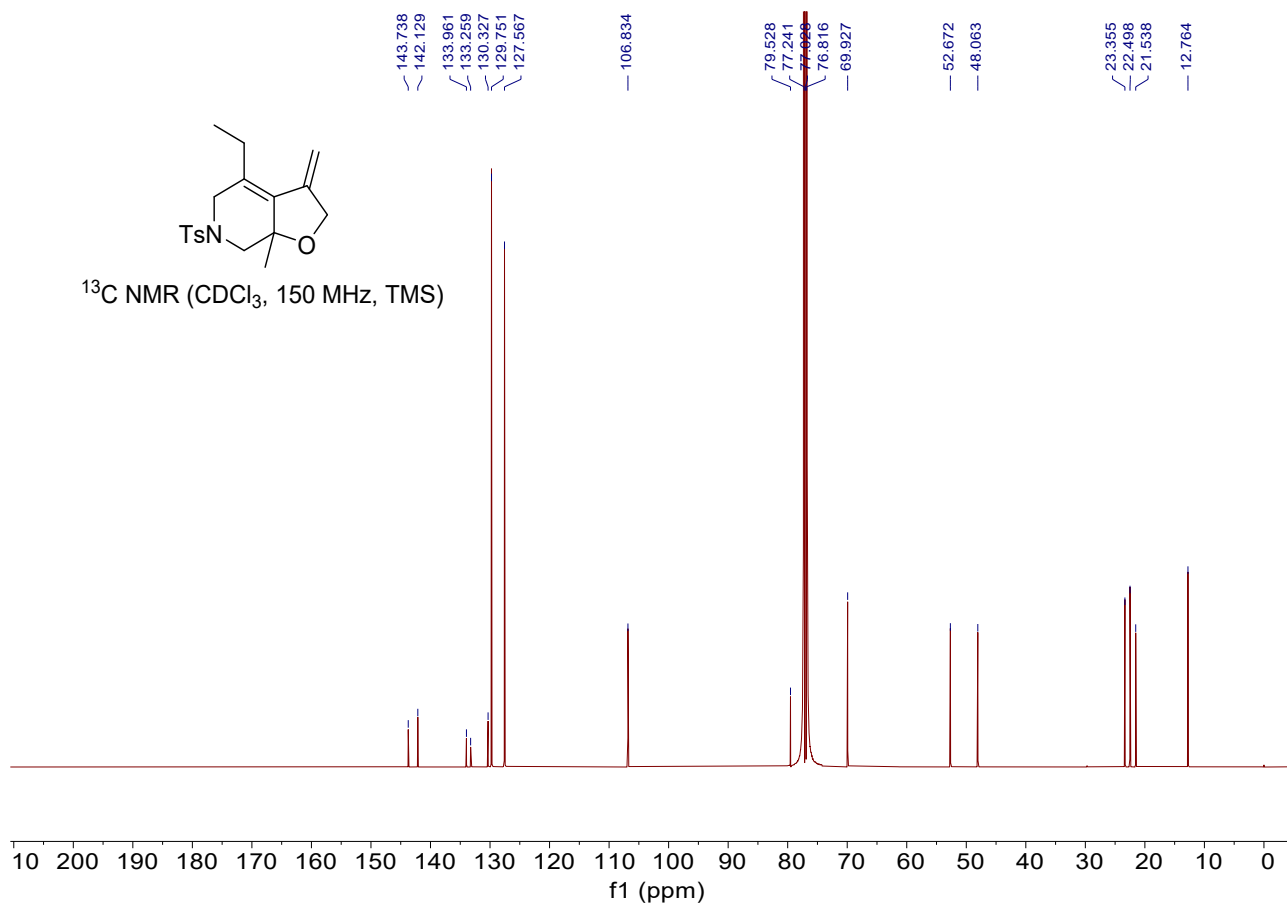
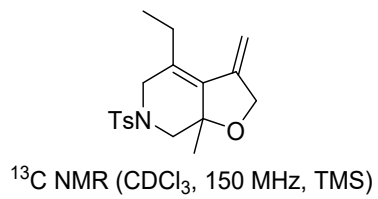
#### 4-ethyl-7a-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3b)

A colorless oil, 80% yield, 26.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 5.18 (s, 1H), 5.08 (s, 1H), 4.51 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.36 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.19 (d,  $J = 17.2$  Hz, 1H), 3.91 (d,  $J = 10.0$  Hz, 1H), 3.01 (d,  $J = 17.2$  Hz, 1H), 2.49 – 2.34 (m, 4H), 2.27 (d,  $J = 10.0$  Hz, 1H), 1.92 (q,  $J = 7.6$  Hz, 1H), 1.34 (s, 3H), 1.07 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.7, 142.1, 134.0, 133.3, 130.3, 129.8, 127.6, 106.8, 79.5, 69.9, 52.7, 48.1, 23.4, 22.5, 21.5, 12.8. IR (neat)  $\nu$  668, 815, 1162, 1350, 1598, 2869, 2927, 2976  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 356.1291, Found: 356.1289.

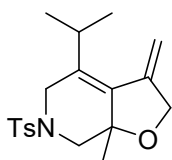


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



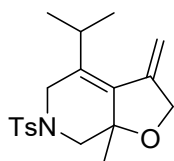




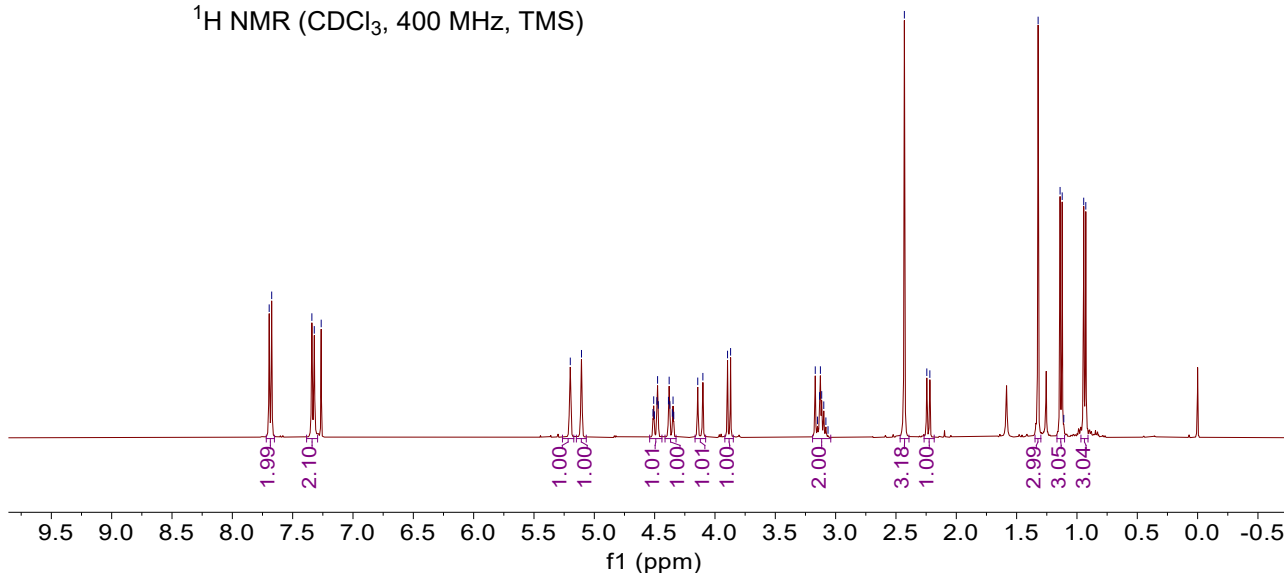


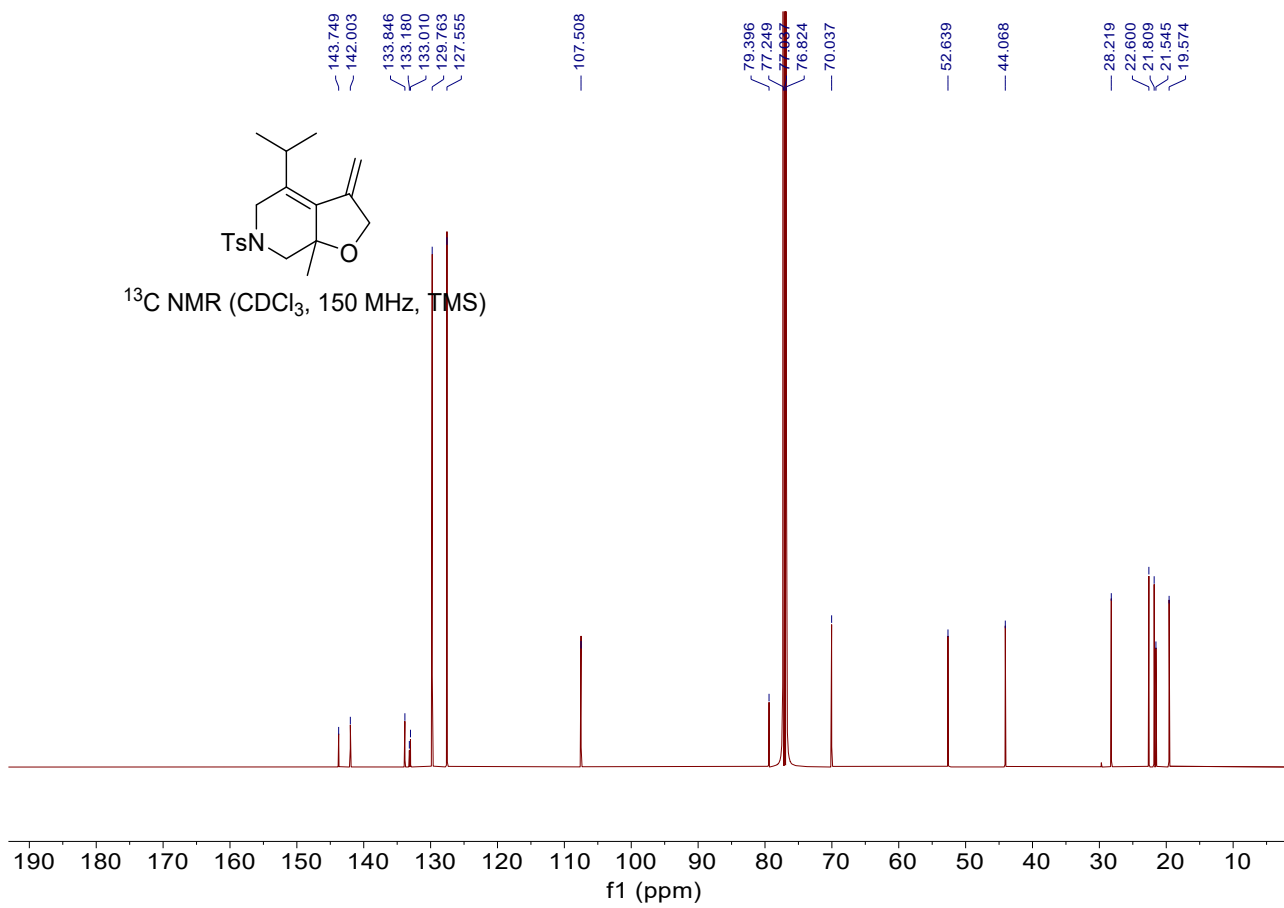
#### 4-isopropyl-7a-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3c)

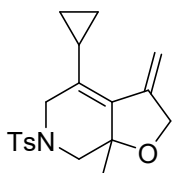
A colorless oil, 82% yield, 28.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.68 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 5.20 (s, 1H), 5.11 (s, 1H), 4.49 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.36 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.12 (d,  $J = 17.2$  Hz, 1H), 3.88 (d,  $J = 10.0$  Hz, 1H), 3.19 – 3.04 (m, 2H), 2.43 (s, 3H), 2.23 (d,  $J = 10.0$  Hz, 1H), 1.32 (s, 3H), 1.13 (d,  $J = 7.0$  Hz, 3H), 0.94 (d,  $J = 7.0$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.7, 142.0, 133.8, 133.2, 133.0, 129.8, 127.6, 107.5, 79.4, 70.0, 52.6, 44.1, 28.2, 22.6, 21.8, 21.5, 19.6. IR (neat)  $\nu$  668, 813, 1164, 1351, 1597, 2853, 2927, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 370.1447, Found: 370.1448.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

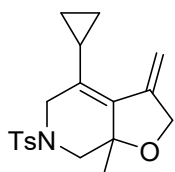




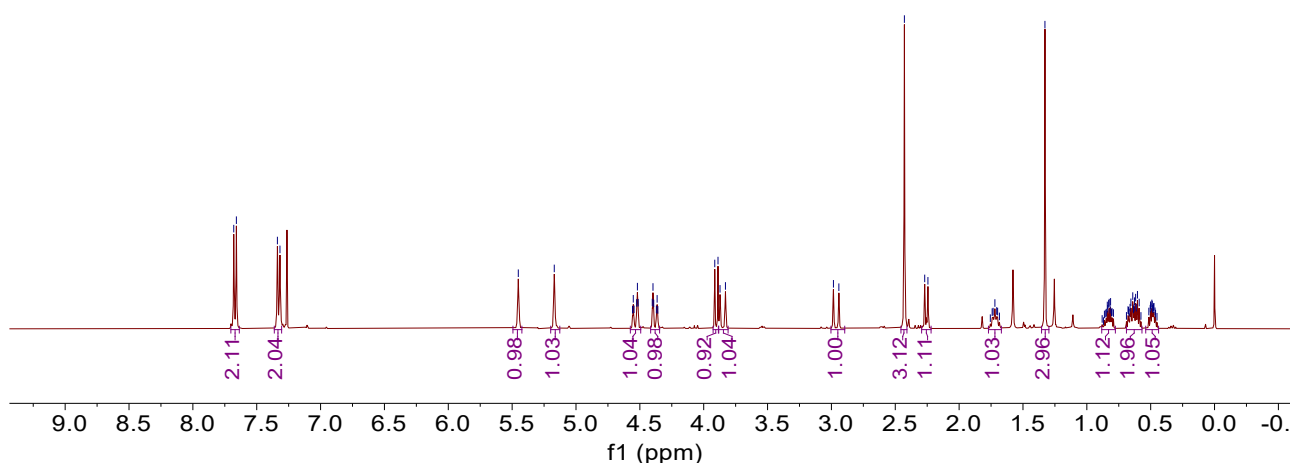


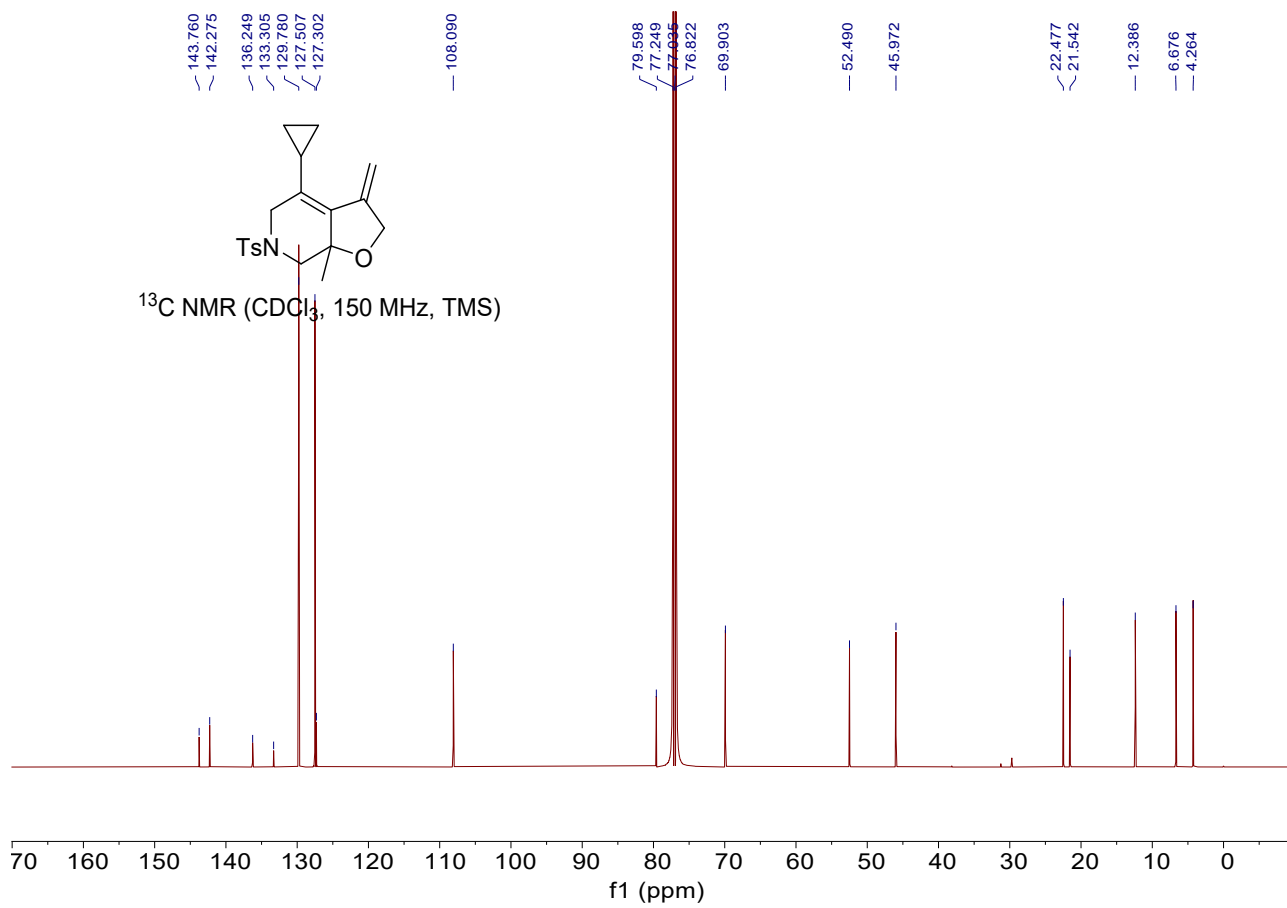
### 4-cyclopropyl-7a-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3d)

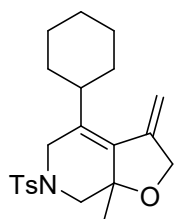
A colorless oil, 86% yield, 29.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.67 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 5.45 (s, 1H), 5.17 (s, 1H), 4.54 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.38 (dt,  $J = 12.8, 2.4$  Hz, 1H), 3.90 (d,  $J = 10.0$  Hz, 1H), 3.85 (d,  $J = 17.2$  Hz, 1H), 2.96 (d,  $J = 17.2$  Hz, 1H), 2.43 (s, 3H), 2.26 (d,  $J = 10.0$  Hz, 1H), 1.77 – 1.67 (m, 1H), 1.33 (s, 3H), 0.88 – 0.78 (m, 1H), 0.69 – 0.57 (m, 2H), 0.54 – 0.44 (m, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.8, 142.3, 136.2, 133.3, 129.8, 127.5, 127.3, 108.1, 79.6, 69.9, 52.5, 46.0, 22.5, 21.5, 12.4, 6.7, 4.3. IR (neat)  $\nu$  663, 816, 1166, 1351, 1586, 2872, 2916, 2963  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 368.1291, Found: 368.1288.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

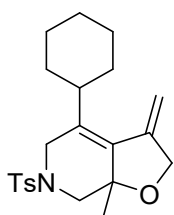




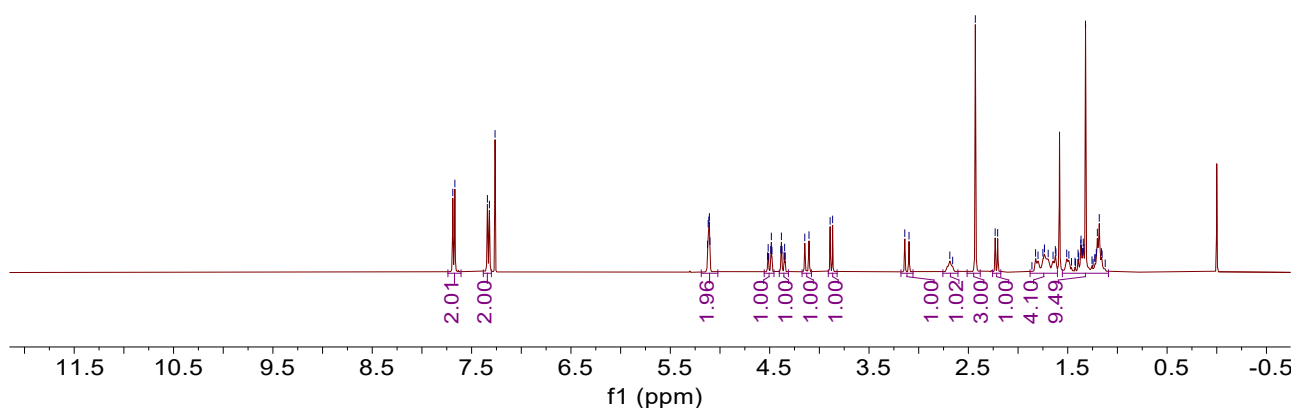


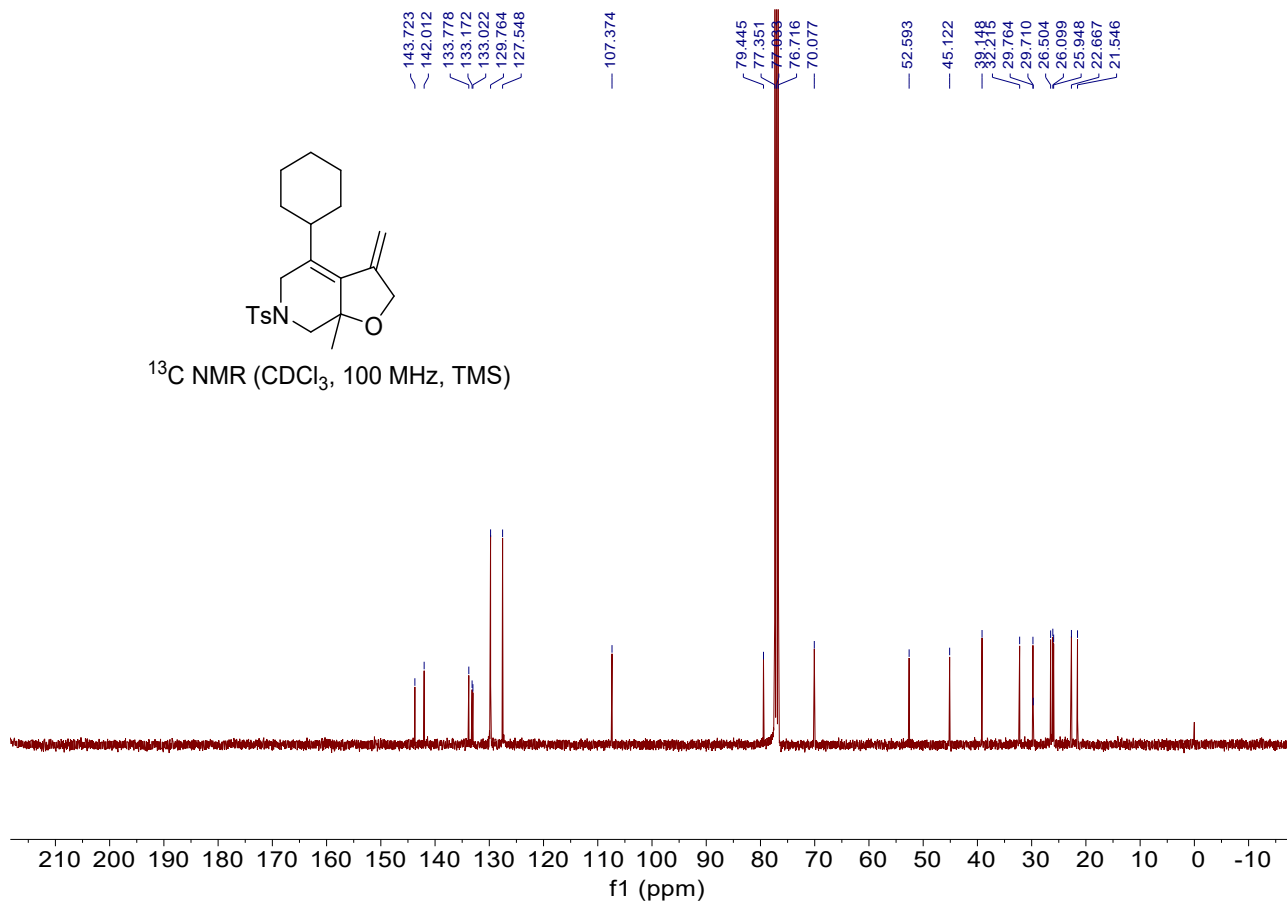
#### 4-cyclohexyl-7a-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3e)

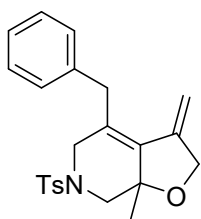
A colorless oil, 82% yield, 31.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.68 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 5.19 – 5.02 (m, 2H), 4.50 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.37 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.13 (d,  $J = 17.0$  Hz, 1H), 3.88 (d,  $J = 10.0$  Hz, 1H), 3.12 (d,  $J = 17.2$  Hz, 1H), 2.76 – 2.61 (m, 1H), 2.43 (s, 3H), 2.22 (d,  $J = 10.0$  Hz, 1H), 1.88 – 1.60 (m, 4H), 1.55 – 1.09 (m, 9H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz) 143.7, 142.0, 133.8, 133.2, 133.0, 129.8, 127.5, 107.4, 79.4, 70.1, 52.6, 45.1, 39.1, 32.2, 29.8, 29.7, 26.5, 26.1, 25.9, 22.7, 21.5. IR (neat)  $\nu$  668, 815, 1164, 1351, 1597, 2853, 2927, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{29}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 410.1760, Found: 410.1767.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

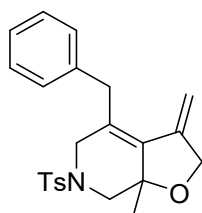




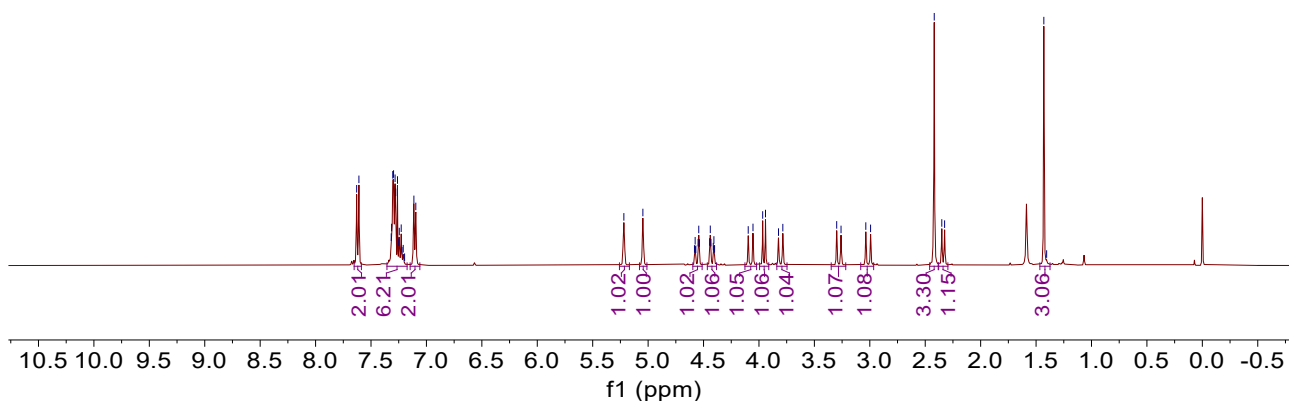


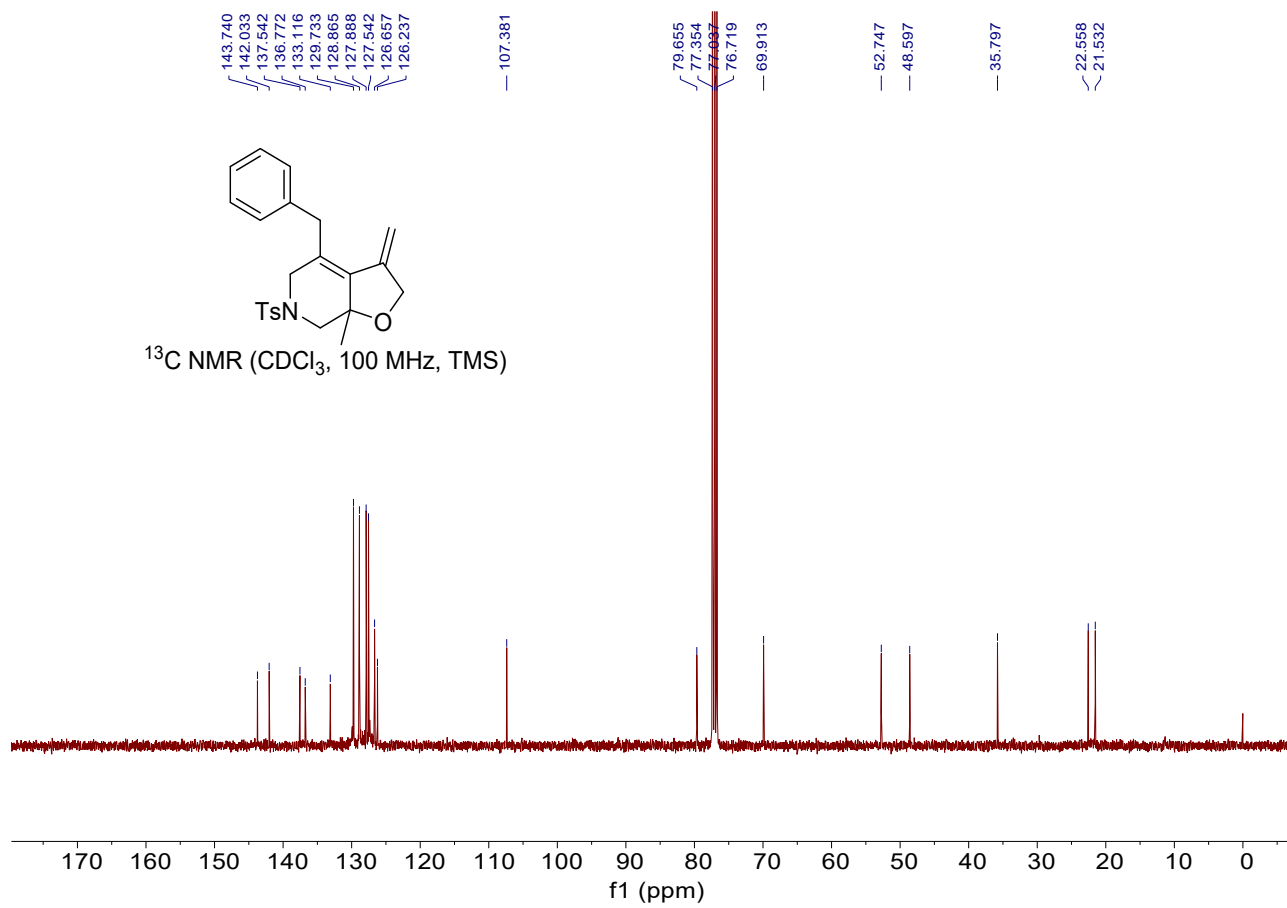
#### 4-cyclohexyl-7a-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3f)

A yellow oil, 86% yield, 33.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.62 (d,  $J = 8.4$  Hz, 2H), 7.36 – 7.17 (m, 5H), 7.10 (d,  $J = 6.8$  Hz, 2H), 5.22 (s, 1H), 5.05 (s, 1H), 4.56 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.42 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.08 (d,  $J = 17.4$  Hz, 1H), 3.95 (d,  $J = 10.0$  Hz, 1H), 3.80 (d,  $J = 15.6$  Hz, 1H), 3.28 (d,  $J = 15.6$  Hz, 1H), 3.01 (d,  $J = 17.4$  Hz, 1H), 2.42 (s, 3H), 2.34 (d,  $J = 10.0$  Hz, 1H), 1.43 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.7, 142.0, 137.5, 136.8, 133.1, 129.7, 128.9, 127.9, 127.5, 126.7, 126.2, 107.4, 79.7, 69.9, 52.7, 48.6, 35.8, 22.6, 21.5. IR (neat)  $\nu$  668, 815, 1162, 1351, 1557, 2869, 2927, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1444.

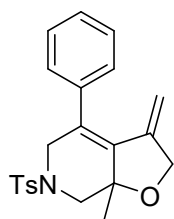


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



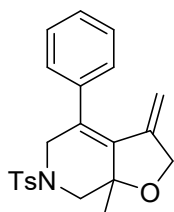




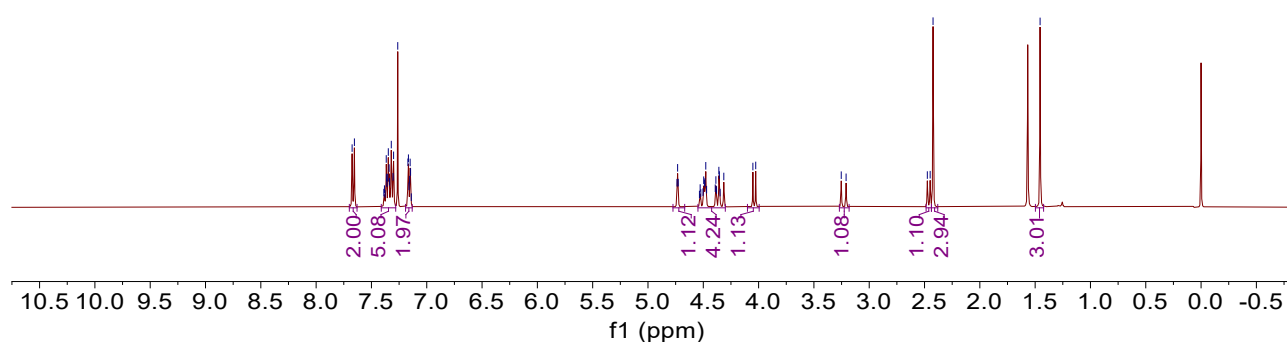


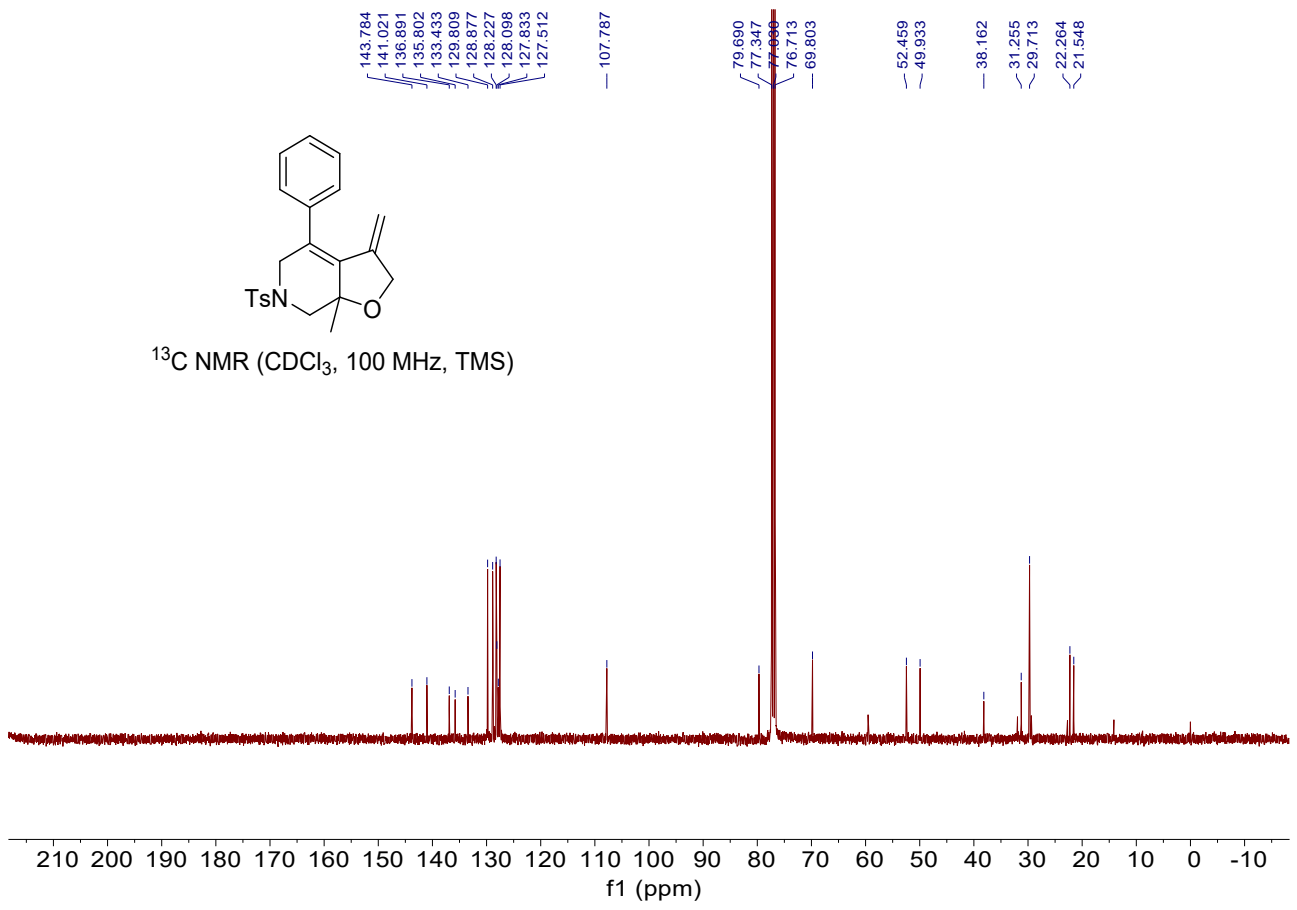
**7a-methyl-3-methylene-4-phenyl-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3i)**

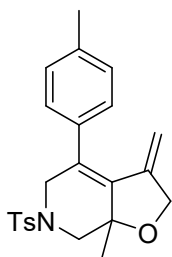
A yellow oil, 76% yield, 29.0 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.66 (d,  $J = 8.4$  Hz, 2H), 7.41 – 7.28 (m, 5H), 7.19 – 7.13 (m, 2H), 4.73 (d,  $J = 2.4$  Hz, 1H), 4.55 – 4.30 (m, 4H), 4.04 (d,  $J = 10.4$  Hz, 1H), 3.23 (d,  $J = 17.6$  Hz, 1H), 2.46 (d,  $J = 10.4$  Hz, 1H), 2.42 (s, 3H), 1.46 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.8, 141.0, 136.9, 135.8, 133.4, 129.8, 128.9, 128.2, 128.1, 127.8, 127.5, 107.8, 79.7, 69.8, 52.5, 49.9, 38.2, 31.3, 29.7, 22.3, 21.5. IR (neat)  $\nu$  668, 816, 1162, 1351, 1558, 2872, 2919, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 404.1291, Found: 404.1292.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

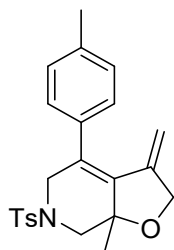




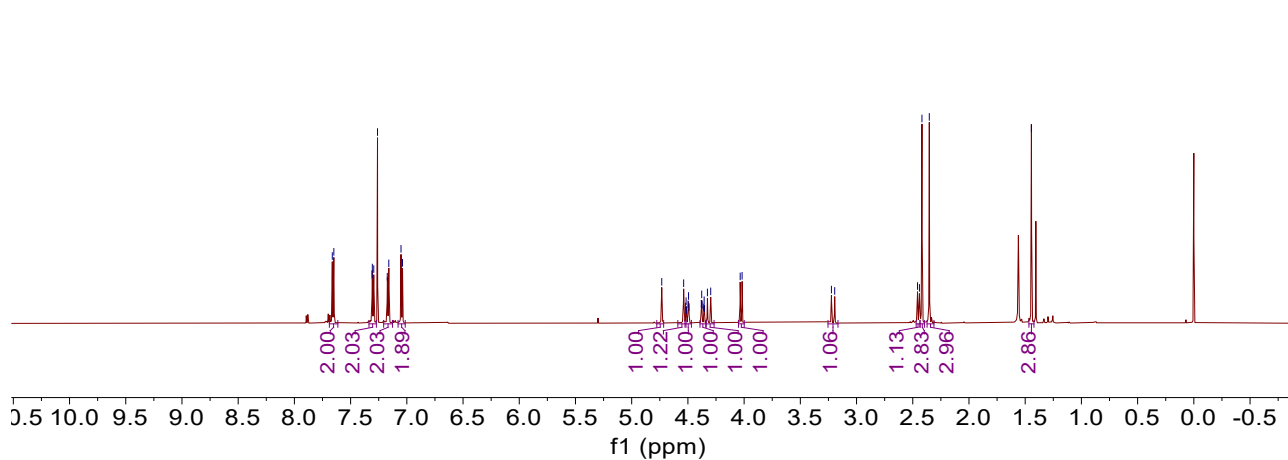


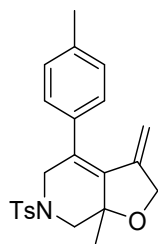
**7a-methyl-3-methylene-4-(p-tolyl)-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3j)**

A colorless oil, 72% yield, 28.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.66 (d,  $J = 8.2$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 7.17 (d,  $J = 8.2$  Hz, 2H), 7.05 (d,  $J = 8.0$  Hz, 2H), 4.73 (s, 1H), 4.54 (s, 1H), 4.51 (dt,  $J = 13.0, 2.4$  Hz, 1H), 4.37 (dt,  $J = 13.0, 2.4$  Hz, 1H), 4.31 (d,  $J = 17.6$  Hz, 1H), 4.03 (d,  $J = 10.2$  Hz, 1H), 3.21 (d,  $J = 17.6$  Hz, 1H), 2.45 (d,  $J = 10.2$  Hz, 1H), 2.42 (s, 3H), 2.35 (s, 3H), 1.45 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.7, 141.1, 137.9, 135.6, 133.9, 133.4, 132.3, 129.8, 129.5, 128.1, 127.8, 127.5, 107.6, 79.7, 69.8, 52.5, 50.0, 22.3, 21.5, 21.3. IR (neat)  $\nu$  680, 1218, 1364, 1569, 2963, 3021  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1449.

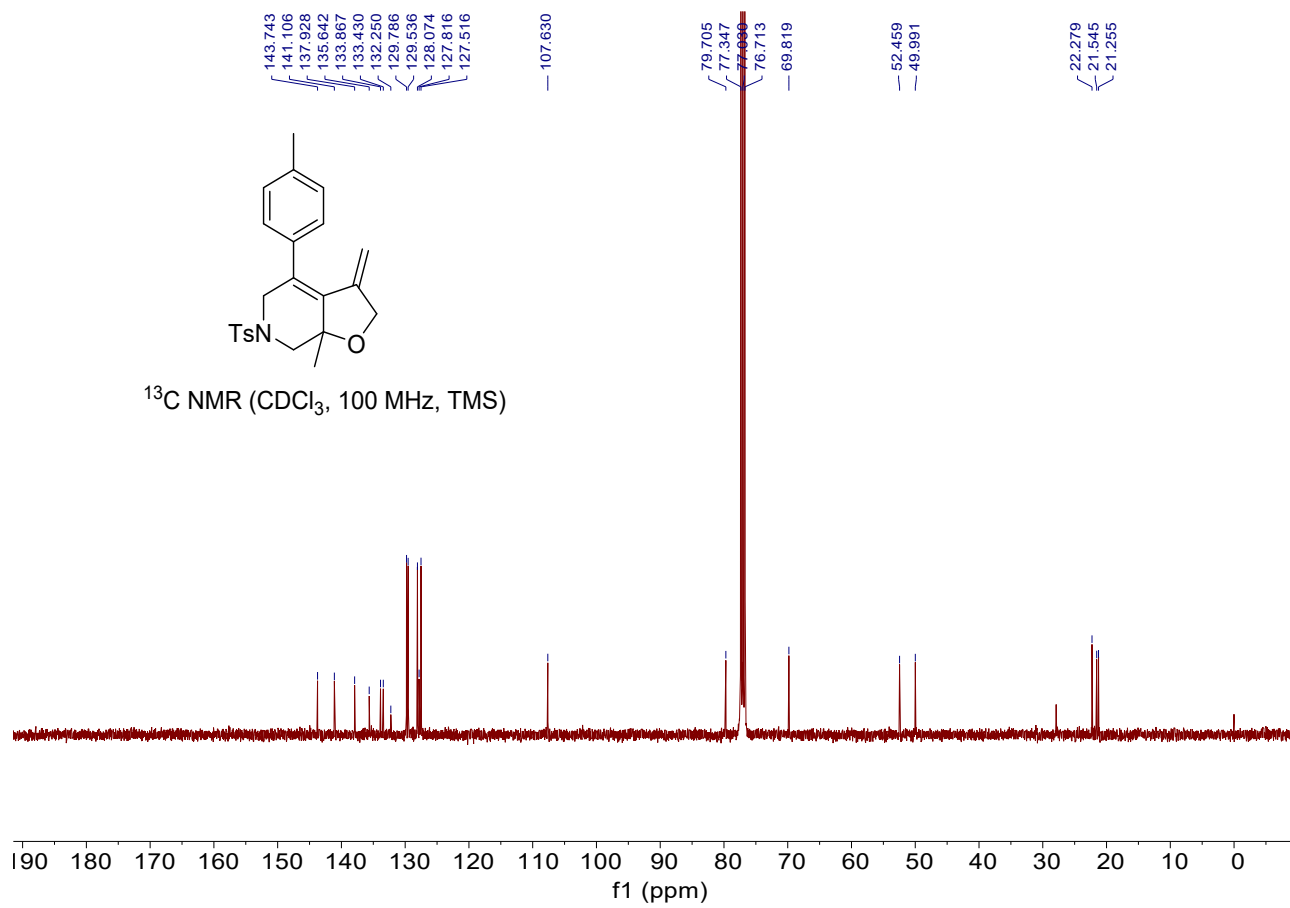


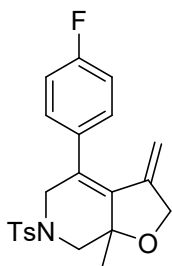
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





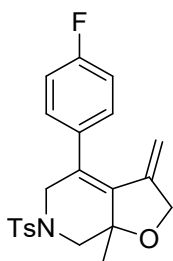
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



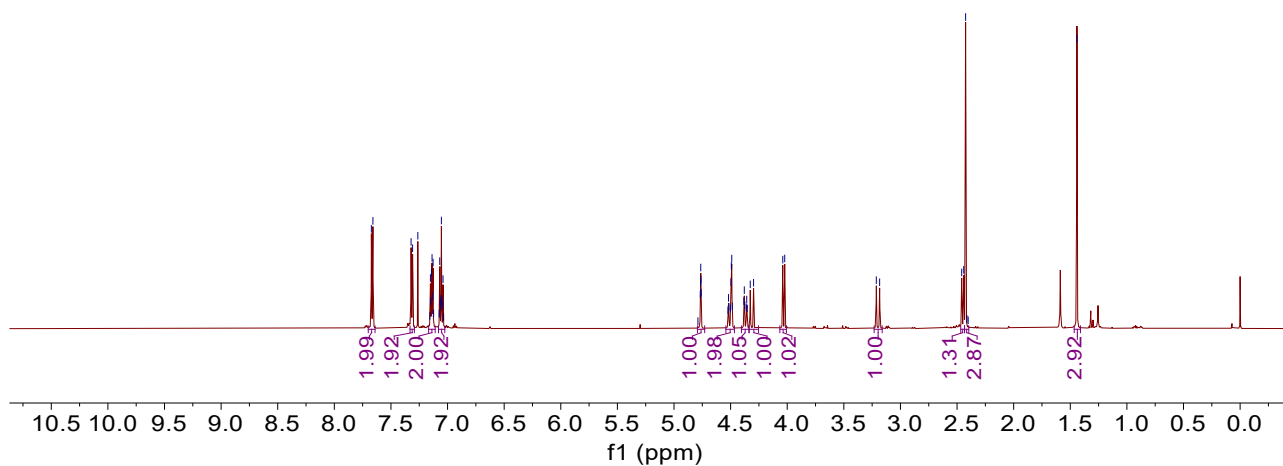


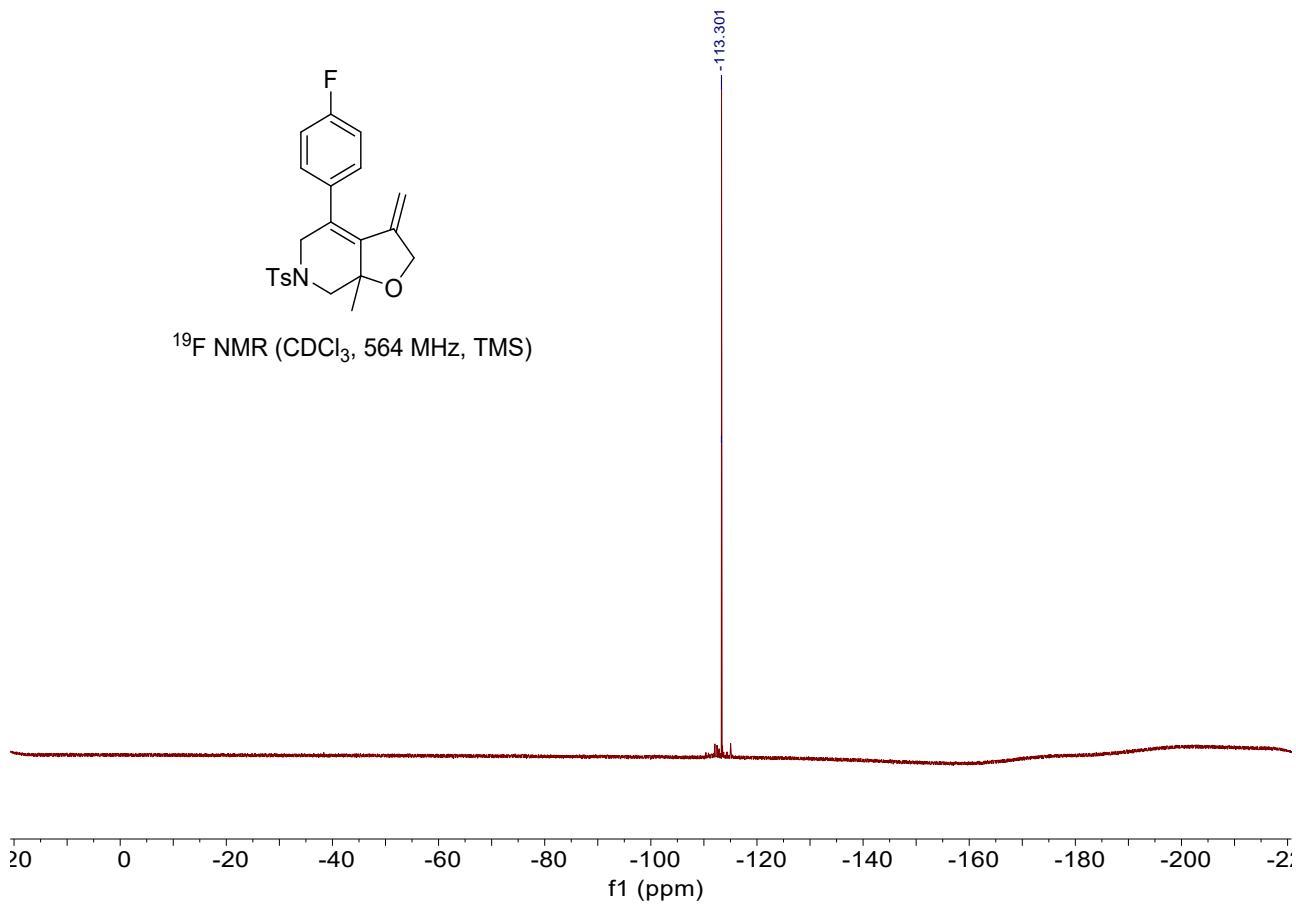
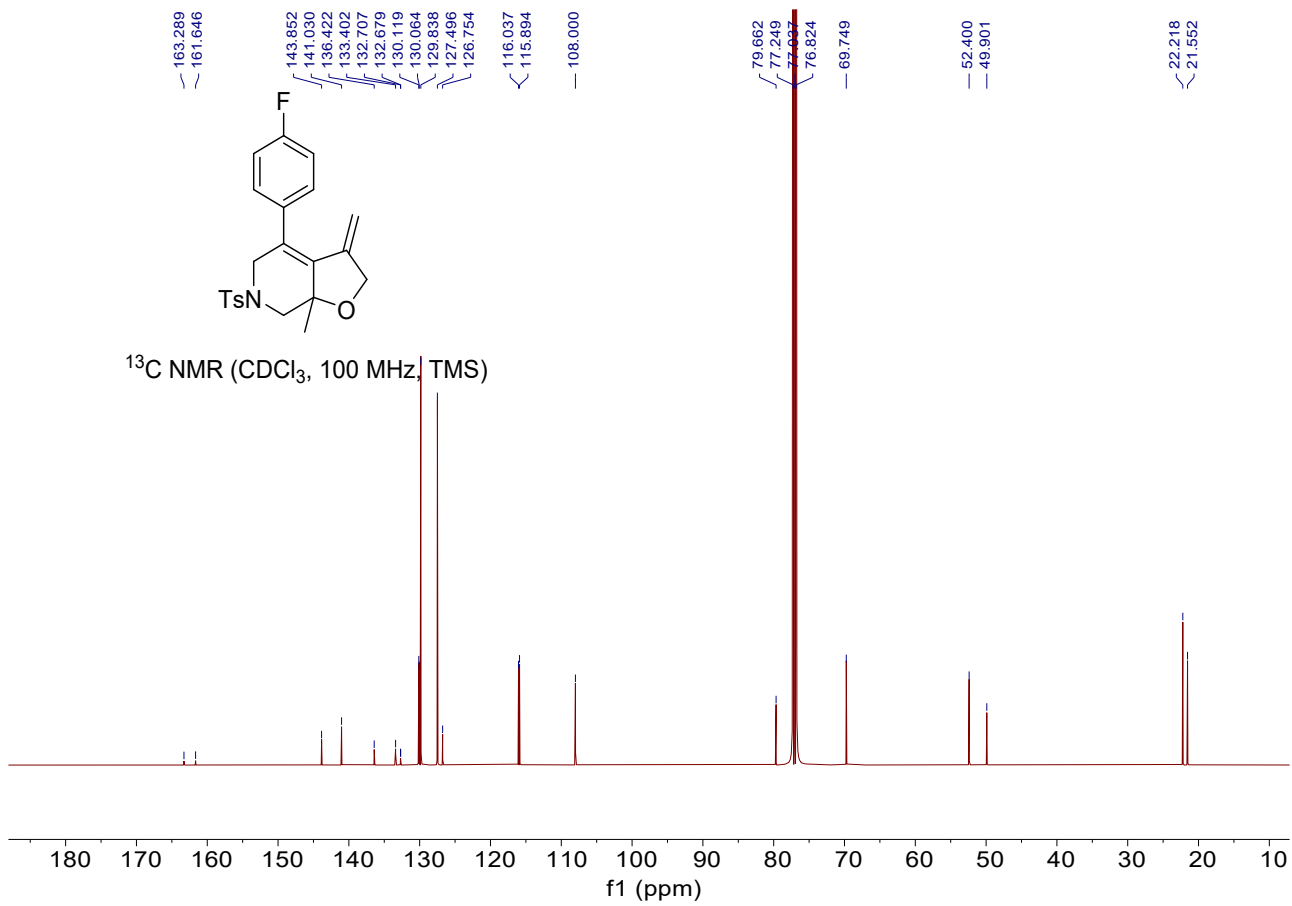
**4-(4-fluorophenyl)-7a-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3k)**

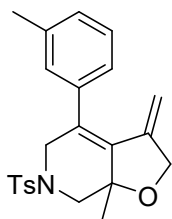
A yellow oil, 76% yield, 30.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.67 (d,  $J = 8.4$  Hz, 2H), 7.32 (d,  $J = 8.4$  Hz, 2H), 7.17 – 7.11 (m, 2H), 7.08 – 7.02 (m, 2H), 4.79 – 4.73 (m, 1H), 4.54 – 4.47 (m, 2H), 4.37 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.31 (d,  $J = 17.6$  Hz, 1H), 4.03 (d,  $J = 10.4$  Hz, 1H), 3.20 (d,  $J = 17.6$  Hz, 1H), 2.45 (d,  $J = 10.8$  Hz, 1H), 2.42 (s, 3H), 1.44 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  162.5 (d,  $J_{\text{C-F}} = 248.9$  Hz), 143.9, 141.0, 136.4, 133.4, 132.70, 132.67, 130.1 (d,  $J_{\text{C-F}} = 8.3$  Hz), 129.8, 127.5, 126.8, 116.0 (d,  $J_{\text{C-F}} = 21.6$  Hz), 108.0, 79.7, 69.7, 52.4, 49.9, 22.2, 21.6.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.3. IR (neat)  $\nu$  660, 837, 1022, 1351, 2858, 2918  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{FSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1192.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

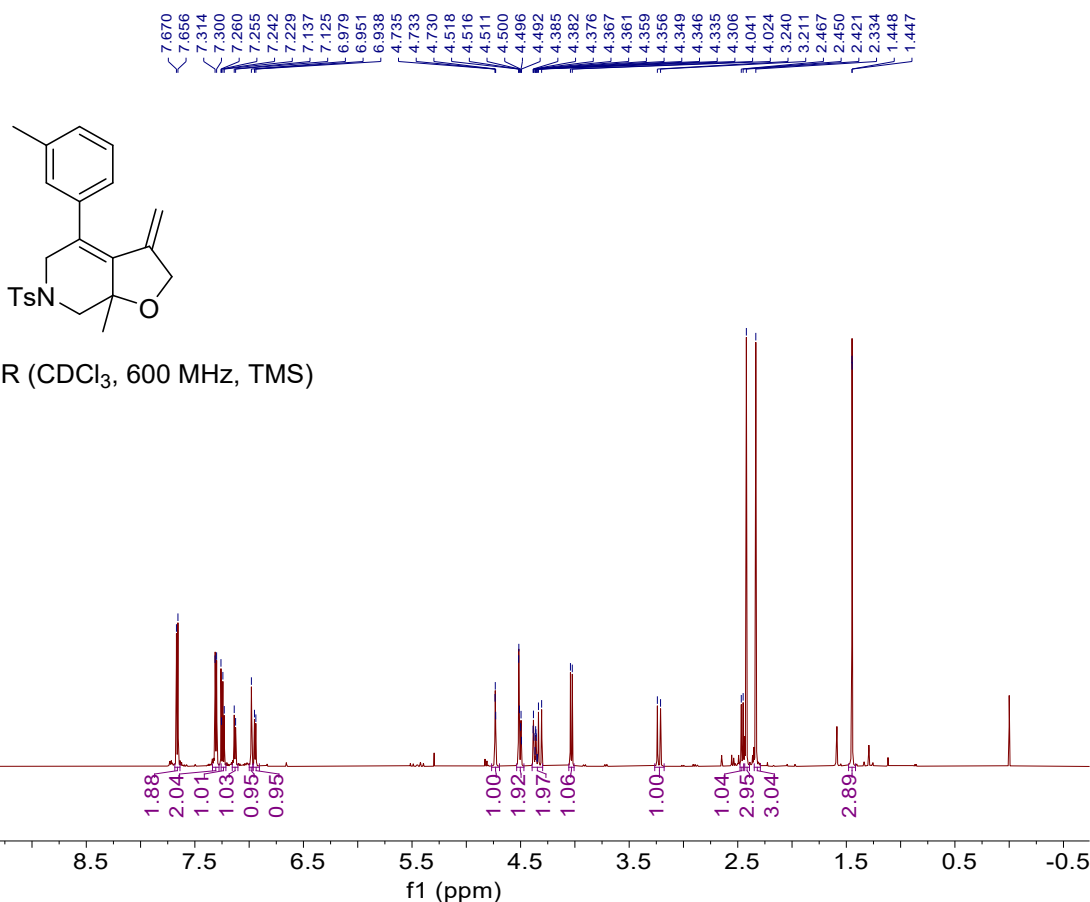


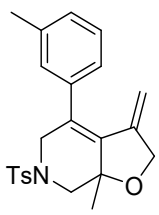




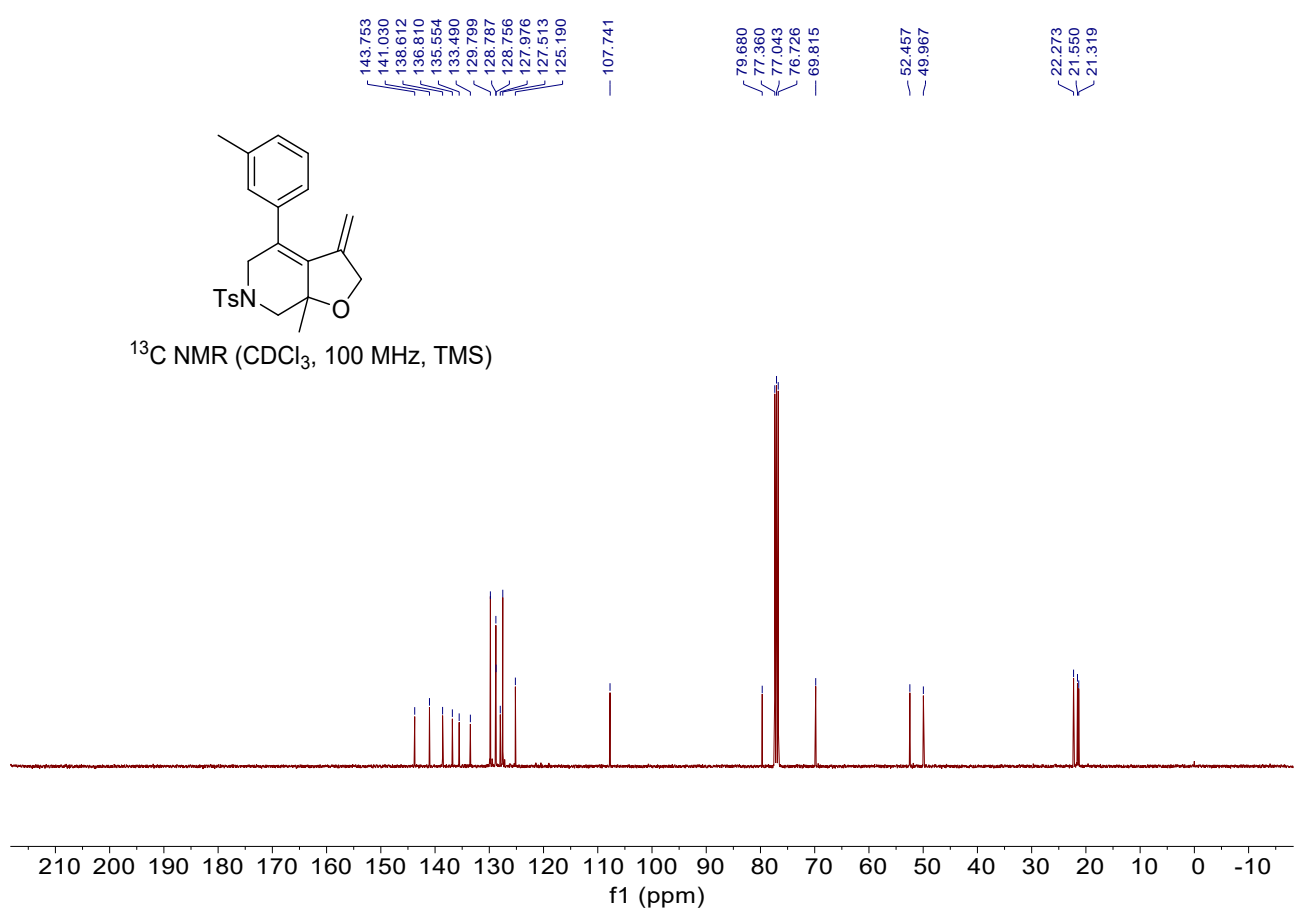
**7a-methyl-3-methylene-4-(m-tolyl)-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3l)**

A colorless oil, 70% yield, 27.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.66 (d,  $J = 8.4$  Hz, 2H), 7.31 (d,  $J = 8.4$  Hz, 2H), 7.24 (t,  $J = 7.6$  Hz, 1H), 7.13 (d,  $J = 7.6$  Hz, 1H), 6.98 (s, 1H), 6.94 (d,  $J = 7.6$  Hz, 1H), 4.77 – 4.69 (m, 1H), 4.54 – 4.47 (m, 2H), 4.39 – 4.30 (m, 2H), 4.03 (d,  $J = 10.4$  Hz, 1H), 3.23 (d,  $J = 17.6$  Hz, 1H), 2.46 (d,  $J = 10.4$  Hz, 1H), 2.42 (s, 3H), 2.33 (s, 3H), 1.45 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.8, 141.0, 138.6, 136.8, 135.6, 133.5, 129.8, 128.78, 128.75, 128.0, 127.5, 125.2, 107.7, 79.7, 69.8, 52.5, 50.0, 22.3, 21.5, 21.3. IR (neat)  $\nu$  667, 778, 1164, 1350, 1598, 2864, 2927, 2971  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1450.

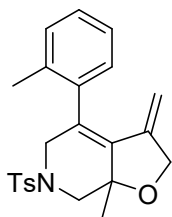




<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)

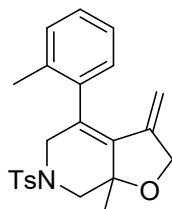




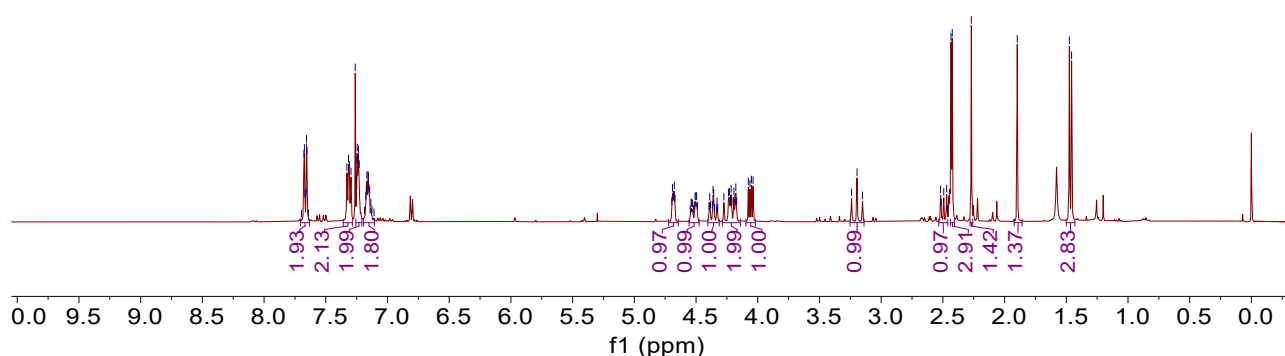


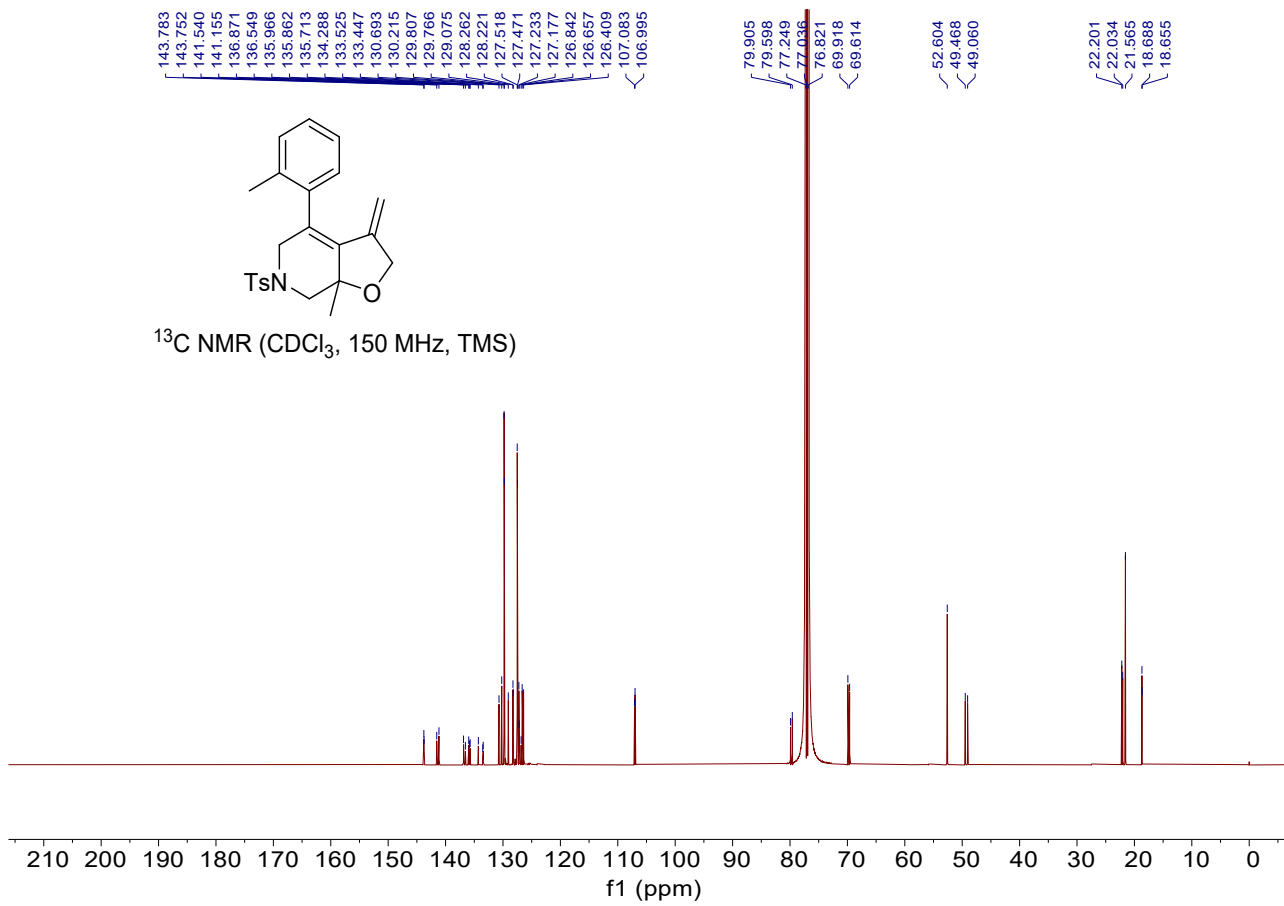
**7a-methyl-3-methylene-4-(o-tolyl)-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3m)**

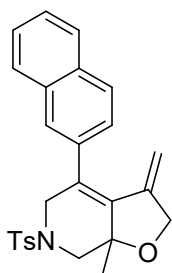
A colorless oil, 68% yield, 27.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.70 – 7.63 (m, 2H), 7.36 – 7.28 (m, 2H), 7.26 – 7.21 (m, 2H), 7.19 – 7.11 (m, 2H), 4.72 – 4.64 (m, 1H), 4.56 – 4.48 (m, 1H), 4.40 – 4.31 (m, 1H), 4.29 – 4.14 (m, 2H), 4.10 – 4.02 (m, 1H), 3.25 – 3.14 (m, 1H), 2.53 – 2.46 (m, 1H), 2.44 – 2.41 (m, 3H), 2.27 (s, 1.5 H), 1.90 (s, 1.5 H), 1.43 – 1.50 (m, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.78, 143.75, 141.5, 141.2, 136.9, 136.5, 136.0, 135.9, 135.7, 134.3, 133.5, 133.4, 130.7, 130.2, 129.80, 129.76, 129.1, 128.3, 128.2, 127.51, 127.47, 127.23, 127.17, 126.8, 126.7, 126.4, 107.1, 107.0, 79.9, 79.6, 69.9, 69.6, 52.6, 49.5, 49.1, 22.2, 22.0, 21.6, 18.68, 18.65. IR (neat)  $\nu$  662, 778, 815, 1167, 13506, 1598, 2866, 2927, 2971  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.1447, Found: 418.1454.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

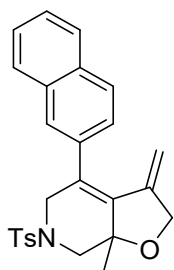




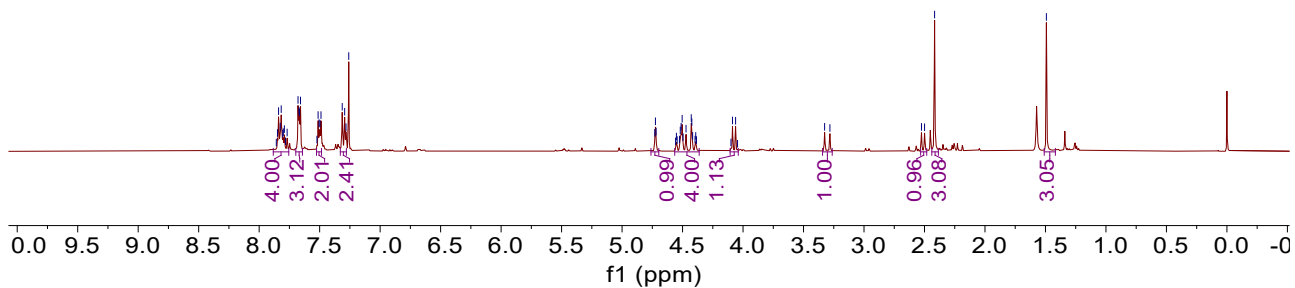


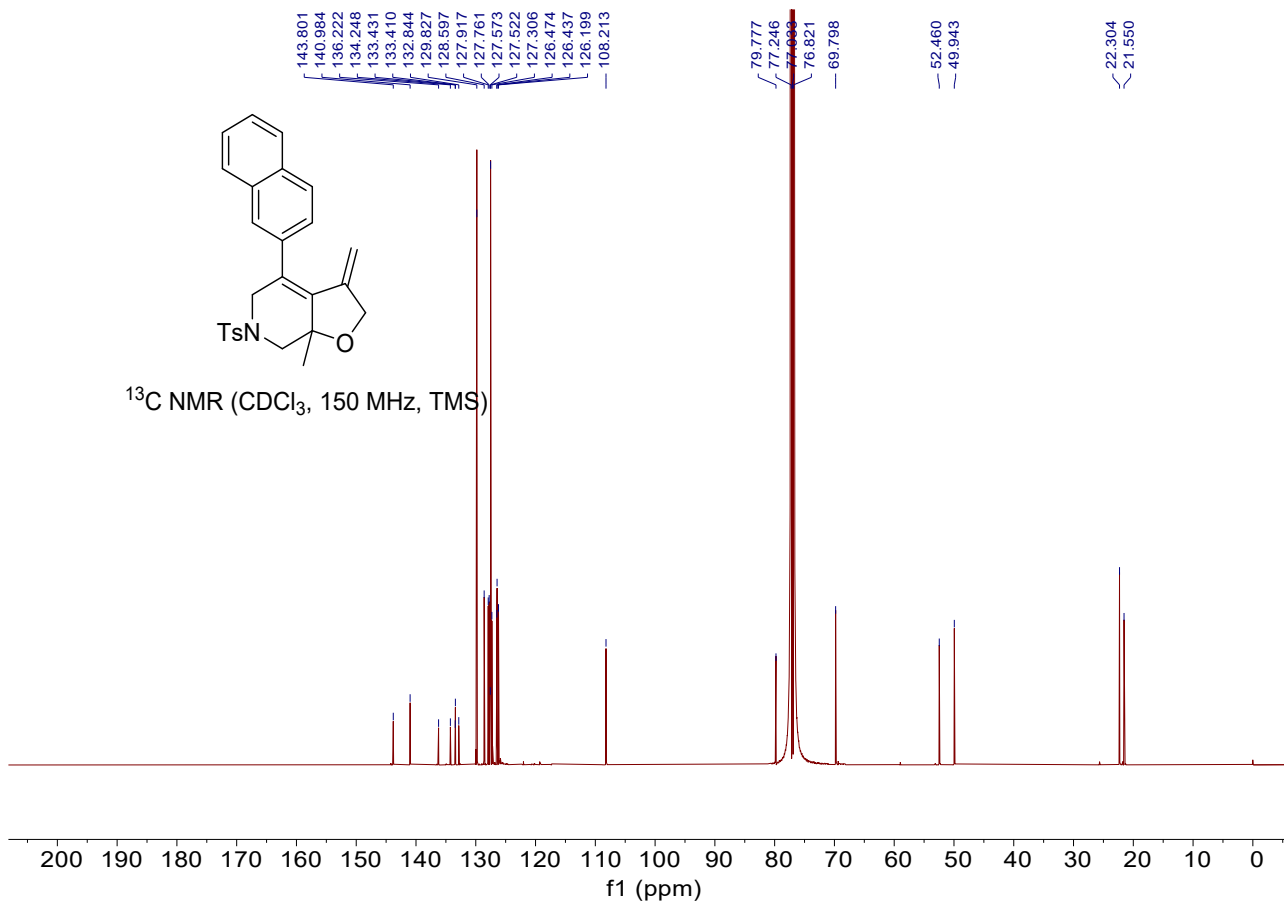
**7a-methyl-3-methylene-4-(naphthalen-2-yl)-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3n)**

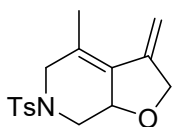
A colorless oil, 68% yield, 27.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.88 – 7.76 (m, 4H), 7.70 – 7.64 (m, 3H), 7.53 – 7.48 (m, 2H), 7.33 – 7.28 (m, 2H), 4.72 (d,  $J = 2.0$  Hz, 1H), 4.56 – 4.36 (m, 4H), 4.07 (d,  $J = 10.2$  Hz, 1H), 3.30 (d,  $J = 17.4$  Hz, 1H), 2.51 (d,  $J = 10.4$  Hz, 1H), 2.42 (s, 3H), 1.49 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.8, 141.0, 136.2, 134.2, 133.43, 133.41, 132.8, 129.8, 128.6, 127.9, 127.8, 127.6, 127.5, 127.3, 126.5, 126.4, 126.2, 108.2, 79.8, 69.8, 52.5, 49.9, 22.3, 21.5. IR (neat)  $\nu$  660, 817, 1159, 1350, 1597, 2858, 2922  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{26}\text{H}_{25}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 454.1447, Found: 454.1452.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

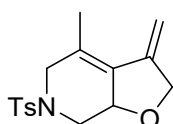




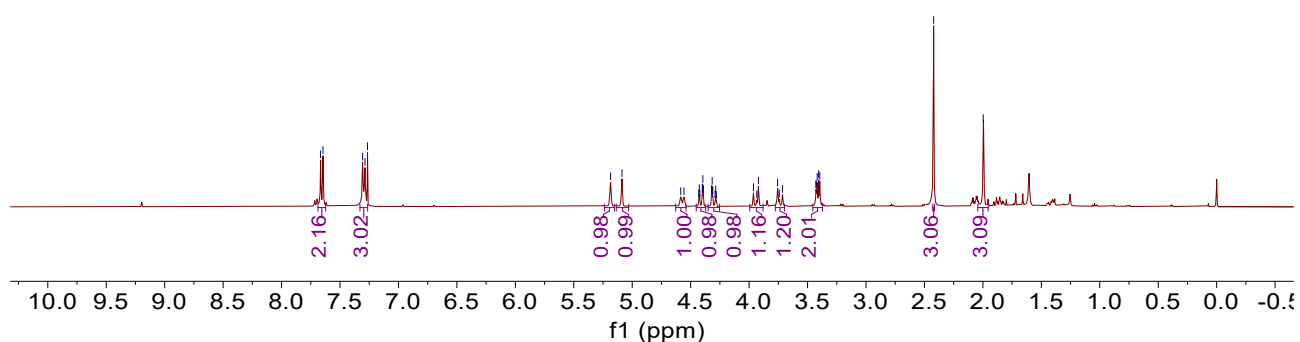


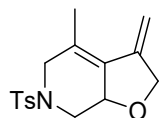
#### 4-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3o)

A colorless oil, 72% yield, 21.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.66 (d,  $J = 8.2$  Hz, 2H), 7.30 (d,  $J = 8.2$  Hz, 2H), 5.19 (s, 1H), 5.09 (s, 1H), 4.57 (d,  $J = 10.8$  Hz, 1H), 4.41 (dt,  $J = 12.0, 2.0$  Hz, 1H), 4.30 (dt,  $J = 12.0, 2.0$  Hz, 1H), 3.99 – 3.88 (m, 1H), 3.78 – 3.70 (m, 1H), 3.46 – 3.37 (m, 2H), 2.42 (s, 3H), 2.00 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  145.2, 143.4, 137.0, 136.1, 130.5, 129.74, 129.69, 127.1, 107.5, 81.2, 72.5, 53.2, 46.4, 32.8, 21.5, 20.3. IR (neat)  $\nu$  668, 814, 1162, 1325, 1596, 2848, 2929, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{19}\text{NO}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 328.0978, Found: 328.0976.

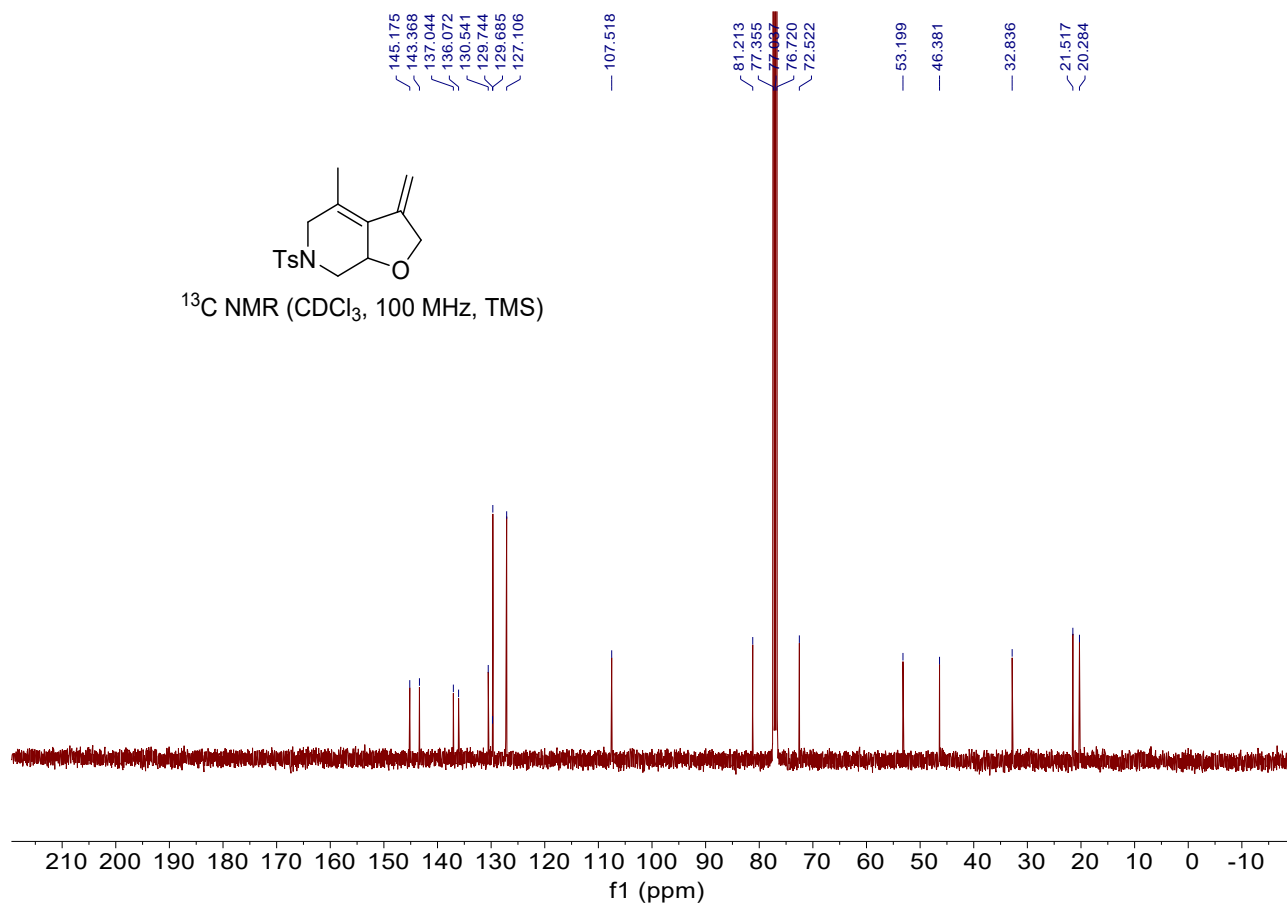


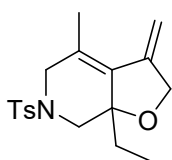
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





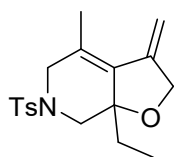
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



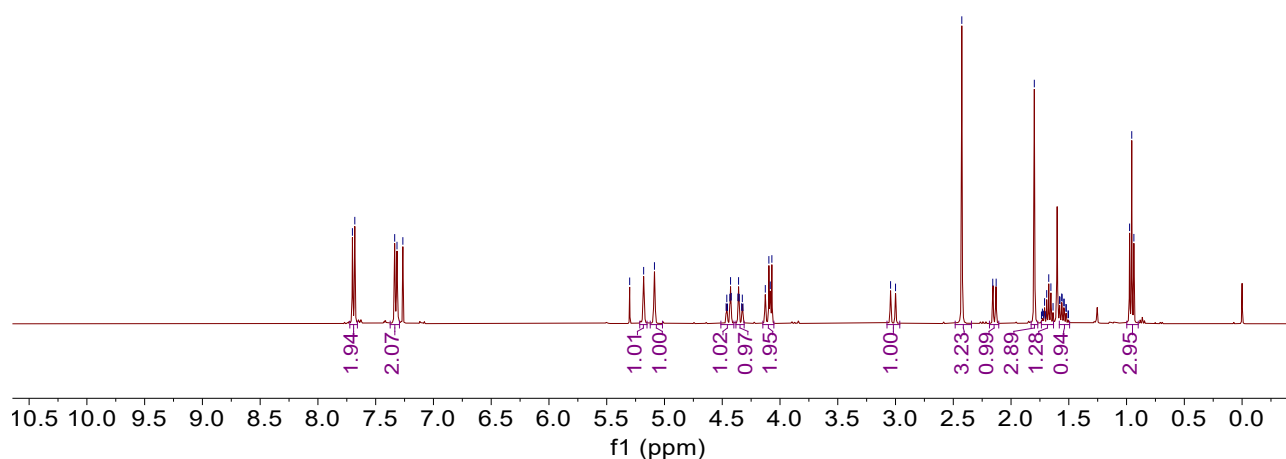


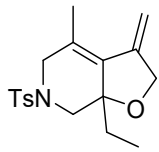
**7a-ethyl-4-methyl-3-methylene-6-tosyl-2,3,5,6,7a-hexahydrofuro[2,3-c]pyridine (3p)**

A colorless oil, 72% yield, 23.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.69 (d,  $J = 8.4$  Hz, 2H), 7.33 (d,  $J = 8.4$  Hz, 2H), 5.18 (s, 1H), 5.09 (s, 1H), 4.44 (dt,  $J = 13.0, 2.4$  Hz, 1H), 4.34 (dt,  $J = 13.0, 2.4$  Hz, 1H), 4.15 – 4.05 (m, 2H), 3.02 (d,  $J = 17.2$  Hz, 1H), 2.43 (s, 3H), 2.14 (d,  $J = 11.8$  Hz, 1H), 1.80 (s, 3H), 1.74 – 1.63 (m, 1H), 1.58 – 1.49 (m, 1H), 0.96 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.7, 143.1, 134.9, 133.3, 129.7, 127.5, 124.2, 107.2, 81.8, 70.0, 49.6, 48.6, 26.6, 21.5, 16.3, 7.4. IR (neat)  $\nu$  667, 817, 1166, 1345, 1596, 2868, 2929, 2964  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{24}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 334.1471, Found: 334.1462.

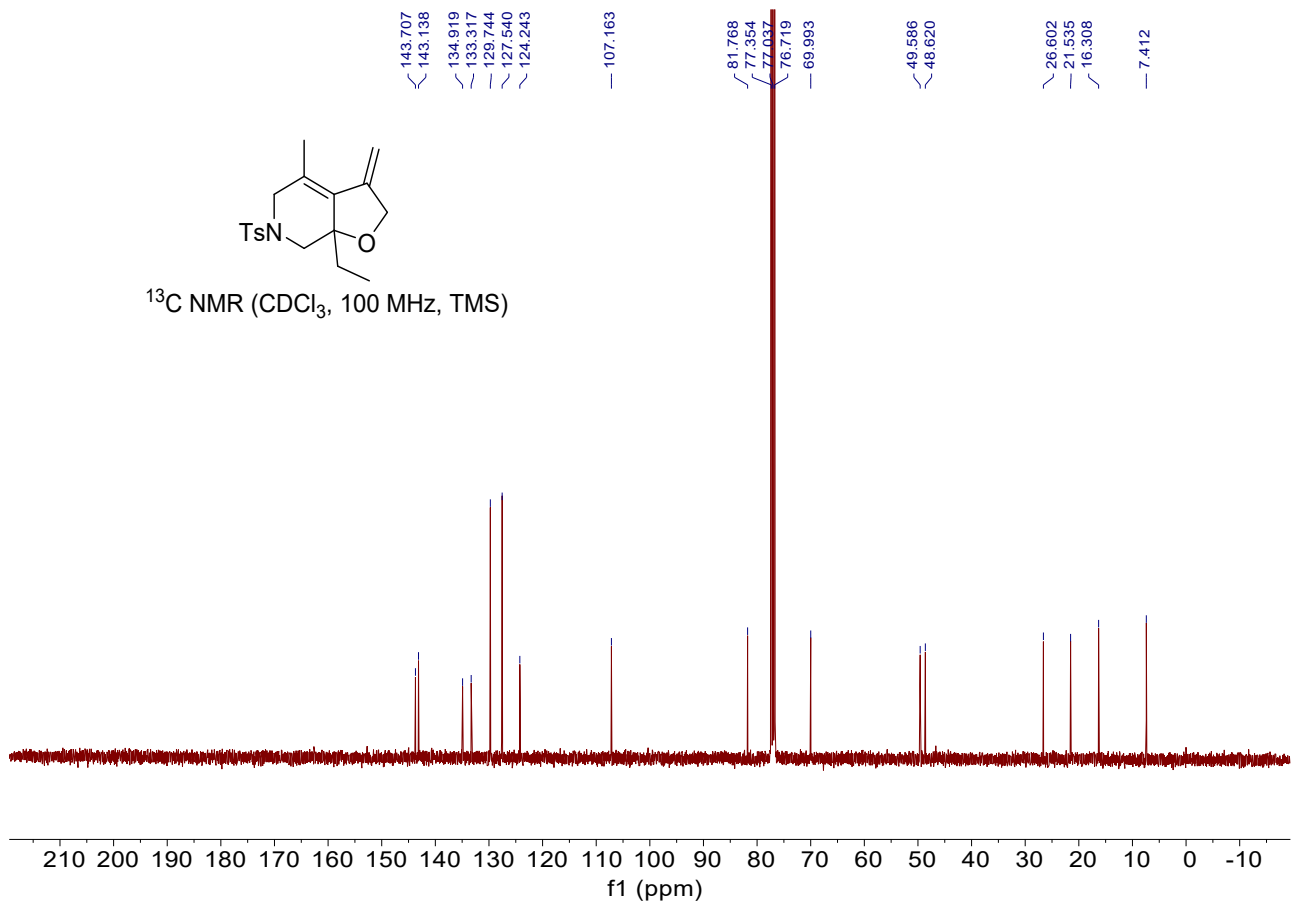


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

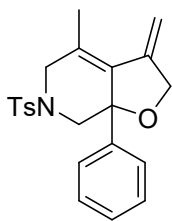




<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)

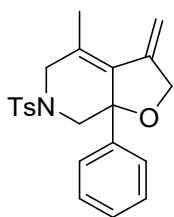




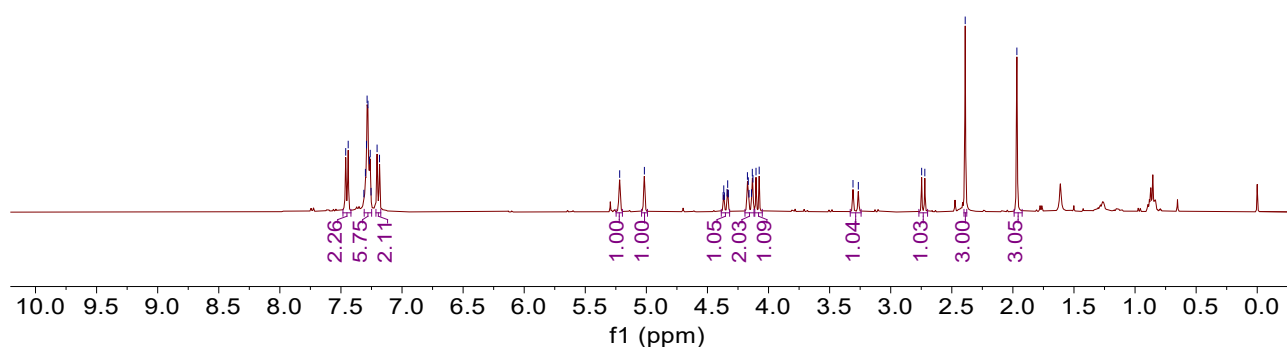


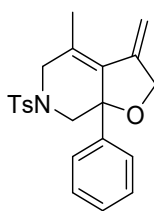
#### 4-methyl-3-methylene-7a-phenyl-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3r)

A colorless oil, 50% yield, 19.1 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.45 (d,  $J = 8.0$  Hz, 2H), 7.31 – 7.25 (m, 5H), 7.19 (d,  $J = 8.0$  Hz, 2H), 5.22 (s, 1H), 5.02 (s, 1H), 4.35 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.19 – 4.12 (m, 2H), 4.09 (d,  $J = 10.4$  Hz, 1H), 3.29 (d,  $J = 17.6$  Hz, 1H), 2.73 (d,  $J = 10.4$  Hz, 1H), 2.39 (s, 3H), 1.97 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.5, 142.9, 140.9, 133.8, 132.6, 129.6, 128.1, 127.7, 127.5, 126.7, 126.3, 107.3, 83.0, 69.9, 53.4, 49.5, 21.5, 16.4. IR (neat)  $\nu$  668, 814, 1163, 1328, 1585, 2848, 2919, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{24}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 382.1471, Found: 382.1464.

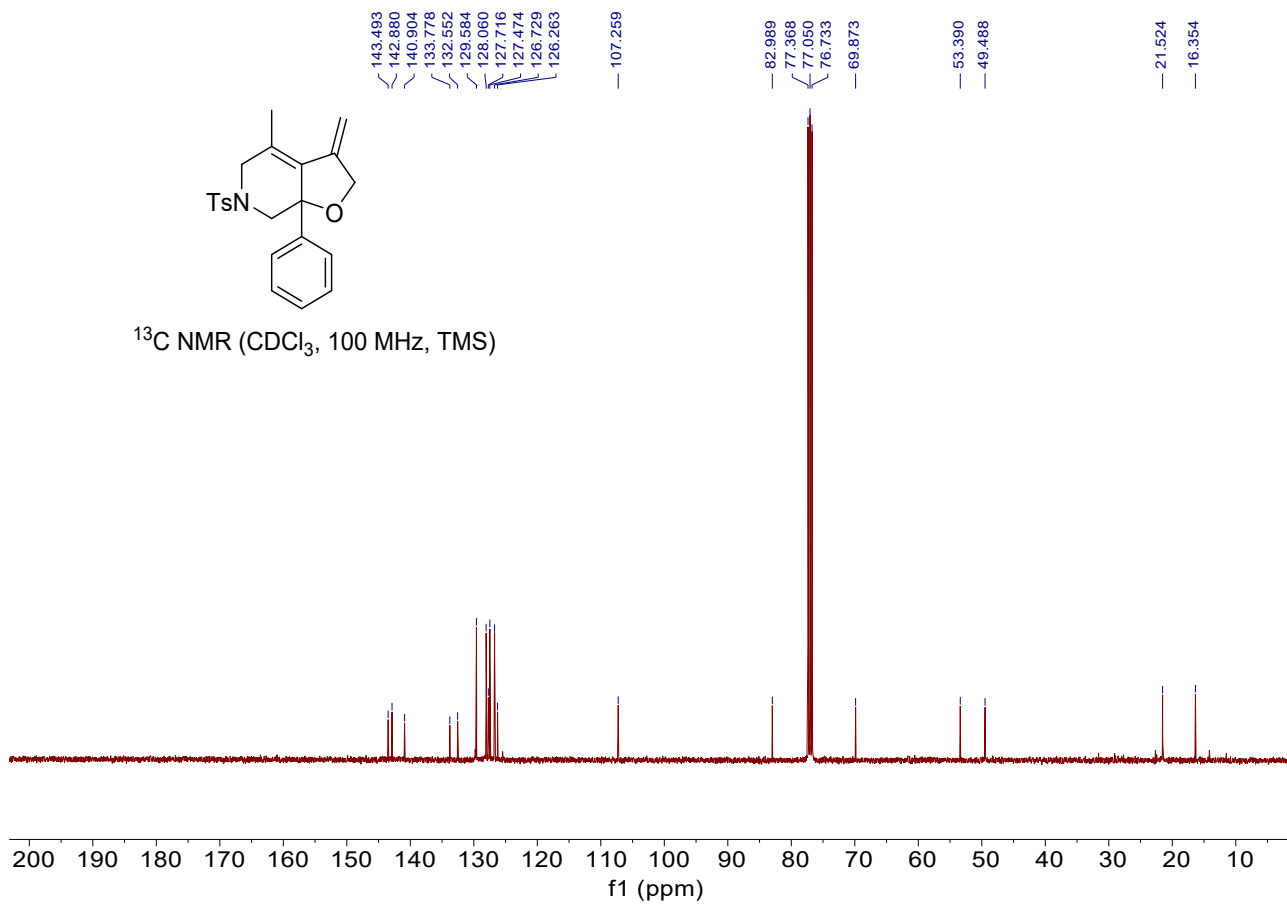


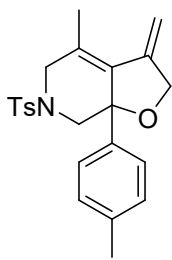
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





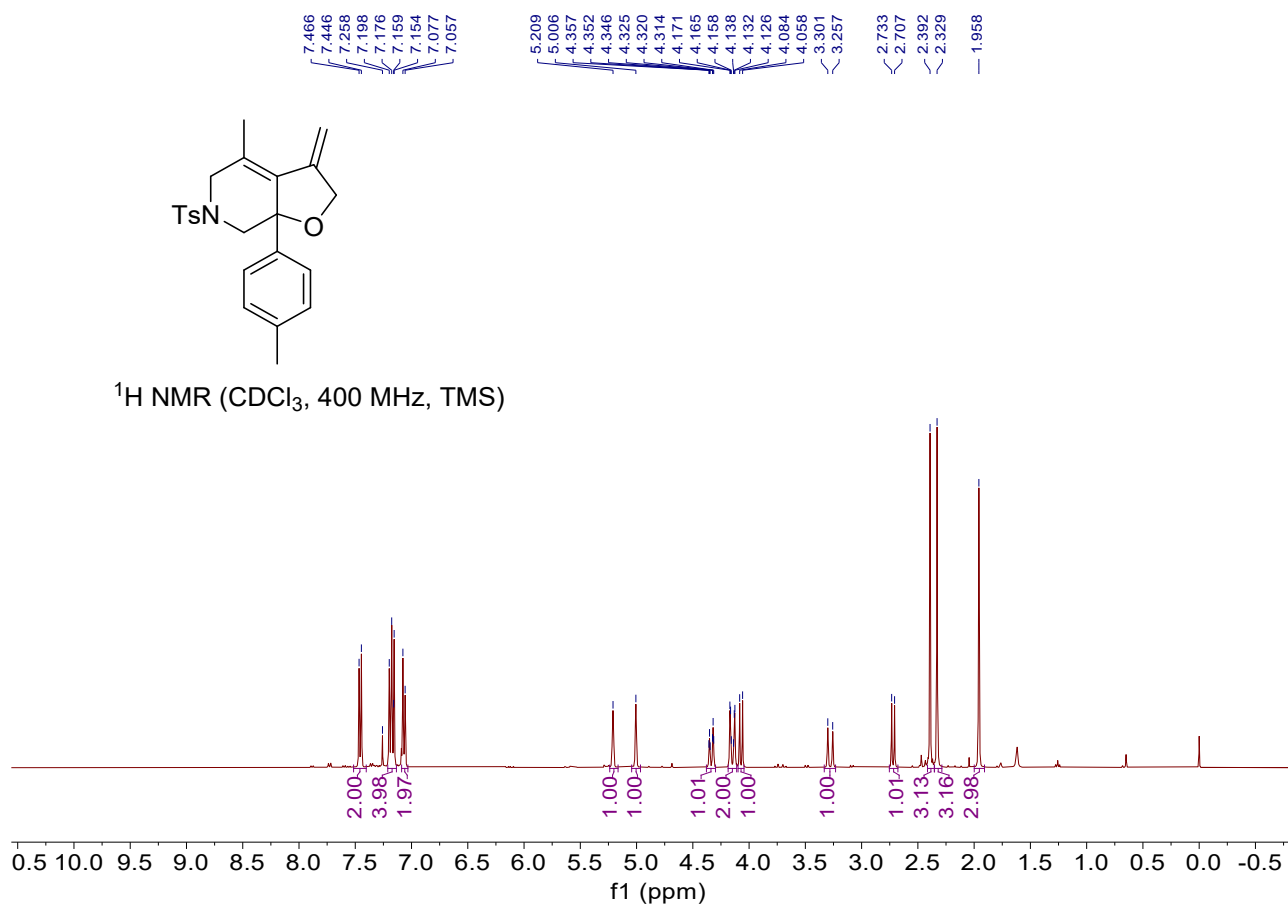
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)





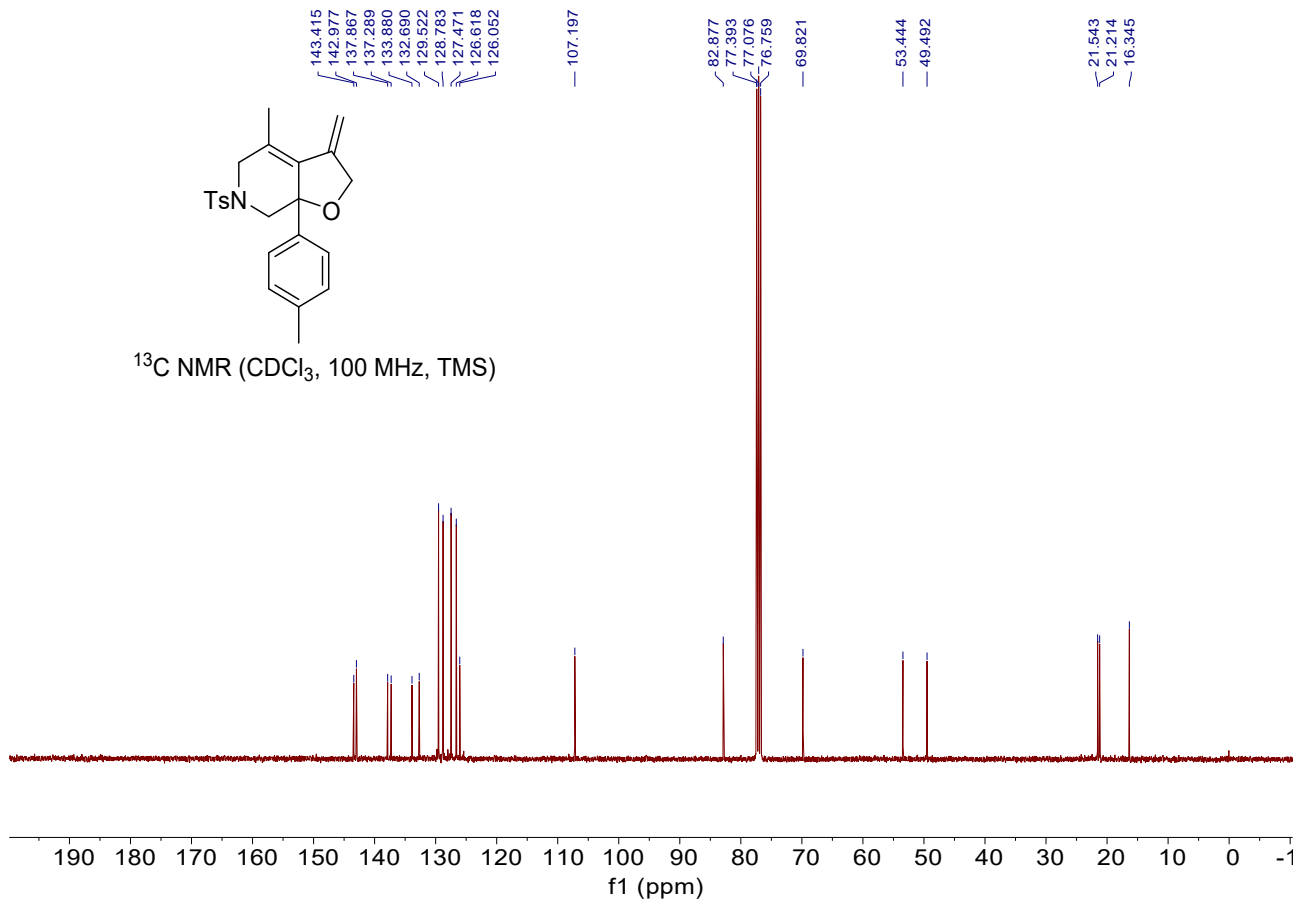
#### 4-methyl-3-methylene-7a-(p-tolyl)-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3s)

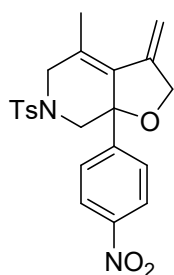
A colorless oil, 48% yield, 19.0 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.46 (d,  $J = 8.0$  Hz, 2H), 7.21 – 7.13 (m, 4H), 7.07 (d,  $J = 8.0$  Hz, 2H), 5.21 (s, 1H), 5.01 (s, 1H), 4.34 (dt,  $J = 12.8, 2.2$  Hz, 1H), 4.19 – 4.11 (m, 2H), 4.07 (d,  $J = 10.4$  Hz, 1H), 3.28 (d,  $J = 17.6$  Hz, 1H), 2.72 (d,  $J = 10.4$  Hz, 1H), 2.39 (s, 3H), 2.33 (s, 3H), 1.96 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.4, 143.0, 137.9, 137.3, 133.9, 132.7, 129.5, 128.8, 127.5, 126.6, 126.1, 107.2, 82.9, 69.8, 53.4, 49.5, 21.5, 21.2, 16.3. IR (neat)  $\nu$  663, 814, 1165, 1328, 1595, 2849, 2939, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{26}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 396.1628, Found: 396.1620.





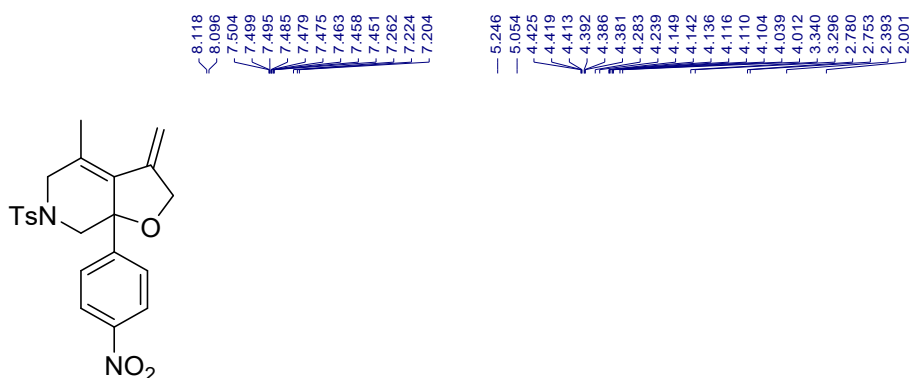
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



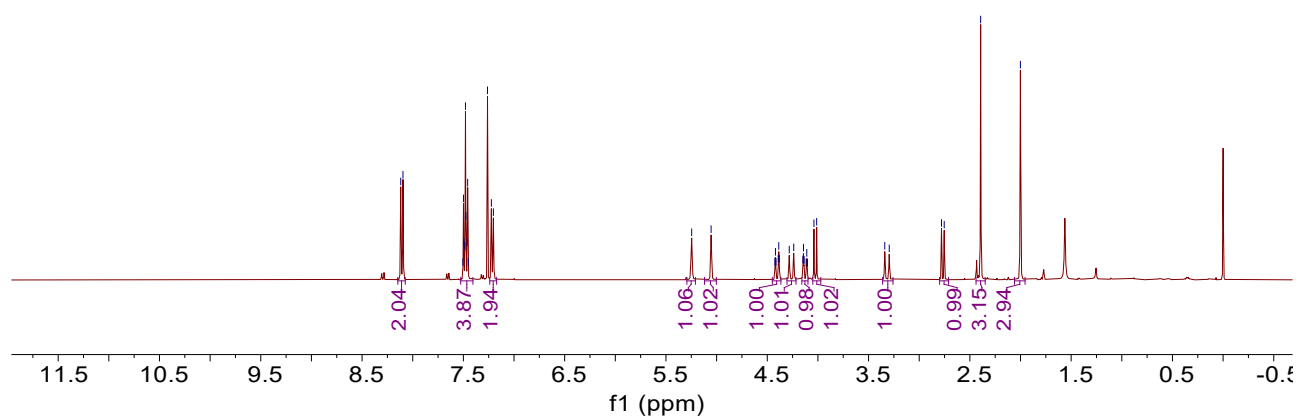


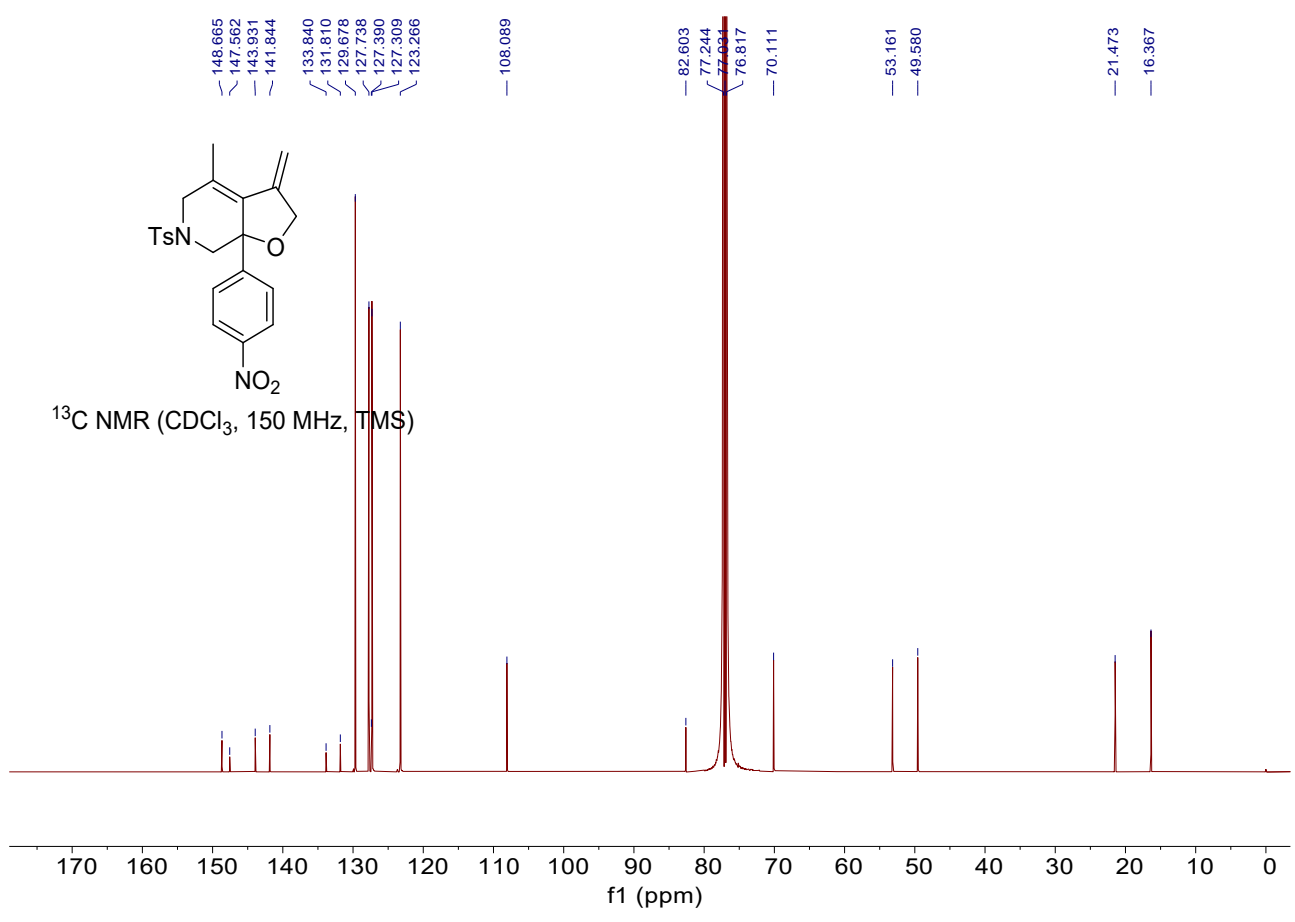
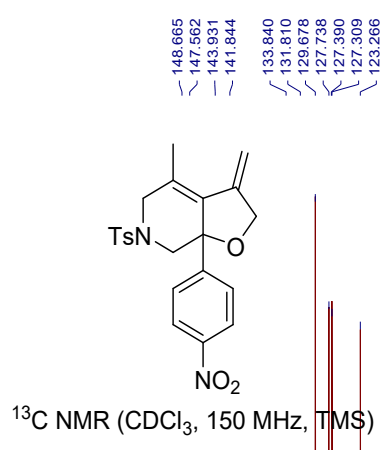
**4-methyl-3-methylene-7a-(4-nitrophenyl)-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3t)**

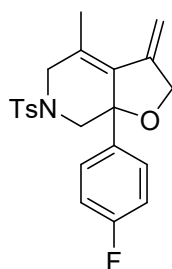
A colorless oil, 62% yield, 26.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  8.11 (d,  $J = 8.0$  Hz, 2H), 7.53 – 7.41 (m, 4H), 7.21 (d,  $J = 8.0$  Hz, 2H), 5.25 (s, 1H), 5.05 (s, 1H), 4.40 (dt,  $J = 13.2, 2.2$  Hz, 1H), 4.26 (d,  $J = 17.6$  Hz, 1H), 4.13 (dt,  $J = 13.2, 2.4$  Hz, 1H), 4.03 (d,  $J = 10.8$  Hz, 1H), 3.32 (d,  $J = 17.6$  Hz, 1H), 2.77 (d,  $J = 10.8$  Hz, 1H), 2.39 (s, 3H), 2.00 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  148.7, 147.6, 143.9, 141.8, 133.8, 131.8, 129.7, 127.7, 127.4, 127.3, 123.3, 108.1, 82.6, 70.1, 53.2, 49.6, 21.5, 16.4. IR (neat)  $\nu$  668, 814, 1162, 1325, 1595, 2848, 2929, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{N}_2\text{O}_5\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 449.1142, Found: 449.1146.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

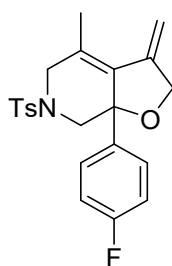




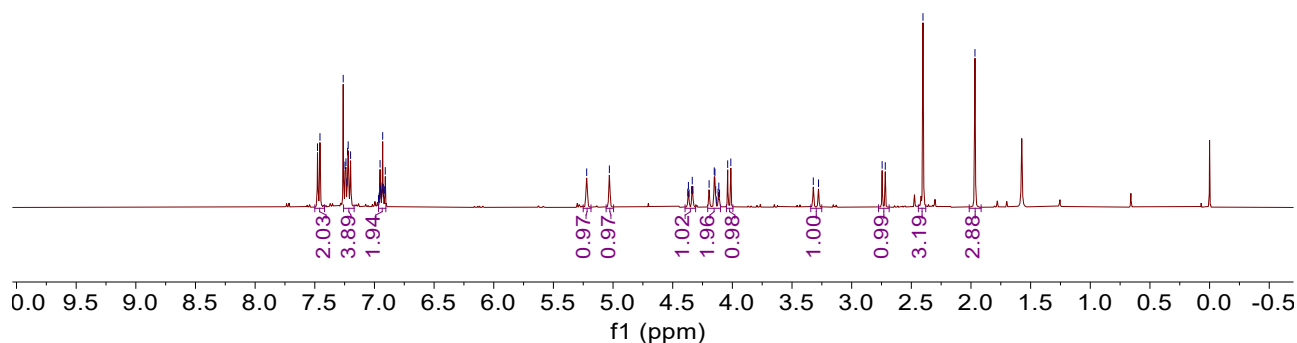


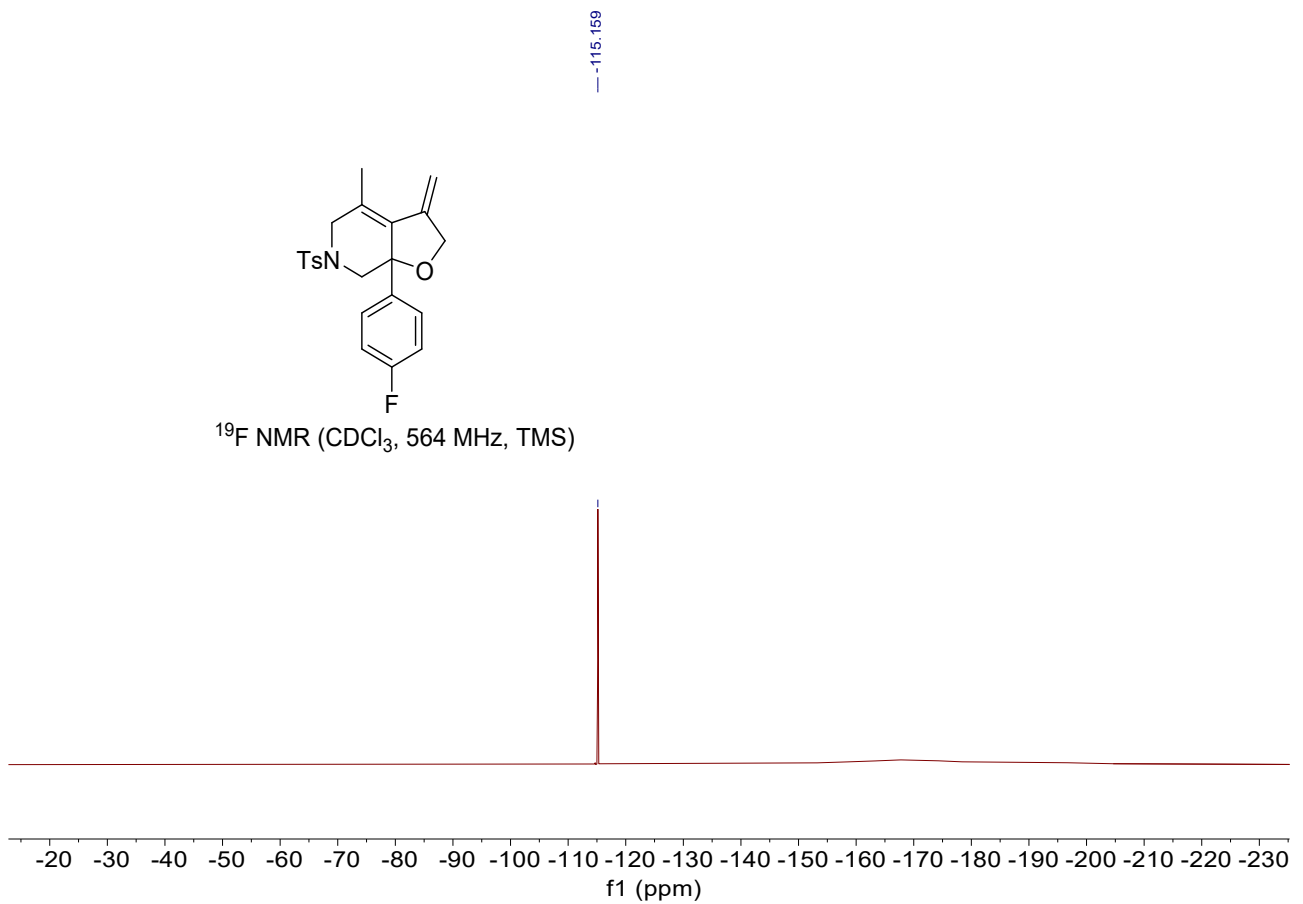
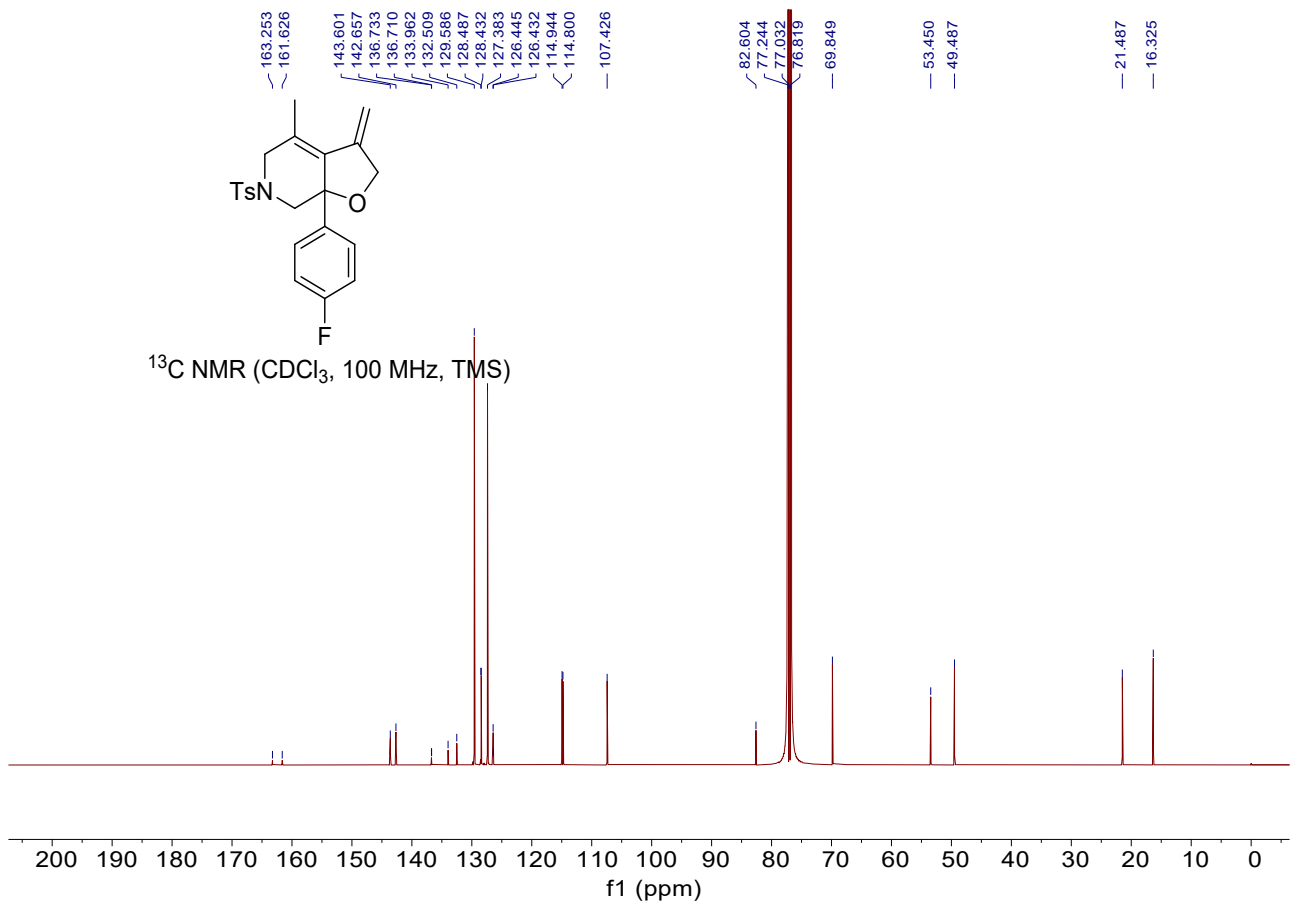
**7a-(4-fluorophenyl)-4-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3u)**

A colorless oil, 58% yield, 23.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.47 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.17 (m, 4H), 6.97 – 6.90 (m, 2H), 5.22 (s, 1H), 5.03 (s, 1H), 4.35 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.21 – 4.10 (m, 2H), 4.03 (d,  $J = 10.4$  Hz, 1H), 3.30 (d,  $J = 17.6$  Hz, 1H), 2.73 (d,  $J = 10.4$  Hz, 1H), 2.40 (s, 3H), 1.97 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  163.2 (d,  $J_{\text{C-F}} = 245.8$  Hz), 143.6, 142.7, 136.73, 136.71, 134.0, 132.5, 129.6, 128.5 (d,  $J_{\text{C-F}} = 8.3$  Hz), 127.4, 126.45, 126.43, 114.9 (d,  $J_{\text{C-F}} = 21.7$  Hz), 107.4, 82.6, 69.8, 53.4, 49.5, 21.5, 16.3.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.2. IR (neat)  $\nu$  667, 817, 1220, 1355, 1506, 2868, 2919, 2963  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{FSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 422.1197, Found: 422.1192.

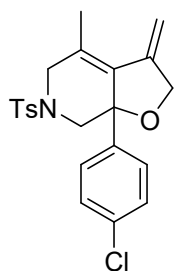


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



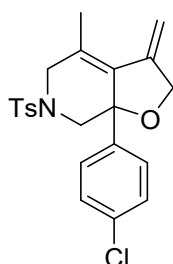




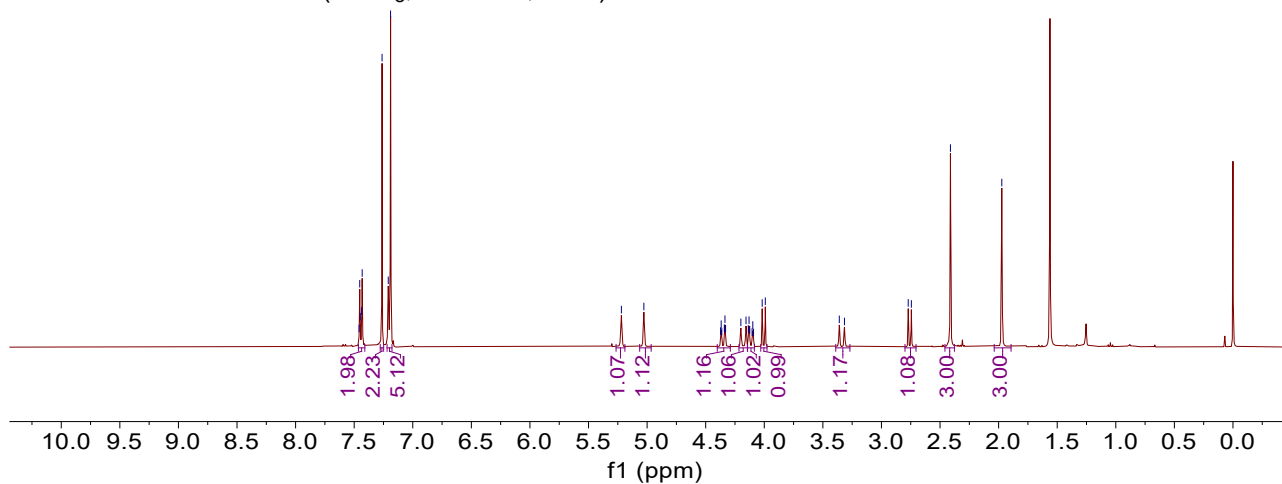


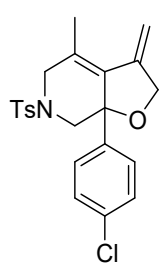
**7a-(4-chlorophenyl)-4-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3v)**

A colorless oil, 60% yield, 26.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.46 – 7.41 (m, 2H), 7.26 (s, 2H), 7.22 – 7.18 (m, 4H), 5.22 (s, 1H), 5.03 (s, 1H), 4.35 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.18 (d,  $J = 17.6$  Hz, 1H), 4.11 (dt,  $J = 12.8, 2.4$  Hz, 1H), 4.00 (d,  $J = 10.4$  Hz, 1H), 3.34 (d,  $J = 17.6$  Hz, 1H), 2.76 (d,  $J = 10.4$  Hz, 1H), 2.41 (s, 3H), 1.97 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.6, 142.5, 134.0, 129.6, 128.19, 128.15, 127.3, 107.5, 82.6, 69.9, 53.3, 49.4, 21.5, 16.3. IR (neat)  $\nu$  663, 825, 1027, 1347, 1492, 1595, 2923, 2966  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{22}\text{NO}_3\text{ClSNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 438.0901, Found: 438.0907.

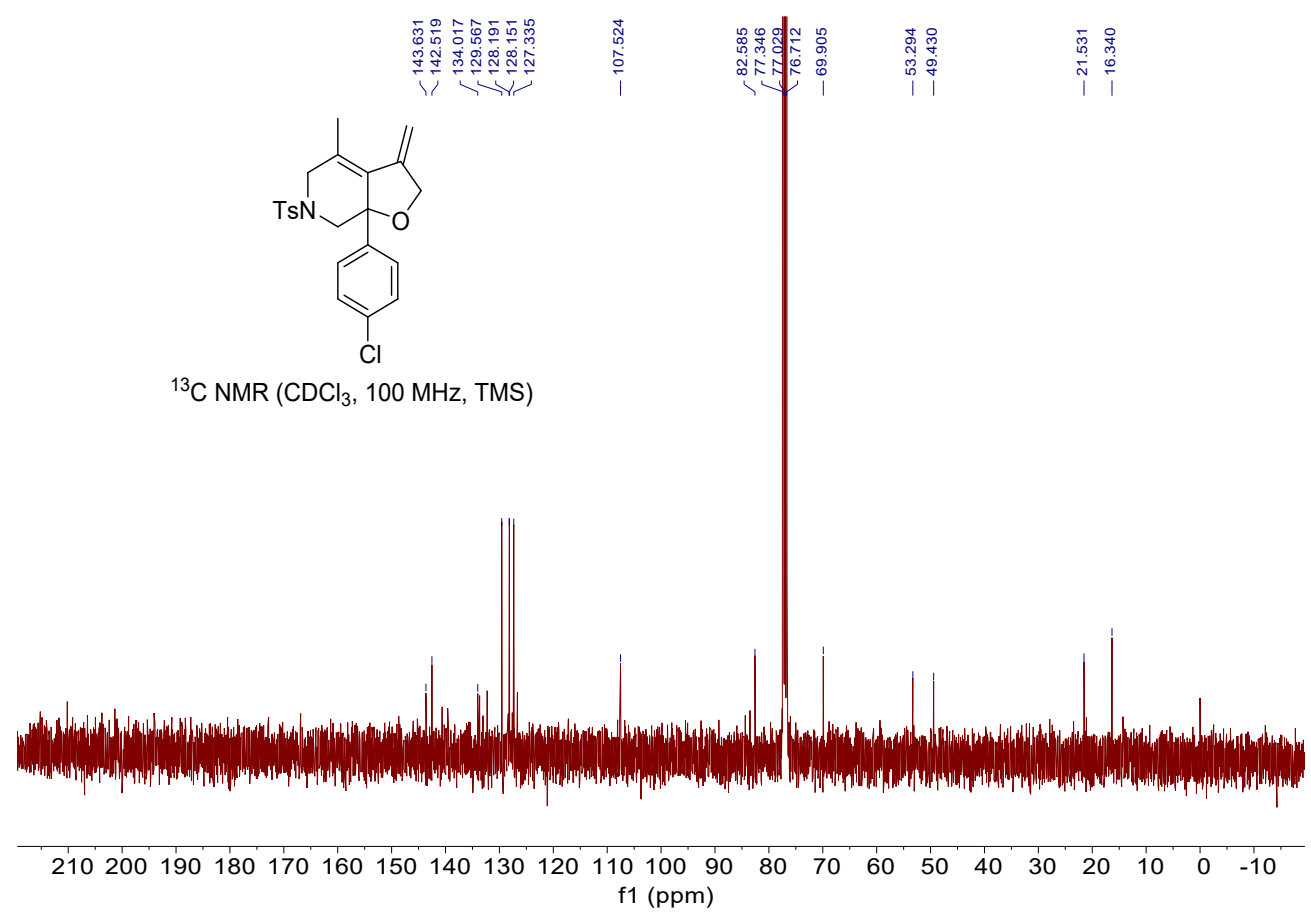


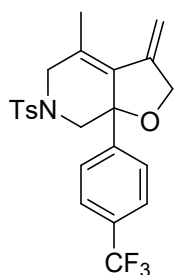
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





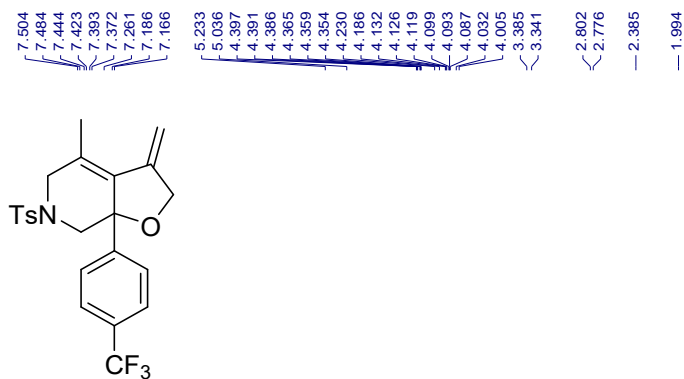
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



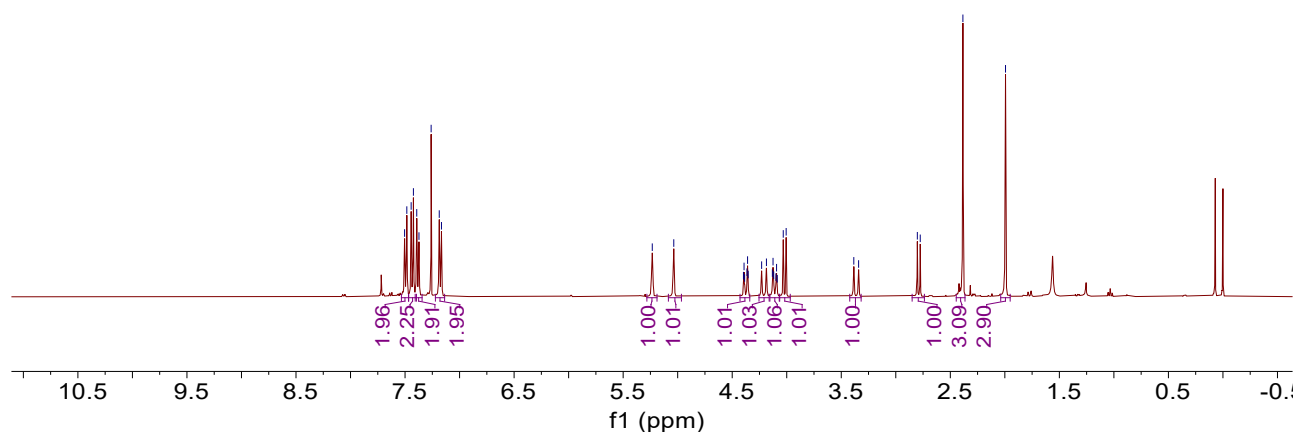


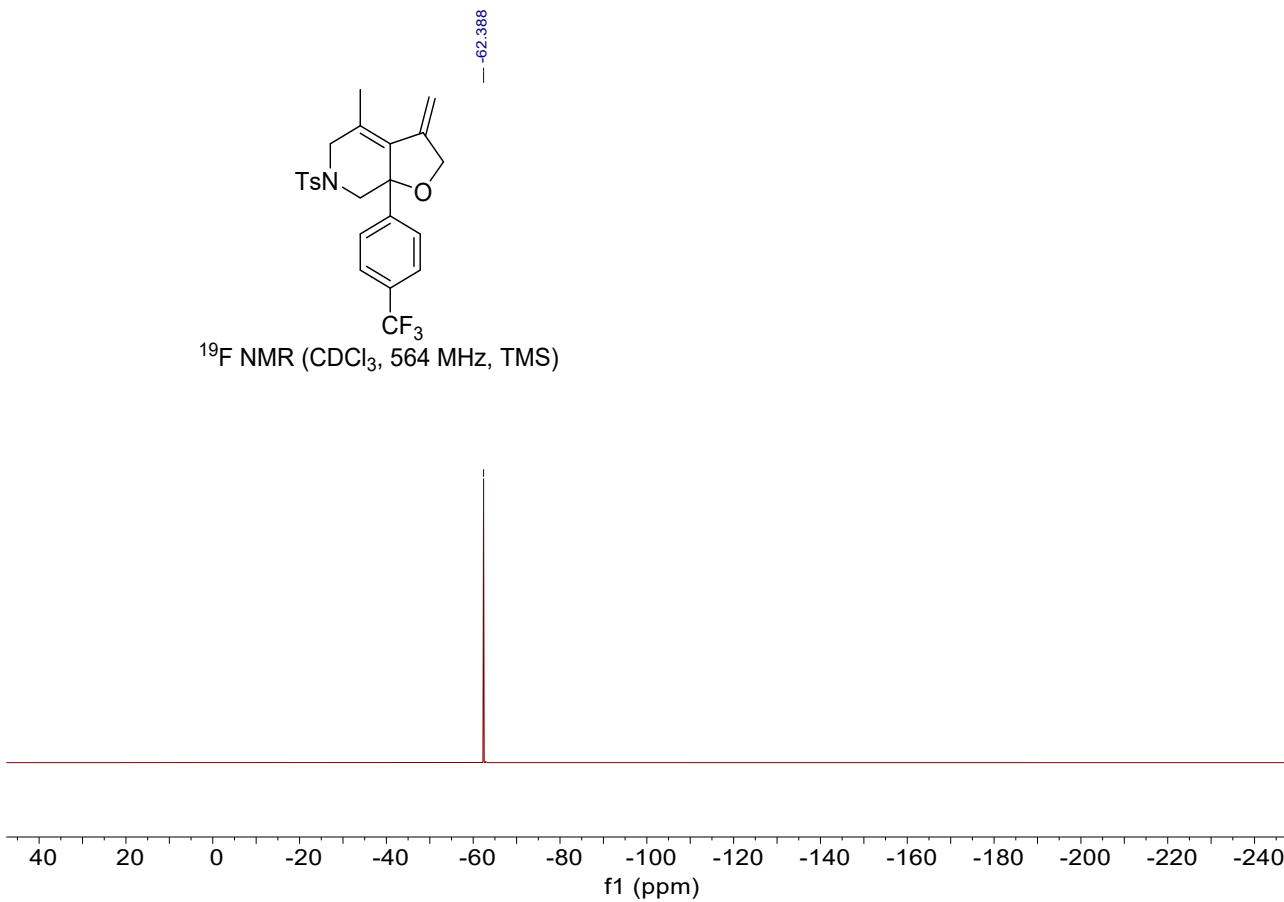
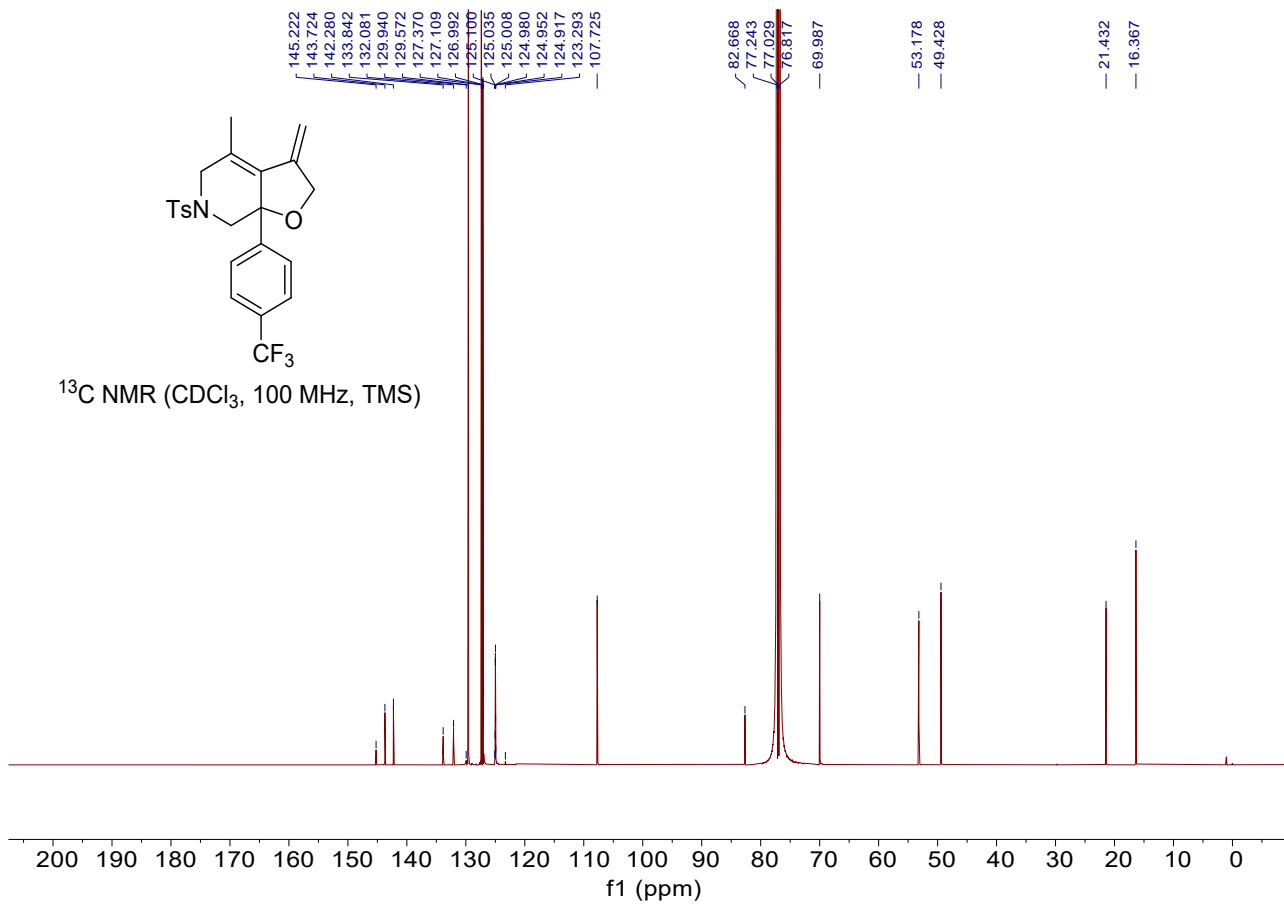
**4-methyl-3-methylene-6-tosyl-7a-(4-(trifluoromethyl)phenyl)-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3w)**

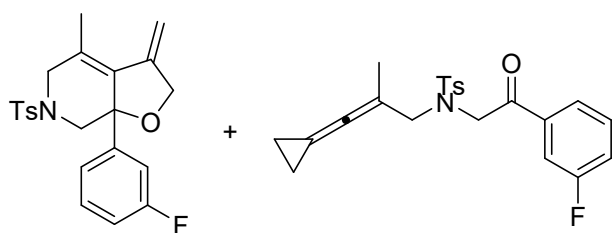
A colorless oil, 76% yield, 32.3 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.49 (d,  $J = 8.2$  Hz, 2H), 7.43 (d,  $J = 8.2$  Hz, 2H), 7.38 (d,  $J = 8.2$  Hz, 2H), 7.18 (d,  $J = 8.2$  Hz, 2H), 5.23 (s, 1H), 5.04 (s, 1H), 4.38 (dt,  $J = 13.0, 2.2$  Hz, 1H), 4.21 (d,  $J = 17.6$  Hz, 1H), 4.11 (dt,  $J = 13.0, 2.4$  Hz, 1H), 4.02 (d,  $J = 10.8$  Hz, 1H), 3.36 (d,  $J = 17.6$  Hz, 1H), 2.79 (d,  $J = 10.8$  Hz, 1H), 2.38 (s, 3H), 1.99 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  145.2, 143.7, 142.3, 133.8, 132.1, 129.8 (q,  $J_{\text{C-F}} = 32.6$  Hz), 129.0, 127.4, 127.1, 127.0, 126.7 (q,  $J_{\text{C-F}} = 272.9$  Hz), 125.0 (q,  $J_{\text{C-F}} = 4.0$  Hz), 107.7, 82.7, 70.0, 53.2, 49.4, 21.4, 16.4.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.4. IR (neat)  $\nu$  668, 814, 1162, 1325, 1595, 2848, 2929, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{22}\text{NO}_3\text{F}_3\text{SNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 472.1165, Found: 472.1162.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

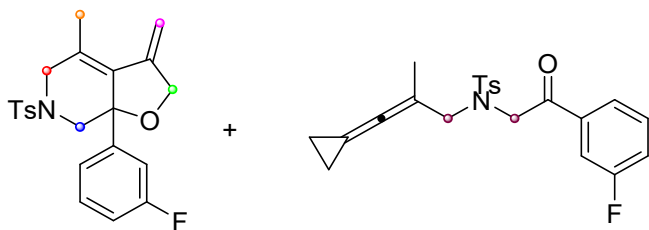






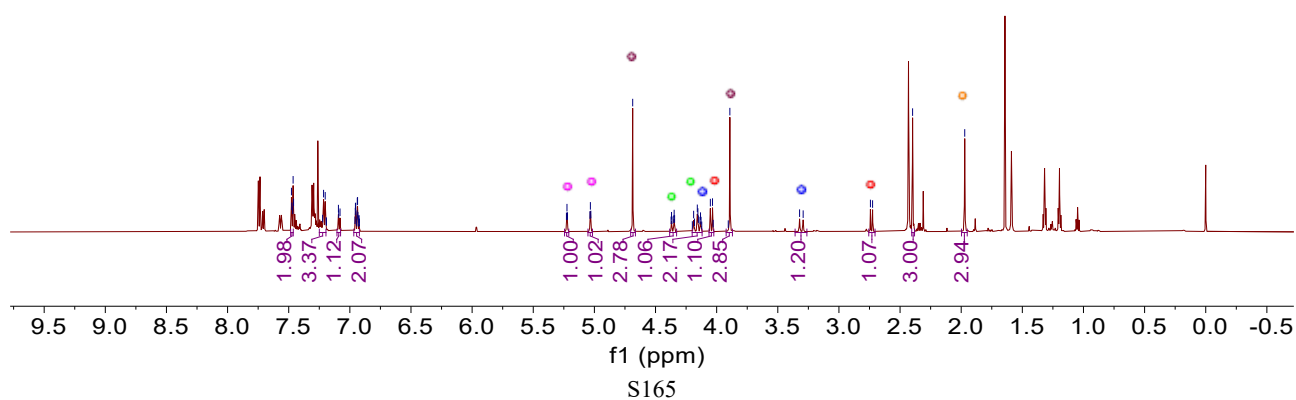
**7a-(3-fluorophenyl)-4-methyl-3-methylene-6-tosyl-2,3,5,6,7,7a-hexahydrofuro[2,3-c]pyridine (3y:1y = 1:2.8)**

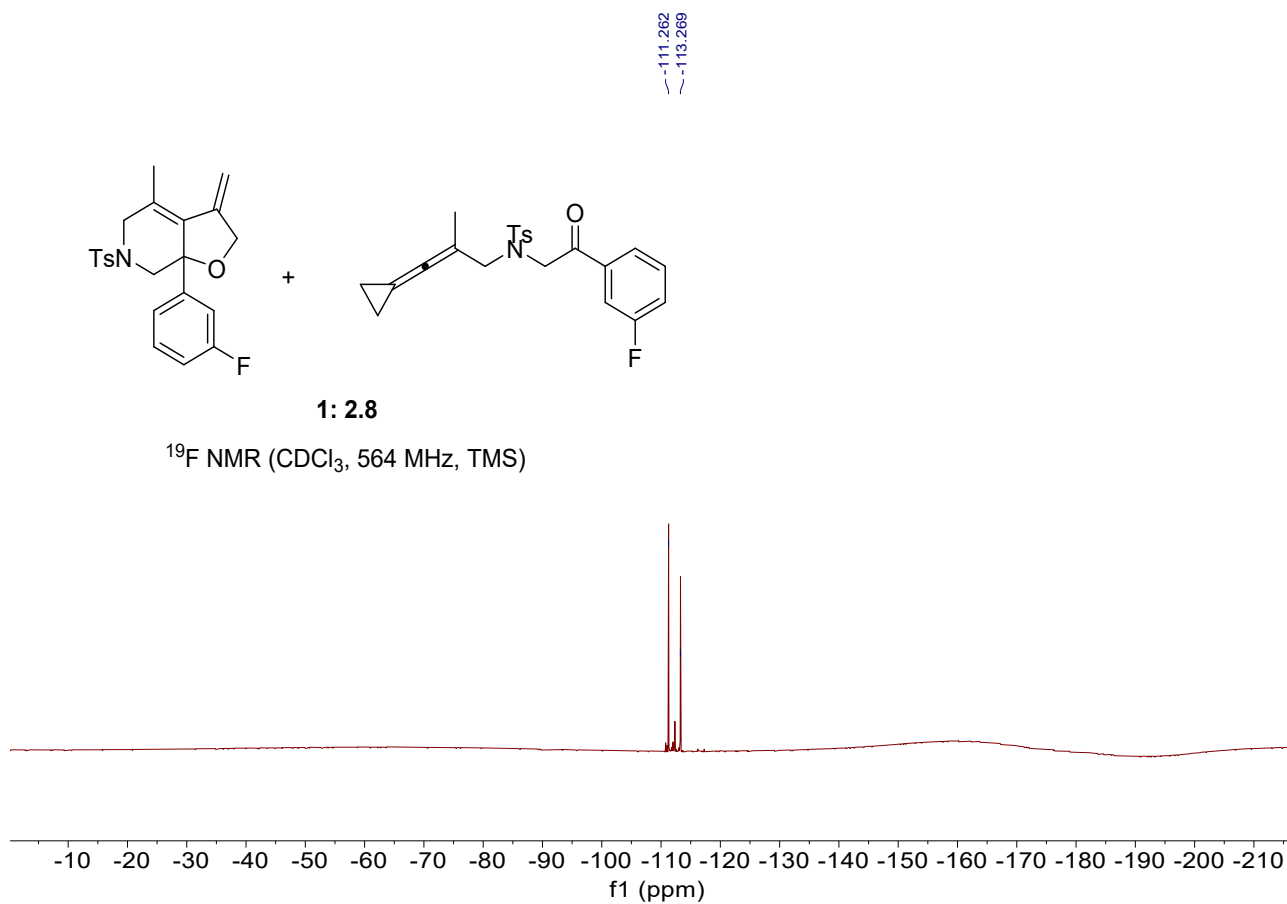
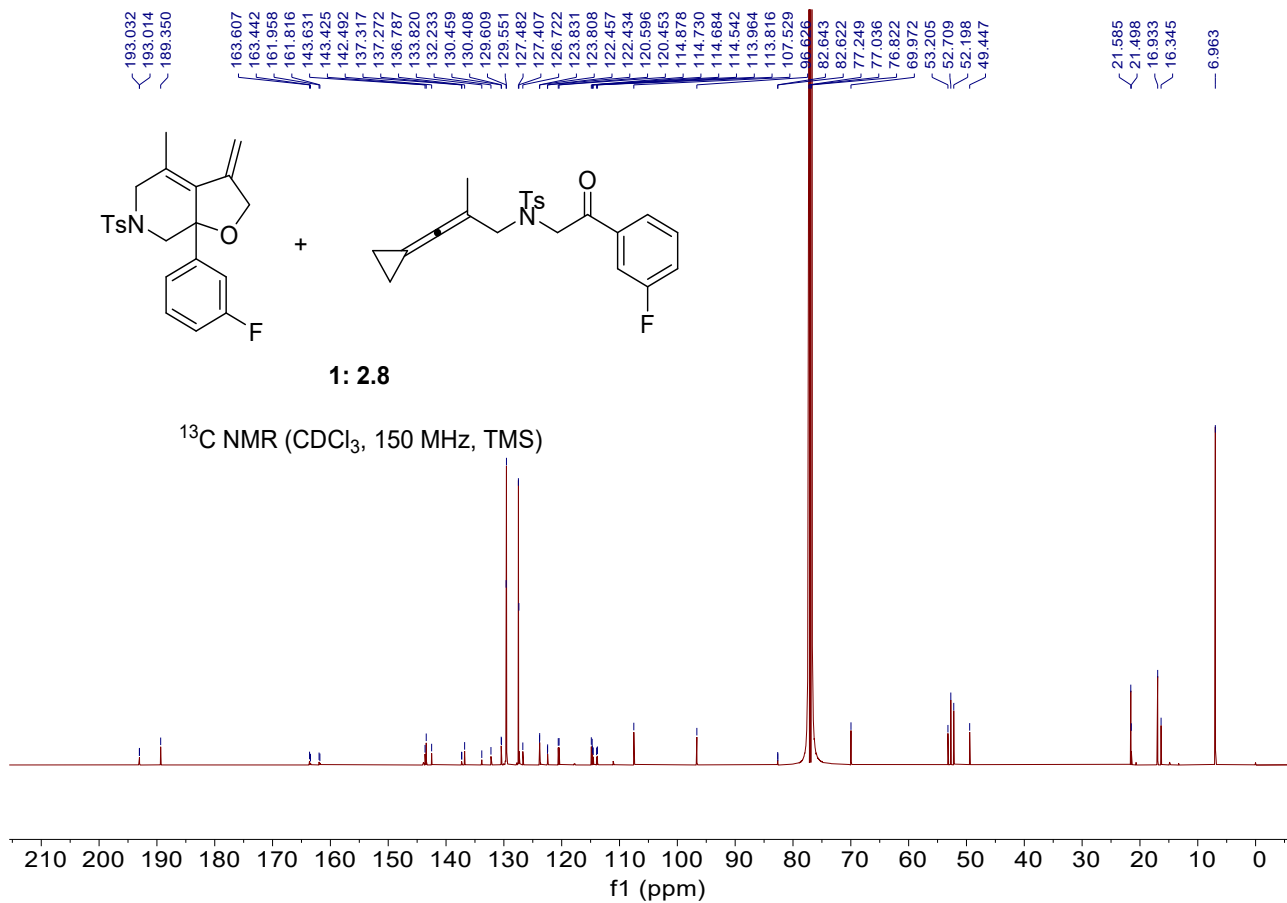
A colorless oil, 26% yield, 10.4 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.48 – 7.46 (m, 2H), 7.21 (d,  $J = 8.0$  Hz, 3H), 7.11 – 7.08 (m, 1H), 6.97 – 6.92 (m, 2H), 5.24 – 5.21 (m, 1H), 5.03 (d,  $J = 2.2$  Hz, 1H), 4.69 (s, 3H), 4.36 (dt,  $J = 12.9, 2.2$  Hz, 1H), 4.20 – 4.12 (m, 2H), 4.04 (d,  $J = 10.6$  Hz, 1H), 3.89 (s, 3H), 3.31 (d,  $J = 17.6$  Hz, 1H), 2.73 (d,  $J = 10.6$  Hz, 1H), 2.40 (s, 3H), 1.97 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  193.0, 193.0, 189.4, 163.6, 163.4, 162.0, 161.8, 143.6, 143.4, 142.5, 137.3, 137.3, 136.8, 133.8, 132.2, 130.5, 130.4, 129.6, 129.6, 127.5, 127.4, 126.7, 123.8, 123.8, 122.5, 122.4, 120.6, 120.5, 114.9, 114.7, 114.7, 114.5, 114.0, 113.8, 107.5, 96.6, 82.6, 82.6, 70.0, 53.2, 52.7, 52.2, 49.4, 21.6, 21.5, 16.9, 16.3, 7.0.  $^{19}\text{F}$  NMR (564 MHz,  $\text{CDCl}_3$ )  $\delta$  -111.26, -111.29. IR (neat)  $\nu$  667, 817, 1220, 1355, 1506, 2868, 2919, 2963  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{23}\text{NO}_3\text{FSN}$  (M+H) $^+$ : 400.1377, Found: 400.1367.

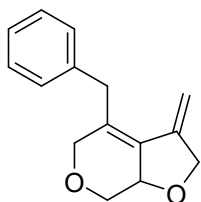


**1: 2.8**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)

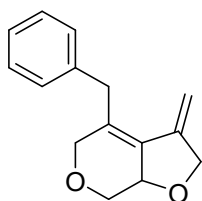




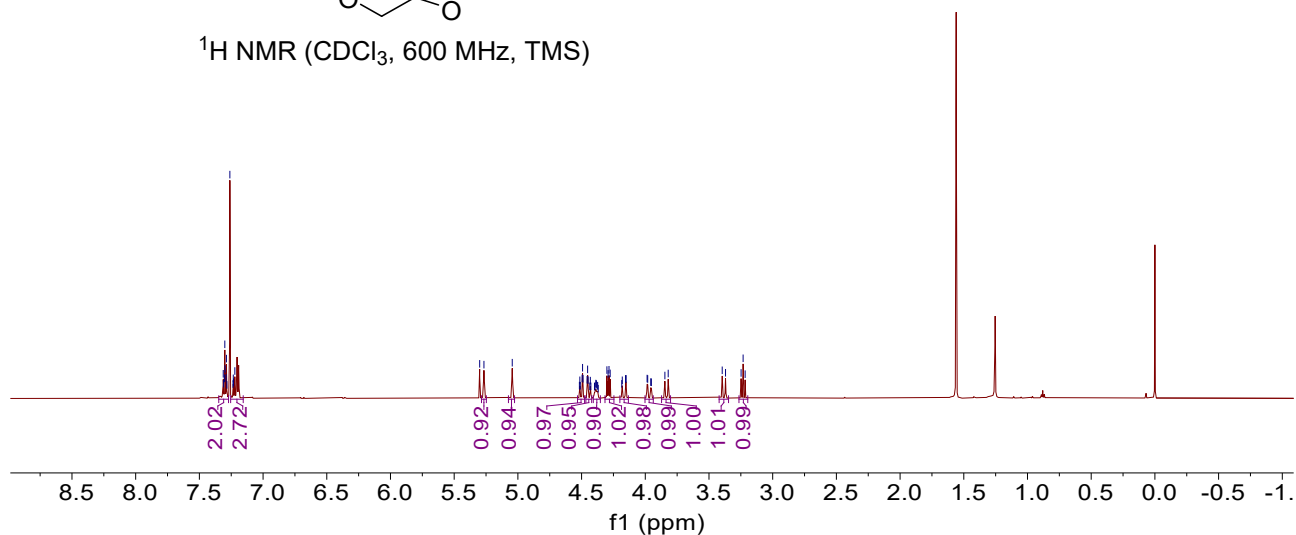


#### 4-benzyl-3-methylene-3,5,7,7a-tetrahydro-2H-furo[2,3-c]pyran (3ad)

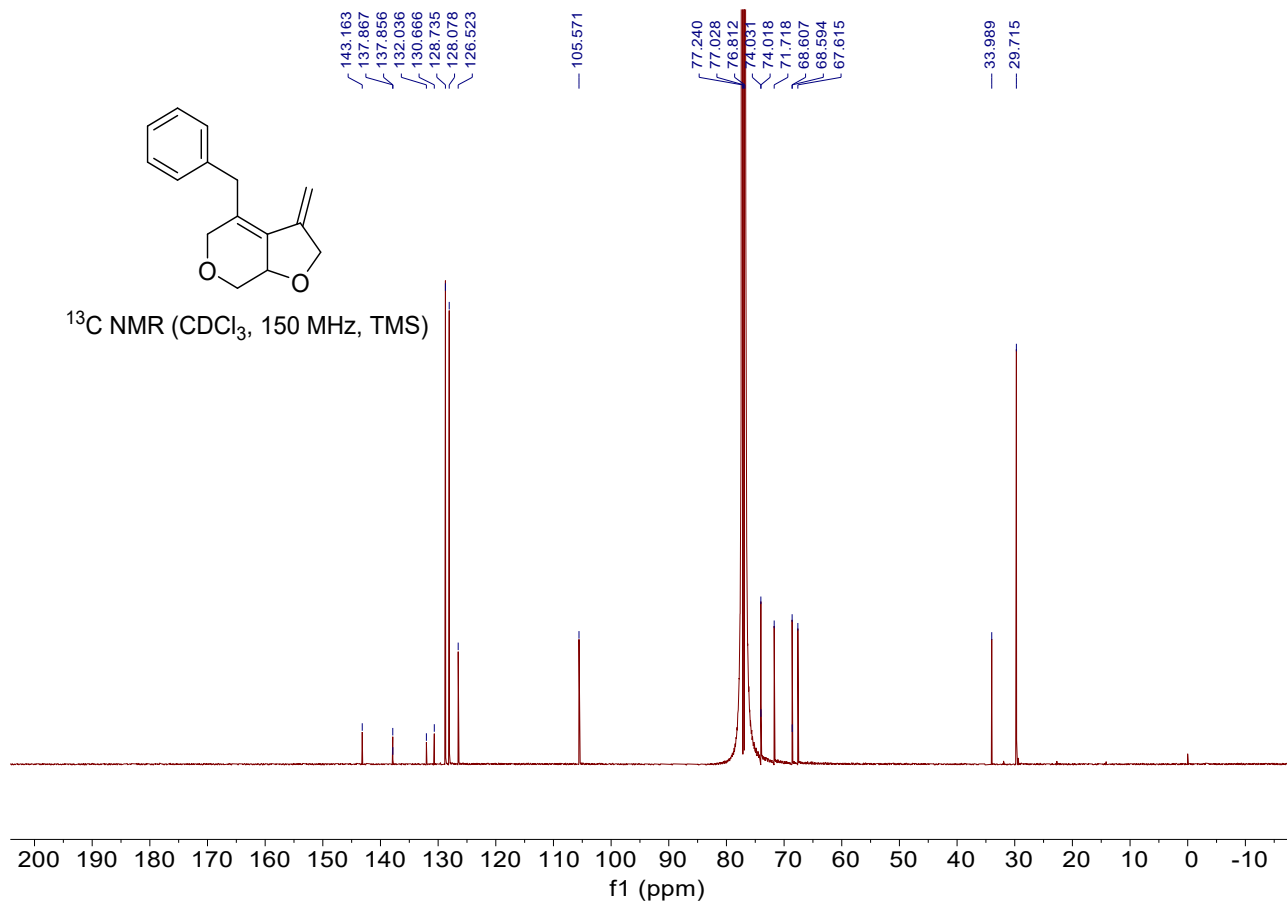
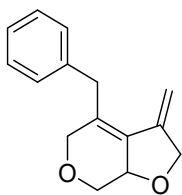
A colorless oil, 42% yield, 9.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.35 – 7.27 (m, 2H), 7.25 – 7.16 (m, 3H), 5.27 (s, 1H), 5.04 (s, 1H), 4.50 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.44 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.41 – 4.35 (m, 1H), 4.29 (dd,  $J = 9.8, 5.6$  Hz, 1H), 4.20 – 4.13 (m, 1H), 3.97 (dd,  $J = 17.2, 2.8$  Hz, 1H), 3.83 (d,  $J = 15.6$  Hz, 1H), 3.38 (d,  $J = 15.6$  Hz, 1H), 3.23 (t,  $J = 9.6$  Hz, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.2, 137.9, 132.0, 130.7, 128.7, 128.1, 126.5, 105.6, 74.03, 74.01, 71.7, 68.60, 68.59, 67.6, 34.0, 29.7. IR (neat)  $\nu$  669, 834, 1152, 1325, 1588, 2898, 2922, 2964  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{15}\text{H}_{19}\text{O}_2$  ( $\text{M}+\text{H}$ ) $^+$ : 229.1224, Found: 229.1220



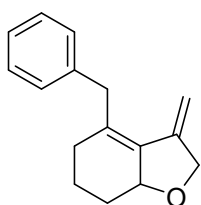
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)



<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, TMS)

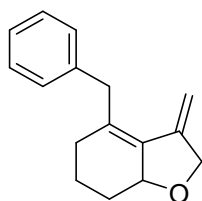




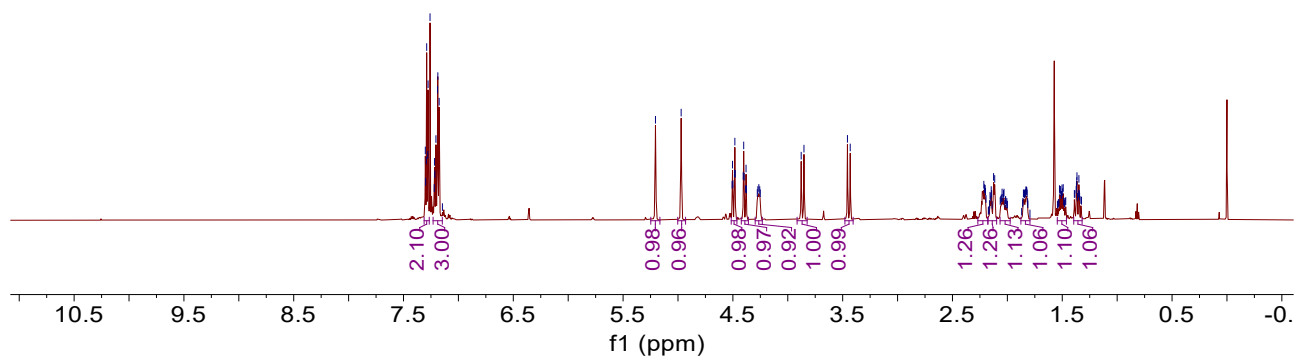


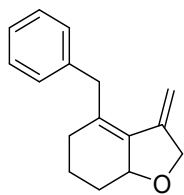
### 4-benzyl-3-methylene-2,3,5,6,7,7a-hexahydrobenzofuran (3ae)

A colorless oil, 40% yield, 9.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 600 MHz)  $\delta$  7.31 – 7.27 (m, 2H), 7.23 – 7.15 (m, 3H), 5.21 (s, 1H), 4.97 (s, 1H), 4.49 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.39 (dt,  $J = 12.8, 2.0$  Hz, 1H), 4.30 – 4.23 (m, 1H), 3.87 (d,  $J = 15.2$  Hz, 1H), 3.44 (d,  $J = 15.2$  Hz, 1H), 2.20 (d,  $J = 4.8$  Hz, 1H), 2.18 – 2.10 (m, 1H), 2.07 – 1.97 (m, 1H), 1.88 – 1.79 (m, 1H), 1.55 – 1.46 (m, 1H), 1.40 – 1.32 (m, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  144.4, 139.0, 133.9, 128.5, 128.4, 126.2, 104.6, 79.4, 71.7, 38.4, 30.8, 28.6, 19.7. IR (neat)  $\nu$  668, 814, 1162, 1325, 1595, 2848, 2929, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{19}\text{O}$  ( $\text{M}+\text{H}$ ) $^+$ : 227.1430, Found: 227.1428.

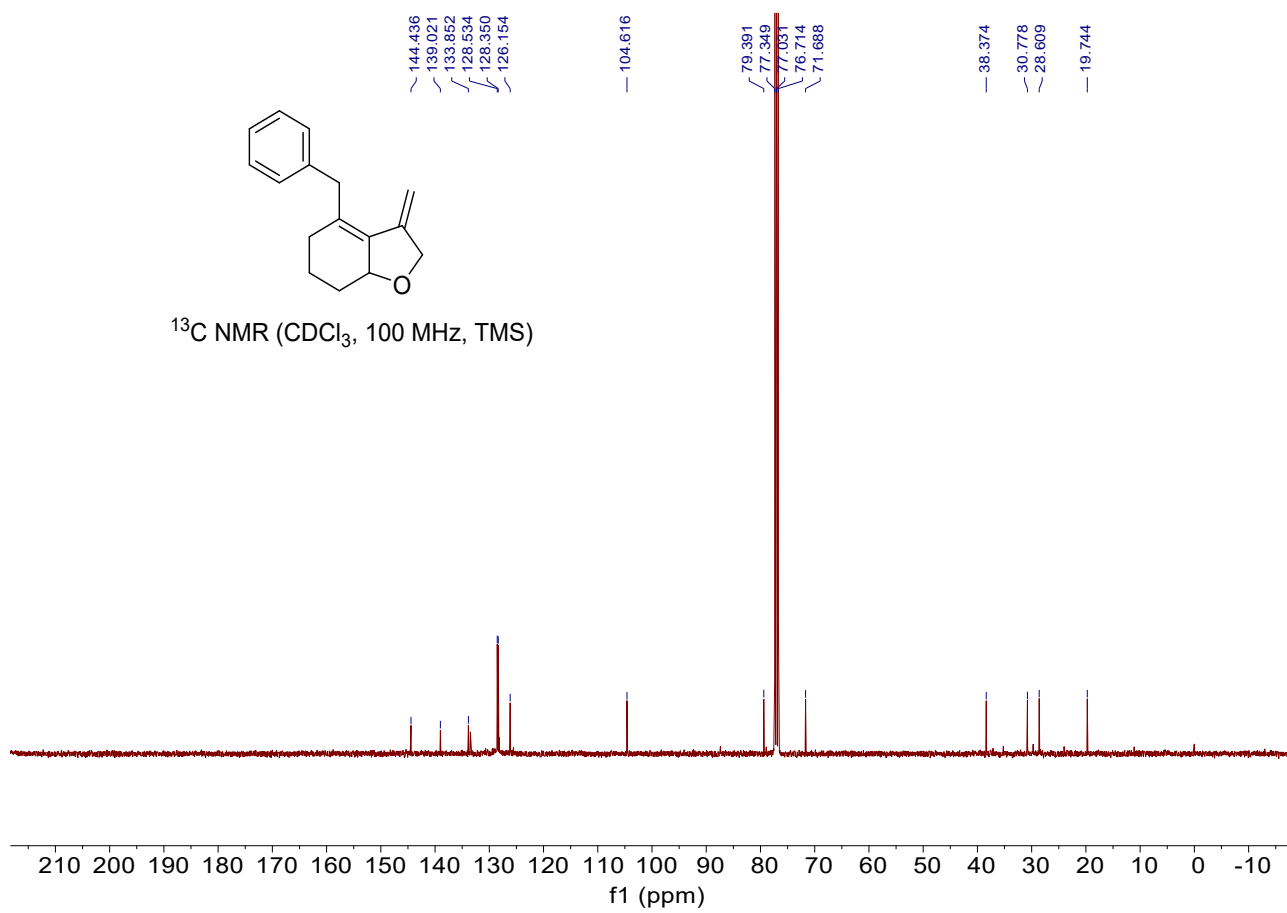


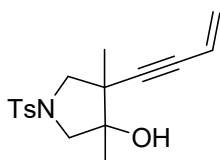
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz, TMS)





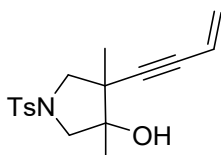
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



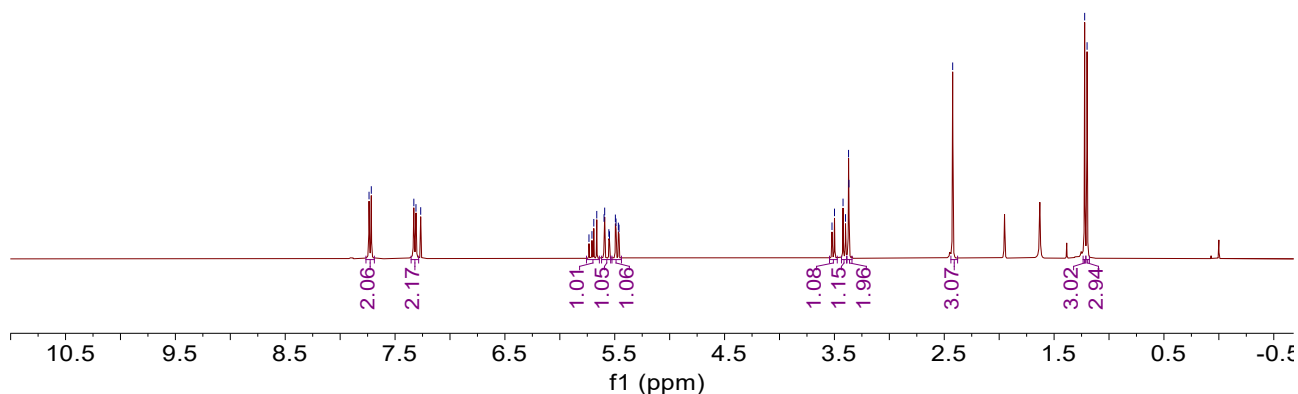


#### 4-(but-3-en-1-yn-1-yl)-3,4-dimethyl-1-tosylpyrrolidin-3-ol (4)

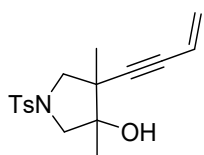
A colorless oil, 82% yield, 26.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 5.70 (dd,  $J = 17.6, 10.8$  Hz, 1H), 5.57 (dd,  $J = 17.6, 2.4$  Hz, 1H), 5.48 (dd,  $J = 10.8, 2.4$  Hz, 1H), 3.51 (d,  $J = 9.2$  Hz, 1H), 3.41 (d,  $J = 9.2$  Hz, 1H), 3.37 (d,  $J = 1.2$  Hz, 2H), 2.42 (s, 3H), 1.22 (s, 3H), 1.20 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.5, 134.0, 129.6, 127.9, 127.5, 116.2, 88.3, 84.2, 79.7, 57.9, 57.2, 47.0, 22.1, 21.6, 20.0. IR (neat)  $\nu$  664, 760, 1029, 1092, 1162, 1346, 1596, 2853, 2924, 2956  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{22}\text{NO}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 320.1315, Found: 320.1308.



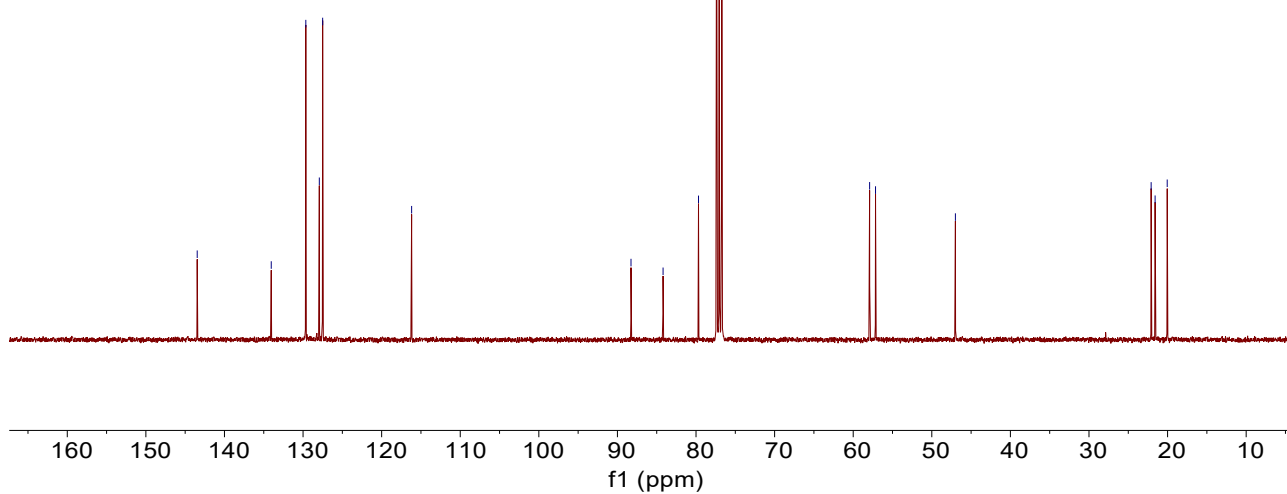
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

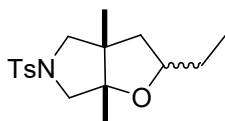


143.467  
134.047  
129.649  
127.931  
127.506  
116.186  
88.273  
84.193  
79.683  
77.366  
77.048  
76.730  
57.912  
57.160  
46.997  
22.091  
21.587  
20.047



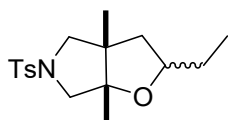
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



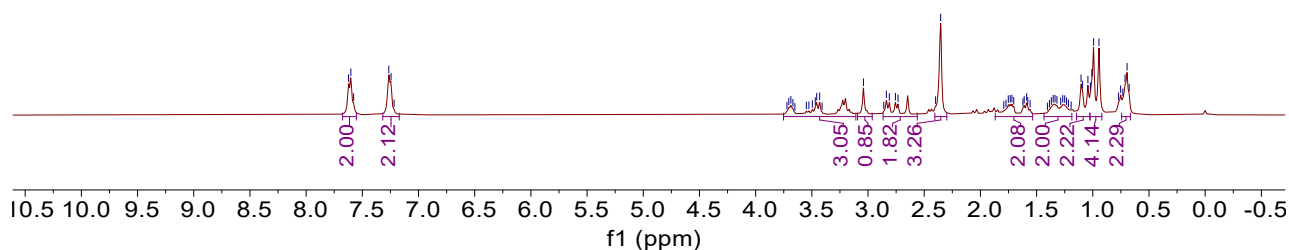


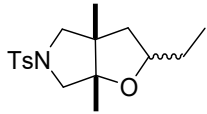
### 2-ethyl-3a,6a-dimethyl-5-tosylhexahydro-2H-furo[2,3-c]pyrrole (5)

A colorless oil, 96% yield, 31.0 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.68 – 7.55 (m, 2H), 7.32 – 7.17 (m, 2H), 3.75 – 3.11 (m, 3H), 3.09 – 2.96 (m, 1H), 2.87 – 2.56 (m, 2H), 2.35 (s, 3H), 1.87 – 1.54 (m, 2H), 1.43 – 1.19 (m, 2H), 1.15 – 1.02 (m, 2H), 1.03 – 0.92 (m, 4H), 0.74 – 0.67 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.5, 132.8, 129.6, 127.8, 89.7, 78.4, 78.1, 60.1, 59.6, 50.9, 44.2, 28.9, 21.6, 20.4, 18.9, 10.3. IR (neat)  $\nu$  666, 762, 1092, 1162, 1346, 1596, 2863, 2954  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{24}\text{NO}_3\text{S}$  (M-H) $^+$ : 322.1471, Found: 322.1465.

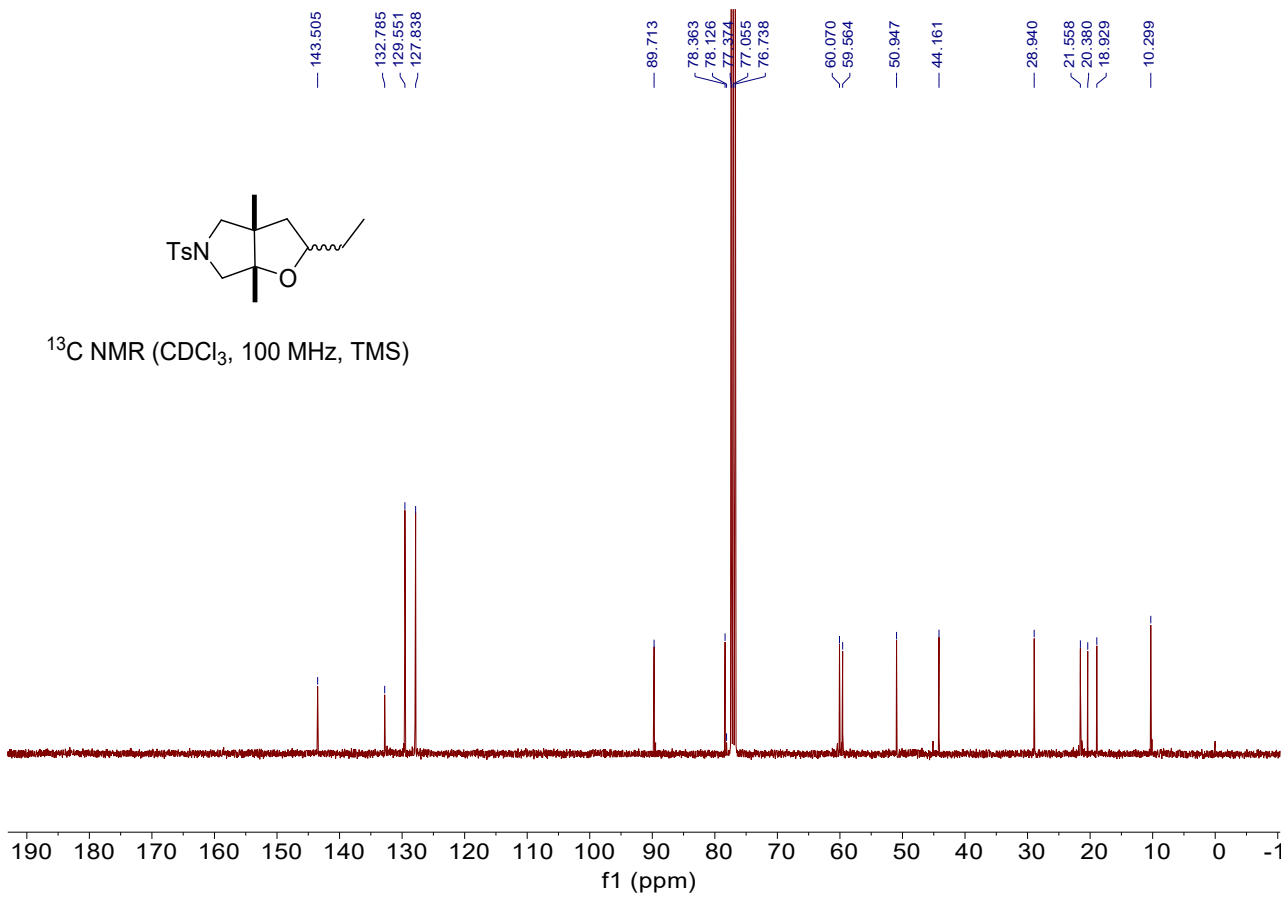


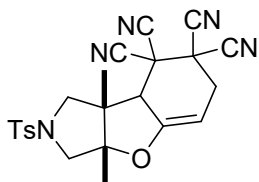
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





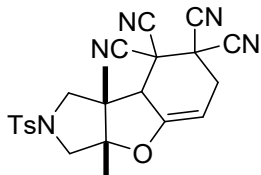
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



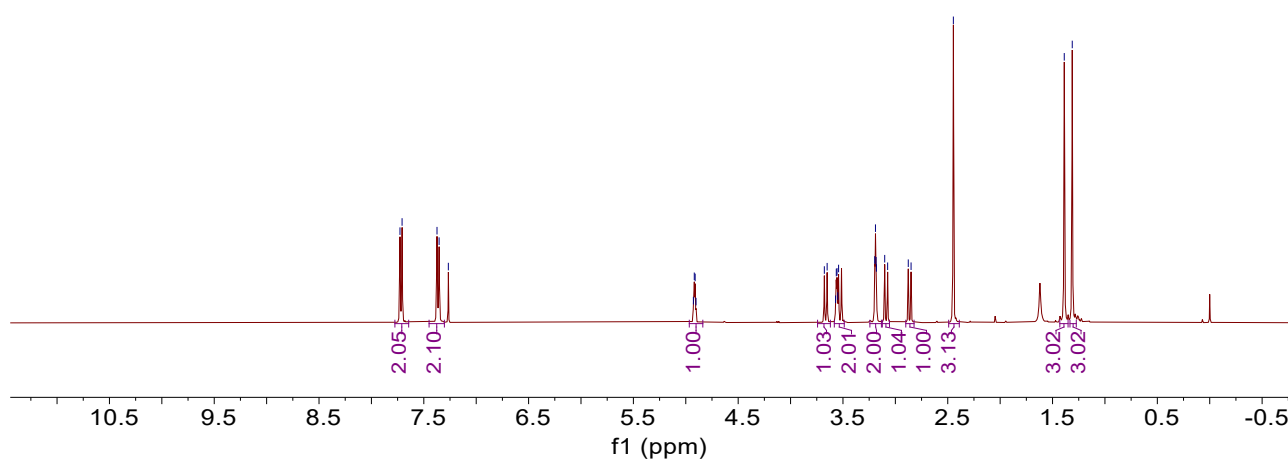


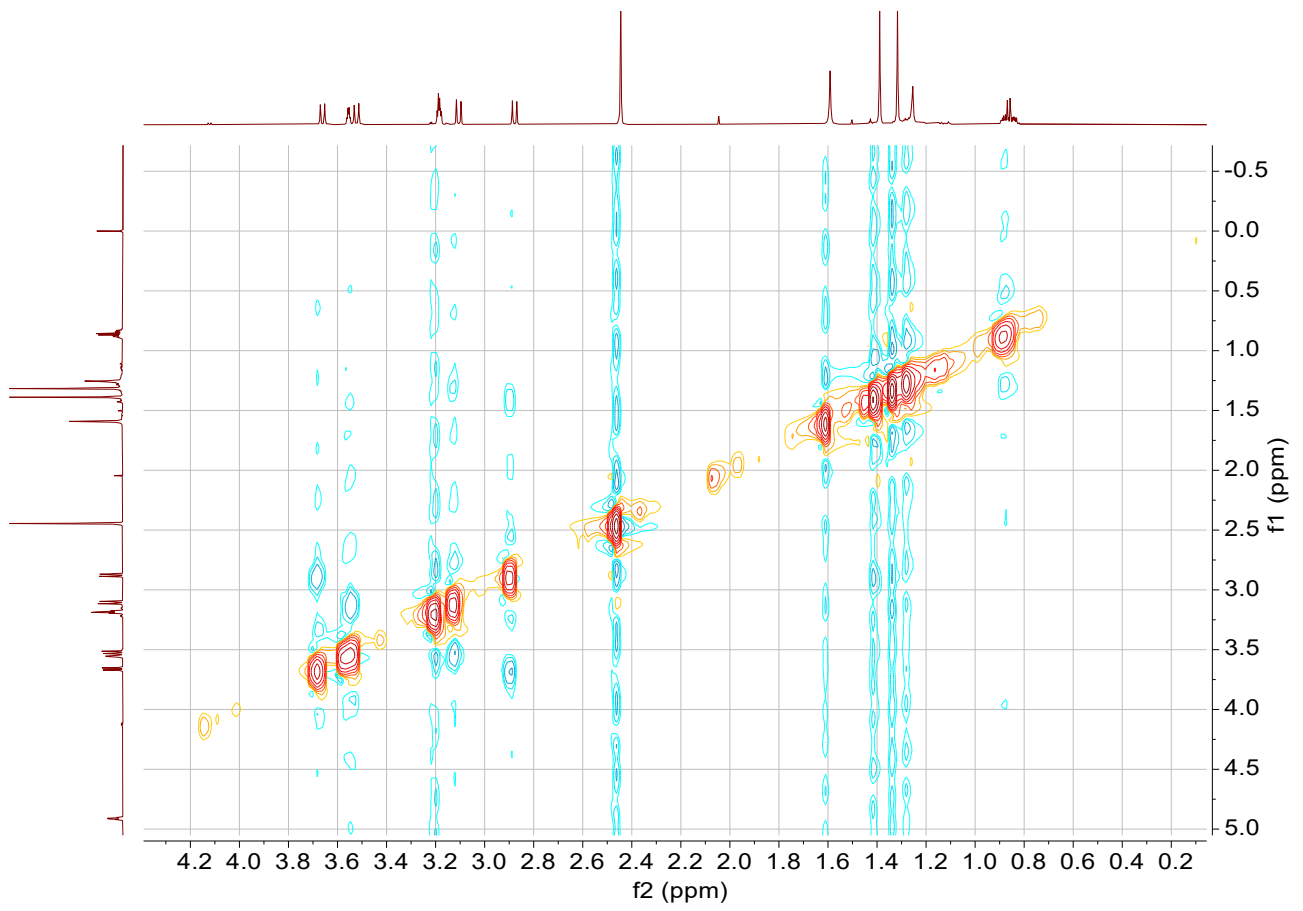
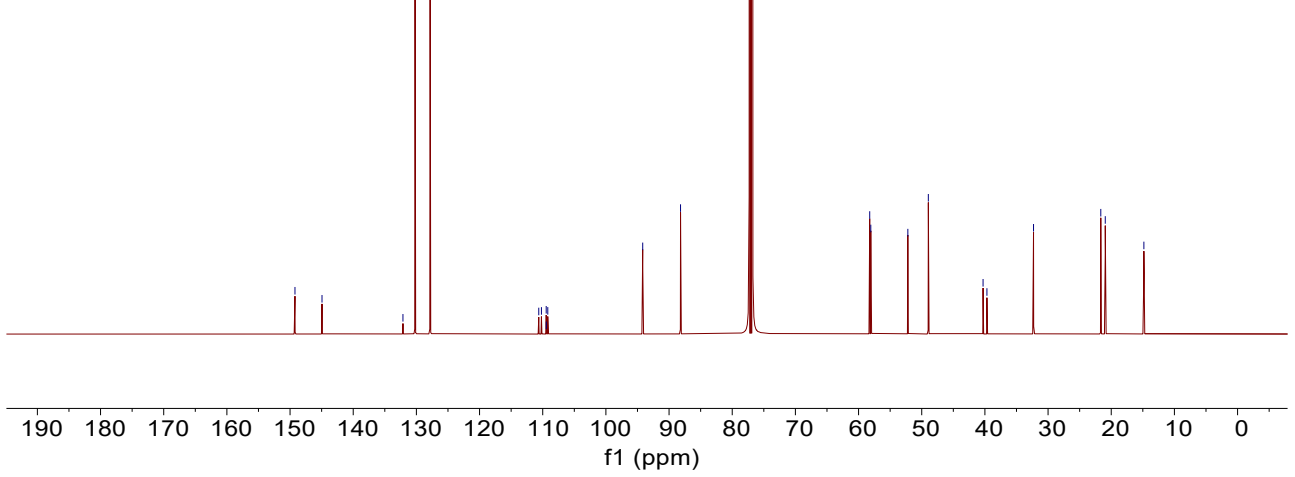
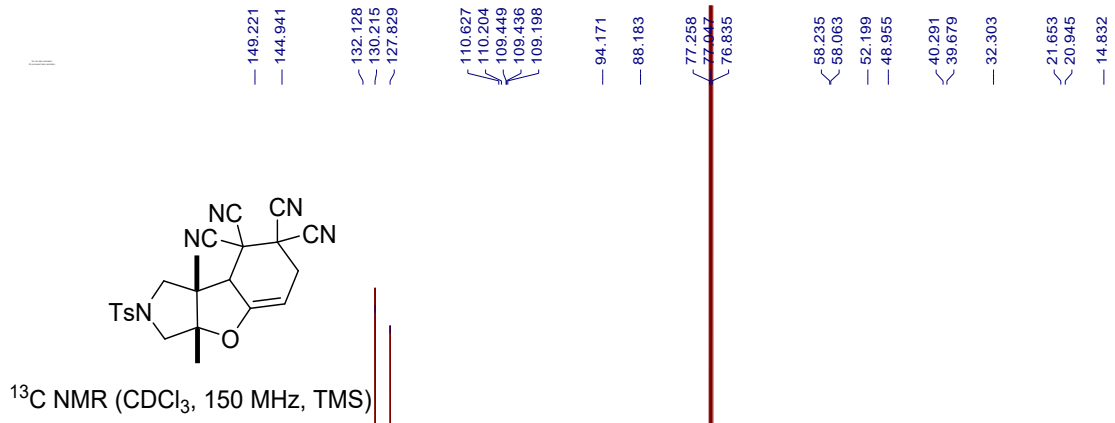
**3a,8b-dimethyl-2-tosyl-2,3,3a,6,8a,8b-hexahydro-1H-benzofuro[2,3-c]pyrrole-7,7,8,8-tetracarbonitrile (6)**

A colorless oil, 90% yield, 40.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 4.97 – 4.84 (m, 1H), 3.66 (d,  $J = 10.8$  Hz, 1H), 3.58 – 3.49 (m, 2H), 3.24 – 3.13 (m, 2H), 3.09 (d,  $J = 11.2$  Hz, 1H), 2.86 (d,  $J = 10.8$  Hz, 1H), 2.45 (s, 3H), 1.39 (s, 3H), 1.31 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  149.2, 144.9, 132.1, 130.2, 127.8, 110.6, 110.2, 109.44, 109.43, 109.2, 94.2, 88.2, 58.2, 58.1, 52.2, 49.0, 40.3, 39.7, 32.3, 21.7, 20.9, 14.8. IR (neat)  $\nu$  665, 828, 1092, 1164, 1351, 1592, 2159, 2165, 2848, 2869, 2916, 2969  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{22}\text{N}_5\text{O}_3\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 448.1438, Found: 448.1432.

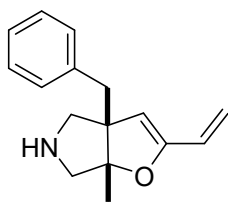


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



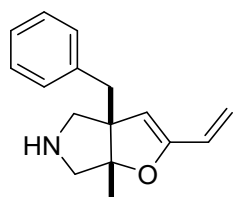




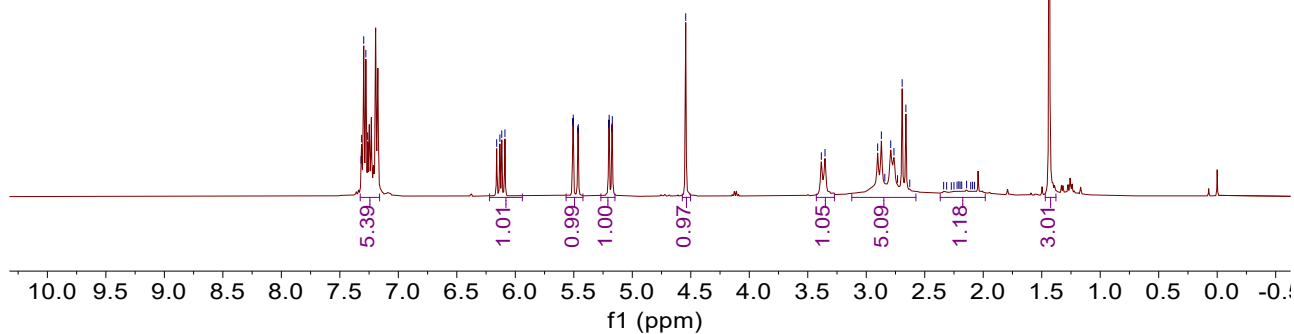


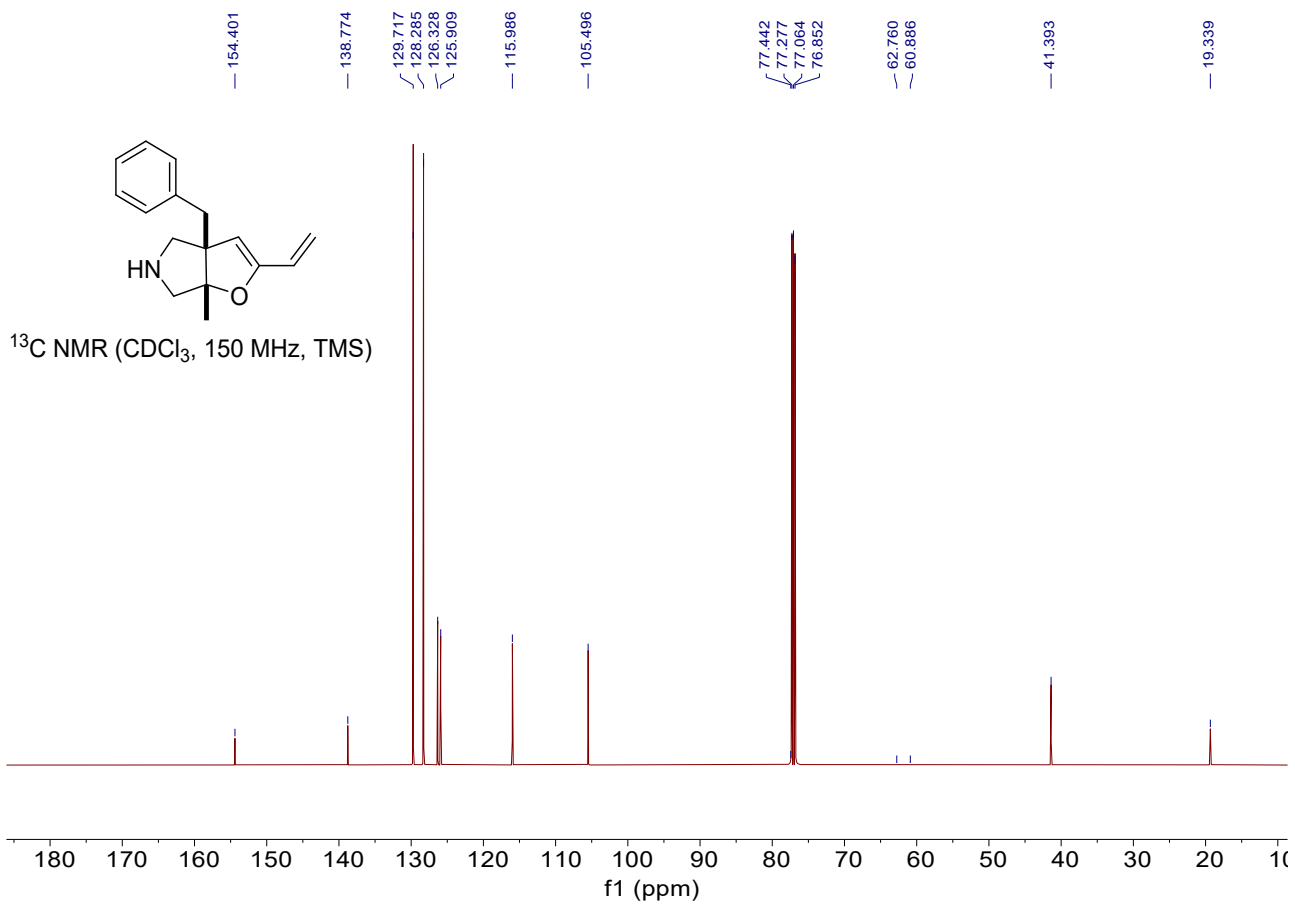
**3a-benzyl-6a-methyl-2-vinyl-3a,5,6,6a-tetrahydro-4H-furo[2,3-c]pyrrole (7)**

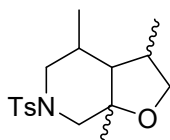
A brown oil, 90% yield, 31.2 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.33 – 7.16 (m, 5H), 6.12 (dd,  $J = 17.4, 10.8$  Hz, 1H), 5.49 (dd,  $J = 17.4, 1.6$  Hz, 1H), 5.19 (dd,  $J = 10.8, 1.6$  Hz, 1H), 4.54 (s, 1H), 3.37 (d,  $J = 12.6$  Hz, 1H), 3.12 – 2.58 (m, 5H), 2.37 – 1.98 (m, 1H), 1.44 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  154.4, 138.8, 129.7, 128.3, 126.3, 125.9, 116.0, 105.5, 77.4, 62.8, 60.9, 41.4, 19.3. IR (neat)  $\nu$  663, 815, 1092, 1161, 1341, 1597, 2848, 2867, 2932, 2968  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{20}\text{NO}$  ( $\text{M}+\text{H}$ ) $^+$ : 242.1539, Found: 242.1535.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

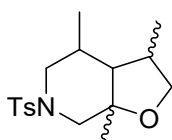




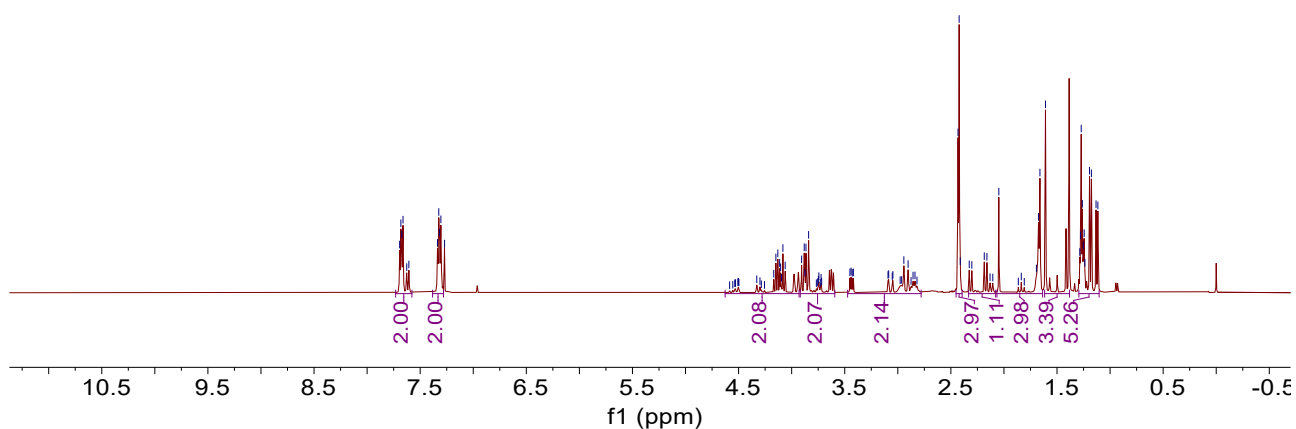


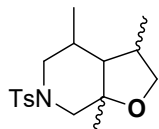
### 3,4,7a-trimethyl-6-tosyloctahydrofuro[2,3-c]pyridine (8)

A colorless oil, 80% yield, 26.0 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.73 – 7.58 (m, 2H), 7.38 – 7.28 (m, 2H), 4.63 – 3.93 (m, 2H), 3.92 – 3.59 (m, 2H), 3.47 – 2.78 (m, 2H), 2.45 – 2.39 (m, 3H), 2.33 – 2.08 (m, 1H), 2.07 – 1.64 (m, 3H), 1.62 – 1.38 (m, 3H), 1.29 – 1.10 (m, 5H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 150 MHz)  $\delta$  143.6, 143.5, 143.5, 140.7, 140.4, 133.8, 133.6, 129.7, 129.7, 127.5, 127.5, 127.5, 119.8, 119.5, 88.0, 79.4, 78.0, 73.6, 72.8, 60.4, 57.3, 54.2, 53.3, 52.9, 48.6, 48.5, 35.0, 34.8, 32.4, 27.9, 23.2, 23.2, 22.7, 22.7, 21.5, 21.5, 21.1, 19.2, 18.4, 16.6, 15.8, 15.7, 14.2, 10.3. IR (neat)  $\nu$  666, 814, 1062, 1163, 1347, 1593, 2849, 2869, 2928  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{24}\text{NO}_3\text{S}$  (M-H) $^+$ : 324.1628, Found: 324.1621.

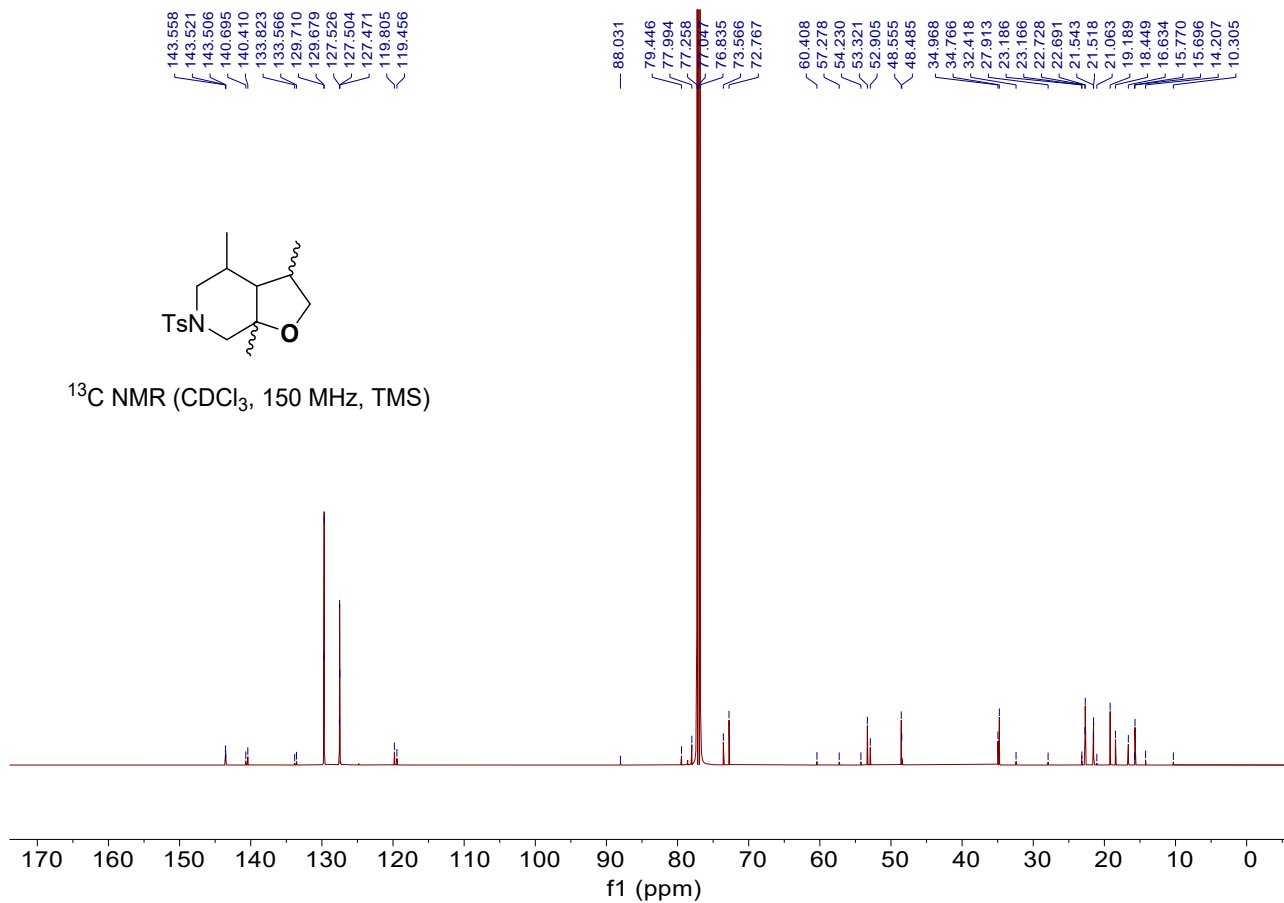


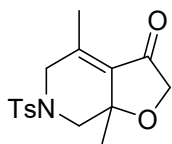
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





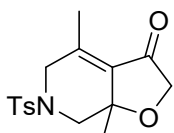
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, TMS)



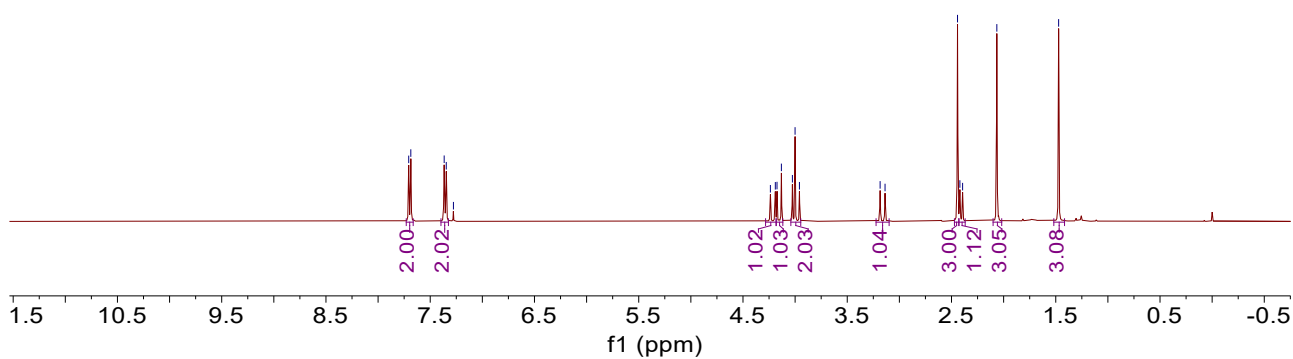


**4,7a-dimethyl-6-tosyl-5,6,7,7a-tetrahydrofuro[2,3-c]pyridin-3(2H)-one (9)**

A colorless oil, 90% yield, 28.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 4.21 (d,  $J = 19.0$  Hz, 1H), 4.15 (d,  $J = 16.8$  Hz, 1H), 4.04 – 3.95 (m, 2H), 3.16 (d,  $J = 18.8$  Hz, 1H), 2.44 (s, 3H), 2.41 (d,  $J = 10.4$  Hz, 1H), 2.07 (s, 3H), 1.47 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  201.7, 144.2, 141.3, 133.2, 132.4, 130.0, 127.4, 79.0, 70.2, 52.8, 49.7, 22.9, 21.6, 15.2. IR (neat)  $\nu$  666, 815, 1092, 1163, 1347, 1592, 1692, 2852, 2929  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{20}\text{NO}_4\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 322.1108, Found: 322.1100.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



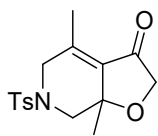
— 201.731

— 144.183  
— 141.281  
— 133.199  
— 132.449  
— 129.972  
— 127.438

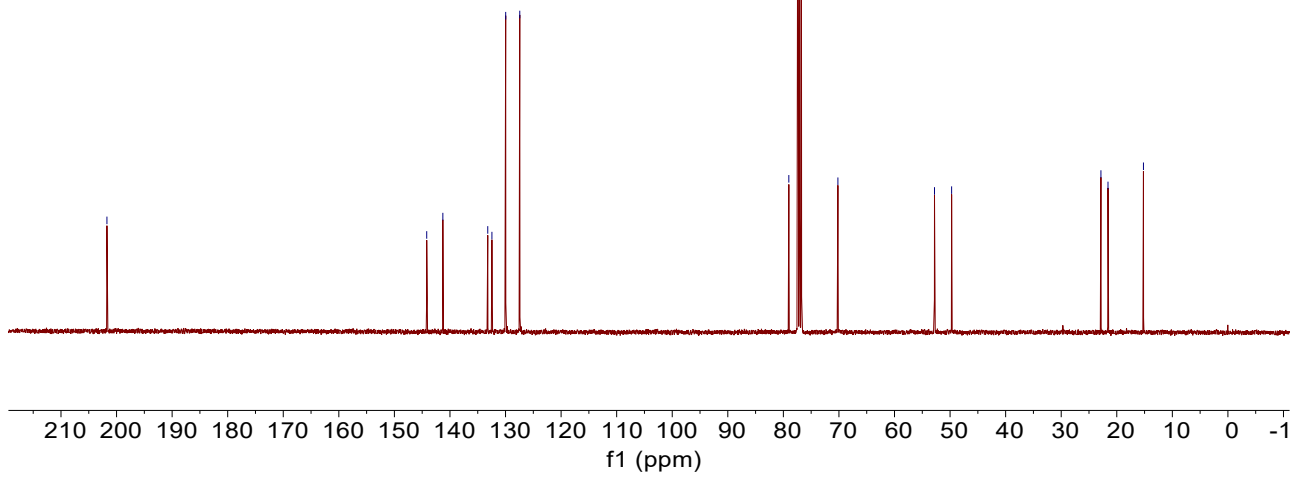
79.018  
77.397  
77.076  
76.759  
— 70.185

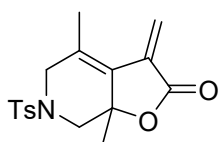
— 52.803  
— 49.721

— 22.852  
— 21.579  
— 15.199



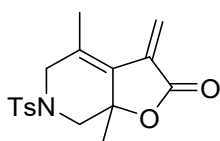
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, TMS)



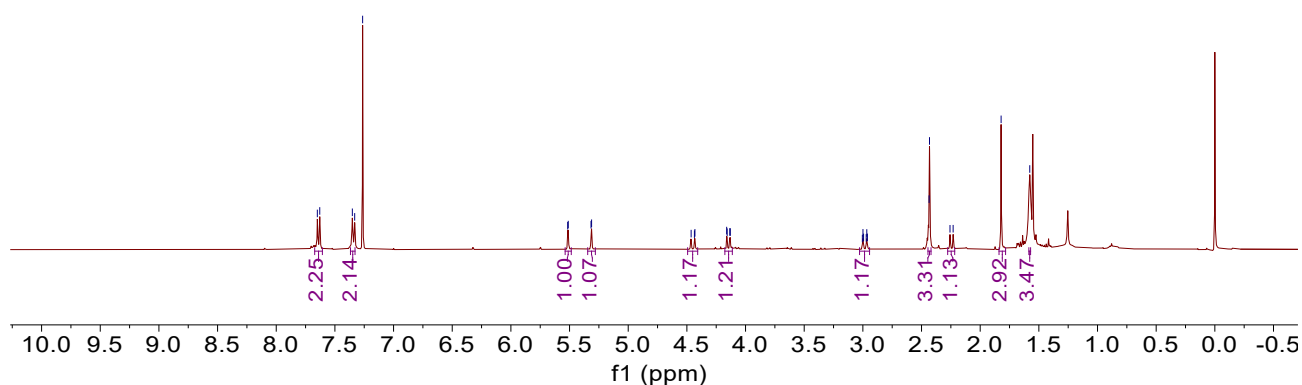


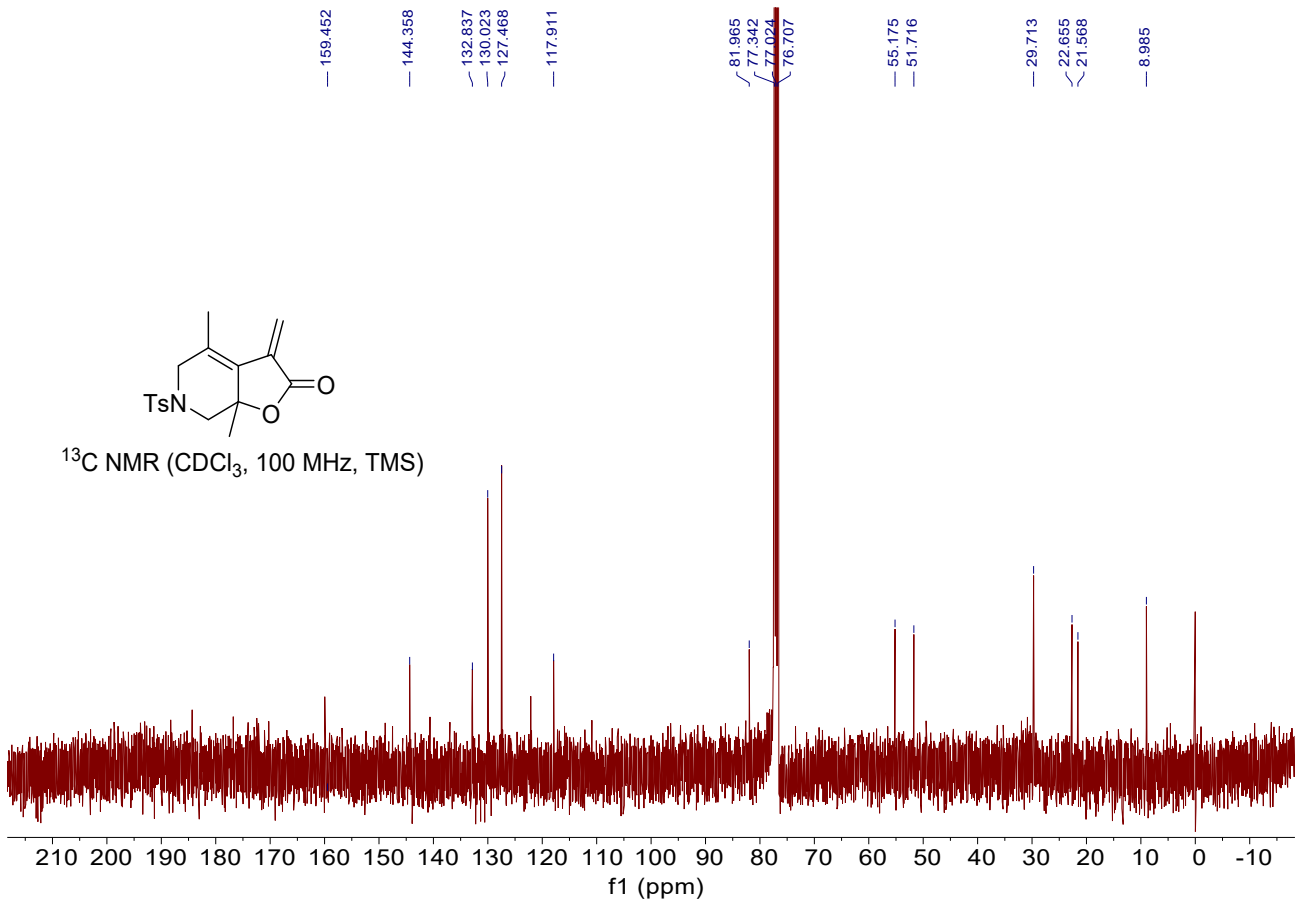
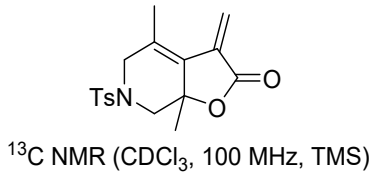
**4,7a-dimethyl-3-methylene-6-tosyl-5,6,7,7a-tetrahydrofuro[2,3-c]pyridin-2(3H)-one (10)**

A yellow oil, 36% yield, 11.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.64 (d,  $J = 8.0$  Hz, 2H), 7.34 (d,  $J = 8.0$  Hz, 2H), 5.51 (d,  $J = 2.0$  Hz, 1H), 5.31 (d,  $J = 2.0$  Hz, 1H), 4.49 – 4.41 (m, 1H), 4.15 (dd,  $J = 10.8, 1.6$  Hz, 1H), 2.98 (dt,  $J = 13.2, 2.0$  Hz, 1H), 2.44 – 2.42 (m, 3H), 2.24 (d,  $J = 10.8$  Hz, 1H), 1.82 (s, 3H), 1.58 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  159.5, 144.4, 132.8, 130.0, 127.5, 117.9, 82.0, 55.2, 51.7, 22.7, 21.6, 9.0. IR (neat)  $\nu$  666, 977, 1210, 1345, 1592, 1672, 2869, 2907  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{20}\text{NO}_4\text{S}$  ( $\text{M}+\text{H}$ ) $^+$ : 334.1108, Found: 334.1099.

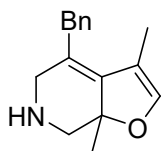


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)



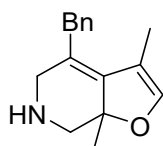




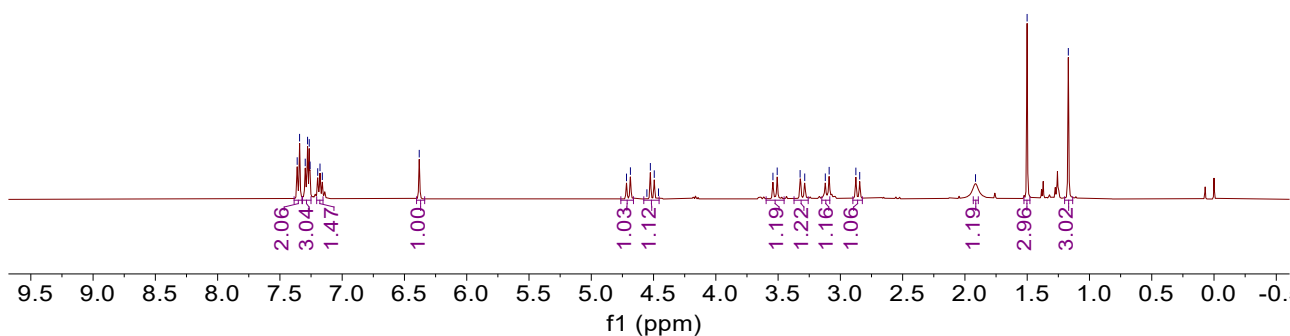


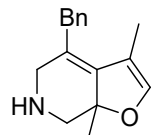
#### 4-benzyl-3,7a-dimethyl-5,6,7,7a-tetrahydrofuro[2,3-c]pyridine (11)

A brown oil, 62% yield, 14.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.39 – 7.32 (m, 2H), 7.32 – 7.25 (m, 2H), 7.20 – 7.15 (m, 1H), 6.38 (s, 1H), 4.70 (d,  $J = 12.6$  Hz, 1H), 4.51 (d,  $J = 12.6$  Hz, 1H), 3.52 (d,  $J = 13.6$  Hz, 1H), 3.30 (d,  $J = 14.8$  Hz, 1H), 3.11 (d,  $J = 12.4$  Hz, 1H), 2.86 (d,  $J = 12.4$  Hz, 1H), 1.92 (brs, 1H), 1.50 (s, 3H), 1.17 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  137.2, 134.3, 128.3, 128.0, 126.74, 126.65, 125.5, 77.9, 59.1, 55.7, 55.6, 29.7, 23.0, 11.3. IR (neat)  $\nu$  665, 987, 1347, 1640, 2851, 2869, 2926, 2974  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{20}\text{NO}$  ( $\text{M}+\text{H}$ ) $^+$ : 242.1539, Found: 242.1534.

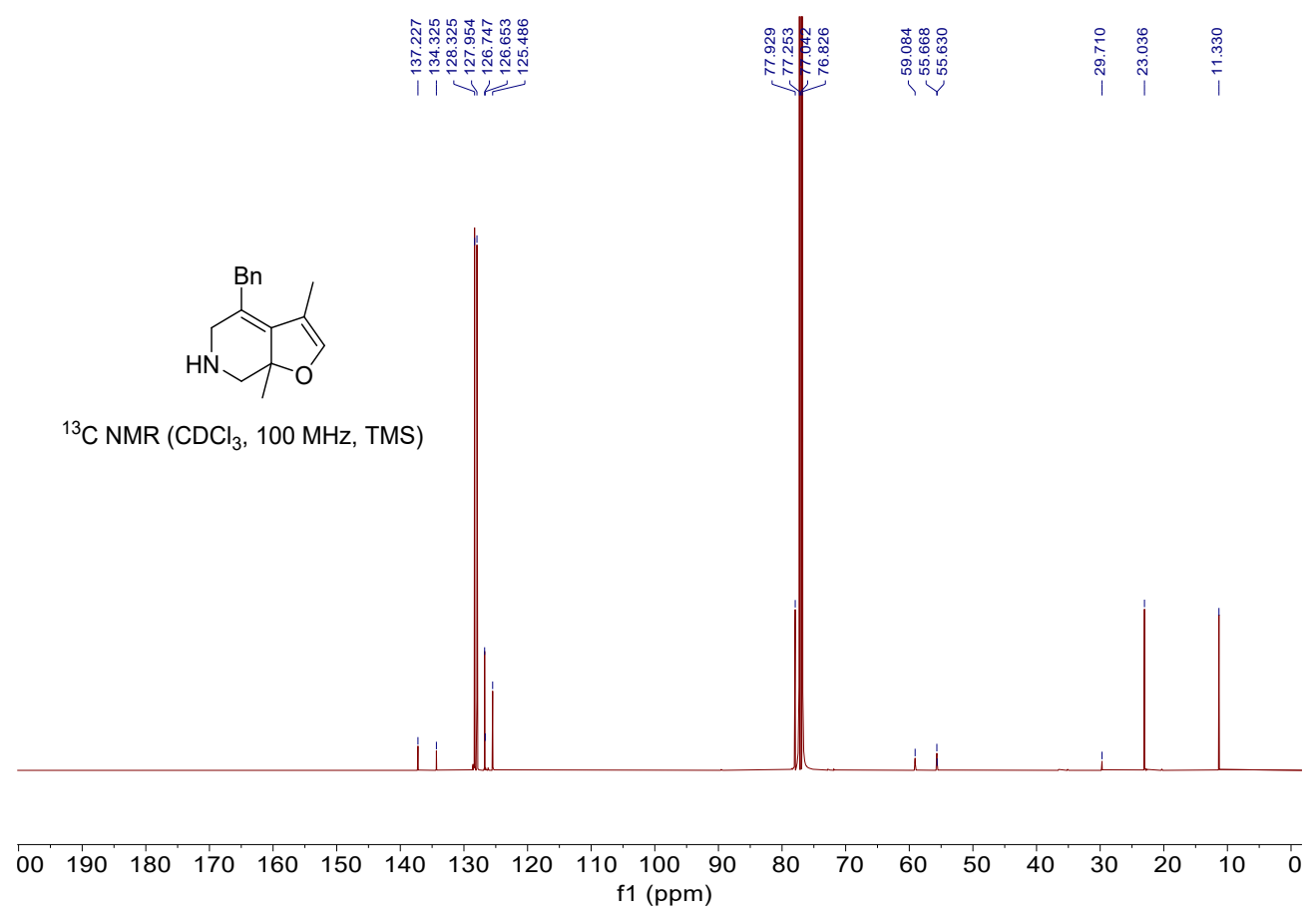


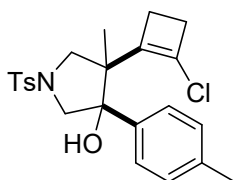
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)





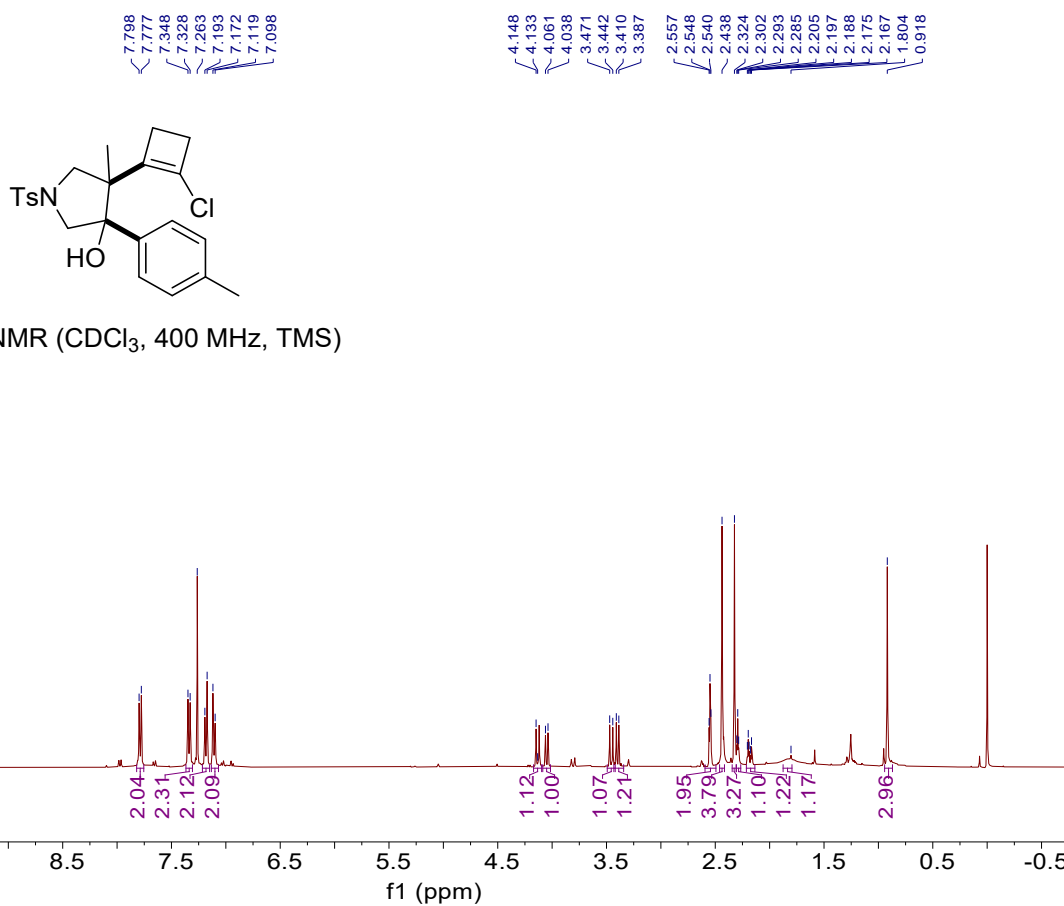
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)



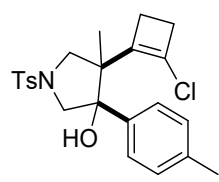


#### 4-(2-chlorocyclobut-1-en-1-yl)-4-methyl-3-(p-tolyl)-1-tosylpyrrolidin-3-ol (12)

A colorless oil, 46% yield, 19.8 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.79 (d,  $J = 8.2$  Hz, 2H), 7.34 (d,  $J = 8.0$  Hz, 2H), 7.18 (d,  $J = 8.2$  Hz, 2H), 7.11 (d,  $J = 8.0$  Hz, 2H), 4.15 (s, 1H), 4.05 (d,  $J = 9.2$  Hz, 1H), 3.46 (d,  $J = 11.4$  Hz, 1H), 3.40 (d,  $J = 9.2$  Hz, 1H), 2.55 (t,  $J = 3.2$  Hz, 2H), 2.44 (s, 4H), 2.32 (s, 3H), 2.31 – 2.27 (m, 1H), 2.21 – 2.14 (m, 1H), 1.80 (brs, 1H), 0.92 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.6, 141.3, 138.0, 135.5, 134.0, 129.7, 128.8, 127.6, 126.2, 123.9, 84.4, 57.7, 56.0, 51.3, 33.5, 28.5, 21.6, 21.2, 21.0. IR (neat)  $\nu$  668, 814, 1038, 1163, 1343, 1463, 2869, 2936  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{23}\text{H}_{27}\text{NO}_3\text{SCl}$  ( $\text{M}+\text{H}$ ) $^+$ : 432.1395, Found: 432.1394.



143.598  
141.338  
138.004  
135.470  
134.040  
129.677  
128.847  
127.569  
126.202  
123.924



<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)

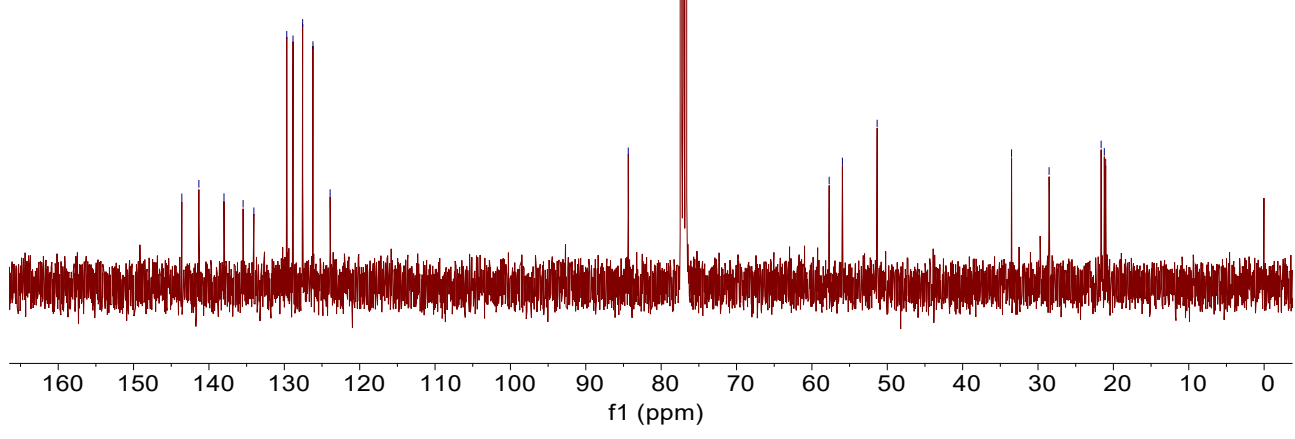
84.365  
77.357  
77.046  
76.722

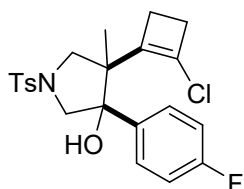
57.710  
55.953  
51.345

33.511

28.530

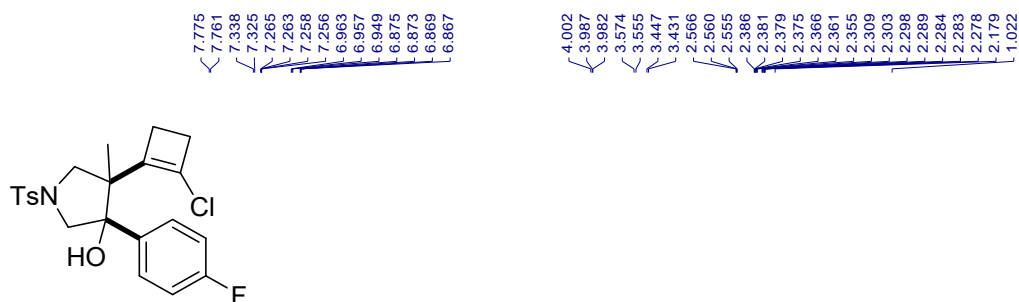
21.626  
21.203  
21.020



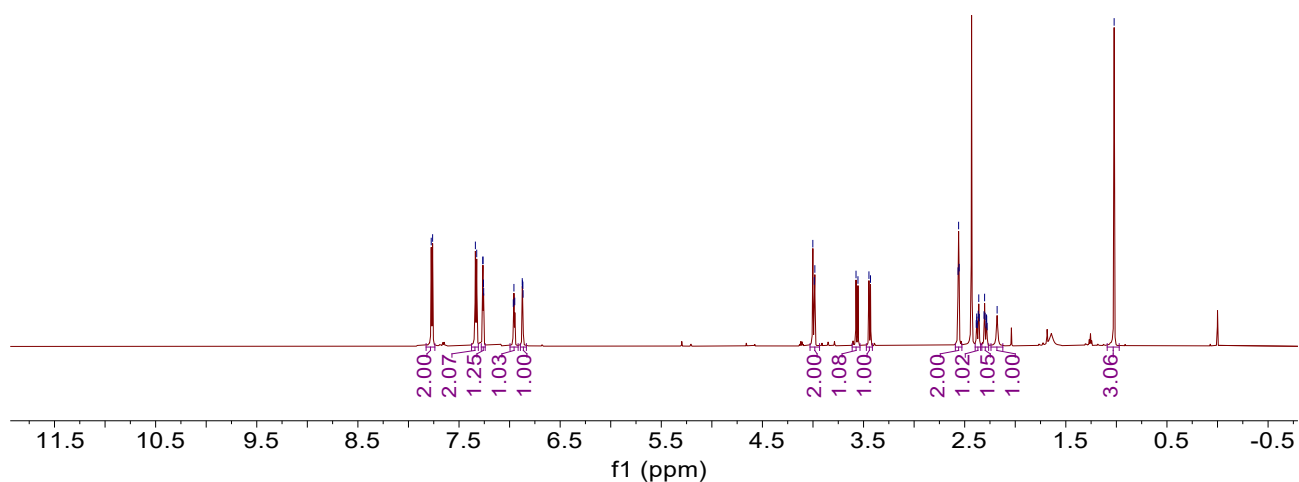


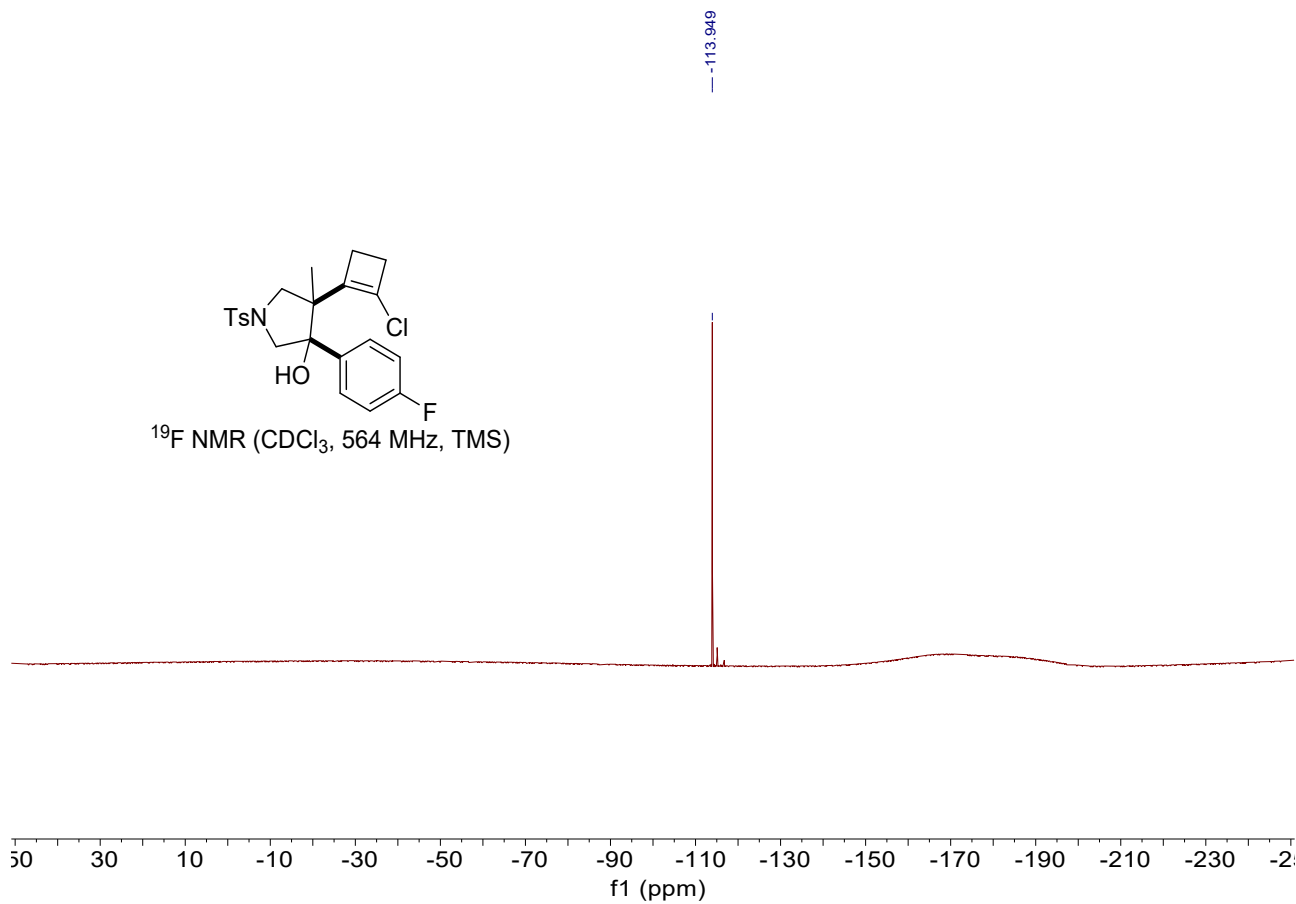
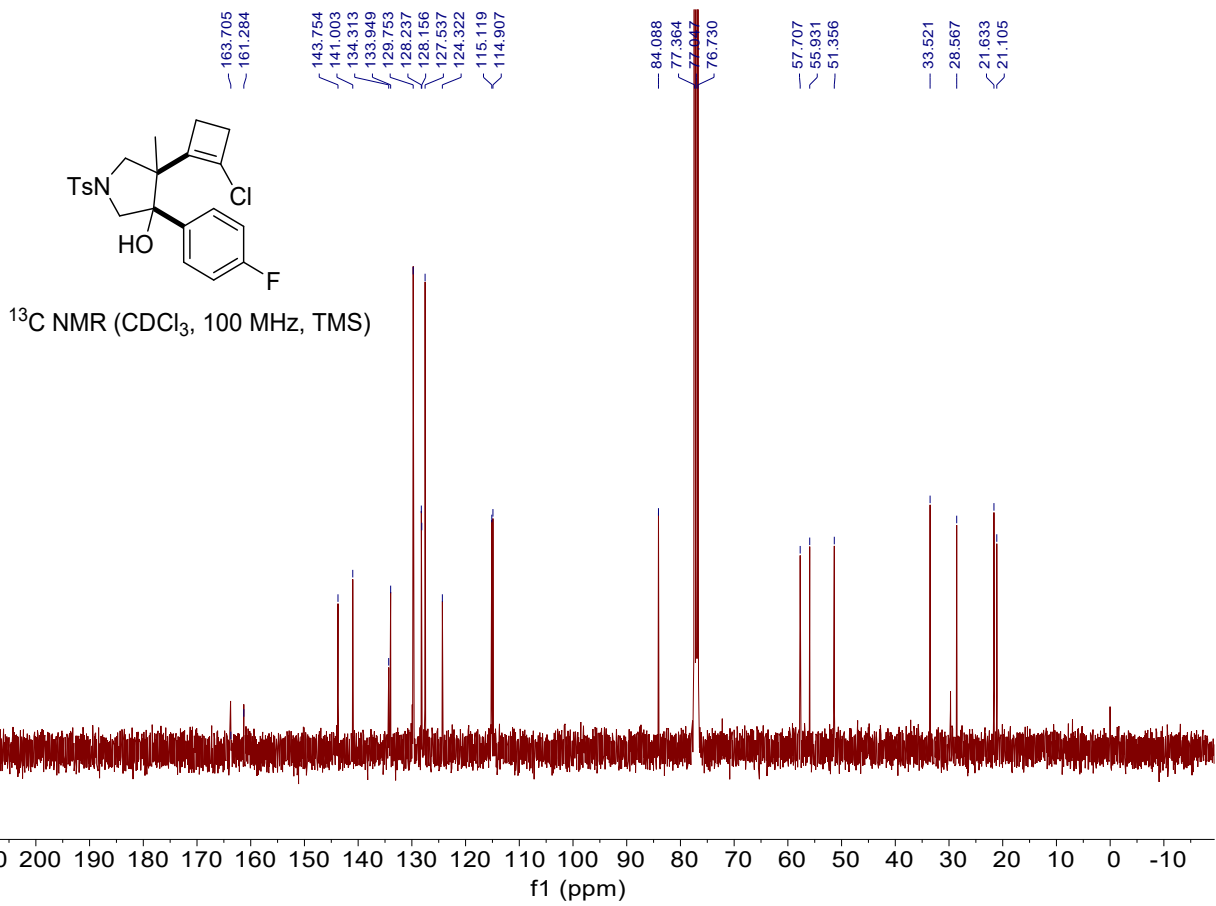
#### 4-(2-chlorocyclobut-1-en-1-yl)-3-(4-fluorophenyl)-4-methyl-1-tosylpyrrolidin-3-ol (13)

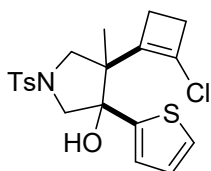
A colorless oil, 38% yield, 16.6 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.78 (d,  $J = 8.2$  Hz, 2H), 7.35 (d,  $J = 8.0$  Hz, 2H), 7.31 – 7.27 (m, 2H), 7.03 – 6.94 (m, 2H), 4.10 (d,  $J = 11.4$  Hz, 1H), 4.01 (d,  $J = 9.4$  Hz, 1H), 3.47 (d,  $J = 11.4$  Hz, 1H), 3.39 (d,  $J = 9.4$  Hz, 1H), 2.56 (dd,  $J = 4.2, 2.8$  Hz, 2H), 2.44 (s, 3H), 2.37 – 2.28 (m, 1H), 2.23 – 2.10 (m, 1H), 1.81 (brs, 1H), 0.91 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  162.5 (d,  $J_{\text{C-F}} = 242.1$  Hz), 143.8, 141.0, 134.2 (d,  $J_{\text{C-F}} = 3.3$  Hz), 129.8, 128.2 (d,  $J_{\text{C-F}} = 8.1$  Hz), 127.5, 124.3, 115.0 (d,  $J_{\text{C-F}} = 21.2$  Hz), 84.1, 57.7, 55.9, 51.4, 33.5, 28.6, 21.6, 21.1.  $^{19}\text{F}$  NMR ( $\text{CDCl}_3$ , TMS, 564 MHz)  $\delta$  -113.9 IR (neat)  $\nu$  668, 810, 1039, 1092, 1232, 1334, 1506, 2841, 2930  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{20}\text{H}_{22}\text{NO}_3\text{S}_2\text{Cl}$  ( $\text{M}+\text{H}$ ) $^+$ : 436.1144, Found: 436.1139.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, TMS)

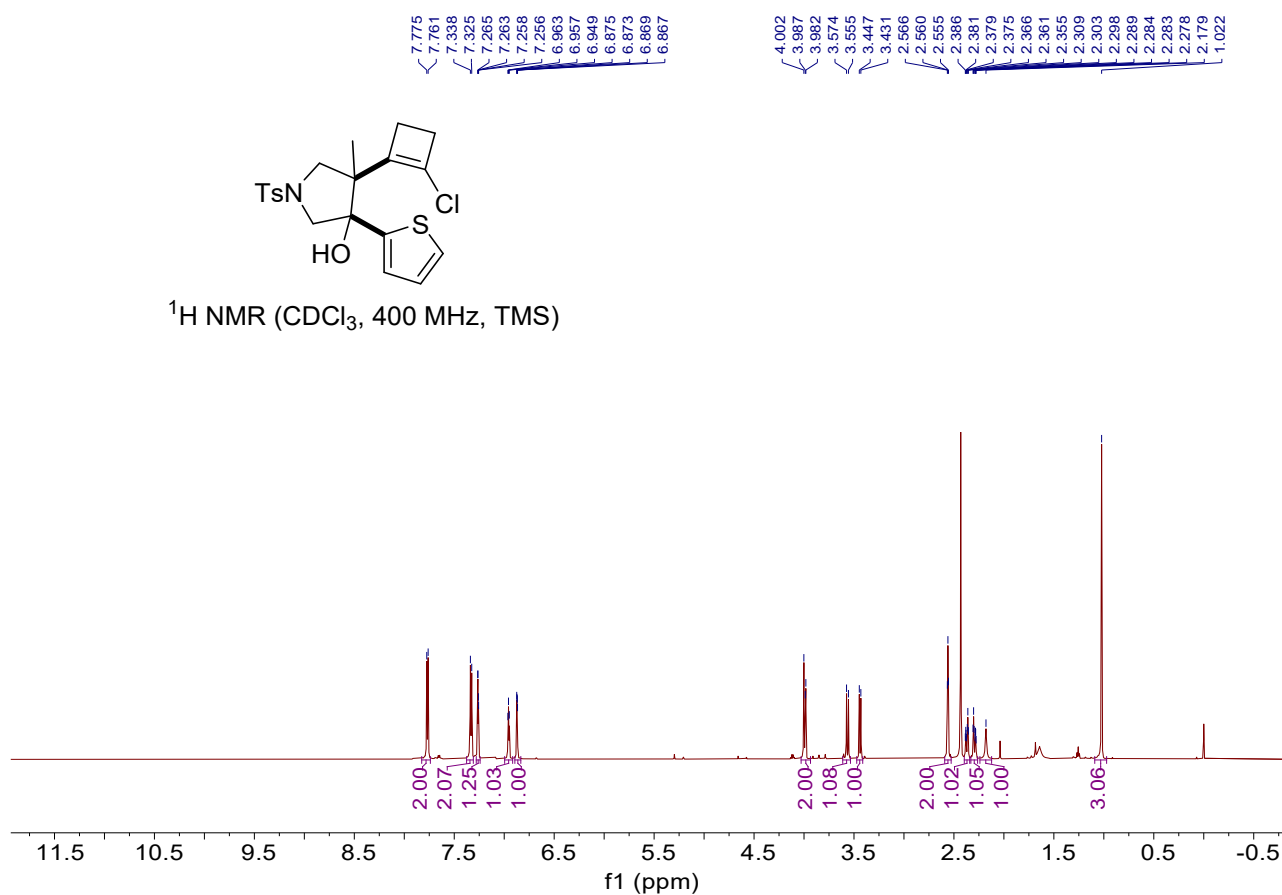


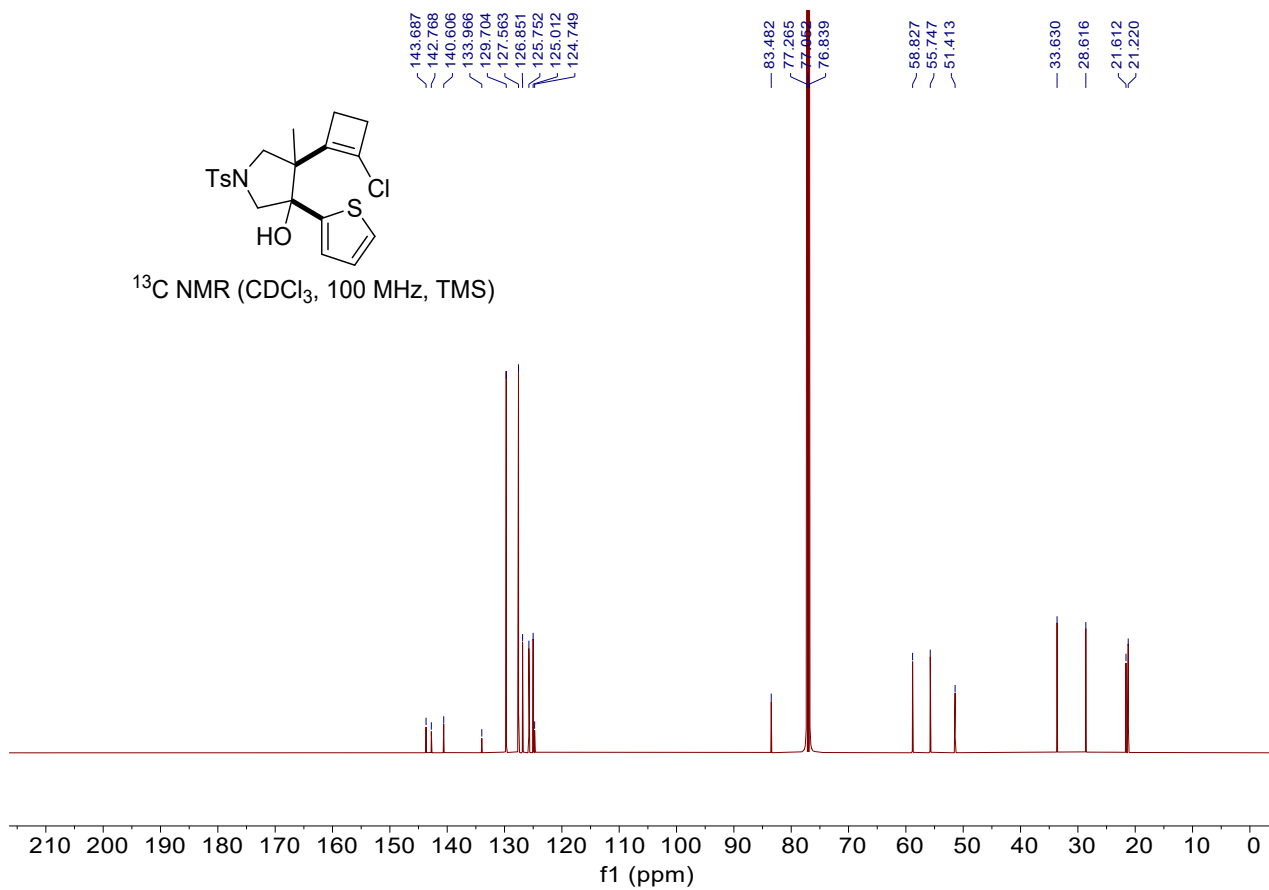




#### 4-(2-chlorocyclobut-1-en-1-yl)-4-methyl-3-(thiophen-2-yl)-1-tosylpyrrolidin-3-ol (14)

A colorless oil, 40% yield, 16.9 mg.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS, 400 MHz)  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H), 7.33 (d,  $J = 8.4$  Hz, 2H), 7.28 – 7.24 (m, 1H), 7.00 – 6.92 (m, 1H), 6.87 (dd,  $J = 3.6, 1.2$  Hz, 1H), 4.03 – 3.94 (m, 2H), 3.56 (d,  $J = 11.6$  Hz, 1H), 3.44 (d,  $J = 9.2$  Hz, 1H), 2.56 (t,  $J = 3.2$  Hz, 2H), 2.37 (dt,  $J = 11.6, 3.2$  Hz, 1H), 2.29 (dt,  $J = 11.6, 3.6$  Hz, 1H), 2.18 (brs, 1H), 1.02 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , TMS, 100 MHz)  $\delta$  143.7, 142.8, 140.6, 134.0, 129.7, 127.6, 126.9, 125.8, 125.0, 124.7, 83.5, 58.8, 55.7, 51.4, 33.6, 28.6, 21.6, 21.2. IR (neat)  $\nu$  668, 767, 1039, 1042, 1192, 1356, 1596, 2899, 2933  $\text{cm}^{-1}$ . HRMS (ESI) calcd. for  $\text{C}_{20}\text{H}_{22}\text{NO}_3\text{S}_2\text{ClNa}$  ( $\text{M}+\text{Na}$ ) $^+$ : 446.0622, Found: 446.0621.







## 10. Computational studies

### 10.1 DFT calculations of proximal C-C bond cleavage.

All quantum mechanical calculations have been performed with Gaussian 16.<sup>[4]</sup> The geometries of all species have been optimized at B3LYP/6-31G(d)/Lanl2dz level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the SMD(toluene)/B3LYP/6-311+G(d,p)/Lanl2dz//B3LYP/6-31G(d)/Lanl2dz level to yield free energy  $G_{298}$  at 298.15 K. The solvent effect was estimated by the IEFPCM method with radii and nonelectrostatic terms for SMD salvation model in toluene ( $\epsilon = 2.3741$ ).

**Table S4.** The total energies, enthalpies and free energies of all species in toluene shown in Schemes S1 & S2 & Scheme 7a

	$E_{\text{tot}}$	$H_{298}$	$G_{298}$
<b>2-Int1</b>	-2279.787277	-2279.917073	-2280.556690
<b>2-Ts1</b>	-2279.754786	-2279.882268	-2280.522494
<b>2-Ts1'</b>	-2279.722047	-2279.843055	-2280.489357
<b>2-Int2</b>	-2279.781835	-2279.905456	-2280.551696
<b>2-Int2''</b>	-2279.764780	-2279.885805	-2280.535000
<b>2-Ts2</b>	-2279.765803	-2279.884554	-2280.534763
<b>2-Ts2'</b>	-2279.753803	-2279.871081	-2280.522647
<b>2-Ts2''</b>	-2279.703396	-2279.830765	-2280.467525
<b>2-Int3</b>	-2279.776141	-2279.894637	-2280.547360
<b>2-Int3''</b>	-2279.766920	-2279.896828	-2280.531604
<b>2-Ts3</b>	-2279.758423	-2279.879797	-2280.522665
<b>2-Ts3''</b>	-2279.753001	-2279.875682	-2280.518514
<b>2-Int4</b>	-2279.758772	-2279.887644	-2280.525212
<b>2-Int4''</b>	-2279.765497	-2279.897132	-2280.530848
<b>2-Ts4</b>	-2279.751243	-2279.874953	-2280.514939
<b>2-Int5</b>	-2279.795379	-2279.914305	-2280.565817
<b>2-Int5''</b>	-2279.772338	-2279.897992	-2280.538573
<b>2-TS5</b>	-2279.774145	-2279.892923	-2280.542442
<b>2-Int6</b>	-2279.830847	-2279.955917	-2280.602512

## 10.2 DFT calculations of distal C-C bond cleavage.

All quantum mechanical calculations have been performed with Gaussian 16. The geometries of all species have been optimized at  $\omega$ B97X-D/6-31G(d)/Lanl2dz level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the SMD(toluene)/ $\omega$ B97X-D/6-311+G(d,p)/Lanl2dz// $\omega$ B97X-D/6-31G(d)/Lanl2dz level to yield free energy  $G_{298}$  at 298.15 K. The solvent effect was estimated by the IEFPCM method with radii and nonelectrostatic terms for SMD salvation model in toluene ( $\epsilon = 2.3741$ ).

**Table S5.** The total energies, enthalpies and free energies of all species in toluene shown in **Scheme 7b**

	$E_{\text{tot}}$	$H_{298}$	$G_{298}$
<b>1a</b>	-1338.596349	-1338.217969	-1338.298770
<b>Pd</b>	-1600.000258	-1599.280868	-1599.381149
<b>3-Int1-a</b>	-2938.604443	-2937.503807	-2937.664189
<b>3-Ts1-a</b>	-2938.606983	-2937.508634	-2937.660200
<b>3-Int2-a</b>	-2938.632893	-2937.532573	-2937.684914
<b>3-Ts2-a</b>	-2938.581311	-2937.482359	-2937.635790
<b>3-Int3-a</b>	-2938.624503	-2937.523519	-2937.679753
<b>3-Ts3-a</b>	-2938.595560	-2937.495434	-2937.640581
<b>3-Int4</b>	-2938.653535	-2937.550349	-2937.698454
<b>3-Ts4</b>	-2938.62696	-2937.525973	-2937.672988
<b>3+PdL</b>	-2938.690222	-2937.586547	-2937.740068
<b>1a+ZnCl<sub>2</sub></b>	-2324.612067	-2324.223978	-2324.317312
<b>3-Int1-b</b>	-3924.637201	-3923.527787	-3923.700862
<b>3-Ts1-b</b>	-3924.636696	-3923.529061	-3923.696093
<b>3-Int2-b</b>	-3924.665652	-3923.556361	-3923.723694
<b>3-Ts2-b</b>	-3924.612247	-3923.503978	-3923.672031
<b>3-Int3-b</b>	-3924.658858	-3923.549119	-3923.719918
<b>3-Ts3-b</b>	-3924.630202	-3923.521235	-3923.683495
<b>3-Int1'</b>	-2938.568733	-2937.469431	-2937.639441
<b>3-Ts1'</b>	-2938.564112	-2937.466122	-2937.629710
<b>3-Int2'</b>	-2938.595629	-2937.495439	-2937.647003
<b>3-Ts2'</b>	-2938.543815	-2937.445669	-2937.601274

<b>3-Int3'</b>	-2938.600183	-2937.499586	-2937.658239
<b>3-Ts3'</b>	-2938.565605	-2937.467803	-2937.619657
<b>3-Int4'</b>	-2938.63036	-2937.527644	-2937.680249
<b>3-Ts4'</b>	-2938.596441	-2937.495604	-2937.649678
<b>3+PdL'</b>	-2938.667115	-2937.563082	-2937.715840

## Archive entries

<b>2-Int1</b>				C	8.02929600	1.46059900	-0.68026400
Zero-point correction= 0.723023 (Hartree/Particle)				H	7.24724300	1.91977500	-2.63645400
Thermal correction to Energy= 0.768470				H	8.57716100	0.72219600	1.27015200
Thermal correction to Enthalpy= 0.769414				C	9.12927300	2.49383500	-0.73780600
Thermal correction to Gibbs Free Energy= 0.639617				H	9.45038500	2.68094500	-1.76768100
Sum of electronic and zero-point Energies= -2279.833667				H	8.79010600	3.45237200	-0.32269800
Sum of electronic and thermal Energies= -2279.788221				H	10.00444000	2.18066400	-0.15916700
Sum of electronic and thermal Enthalpies= -2279.787277				C	1.56018300	-2.42943800	2.09955700
Sum of electronic and thermal Free Energies= -2279.917073				H	0.89658400	-2.32312800	1.23415800
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.062436				H	2.36505500	-3.11308000	1.81039900
N	3.28362700	-0.78622400	0.25679100	H	0.98579900	-2.83320300	2.93655400
C	3.32311100	-0.54991700	1.69956000	C	0.65570700	-1.22229800	-1.49659700
H	4.18024500	-1.08926500	2.11729700	H	0.89552400	-1.02600500	-2.55131800
H	3.44197900	0.51711100	1.92719400	H	1.20576900	-2.13044200	-1.22058200
C	2.10062500	-1.06790300	2.47462000	H	-0.41709700	-1.41304300	-1.41711500
C	2.55455100	0.22038900	-0.55367100	Pd	-1.89772000	0.76144600	0.16422400
H	2.97026800	0.19158700	-1.56496100	P	-4.15221300	-0.02876100	-0.27187900
H	2.74234300	1.21611100	-0.13298500	C	-4.61887200	0.20248900	-2.14698000
C	1.06101700	-0.05650600	-0.62878100	C	-3.40296500	-0.24775800	-2.99352000
C	0.21404500	0.73473900	0.02459300	H	-2.49489700	0.28091800	-2.68515700
C	-0.13763300	1.77389400	0.81949400	H	-3.20668200	-1.31867500	-2.93617500
C	0.07885800	2.32930000	2.18597500	H	-3.60016700	-0.00786900	-4.04722100
C	0.03173700	3.24965200	0.96909700	C	-4.79300200	1.70824200	-2.44486900
H	1.03041700	2.12375900	2.67125900	H	-4.86297700	1.84090300	-3.53246000
H	-0.76677600	2.36549800	2.86918500	H	-5.70372100	2.12873400	-2.01232200
H	-0.83914000	3.89232800	0.85965600	H	-3.93348400	2.29054800	-2.09651200
H	0.96028300	3.69372800	0.61142300	C	-5.87947800	-0.54263500	-2.62898300
S	4.59279500	-1.58966400	-0.44662000	H	-6.77556300	-0.26185200	-2.06923500
O	4.98301600	-2.62995300	0.51205400	H	-6.06091700	-0.29352100	-3.68354300
O	4.18568000	-1.90917700	-1.81710600	H	-5.77093700	-1.62875200	-2.57283100
C	5.95311300	-0.42032100	-0.55009700	C	-5.37676400	1.02616700	0.81439900
C	6.09535900	0.37571100	-1.68992800	C	-4.36140300	-1.90599000	0.20006300
C	6.84704600	-0.30105600	0.51759300	C	-6.86303300	0.96628500	0.40859700
C	7.12990500	1.30783700	-1.74541200	H	-7.45185500	1.56108600	1.12042200
H	5.42351800	0.24159300	-2.53085900	H	-7.04363900	1.38657200	-0.58399300
C	7.87532500	0.63667600	0.44413900	H	-7.26346700	-0.05065900	0.42486000
H	6.75564600	-0.95685400	1.37671200	C	-4.89832400	2.49875600	0.77354600

H	-5.50753000	3.08650300	1.47375000	H	-1.05428600	-4.26568000	-3.25192600
H	-3.85006200	2.57991700	1.08320500	H	-1.62998400	-2.68194600	-3.93504800
H	-4.99363900	2.96014100	-0.20933900	S	4.55868900	-0.82033500	0.81460500
C	-5.25369000	0.59257800	2.29227700	O	4.67547100	-0.43920900	2.22625700
H	-4.21175500	0.58690900	2.62870600	O	5.37940000	-1.88414300	0.23078400
H	-5.79836500	1.31662300	2.91243800	C	4.80801700	0.66668300	-0.15850200
H	-5.69059600	-0.38888600	2.48868100	C	5.22173400	0.56062500	-1.48970700
C	-5.81219300	-2.39859000	0.37248800	C	4.56131600	1.91669300	0.41688400
H	-5.80064700	-3.47618900	0.58616600	C	5.37978900	1.71919900	-2.24677000
H	-6.32235900	-1.91395900	1.20862700	H	5.43788800	-0.41421900	-1.91366200
H	-6.41691500	-2.25107600	-0.52609400	C	4.72398300	3.06438600	-0.35816700
C	-3.57672400	-2.15561200	1.51122900	H	4.26608300	1.98533600	1.45854300
H	-4.01631300	-1.66420400	2.37938500	C	5.13382100	2.98632600	-1.69652600
H	-3.56852500	-3.23482200	1.71567300	H	5.70633100	1.63923200	-3.28081600
H	-2.54065400	-1.81305600	1.42087700	H	4.53464700	4.03762700	0.08781100
C	-3.67335800	-2.78261500	-0.86989800	C	5.34007900	4.23675400	-2.51802200
H	-2.64120800	-2.46708400	-1.05255300	H	4.72712300	5.06510100	-2.14858000
H	-3.64061200	-3.81637100	-0.50192000	H	6.38798400	4.56276100	-2.47979500
H	-4.20904100	-2.79836700	-1.82159900	H	5.09055900	4.07027200	-3.57129400
O	1.66063800	-0.40863400	3.39726600	C	1.99815100	-1.63206000	3.47211400
<b>2-Ts1</b>				H	1.42874700	-2.44874900	3.01228800
Zero-point correction= 0.721711 (Hartree/Particle)				H	3.05424800	-1.91592700	3.45320100
Thermal correction to Energy= 0.766764				H	1.67255800	-1.48253800	4.50369000
Thermal correction to Enthalpy= 0.767708				C	1.79107200	-4.13157600	0.10654700
Thermal correction to Gibbs Free Energy= 0.640226				H	2.60992400	-4.67632900	-0.38368400
Sum of electronic and zero-point Energies= -2279.800783				H	2.12729600	-3.90951400	1.12623700
Sum of electronic and thermal Energies= -2279.755730				H	0.92151800	-4.79213700	0.16008600
Sum of electronic and thermal Enthalpies= -2279.754786				Pd	-2.00080100	-1.08715600	-0.92786400
Sum of electronic and thermal Free Energies= -2279.882268				P	-3.13708100	0.74022600	0.15060800
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.027408				C	-3.42385300	0.36473600	2.04105000
N	2.93882900	-1.29068700	0.60526700	C	-2.13614800	-0.29504600	2.59133400
C	1.94520900	-0.37289100	1.17330400	H	-1.85508600	-1.16199700	1.98270900
H	2.07547500	0.66281500	0.83070500	H	-1.28240800	0.38074600	2.64014200
H	0.97423000	-0.71583600	0.79128200	H	-2.33008800	-0.64345300	3.61490400
C	1.80303500	-0.34780800	2.69994700	C	-4.53132900	-0.70299400	2.18332200
C	2.58462300	-1.82773400	-0.73591200	H	-4.54688500	-1.05094500	3.22444900
H	3.48556000	-2.31081000	-1.12524500	H	-5.52915000	-0.31793800	1.96035800
H	2.29771100	-1.01475700	-1.41642800	H	-4.33813300	-1.57310500	1.54701200
C	1.47198900	-2.85438500	-0.64642600	C	-3.79199700	1.57052700	2.92914500
C	0.31132500	-2.66423600	-1.24970000	H	-4.70386400	2.07533900	2.60006200
C	-0.80885400	-2.53193500	-1.90915800	H	-3.96610200	1.21729200	3.95476500
C	-2.46897800	-3.08151300	-1.94641700	H	-2.99159300	2.31245700	2.98135100
C	-1.42426000	-3.26228700	-3.03376900	C	-4.87534800	1.05473500	-0.68224800
H	-3.38099000	-2.55445800	-2.22819900	C	-2.09764900	2.38302700	-0.00154800
H	-2.61659800	-3.90005400	-1.24914000	C	-5.85365300	1.94080000	0.11596600
				H	-6.76096800	2.10022600	-0.48303000

H	-6.16900500	1.47365600	1.05244900	C	0.69630500	1.25302600	-3.47951100
H	-5.44107900	2.92477100	0.34998900	H	2.10432000	-0.46022200	-3.27423300
C	-5.55110400	-0.31124700	-0.94912100	H	2.88469600	1.16329800	-3.13953100
H	-6.48895800	-0.13810500	-1.49437400	H	0.87996900	2.14457300	-4.09598900
H	-4.91146300	-0.94858400	-1.56615200	H	0.06063700	0.57245000	-4.06355600
H	-5.79767600	-0.86129200	-0.04115900	S	-4.54350500	0.76468700	1.25835700
C	-4.66200200	1.68602800	-2.07594000	O	-4.14711100	0.42498400	2.63168700
H	-3.94447900	1.11243500	-2.67237100	O	-5.56305900	1.77700900	0.97573200
H	-5.61997400	1.68040500	-2.61268200	C	-5.05931600	-0.75971800	0.46014700
H	-4.32735100	2.72440200	-2.02959300	C	-5.84987800	-0.70195100	-0.69136900
C	-2.85297000	3.70074000	0.26508500	C	-4.64903600	-1.98929000	0.98124700
H	-2.14167600	4.53604400	0.20538900	C	-6.21403900	-1.88663100	-1.32777000
H	-3.63544300	3.89649000	-0.47229400	H	-6.19648900	0.25645200	-1.06284600
H	-3.30622300	3.73163600	1.25934600	C	-5.02430000	-3.16424700	0.33159800
C	-1.49074600	2.42408600	-1.42571600	H	-4.07270700	-2.02117800	1.89960300
H	-0.80078900	3.27660300	-1.49069700	C	-5.80286600	-3.13362100	-0.83399200
H	-0.92616200	1.50972100	-1.63909200	H	-6.83686500	-1.84268700	-2.21791600
H	-2.23562000	2.54644800	-2.21251300	H	-4.71541800	-4.12203400	0.74323200
C	-0.89443200	2.31492300	0.96252200	C	-6.17988900	-4.40965600	-1.54844400
H	-0.32719300	1.38914200	0.84258200	H	-7.16182800	-4.32664200	-2.02601100
H	-0.21553900	3.14675200	0.73294300	H	-5.45377300	-4.64741900	-2.33730200
H	-1.17183700	2.41201000	2.01343700	H	-6.20580100	-5.26163600	-0.86143600
O	1.44088500	0.68926200	3.22579000	C	-1.18907400	2.51684500	2.34602700
<b>2-Int2</b>				H	-1.65931100	3.36757600	1.84096300
Zero-point correction= 0.724491 (Hartree/Particle)				H	-1.93545500	2.11341000	3.03852700
Thermal correction to Energy= 0.768916				H	-0.30222000	2.86502500	2.87985700
Thermal correction to Enthalpy= 0.769861				C	-2.25608300	4.18334800	-0.91614300
Thermal correction to Gibbs Free Energy= 0.646240				H	-2.98286700	4.65626600	-1.59290000
Sum of electronic and zero-point Energies= -2279.827205				H	-2.64078000	4.33471400	0.10247400
Sum of electronic and thermal Energies= -2279.782780				H	-1.30859200	4.72149500	-1.01208500
Sum of electronic and thermal Enthalpies= -2279.781835				Pd	1.50788100	0.66624100	-0.96261600
Sum of electronic and thermal Free Energies= -2279.905456				P	3.41843900	-0.56360600	0.21983300
HF(B3LYP/6-311+G(d,p)/LanL2dz, SMD[toluene])= -2281.051946				C	4.49039100	0.72022800	1.21993800
N	-3.13399300	1.28753600	0.48721500	C	3.53117200	1.78879300	1.79555100
C	-1.89216100	0.56785400	0.78397700	H	2.94501900	2.26493000	1.00404000
H	-2.08632400	-0.15931400	1.58126700	H	2.83082500	1.39422600	2.53080500
H	-1.51174600	0.03645000	-0.09496800	H	4.13145200	2.56400900	2.29122200
C	-0.79442700	1.48206000	1.32363200	C	5.42552000	1.47836800	0.25136700
C	-3.24883600	1.79378700	-0.91250000	H	5.85125000	2.33846900	0.78456800
H	-4.19941800	2.32840100	-0.97520000	H	6.26491200	0.87003600	-0.09357800
H	-3.27061200	0.94343200	-1.60773400	H	4.88685000	1.86660000	-0.61916200
C	-2.08439100	2.71241900	-1.23164300	C	5.34949400	0.14213900	2.36334000
C	-0.97630300	2.18973400	-1.74774800	H	6.05946400	-0.61319200	2.01861300
C	0.09005600	1.57863000	-2.13908700	H	5.93265400	0.95691400	2.81433200
C	1.97652300	0.58131200	-2.97031700	H	4.74798100	-0.29781000	3.16204700
				C	4.62809800	-1.60234500	-0.91129800

C	2.61006300	-1.81299900	1.49238500	C	-1.17261500	-1.39105300	2.13850400
C	5.91848500	-2.10644400	-0.22971500	C	-0.35644400	-0.53683500	2.53657000
H	6.45852600	-2.75226600	-0.93586500	C	1.25258400	1.17959800	2.52833500
H	6.59331900	-1.28556200	0.02748800	C	0.27533500	0.45497700	3.45693400
H	5.73605200	-2.69222700	0.67244400	H	0.85700100	2.13510400	2.17640300
C	5.05075700	-0.76302400	-2.14080700	H	2.25912600	1.30029300	2.92863500
H	5.69757500	-1.38722600	-2.77246100	H	0.79511600	-0.07537800	4.26504000
H	4.19388900	-0.46270100	-2.74081600	H	-0.47364700	1.11181600	3.92250800
H	5.61787300	0.13115200	-1.88554500	S	-4.42663700	-0.87503900	-1.30248800
C	3.85738400	-2.81443200	-1.48275500	O	-4.07947300	-0.79712700	-2.72437300
H	2.90885900	-2.51380600	-1.93937000	O	-5.61659100	-1.58728500	-0.82870100
H	4.46949900	-3.27870300	-2.26715500	C	-4.53618500	0.81031900	-0.68705400
H	3.65540800	-3.58604900	-0.73709900	C	-5.34266500	1.09346100	0.41828800
C	3.53160500	-2.91147600	2.06079000	C	-3.78412500	1.81963600	-1.29554200
H	2.96363800	-3.50139400	2.79340200	C	-5.38523300	2.39491500	0.91732400
H	3.88544700	-3.60881300	1.29845900	H	-5.94387600	0.30622200	0.86034600
H	4.40146800	-2.50082900	2.58057600	C	-3.83881200	3.11454700	-0.78345800
C	1.41039800	-2.48033500	0.77551700	H	-3.18633000	1.59323200	-2.17210000
H	0.88102100	-3.12165400	1.49369400	C	-4.63663000	3.42343600	0.32849600
H	0.70642000	-1.72926100	0.40302100	H	-6.01618300	2.61628500	1.77487200
H	1.70335100	-3.10728400	-0.06757400	H	-3.25883200	3.90131700	-1.26023600
C	2.01207200	-1.04562900	2.69312300	C	-4.71600400	4.83763500	0.85359000
H	1.35586700	-0.23349500	2.37750200	H	-4.95220100	4.85598400	1.92257800
H	1.41224600	-1.75082500	3.28435800	H	-3.77359000	5.37490600	0.70338700
H	2.77439900	-0.64012900	3.36183400	H	-5.50053900	5.40607300	0.33640000
O	0.38440200	1.31466400	1.01525700	C	-1.00551200	-3.62832300	-0.96099700
<b>2-Ts2</b>				H	-2.05789900	-3.91159300	-1.03649400
Zero-point correction= 0.725139 (Hartree/Particle)				H	-0.58664400	-3.60504500	-1.97611900
Thermal correction to Energy= 0.768017				H	-0.45512000	-4.38245500	-0.39306100
Thermal correction to Enthalpy= 0.768961				C	-1.80216600	-3.77886700	1.97364400
Thermal correction to Gibbs Free Energy= 0.650209				H	-2.32040300	-3.87669100	2.93727300
Sum of electronic and zero-point Energies= -2279.809625				H	-2.26212900	-4.49099600	1.28178700
Sum of electronic and thermal Energies= -2279.766747				H	-0.75819100	-4.07235600	2.12748900
Sum of electronic and thermal Enthalpies= -2279.765803				Pd	1.10218400	-0.15976500	0.95565800
Sum of electronic and thermal Free Energies= -2279.884554				P	3.09034800	0.40356100	-0.34481300
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.033935				C	4.57994400	-0.48695100	0.54597400
N	-3.12411600	-1.58630100	-0.52786800	C	4.06503900	-1.84194600	1.08932700
C	-1.76776200	-1.18070900	-0.88716300	H	3.22620800	-1.69978300	1.77820400
H	-1.69554100	-1.13779700	-1.97792900	H	3.73546400	-2.52593200	0.30768300
H	-1.48601800	-0.20113100	-0.47003900	H	4.88181400	-2.33001400	1.63830400
C	-0.80804500	-2.24811600	-0.34561300	C	5.03045300	0.32499600	1.78048100
C	-3.26114700	-1.90253500	0.91697500	H	5.74733400	-0.28328200	2.34726400
H	-4.00970000	-2.69077500	1.02434600	H	5.53823100	1.25639000	1.51957200
H	-3.61411900	-1.02149100	1.47080700	H	4.19679300	0.55262700	2.44986200
C	-1.88745000	-2.35347500	1.43045400	C	5.82405100	-0.73734000	-0.33286400
				H	6.24787300	0.18341400	-0.74051100

H	6.59985700	-1.20579100	0.28771700	H	3.49128500	-3.11916000	-1.21435400
H	5.62584600	-1.41882500	-1.16221800	H	3.73533100	-1.40687600	-1.58147200
C	3.54250400	2.29126300	-0.56778900	C	1.61447400	-2.02416200	-1.47998100
C	2.90377300	-0.36379800	-2.13524200	C	1.28309300	-0.63467000	-1.82538200
C	4.98225200	2.56190700	-1.05711400	C	1.05689700	0.53823400	-2.08828100
H	5.09042200	3.63961300	-1.24007700	C	-0.85122100	1.91932600	-1.85128900
H	5.73109300	2.29093500	-0.30848900	C	0.61311000	1.92758000	-2.32342100
H	5.22868200	2.04811100	-1.98712300	H	-1.08237000	2.76976100	-1.20976300
C	3.34525400	3.04602100	0.76617600	H	-1.54080500	1.87033500	-2.69681200
H	3.65138900	4.09004900	0.61600900	H	0.73955300	2.20792100	-3.37763700
H	2.29803000	3.04913100	1.06780600	H	1.23501900	2.60781200	-1.72935900
H	3.93707000	2.64951500	1.59065400	S	4.37251000	-1.11054600	1.14817700
C	2.54990900	2.94492300	-1.55555800	O	4.13794300	-1.20272400	2.59130100
H	1.50985600	2.73987000	-1.28101100	O	5.56645100	-1.67061000	0.50755100
H	2.69214700	4.03291000	-1.51805600	C	4.31668000	0.63548900	0.71811500
H	2.70534700	2.63716500	-2.59100400	C	5.01469600	1.09674500	-0.40152800
C	3.95473800	0.09687900	-3.16789700	C	3.55071100	1.51522100	1.48832800
H	3.78209900	-0.45680900	-4.10033600	C	4.93180700	2.44327400	-0.75282000
H	3.87671500	1.15871900	-3.41235900	H	5.63419700	0.40997700	-0.96836600
H	4.98107900	-0.10982900	-2.85530300	C	3.47809800	2.85892000	1.12242700
C	1.49473600	-0.00884500	-2.66705400	H	3.04338000	1.15280800	2.37597500
H	1.36924000	-0.47956600	-3.65135700	C	4.16471900	3.34475600	-0.00018200
H	0.72579400	-0.40595200	-2.00305000	H	5.48164700	2.80282200	-1.61955900
H	1.33064000	1.06119900	-2.79639000	H	2.88948600	3.54488100	1.72730500
C	2.95027500	-1.90784200	-2.05987200	C	4.11828800	4.81094400	-0.36290300
H	2.22213900	-2.29942700	-1.34598600	H	4.95181500	5.35686200	0.09884100
H	2.68426300	-2.29760100	-3.05176400	H	4.19458100	4.95994100	-1.44529900
H	3.94468300	-2.29461500	-1.82675300	H	3.19160000	5.28152400	-0.01800800
O	0.42339200	-1.92614900	-0.13411300	C	0.81242600	-3.85717900	0.17437400
<b>2-Int3</b>				H	0.22084800	-4.39916900	-0.56869800
Zero-point correction= 0.727328 (Hartree/Particle)				H	1.82340200	-4.28035100	0.20959100
Thermal correction to Energy= 0.770274				H	0.34491200	-4.01646200	1.15157200
Thermal correction to Enthalpy= 0.771219				C	1.26956900	-2.94887200	-2.65847900
Thermal correction to Gibbs Free Energy= 0.652723				H	1.75685900	-2.61604600	-3.58163300
Sum of electronic and zero-point Energies= -2279.820032				H	1.59233900	-3.97362400	-2.45278700
Sum of electronic and thermal Energies= -2279.777085				H	0.18702200	-2.94923200	-2.82028700
Sum of electronic and thermal Enthalpies= -2279.776141				Pd	-0.90271400	0.07711200	-0.86179000
Sum of electronic and thermal Free Energies= -2279.894637				P	-3.01761400	0.25890300	0.26842000
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.046202				C	-4.21700900	-1.11994100	-0.41953600
N	3.06636500	-1.82904800	0.41084000	C	-3.40263600	-2.39445800	-0.73372800
C	1.69947900	-1.60773900	0.90671600	H	-2.61067400	-2.20153500	-1.45942900
H	1.59249300	-2.01326500	1.91471600	H	-2.92319000	-2.83267500	0.13844600
H	1.43508200	-0.54067500	0.92055300	H	-4.09441900	-3.13668400	-1.15542900
C	0.79931000	-2.34554000	-0.13066200	C	-4.82617600	-0.66248100	-1.76345000
C	3.09674100	-2.11223600	-1.04009800	H	-5.31726000	-1.52777900	-2.22648300
				H	-5.58839500	0.11150500	-1.64801200

H	-4.06139000	-0.30907300	-2.46291600	C	-3.10985800	3.83559600	0.24150300
C	-5.37168800	-1.49911200	0.53336500	C	-3.81594900	3.27035500	-0.83011600
H	-6.01119000	-0.65477200	0.79746900	C	-4.33372800	1.97900100	-0.75210300
H	-6.00432200	-2.24047700	0.02705200	C	-2.58897000	5.25176800	0.16182400
H	-5.01602000	-1.96209500	1.45610900	S	-4.77057900	-0.44821200	0.51015100
C	-3.97442600	1.96882500	0.19025300	O	-5.85644500	-0.55670200	-0.46810800
C	-2.62999500	-0.10745700	2.15126600	O	-4.96502900	-0.75078100	1.93217100
C	-5.41969900	1.91908200	0.73753000	H	-3.33426600	1.19793200	2.40864900
H	-5.80754000	2.94608600	0.77281400	H	-2.40260500	3.49524400	2.24980500
H	-6.08574800	1.35229700	0.08217300	H	-3.96960300	3.85225300	-1.73594000
H	-5.49782800	1.50837000	1.74407200	H	-4.90267300	1.55677400	-1.57324600
C	-4.06894100	2.50569100	-1.25867800	H	-3.35551000	5.97293000	0.47598900
H	-4.64460500	3.44071100	-1.23015200	H	-1.72013200	5.39731600	0.81246600
H	-3.09471800	2.73714000	-1.67956400	H	-2.29703000	5.51454800	-0.86060800
H	-4.58386600	1.83314900	-1.94219900	C	-2.39521200	-1.72734200	0.84024800
C	-3.18307200	3.02852800	0.99076000	C	-3.21372800	-1.54394700	-1.45208000
H	-2.12990200	3.06486700	0.69838500	C	-1.52667300	-2.60850000	-0.08732700
H	-3.61850600	4.01504700	0.78480800	H	-2.70307800	-2.24454900	1.75134900
H	-3.23561500	2.87455500	2.07009100	H	-1.85760600	-0.80699500	1.09990400
C	-3.74667900	0.25982500	3.15113300	C	-1.67841100	-1.80473400	-1.45236700
H	-3.42481700	-0.06451800	4.14948900	H	-3.40351400	-0.60638900	-1.97941900
H	-3.93846300	1.33347000	3.21363500	H	-3.79398700	-2.34074100	-1.93057500
H	-4.68991300	-0.24927000	2.93691900	N	-3.56411000	-1.46496500	-0.01754300
C	-1.34601000	0.67028000	2.52664800	C	-2.11680200	-4.03776000	-0.15858700
H	-1.08883200	0.43292700	3.56741600	H	-1.52434700	-4.67498000	-0.82073700
H	-0.50799500	0.36650600	1.89385600	H	-2.11708200	-4.49346200	0.83667000
H	-1.45387400	1.75372200	2.45465400	H	-3.14921100	-4.01877400	-0.51765300
C	-2.29899300	-1.60553300	2.33767000	C	-1.20628800	-2.58166100	-2.68964600
H	-1.55381600	-1.94352700	1.61095600	H	-1.34799300	-1.95388600	-3.57587300
H	-1.88958200	-1.73359000	3.34898700	H	-0.13539200	-2.79942500	-2.60352500
H	-3.18543500	-2.24180500	2.27338800	H	-1.74377400	-3.52374300	-2.84407900
O	-0.50398800	-1.91679300	-0.17269200	C	0.67157900	-3.49575700	1.00592600
				O	-1.09466900	-0.55205500	-1.38341300
<b>2-Ts3</b>				C	1.66372500	-4.23824400	1.67013200
Zero-point correction= 0.719825 (Hartree/Particle)				H	1.69707400	-4.14687700	2.75635900
Thermal correction to Energy= 0.763297				C	2.54425000	-5.05834500	1.05380400
Thermal correction to Enthalpy= 0.764242				H	2.54229700	-5.18821000	-0.02394100
Thermal correction to Gibbs Free Energy= 0.642868				H	3.27879600	-5.61682900	1.62541900
Sum of electronic and zero-point Energies= -2279.802840				Pd	0.74039400	-0.09791400	-0.70768800
Sum of electronic and thermal Energies= -2279.759367				P	2.81760400	0.68764000	0.01109700
Sum of electronic and thermal Enthalpies= -2279.758423				C	3.04618300	0.62933800	1.93935200
Sum of electronic and thermal Free Energies= -2279.879797				C	4.27017800	-0.28961600	-0.83285700
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.029369				C	2.88120900	2.54459000	-0.57251500
C	-4.14126900	1.23290600	0.41343800	C	4.28180500	3.18665500	-0.62739900
C	-3.44644600	1.77534000	1.49725300	H	4.93419700	2.71136500	-1.36399600
C	-2.93541900	3.06910700	1.40266400	H	4.17950400	4.23991600	-0.92243400



H	4.79086800	3.16797000	0.33987900	C	-5.71047900	-0.05674400	-0.16134300
C	2.23136200	2.61627800	-1.97749100	C	-5.98512500	0.93136100	0.78727300
H	2.78328800	2.07340600	-2.74415900	C	-6.42712200	2.18298200	0.36034900
H	1.20355600	2.23100100	-1.96490400	C	-6.59638400	2.46735700	-1.00186700
H	2.18153900	3.66837200	-2.28907900	C	-6.32344700	1.45480500	-1.93356100
C	1.98309100	3.40892500	0.34123600	C	-5.88174200	0.19803900	-1.52514400
H	0.97661000	2.98938300	0.43953000	C	-7.04735200	3.83457700	-1.45902800
H	2.40204500	3.55548500	1.33904700	S	-5.09846800	-1.65887200	0.37446000
H	1.88339200	4.40280900	-0.11448800	O	-5.44569200	-2.63164200	-0.66377100
C	4.28947900	0.03199800	-2.34427400	O	-5.49950200	-1.83595500	1.77347800
H	4.99016200	-0.65585000	-2.83500400	H	-5.88144600	0.70694100	1.84358800
H	3.30624800	-0.11902600	-2.80198500	H	-6.65268400	2.94893500	1.09850300
H	4.63025900	1.04600600	-2.56492400	H	-6.46599300	1.65060300	-2.99364800
C	5.67663100	-0.03070900	-0.25631500	H	-5.69683200	-0.58945400	-2.24785000
H	6.41224200	-0.59283900	-0.84744200	H	-7.59750300	4.35988700	-0.67167100
H	5.96350100	1.02329700	-0.29738700	H	-6.18791900	4.46116500	-1.73268100
H	5.77371400	-0.36970000	0.77823200	H	-7.69376000	3.76939000	-2.34087200
C	3.94907700	-1.80093200	-0.73592700	C	-2.76333800	-0.69526400	1.36494200
H	3.97231000	-2.18885800	0.28225500	C	-2.69435500	-1.38245200	-0.88439000
H	2.96318500	-2.01980400	-1.15728300	C	-1.25884300	-1.03604100	1.13828300
H	4.70084100	-2.35450000	-1.31471200	H	-3.10780700	-0.93324600	2.37277400
C	4.15451100	1.54108500	2.50403300	H	-2.95233300	0.36905800	1.15768000
H	4.22297600	1.38596900	3.58929600	C	-1.18858400	-1.37982000	-0.46442100
H	5.13835900	1.32157000	2.08145100	H	-2.91283300	-0.41087200	-1.35048700
H	3.94643500	2.60230000	2.34679300	H	-2.94535000	-2.18771600	-1.57626400
C	1.69421400	1.00113600	2.59563000	N	-3.42139000	-1.55952200	0.38055300
H	1.77776400	0.84681700	3.67981100	C	-0.84889000	-2.18465700	2.08395200
H	1.40690500	2.04046300	2.43669200	H	0.17121900	-2.52759700	1.88904300
H	0.88581800	0.36680200	2.21950400	H	-0.89951700	-1.85216400	3.12706400
C	3.33704700	-0.82283400	2.37638400	H	-1.53075500	-3.03109100	1.96313900
H	4.33301300	-1.16613000	2.08811300	C	-0.58399800	-2.77212000	-0.73451400
H	3.28519800	-0.87040100	3.47200800	H	-0.55608900	-2.91378700	-1.82028200
H	2.59542200	-1.52269700	1.98086900	H	0.44457100	-2.83800300	-0.36517100
C	-0.11910700	-2.73347600	0.42093900	H	-1.17264400	-3.58437300	-0.29318700
H	0.60637100	-1.49471300	0.12353600	C	0.05286200	1.24793300	1.62266500
				O	-0.54408000	-0.38603900	-1.16837700
<b>2-Int4</b>				C	0.46627500	2.58480300	1.89905000
Zero-point correction= 0.722088 (Hartree/Particle)				H	0.50107600	3.25889000	1.04346300
Thermal correction to Energy= 0.766155				C	0.75768500	3.05562700	3.12240900
Thermal correction to Enthalpy= 0.767099				H	0.72763400	2.42046200	4.00266100
Thermal correction to Gibbs Free Energy= 0.643859				H	1.02585400	4.09771300	3.26771100
Sum of electronic and zero-point Energies= -2279.800173				Pd	1.38017300	-0.04744600	-0.53676600
Sum of electronic and thermal Energies= -2279.756107				P	3.73790200	0.13326100	-0.24092800
Sum of electronic and thermal Enthalpies= -2279.755162				C	4.31822300	1.93003900	-0.71421700
Sum of electronic and thermal Free Energies= -2279.878402				C	4.31273700	-0.26662300	1.57841800
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.030934				C	4.62647500	-1.13493000	-1.43832800

C	6.12086900	-1.37584100	-1.13081200	Sum of electronic and thermal Enthalpies=	-2279.751243		
H	6.27696500	-1.87453600	-0.17161000	Sum of electronic and thermal Free Energies=	-2279.874953		
H	6.53239400	-2.03817100	-1.90366600	HF(B3LYP/6-311+G(d,p)/LanL2dz, SMD[toluene])=	-2281.023499		
H	6.71404400	-0.45871300	-1.14101600	C	-4.14126900	1.23290600	0.41343800
C	3.89140300	-2.49671400	-1.38038400	C	-3.44644600	1.77534000	1.49725300
H	3.95287900	-2.98276600	-0.40690900	C	-2.93541900	3.06910700	1.40266400
H	2.83574800	-2.39538100	-1.64326100	C	-3.10985800	3.83559600	0.24150300
H	4.35957400	-3.16996800	-2.11058100	C	-3.81594900	3.27035500	-0.83011600
C	4.51405100	-0.65554400	-2.90350400	C	-4.33372800	1.97900100	-0.75210300
H	3.47930800	-0.44818400	-3.19198200	C	-2.58897000	5.25176800	0.16182400
H	5.12122300	0.22702000	-3.11535600	S	-4.77057900	-0.44821200	0.51015100
H	4.87922400	-1.46027400	-3.55419800	O	-5.85644500	-0.55670200	-0.46810800
C	4.17392200	-1.78246500	1.84441700	O	-4.96502900	-0.75078100	1.93217100
H	4.30517000	-1.95580700	2.92026100	H	-3.33426600	1.19793200	2.40864900
H	3.18180500	-2.15603400	1.57093300	H	-2.40260500	3.49524400	2.24980500
H	4.92793300	-2.38121300	1.32989300	H	-3.96960300	3.85225300	-1.73594000
C	5.75381900	0.16582200	1.92273000	H	-4.90267300	1.55677400	-1.57324600
H	5.98385800	-0.16957500	2.94301700	H	-3.35551000	5.97293000	0.47598900
H	6.50411400	-0.27063400	1.26075900	H	-1.72013200	5.39731600	0.81246600
H	5.87783200	1.25156800	1.91014400	H	-2.29703000	5.51454800	-0.86060800
C	3.34522900	0.41947200	2.56804600	C	-2.39521200	-1.72734200	0.84024800
H	3.34791900	1.50633600	2.49952000	C	-3.21372800	-1.54394700	-1.45208000
H	2.31730200	0.07600200	2.42844500	C	-1.52667300	-2.60850000	-0.08732700
H	3.65232200	0.15421400	3.58870700	H	-2.70307800	-2.24454900	1.75134900
C	5.82024700	2.08979200	-1.02805500	H	-1.85760600	-0.80699500	1.09990400
H	6.02481200	3.15057500	-1.22597300	C	-1.67841100	-1.80473400	-1.45236700
H	6.46073900	1.78589800	-0.19626100	H	-3.40351400	-0.60638900	-1.97941900
H	6.12852000	1.53585500	-1.91727600	H	-3.79398700	-2.34074100	-1.93057500
C	3.49144000	2.38574800	-1.94140300	N	-3.56411000	-1.46496500	-0.01754300
H	3.74856200	3.42944500	-2.16685900	C	-2.11680200	-4.03776000	-0.15858700
H	3.68900200	1.79838700	-2.83831900	H	-1.52434700	-4.67498000	-0.82073700
H	2.41723700	2.33168900	-1.73900700	H	-2.11708200	-4.49346200	0.83667000
C	3.96341300	2.90823500	0.42648800	H	-3.14921100	-4.01877400	-0.51765300
H	4.59374400	2.78164900	1.30972300	C	-1.20628800	-2.58166100	-2.68964600
H	4.12219700	3.93185100	0.06275400	H	-1.34799300	-1.95388600	-3.57587300
H	2.91721800	2.82673300	0.73162800	H	-0.13539200	-2.79942500	-2.60352500
C	-0.44823900	0.15831700	1.38884400	H	-1.74377400	-3.52374300	-2.84407900
H	1.80986900	-0.50359600	-1.92909100	C	0.67157900	-3.49575700	1.00592600
				O	-1.09466900	-0.55205500	-1.38341300
<b>2-Ts4</b>				C	1.66372500	-4.23824400	1.67013200
Zero-point correction=	0.719090	(Hartree/Particle)		H	1.69707400	-4.14687700	2.75635900
Thermal correction to Energy=	0.762752			C	2.54425000	-5.05834500	1.05380400
Thermal correction to Enthalpy=	0.763697			H	2.54229700	-5.18821000	-0.02394100
Thermal correction to Gibbs Free Energy=	0.639986			H	3.27879600	-5.61682900	1.62541900
Sum of electronic and zero-point Energies=	-2279.795849			Pd	0.74039400	-0.09791400	-0.70768800
Sum of electronic and thermal Energies=	-2279.752187			P	2.81760400	0.68764000	0.01109700

C	3.04618300	0.62933800	1.93935200	Thermal correction to Gibbs Free Energy= 0.651512			
C	4.27017800	-0.28961600	-0.83285700	Sum of electronic and zero-point Energies= -2279.839311			
C	2.88120900	2.54459000	-0.57251500	Sum of electronic and thermal Energies= -2279.796323			
C	4.28180500	3.18665500	-0.62739900	Sum of electronic and thermal Enthalpies= -2279.795379			
H	4.93419700	2.71136500	-1.36399600	Sum of electronic and thermal Free Energies= -2279.914305			
H	4.17950400	4.23991600	-0.92243400	HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.068624			
H	4.79086800	3.16797000	0.33987900	C	-5.05503300	0.53614500	-0.23910700
C	2.23136200	2.61627800	-1.97749100	C	-5.26650200	1.24740800	0.94538600
H	2.78328800	2.07340600	-2.74415900	C	-5.14474000	2.63631900	0.94030500
H	1.20355600	2.23100100	-1.96490400	C	-4.81297300	3.33189900	-0.23106000
H	2.18153900	3.66837200	-2.28907900	C	-4.62438200	2.59747900	-1.41064200
C	1.98309100	3.40892500	0.34123600	C	-4.74263200	1.20855500	-1.42404400
H	0.97661000	2.98938300	0.43953000	C	-4.64920800	4.83354200	-0.21899900
H	2.40204500	3.55548500	1.33904700	S	-5.14226600	-1.26027600	-0.22849500
H	1.88339200	4.40280900	-0.11448800	O	-5.52559900	-1.67924500	-1.57911800
C	4.28947900	0.03199800	-2.34427400	O	-5.91107000	-1.64316400	0.96041800
H	4.99016200	-0.65585000	-2.83500400	H	-5.55493400	0.71533800	1.84572500
H	3.30624800	-0.11902600	-2.80198500	H	-5.32118300	3.19045600	1.85939300
H	4.63025900	1.04600600	-2.56492400	H	-4.39076400	3.12107400	-2.33474100
C	5.67663100	-0.03070900	-0.25631500	H	-4.62416900	0.64920900	-2.34587000
H	6.41224200	-0.59283900	-0.84744200	H	-5.29507500	5.30209300	0.53115800
H	5.96350100	1.02329700	-0.29738700	H	-3.61461400	5.11371700	0.02099400
H	5.77371400	-0.36970000	0.77823200	H	-4.88707600	5.27148800	-1.19407900
C	3.94907700	-1.80093200	-0.73592700	C	-2.98392800	-1.76996900	1.36330600
H	3.97231000	-2.18885800	0.28225500	C	-2.57950400	-1.75255700	-1.04623100
H	2.96318500	-2.01980400	-1.15728300	C	-1.47404000	-1.56314200	1.09916800
H	4.70084100	-2.35450000	-1.31471200	H	-3.17774800	-2.71548500	1.88172900
C	4.15451100	1.54108500	2.50403300	H	-3.40732100	-0.96989600	1.97996700
H	4.22297600	1.38596900	3.58929600	C	-1.28985700	-2.23904500	-0.32742900
H	5.13835900	1.32157000	2.08145100	H	-2.41549900	-0.73301100	-1.41887700
H	3.94643500	2.60230000	2.34679300	H	-2.86433500	-2.39827700	-1.87937900
C	1.69421400	1.00113600	2.59563000	N	-3.59515600	-1.80728900	0.01736300
H	1.77776400	0.84681700	3.67981100	C	-0.62157800	-2.17913100	2.22184500
H	1.40690500	2.04046300	2.43669200	H	0.44023400	-2.13047800	1.95697500
H	0.88581800	0.36680200	2.21950400	H	-0.75748400	-1.62529200	3.15855800
C	3.33704700	-0.82283400	2.37638400	H	-0.88831400	-3.22481900	2.40735200
H	4.33301300	-1.16613000	2.08811300	C	-1.29853400	-3.78112900	-0.23385700
H	3.28519800	-0.87040100	3.47200800	H	-1.25705600	-4.18994400	-1.24839000
H	2.59542200	-1.52269700	1.98086900	H	-0.41578100	-4.13606000	0.30609900
C	-0.11910700	-2.73347600	0.42093900	H	-2.19911000	-4.17155700	0.25327200
H	0.60637100	-1.49471300	0.12353600	C	-0.13970500	0.53662700	0.40443500
				O	-0.15388900	-1.87610000	-1.02592800
<b>2-Int5</b>				C	-0.01182300	1.99441500	0.32030700
Zero-point correction= 0.726506 (Hartree/Particle)				H	0.21692800	2.40377000	-0.66322300
Thermal correction to Energy= 0.769494				C	-0.18814700	2.84307000	1.34622000
Thermal correction to Enthalpy= 0.770438				H	-0.39130800	2.48622200	2.35256200

H	-0.14165800	3.91995500	1.20422800	Zero-point correction= 0.724884 (Hartree/Particle)			
Pd	1.26989200	-0.61141100	-0.45786900	Thermal correction to Energy= 0.767352			
P	3.45697100	0.29654000	-0.05501700	Thermal correction to Enthalpy= 0.768296			
C	3.92871300	2.05077500	-0.75181200	Thermal correction to Gibbs Free Energy= 0.649519			
C	3.94539300	0.19791300	1.82026100	Sum of electronic and zero-point Energies= -2279.817558			
C	4.46992300	-1.04711100	-1.05067500	Sum of electronic and thermal Energies= -2279.775089			
C	5.95786700	-1.17848700	-0.66891200	Sum of electronic and thermal Enthalpies= -2279.774145			
H	6.09763700	-1.52874200	0.35658900	Sum of electronic and thermal Free Energies= -2279.892923			
H	6.42764500	-1.92090500	-1.32823400	HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.043116			
H	6.50910500	-0.24273500	-0.78749500	C	5.72073400	-0.09003800	0.29656000
C	3.77945600	-2.42030500	-0.84483400	C	6.25762500	0.41818300	-0.88903100
H	3.76478200	-2.75642300	0.19106200	C	6.67077800	1.74958600	-0.93728500
H	2.74491000	-2.42988400	-1.21724900	C	6.55981700	2.58522100	0.18241200
H	4.32331500	-3.17435200	-1.42958600	C	6.02258200	2.04981900	1.36283000
C	4.37295000	-0.76463900	-2.56789000	C	5.60576000	0.72198700	1.42935200
H	3.33635400	-0.63745000	-2.89743800	C	7.04048500	4.01662300	0.13369700
H	4.94914100	0.10744600	-2.88223600	S	5.12640600	-1.78629100	0.35218000
H	4.78197700	-1.63007000	-3.10501700	O	5.24282400	-2.24086800	1.73983300
C	3.89930800	-1.27424000	2.28687500	O	5.75964500	-2.49977200	-0.76156300
H	3.99523200	-1.29178300	3.38000300	H	6.37199800	-0.23382400	-1.74848100
H	2.94692300	-1.75050400	2.03328200	H	7.09449000	2.14337600	-1.85823400
H	4.71520400	-1.87899100	1.88457600	H	5.93670100	2.68003800	2.24501100
C	5.32813600	0.78064100	2.17763000	H	5.21667600	0.30693900	2.35300100
H	5.50924100	0.62452200	3.24945900	H	7.04595900	4.40368100	-0.89043500
H	6.14470100	0.29653500	1.63609600	H	6.40904000	4.67272800	0.74258900
H	5.39061800	1.85645600	1.99784900	H	8.06455300	4.10183400	0.52103500
C	2.85355100	0.93203200	2.63471500	C	3.06226100	-1.47149800	-1.38372700
H	2.80615800	2.00186300	2.43313800	C	2.53238600	-1.20238000	0.97524600
H	1.86409500	0.50790800	2.44327400	C	1.59362400	-0.99118600	-1.25309000
H	3.07713100	0.80778700	3.70265600	H	3.14565800	-2.39419900	-1.96523000
C	5.43184600	2.25862400	-1.03332100	H	3.68699400	-0.71391500	-1.87689800
H	5.58346900	3.29122300	-1.37523300	C	1.16707600	-1.34990600	0.24152100
H	6.04954100	2.11815500	-0.14257300	H	2.69643900	-0.13956800	1.20146300
H	5.81304400	1.60406500	-1.81985800	H	2.57773400	-1.77833100	1.90110100
C	3.13129100	2.27174300	-2.05969300	N	3.49971200	-1.72932600	0.00411800
H	3.28349700	3.30671100	-2.39304800	C	0.70744400	-1.60266700	-2.35220600
H	3.44865900	1.61903900	-2.87303800	H	-0.34063900	-1.32858900	-2.19025800
H	2.05939300	2.11862600	-1.90780100	H	1.00012000	-1.22774900	-3.34085800
C	3.47672100	3.15633900	0.22870100	H	0.78816700	-2.69455500	-2.37206900
H	4.07597900	3.18386500	1.14147300	C	0.66088100	-2.79775700	0.36690700
H	3.60837500	4.12620200	-0.26874900	H	0.45357300	-3.01304300	1.41998900
H	2.42410500	3.06523100	0.50341000	H	-0.26831300	-2.93669000	-0.19346400
C	-1.18234000	-0.07334300	0.98288700	H	1.40180500	-3.52318900	0.01053900
H	-1.94811600	0.58548300	1.39864700	C	0.61731100	1.17827800	-0.57084300
				O	0.25471900	-0.45424600	0.76029700
				C	-0.04305900	2.36318700	-0.23044100

H	0.19737900	2.84143200	0.71865000
C	-1.22746200	2.74400100	-0.92238100
H	-1.32807000	2.53198700	-1.98445800
H	-1.77100400	3.61711600	-0.57014700
Pd	-1.56186500	0.77171800	-0.05633500
P	-3.83736200	0.08359700	0.12987300
C	-4.01016100	-1.11601100	1.65410400
C	-5.02891800	1.60255200	0.40049800
C	-4.39009700	-0.85841100	-1.48176300
C	-5.91023500	-1.04510300	-1.66307600
H	-6.43811700	-0.09752200	-1.79529200
H	-6.08943000	-1.63998500	-2.56903100
H	-6.37101600	-1.57828300	-0.82752500
C	-3.82248300	-0.09208400	-2.70123100
H	-4.24510600	0.90552700	-2.82366700
H	-2.73473600	0.00879300	-2.62816300
H	-4.05235300	-0.66073100	-3.61229600
C	-3.72463200	-2.25221200	-1.51854200
H	-2.64353700	-2.19388500	-1.35925500
H	-4.14769000	-2.94711500	-0.79022000
H	-3.88901600	-2.68786000	-2.51272200
C	-5.16406400	2.38890000	-0.92249100
H	-5.68398600	3.33307900	-0.71409700
H	-4.18738100	2.63687200	-1.34914800
H	-5.75182000	1.86087400	-1.67653400
C	-6.44384800	1.25914500	0.91107000
H	-7.03605600	2.18294800	0.96316500
H	-6.97697600	0.56789000	0.25408400
H	-6.43211000	0.83229900	1.91703800
C	-4.36371200	2.57603000	1.40371200
H	-4.29988700	2.17669100	2.41566900
H	-3.35364300	2.84515600	1.08322800
H	-4.96554200	3.49352500	1.45173400
C	-5.30157600	-1.95730600	1.70648000
H	-5.29820500	-2.55235400	2.62984500
H	-6.20791800	-1.34659600	1.71648700
H	-5.37615200	-2.66299000	0.87502800
C	-2.78595800	-2.06293500	1.65483500
H	-2.80342900	-2.64874500	2.58395900
H	-2.79362900	-2.77419900	0.82859900
H	-1.83813900	-1.51532700	1.61889000
C	-3.90538700	-0.29716300	2.96043500
H	-4.79142700	0.31079400	3.15724900
H	-3.80439900	-0.99814800	3.79887200
H	-3.02189100	0.34953800	2.96741700
C	1.49078500	0.51586600	-1.30316800

H	2.15484200	1.07999400	-1.95741200
<b>2-Int6</b>			
Zero-point correction= 0.727233 (Hartree/Particle)			
Thermal correction to Energy= 0.770721			
Thermal correction to Enthalpy= 0.771665			
Thermal correction to Gibbs Free Energy= 0.646595			
Sum of electronic and zero-point Energies= -2279.875279			
Sum of electronic and thermal Energies= -2279.831791			
Sum of electronic and thermal Enthalpies= -2279.830847			
Sum of electronic and thermal Free Energies= -2279.955917			
HF(B3LYP/6-311+G(d,p)/LanL2dz, SMD[toluene])= -2281.100487			
C	-5.05503300	0.53614500	-0.23910700
C	-5.26650200	1.24740800	0.94538600
C	-5.14474000	2.63631900	0.94030500
C	-4.81297300	3.33189900	-0.23106000
C	-4.62438200	2.59747900	-1.41064200
C	-4.74263200	1.20855500	-1.42404400
C	-4.64920800	4.83354200	-0.21899900
S	-5.14226600	-1.26027600	-0.22849500
O	-5.52559900	-1.67924500	-1.57911800
O	-5.91107000	-1.64316400	0.96041800
H	-5.55493400	0.71533800	1.84572500
H	-5.32118300	3.19045600	1.85939300
H	-4.39076400	3.12107400	-2.33474100
H	-4.62416900	0.64920900	-2.34587000
H	-5.29507500	5.30209300	0.53115800
H	-3.61461400	5.11371700	0.02099400
H	-4.88707600	5.27148800	-1.19407900
C	-2.98392800	-1.76996900	1.36330600
C	-2.57950400	-1.75255700	-1.04623100
C	-1.47404000	-1.56314200	1.09916800
H	-3.17774800	-2.71548500	1.88172900
H	-3.40732100	-0.96989600	1.97996700
C	-1.28985700	-2.23904500	-0.32742900
H	-2.41549900	-0.73301100	-1.41887700
H	-2.86433500	-2.39827700	-1.87937900
N	-3.59515600	-1.80728900	0.01736300
C	-0.62157800	-2.17913100	2.22184500
H	0.44023400	-2.13047800	1.95697500
H	-0.75748400	-1.62529200	3.15855800
H	-0.88831400	-3.22481900	2.40735200
C	-1.29853400	-3.78112900	-0.23385700
H	-1.25705600	-4.18994400	-1.24839000
H	-0.41578100	-4.13606000	0.30609900
H	-2.19911000	-4.17155700	0.25327200



H	5.63264100	5.26279500	0.49671200
H	4.81515400	5.11123900	-1.06166700
H	3.87065300	5.33547000	0.42274100
C	1.16117900	-3.97779000	0.61915200
H	0.47226700	-4.61655200	0.06141700
H	2.19466800	-4.22239000	0.35305300
H	1.02684300	-4.20154000	1.68456000
C	0.77376200	-3.13938000	-2.20508600
H	0.88293200	-2.88254600	-3.26556600
H	1.32520100	-4.06594000	-2.02521100
H	-0.28752500	-3.30839700	-1.99972800
Pd	-1.12818800	-0.40728700	-0.68449100
P	-3.27922600	0.41280200	0.23804700
C	-4.70487600	-0.40555700	-0.80251000
C	-4.26120500	-1.84995000	-1.14234700
H	-3.30305300	-1.85123400	-1.67490200
H	-4.15526600	-2.49140700	-0.26800500
H	-5.01492000	-2.30501400	-1.79956700
C	-4.84018800	0.31744400	-2.16097500
H	-5.50565700	-0.27416400	-2.80344100
H	-5.28211700	1.31270900	-2.07405400
H	-3.87677200	0.40274400	-2.67403500
C	-6.09292000	-0.44262400	-0.13201600
H	-6.46052700	0.55357000	0.12844200
H	-6.81581900	-0.88592000	-0.83076000
H	-6.10477500	-1.05571900	0.77212400
C	-3.50003800	2.34603400	0.18606200
C	-3.42284400	-0.18755700	2.08301600
C	-4.93756700	2.86558000	0.39023000
H	-4.92611100	3.96436600	0.38809500
H	-5.61231500	2.55237700	-0.41064800
H	-5.36940800	2.54592600	1.34178500
C	-2.96668800	2.85595300	-1.17454100
H	-2.95025900	3.95421300	-1.15696800
H	-1.94856200	2.49673100	-1.35470300
H	-3.58339800	2.55415800	-2.02142500
C	-2.58906800	2.98847900	1.25563700
H	-1.55512400	2.63741200	1.17101600
H	-2.58375500	4.07575400	1.10169500
H	-2.93472400	2.81020500	2.27596800
C	-4.55027700	0.45860900	2.91254800
H	-4.56661300	-0.00366800	3.90889500
H	-4.40050800	1.53129700	3.06257400
H	-5.53937000	0.31239300	2.46997500
C	-2.05972800	0.07014900	2.77401400
H	-1.78580500	1.12438400	2.82691500

H	-2.12189500	-0.30215300	3.80586400
H	-1.26143300	-0.47991200	2.26686700
C	-3.59945200	-1.72374000	2.11061000
H	-2.81287400	-2.23067100	1.54313600
H	-3.51177400	-2.05472600	3.15406700
H	-4.57965400	-2.05144400	1.75605800
O	-0.46356300	-2.23249000	0.59771200

## 2-Int2'

Zero-point correction= 0.726139 (Hartree/Particle)

Thermal correction to Energy= 0.769276

Thermal correction to Enthalpy= 0.770220

Thermal correction to Gibbs Free Energy= 0.649195

Sum of electronic and zero-point Energies= -2279.808861

Sum of electronic and thermal Energies= -2279.765724

Sum of electronic and thermal Enthalpies= -2279.764780

Sum of electronic and thermal Free Energies= -2279.885805

HF(B3LYP/6-311+G(d,p)/LanL2dz, SMD[toluene])= -2281.035638

N	3.00641900	-1.81220800	0.45964400
C	1.69185500	-1.66038100	1.09697000
H	1.70608900	-2.08752100	2.10146500
H	1.37154800	-0.60922400	1.15351700
C	0.75267900	-2.41980200	0.12039200
C	2.89285700	-1.97011800	-1.00795200
H	3.38567900	-2.89997700	-1.31175100
H	3.36812800	-1.14549800	-1.54912400
C	1.36609500	-2.01957500	-1.26121300
C	0.77530700	-0.63341500	-1.54760000
C	1.22154600	0.33819700	-2.31566300
C	0.95973500	1.70358200	-2.85595200
C	2.22435600	0.93296400	-3.22823900
H	1.07040500	2.56018900	-2.19164700
H	0.19688500	1.83027500	-3.62384800
H	2.30451900	0.54175200	-4.24226900
H	3.16706200	1.27670200	-2.80397900
S	4.38330900	-1.18235300	1.13736200
O	4.25677700	-1.36415500	2.58605600
O	5.50906700	-1.72902300	0.37341600
C	4.35884000	0.59016800	0.82695000
C	5.03856900	1.10964300	-0.27780700
C	3.65089100	1.43588700	1.68573300
C	4.99335000	2.48155200	-0.52666800
H	5.62166100	0.44580600	-0.90719600
C	3.61316500	2.80409100	1.42044300
H	3.16710800	1.02779500	2.56683200
C	4.27517900	3.34824500	0.30996100

H	5.53878500	2.88790400	-1.37547900	H	-5.63492000	0.00388500	2.29149300
H	3.07383900	3.46325800	2.09679400	C	-2.20328400	-0.49147200	2.79052500
C	4.21211400	4.82961500	0.01950100	H	-1.89860800	0.51860300	3.06560700
H	5.11879300	5.17802100	-0.48618100	H	-2.35816500	-1.04854900	3.72460000
H	3.36288500	5.06915700	-0.63468100	H	-1.39042100	-0.97157700	2.23860300
H	4.08934100	5.41344100	0.93774500	C	-3.77343700	-2.04727800	1.71414700
C	0.78289500	-3.92440700	0.42920100	H	-2.97709100	-2.48728400	1.10643200
H	0.18912900	-4.48246500	-0.29976400	H	-3.77290000	-2.56369600	2.68308700
H	1.80737900	-4.31408200	0.43440100	H	-4.74274000	-2.24424200	1.25002600
H	0.34709600	-4.09344100	1.41941300	O	-0.58776800	-2.01257600	0.21509900
C	1.00324300	-2.95898400	-2.42231800				
H	1.39751700	-2.56994600	-3.36781400				
H	1.41622800	-3.96187300	-2.26870700	<b>2-Ts2'</b>			
H	-0.08455400	-3.04066800	-2.51787800	Zero-point correction= 0.725473 (Hartree/Particle)			
Pd	-0.97309400	-0.24588900	-0.68059100	Thermal correction to Energy= 0.767900			
P	-3.21343000	0.35146800	0.28187200	Thermal correction to Enthalpy= 0.768844			
C	-4.59416300	-0.17408900	-0.98198500	Thermal correction to Gibbs Free Energy= 0.651566			
C	-4.21985500	-1.57385300	-1.53051400	Sum of electronic and zero-point Energies= -2279.797174			
H	-3.21188300	-1.57525300	-1.95876700	Sum of electronic and thermal Energies= -2279.754747			
H	-4.25970700	-2.36074500	-0.77817300	Sum of electronic and thermal Enthalpies= -2279.753803			
H	-4.92996900	-1.83976400	-2.32521000	Sum of electronic and thermal Free Energies= -2279.871081			
C	-4.56526600	0.76881900	-2.20573700	HF(B3LYP/6-311+G(d,p)/Lan12dz, SMD[toluene])= -2281.021153			
H	-5.22686800	0.35433700	-2.97733800	N	3.13697200	-1.78576300	0.43630800
H	-4.92424200	1.77639700	-1.98464200	C	1.80821100	-1.69630400	1.06400200
H	-3.56331300	0.83998000	-2.64354400	H	1.83469300	-2.12847900	2.06622500
C	-6.03260100	-0.21055300	-0.42838600	H	1.44867400	-0.65865700	1.12907200
H	-6.35500000	0.75519100	-0.02970600	C	0.88201400	-2.48251500	0.08778100
H	-6.72255800	-0.47678800	-1.24080600	C	3.04770200	-2.00655200	-1.02393300
H	-6.15768600	-0.96096300	0.35588700	H	3.54735500	-2.94619000	-1.28422000
C	-3.29282600	2.27420500	0.54330000	H	3.53042600	-1.20439500	-1.59267200
C	-3.51884900	-0.54500500	1.97460500	C	1.52922300	-2.08546600	-1.30124300
C	-4.70148000	2.88198400	0.69530300	C	0.94599000	-0.72795100	-1.59854500
H	-4.61083300	3.96220300	0.87416900	C	1.02907400	0.36130900	-2.26017100
H	-5.31400100	2.75639200	-0.20087400	C	-0.19569500	1.67437500	-2.14237400
H	-5.24767100	2.45603600	1.54109700	C	1.09495400	1.60058400	-2.96952400
C	-2.57469400	2.93090500	-0.66169700	H	-0.15880300	2.39360600	-1.33432000
H	-2.51100600	4.01441800	-0.49338000	H	-1.10602200	1.64417800	-2.73051700
H	-1.54675500	2.55637200	-0.76068400	H	0.96413700	1.55820300	-4.05292600
H	-3.08510900	2.77867300	-1.61275300	H	1.88883900	2.28955400	-2.67354300
C	-2.45821100	2.66535500	1.78323700	S	4.44437100	-0.98300900	1.07478600
H	-1.44555000	2.25133900	1.74106900	O	4.36322900	-1.13864800	2.52898700
H	-2.36724400	3.75934000	1.80869600	O	5.61241000	-1.41560000	0.30113900
H	-2.92103900	2.35916300	2.72348500	C	4.20421700	0.76599800	0.72192300
C	-4.67742300	0.02209200	2.81889300	C	4.75260900	1.32195800	-0.43656800
H	-4.78977600	-0.59232100	3.72234900	C	3.44774300	1.55273700	1.59621400
H	-4.49271500	1.04702000	3.15207500	C	4.53070500	2.66995300	-0.72112300
				H	5.37007400	0.70949700	-1.08502200



C	3.23455500	2.89721100	1.29651700	C	-4.64185100	-0.72641800	2.55497600
H	3.05769000	1.11863000	2.51059000	H	-4.78462500	-1.56011700	3.25556500
C	3.77078800	3.47790000	0.13702300	H	-4.54768000	0.18005100	3.15854900
H	4.97158100	3.10582700	-1.61494000	H	-5.55353400	-0.64562800	1.95803300
H	2.65408400	3.51036600	1.98214200	C	-2.15280300	-1.09871500	2.64667900
C	3.57437300	4.94816400	-0.15162600	H	-1.93946100	-0.16982300	3.17609100
H	4.32239400	5.55550300	0.37509900	H	-2.36098100	-1.86294800	3.40840100
H	3.67370200	5.16569300	-1.22018500	H	-1.27120200	-1.41217000	2.08197700
H	2.58849200	5.29460800	0.17707500	C	-3.51909800	-2.42152100	1.08224100
C	0.97144300	-3.98663500	0.39161300	H	-2.64076000	-2.67402000	0.48207700
H	0.38123300	-4.56078500	-0.32832400	H	-3.57675700	-3.14957300	1.90264800
H	2.00486700	-4.35424400	0.38410700	H	-4.42970200	-2.54147300	0.49008700
H	0.55120100	-4.16738300	1.38620000	O	-0.45364300	-2.09693100	0.16449500
C	1.18335900	-3.02908700	-2.46428200				
H	1.57107100	-2.64239700	-3.41366500	N	3.13697200	-1.78576300	0.43630800
H	1.61579500	-4.02075400	-2.29814500	C	1.80821100	-1.69630400	1.06400200
H	0.09733300	-3.13233500	-2.55270200	H	1.83469300	-2.12847900	2.06622500
Pd	-0.75827400	-0.20518800	-0.69388200	H	1.44867400	-0.65865700	1.12907200
P	-3.00017100	0.28112100	0.30551600	C	0.88201400	-2.48251500	0.08778100
C	-4.29132700	0.02135000	-1.13567200	C	3.04770200	-2.00655200	-1.02393300
C	-3.79831500	-1.16769900	-1.99688200	H	3.54735500	-2.94619000	-1.28422000
H	-2.78818900	-0.98738700	-2.37991000	H	3.53042600	-1.20439500	-1.59267200
H	-3.77896000	-2.11422300	-1.45734900	C	1.52922300	-2.08546600	-1.30124300
H	-4.47490500	-1.28529600	-2.85465800	C	0.94599000	-0.72795100	-1.59854500
C	-4.29239600	1.24736000	-2.07597100	C	1.02907400	0.36130900	-2.26017100
H	-4.89365100	1.00422200	-2.96194400	C	-0.19569500	1.67437500	-2.14237400
H	-4.73388300	2.13853100	-1.62458300	C	1.09495400	1.60058400	-2.96952400
H	-3.28616000	1.49649300	-2.42602800	H	-0.15880300	2.39360600	-1.33432000
C	-5.74750500	-0.24670800	-0.70290300	H	-1.10602200	1.64417800	-2.73051700
H	-6.16297000	0.55882600	-0.09233900	H	0.96413700	1.55820300	-4.05292600
H	-6.37397000	-0.33163900	-1.60162200	H	1.88883900	2.28955400	-2.67354300
H	-5.85354200	-1.18281700	-0.15068200	S	4.44437100	-0.98300900	1.07478600
C	-3.27730000	2.06184800	1.05318100	O	4.36322900	-1.13864800	2.52898700
C	-3.38358600	-1.01424900	1.70966600	O	5.61241000	-1.41560000	0.30113900
C	-4.74853700	2.48586000	1.24691300	C	4.20421700	0.76599800	0.72192300
H	-4.77250000	3.46741700	1.74019700	C	4.75260900	1.32195800	-0.43656800
H	-5.28380700	2.59315400	0.30022500	C	3.44774300	1.55273700	1.59621400
H	-5.30878600	1.79158100	1.87644700	C	4.53070500	2.66995300	-0.72112300
C	-2.57727100	3.09167300	0.13732900	H	5.37007400	0.70949700	-1.08502200
H	-2.75177600	4.09877300	0.53976700	C	3.23455500	2.89721100	1.29651700
H	-1.49743000	2.92325800	0.12675200	H	3.05769000	1.11863000	2.51059000
H	-2.93444300	3.08512300	-0.89275300	C	3.77078800	3.47790000	0.13702300
C	-2.55663400	2.17877400	2.41514500	H	4.97158100	3.10582700	-1.61494000
H	-1.51425800	1.84935900	2.35491800	H	2.65408400	3.51036600	1.98214200
H	-2.55254000	3.23547900	2.71458400	C	3.57437300	4.94816400	-0.15162600
H	-3.05171100	1.62113400	3.21204300	H	4.32239400	5.55550300	0.37509900

H	3.67370200	5.16569300	-1.22018500
H	2.58849200	5.29460800	0.17707500
C	0.97144300	-3.98663500	0.39161300
H	0.38123300	-4.56078500	-0.32832400
H	2.00486700	-4.35424400	0.38410700
H	0.55120100	-4.16738300	1.38620000
C	1.18335900	-3.02908700	-2.46428200
H	1.57107100	-2.64239700	-3.41366500
H	1.61579500	-4.02075400	-2.29814500
H	0.09733300	-3.13233500	-2.55270200
Pd	-0.75827400	-0.20518800	-0.69388200
P	-3.00017100	0.28112100	0.30551600
C	-4.29132700	0.02135000	-1.13567200
C	-3.79831500	-1.16769900	-1.99688200
H	-2.78818900	-0.98738700	-2.37991000
H	-3.77896000	-2.11422300	-1.45734900
H	-4.47490500	-1.28529600	-2.85465800
C	-4.29239600	1.24736000	-2.07597100
H	-4.89365100	1.00422200	-2.96194400
H	-4.73388300	2.13853100	-1.62458300
H	-3.28616000	1.49649300	-2.42602800
C	-5.74750500	-0.24670800	-0.70290300
H	-6.16297000	0.55882600	-0.09233900
H	-6.37397000	-0.33163900	-1.60162200
H	-5.85354200	-1.18281700	-0.15068200
C	-3.27730000	2.06184800	1.05318100
C	-3.38358600	-1.01424900	1.70966600
C	-4.74853700	2.48586000	1.24691300
H	-4.77250000	3.46741700	1.74019700
H	-5.28380700	2.59315400	0.30022500
H	-5.30878600	1.79158100	1.87644700
C	-2.57727100	3.09167300	0.13732900
H	-2.75177600	4.09877300	0.53976700
H	-1.49743000	2.92325800	0.12675200
H	-2.93444300	3.08512300	-0.89275300
C	-2.55663400	2.17877400	2.41514500
H	-1.51425800	1.84935900	2.35491800
H	-2.55254000	3.23547900	2.71458400
H	-3.05171100	1.62113400	3.21204300
C	-4.64185100	-0.72641800	2.55497600
H	-4.78462500	-1.56011700	3.25556500
H	-4.54768000	0.18005100	3.15854900
H	-5.55353400	-0.64562800	1.95803300
C	-2.15280300	-1.09871500	2.64667900
H	-1.93946100	-0.16982300	3.17609100
H	-2.36098100	-1.86294800	3.40840100

H	-1.27120200	-1.41217000	2.08197700
C	-3.51909800	-2.42152100	1.08224100
H	-2.64076000	-2.67402000	0.48207700
H	-3.57675700	-3.14957300	1.90264800
H	-4.42970200	-2.54147300	0.49008700
O	-0.45364300	-2.09693100	0.16449500

## 2-Ts2''

Zero-point correction= 0.717768 (Hartree/Particle)

Thermal correction to Energy= 0.763185

Thermal correction to Enthalpy= 0.764129

Thermal correction to Gibbs Free Energy= 0.636761

Sum of electronic and zero-point Energies= -2279.749758

Sum of electronic and thermal Energies= -2279.704340

Sum of electronic and thermal Enthalpies= -2279.703396

Sum of electronic and thermal Free Energies= -2279.830765

HF(B3LYP/6-311+G(d,p)/LanL2dz, SMD[toluene])= -2280.976104

C	3.10650700	1.48245900	1.12315800
C	2.06930100	-0.29243700	-0.28235900
C	1.85946400	2.04339200	1.78523700
C	-0.43408500	2.38780700	0.57685500
C	2.04631100	2.37513400	3.25070300
C	0.71086000	2.25858300	1.15430000
C	1.22876100	-0.51951100	-1.54808500
O	0.85505300	-1.65843000	-1.77046600
C	0.81712800	0.65650600	-2.39840400
Pd	-1.91897000	0.96143900	0.39921300
C	-1.02993100	3.50692600	-0.23769900
C	-0.23874900	4.11883100	-1.28391900
N	2.90425100	0.91786700	-0.22614300
C	5.41452500	-0.34489900	-0.38475100
C	6.32425200	0.08009500	0.58776700
C	7.14979900	-0.85828000	1.20384000
C	7.08204400	-2.21841700	0.86707000
C	6.17043400	-2.61604400	-0.12136400
C	5.33713300	-1.69230300	-0.75042800
C	7.96117700	-3.23130500	1.56130200
S	4.32343200	0.84775200	-1.16665400
O	3.91877600	0.27705600	-2.45522500
O	4.95510900	2.16568900	-1.06920800
H	3.54632100	0.72542900	1.79830100
H	3.84493600	2.28568600	1.02602000
H	2.63405600	-1.21411900	-0.08455200
H	1.33772200	-0.18603600	0.52560700
H	2.87155700	3.08749900	3.39784400
H	1.13823300	2.81341100	3.67131100

H	2.29714200	1.47585600	3.83256200	C	-5.88745500	1.15355000	-0.27430300
H	0.41795400	1.46129900	-1.77125900	H	-6.72840400	1.69715800	0.17616800
H	1.69098900	1.05051200	-2.92528600	H	-5.11323200	1.88813400	-0.51993200
H	0.06712900	0.32706000	-3.12089000	H	-6.25373400	0.70816900	-1.20176300
H	-0.72840000	4.59119600	-2.13110900	C	-6.50938400	-0.90477400	1.01301500
H	0.81589400	3.88525500	-1.38817400	H	-7.41190300	-0.35949900	1.32220300
H	6.40347000	1.13432100	0.83097400	H	-6.77085900	-1.49246600	0.12954900
H	7.86694500	-0.52737700	1.95110500	H	-6.26414700	-1.59858200	1.82125800
H	6.11795200	-3.66246200	-0.41150200	H	-1.53524500	4.22286400	0.42738400
H	4.65620000	-2.00164200	-1.53608500				
H	8.18012700	-4.08457400	0.91123900				
H	8.91203300	-2.78870800	1.87567300	<b>2-Int3''</b>			
H	7.47103100	-3.62475400	2.46190000	Zero-point correction= 0.717497 (Hartree/Particle)			
H	-1.94376800	3.02450800	-0.73630300	Thermal correction to Energy= 0.763740			
P	-3.69321000	-0.63548400	0.10670200	Thermal correction to Enthalpy= 0.764684			
C	-3.90842000	-1.15844400	-1.75680900	Thermal correction to Gibbs Free Energy= 0.634777			
C	-3.28174600	-2.22469800	1.15002000	Sum of electronic and zero-point Energies= -2279.814107			
C	-5.37817400	0.10765500	0.74226600	Sum of electronic and thermal Energies= -2279.767864			
C	-3.76412800	0.11660300	-2.62294900	Sum of electronic and thermal Enthalpies= -2279.766920			
H	-2.80943400	0.61488500	-2.42497500	Sum of electronic and thermal Free Energies= -2279.896828			
H	-3.78528100	-0.17327200	-3.68216200	HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.044656			
H	-4.56304500	0.84259700	-2.46723800	C	2.67655900	0.99042500	-0.69904500
C	-2.74544100	-2.08268700	-2.18320800	C	1.73052500	-1.29410800	-0.92096800
H	-2.80244800	-2.22287200	-3.27086500	C	1.71985300	1.52372000	0.35071000
H	-1.76165600	-1.65771600	-1.96458200	C	-0.53361800	2.65316200	-0.41708900
H	-2.80153900	-3.07670200	-1.73403900	C	2.16093100	1.42976300	1.79753900
C	-5.23664900	-1.86070100	-2.10571900	C	0.58904900	2.10692800	-0.02143000
H	-5.21866400	-2.14945100	-3.16551800	C	1.53884700	-2.62557500	-0.18817400
H	-5.39539600	-2.77241400	-1.52365100	O	0.78802500	-3.44913100	-0.67911500
H	-6.10607100	-1.21312100	-1.96684500	C	2.20050700	-2.84591700	1.15441300
C	-4.09627000	-3.48953000	0.81228800	Pd	-2.06732500	1.31514100	-0.16014700
H	-3.80426300	-4.29680500	1.49808600	C	-0.65381000	4.06202400	-0.80936600
H	-5.17288200	-3.33777500	0.92779500	C	-1.74536900	4.64253500	-1.32683700
H	-3.91116000	-3.85050800	-0.20197000	N	2.90456000	-0.48012800	-0.54844600
C	-1.77207400	-2.51694000	0.96620000	C	5.61554100	-0.30666500	-0.31637700
H	-1.48637900	-2.75876900	-0.05684800	C	6.48978700	0.62477300	-0.87496400
H	-1.17059400	-1.65655900	1.28278200	C	7.52666600	1.13720400	-0.09350000
H	-1.49826900	-3.37229500	1.59931600	C	7.70369500	0.72881800	1.23400800
C	-3.46333300	-1.91937300	2.65373900	C	6.80927100	-0.21354400	1.76921800
H	-3.03707400	-2.75120200	3.23005200	C	5.77213100	-0.73754900	1.00449800
H	-2.93372300	-1.00802400	2.95081200	C	8.83986400	1.26739100	2.07047500
H	-4.51104900	-1.82876500	2.94991500	S	4.32513200	-1.01332400	-1.34212100
C	-5.08723700	0.89908200	2.04105500	O	4.32906800	-2.47454300	-1.18979300
H	-4.28533500	1.62923600	1.88451100	O	4.44527100	-0.41856200	-2.68132200
H	-5.99600400	1.44229800	2.33447300	H	3.65325600	1.47342300	-0.57489900
H	-4.80284200	0.26387000	2.88014900	H	2.31460200	1.22290300	-1.70741700
				H	0.85880200	-0.68315200	-0.65350200

H	1.65940700	-1.48623400	-1.99921100	C	-3.06186000	0.09014200	2.86898500
H	3.11469400	1.95503300	1.95062000	H	-2.54485200	0.99416200	2.51774600
H	1.41695700	1.87098900	2.46641500	H	-3.32552600	0.26060300	3.92141300
H	2.32621800	0.38776000	2.09964500	H	-2.35610700	-0.73953000	2.83832500
H	3.25671200	-3.08258000	0.98826800	C	-5.22880800	1.09451400	2.27223800
H	2.15513100	-1.94692700	1.77796600	H	-5.34360800	1.25757000	3.35189800
H	1.71753400	-3.68700400	1.65682000	H	-4.76123400	1.99131200	1.85265400
H	0.24134400	4.67180800	-0.66477000	H	-6.23305600	0.99564400	1.85508100
H	-1.74760400	5.69314500	-1.60363500	C	-5.10205400	-1.37756900	2.65188000
H	-2.65712800	4.07687100	-1.49717000	H	-5.37001400	-1.16093500	3.69513300
H	6.35421300	0.93563200	-1.90526300	H	-6.02918100	-1.59891000	2.11635200
H	8.20849600	1.86545300	-0.52520000	H	-4.49056700	-2.28308700	2.65929900
H	6.93175600	-0.54232900	2.79844100				
H	5.09097200	-1.46916500	1.42515000	<b>2-Int4''</b>			
H	9.28380300	2.15924500	1.61782300	Zero-point correction=	0.718212	(Hartree/Particle)	
H	8.50409300	1.52917500	3.08024300	Thermal correction to Energy=	0.764407		
H	9.63646100	0.51982700	2.17890600	Thermal correction to Enthalpy=	0.765351		
H	-2.28368000	1.56700400	-1.66439400	Thermal correction to Gibbs Free Energy=	0.633717		
P	-3.84719700	-0.30715000	0.18875500	Sum of electronic and zero-point Energies=	-2279.812636		
C	-5.40450200	0.01030000	-0.92205300	Sum of electronic and thermal Energies=	-2279.766442		
C	-3.15499300	-2.08859300	-0.16062500	Sum of electronic and thermal Enthalpies=	-2279.765497		
C	-4.35840400	-0.16428100	2.05971200	Sum of electronic and thermal Free Energies=	-2279.897132		
C	-5.66583900	1.53503500	-0.97756300	HF(B3LYP/6-311+G(d,p)/LanL2dz, SMD[ <i>toluene</i> ])=	-2281.042698		
H	-4.77428100	2.07688200	-1.30665800	C	1.78403700	0.52423000	0.40452600
H	-6.46813800	1.72452100	-1.70305100	C	3.10216500	2.58292700	-0.24828800
H	-5.98556600	1.95595000	-0.02421300	C	0.92070000	0.48275500	-0.85473700
C	-5.09097800	-0.41740400	-2.37310900	C	1.53091600	-0.26601200	-2.03578100
H	-5.90555900	-0.06621800	-3.01957300	C	2.45218100	3.57997500	0.71822600
H	-4.16183600	0.02950600	-2.73995800	O	2.12983500	3.27136800	1.84725400
H	-5.03083500	-1.50114700	-2.49278100	C	2.23575900	4.97679800	0.16141800
C	-6.68947700	-0.71152700	-0.46676500	N	3.09621000	1.18755800	0.16776600
H	-7.48861700	-0.50551500	-1.19156400	C	4.87089200	-0.85752400	0.35516300
H	-6.56690500	-1.79649400	-0.41624800	C	4.62648300	-2.07718500	0.98238700
H	-7.04442300	-0.36396400	0.50683800	C	5.03333600	-3.25890200	0.35763900
C	-4.20222100	-3.21698900	-0.23993300	C	5.68636900	-3.23680700	-0.87947500
H	-3.68124300	-4.17090500	-0.39596600	C	5.93074000	-1.99130200	-1.48404700
H	-4.79315900	-3.31246000	0.67520500	C	5.52987900	-0.80618700	-0.87753000
H	-4.89103800	-3.08884200	-1.07908000	C	6.12737700	-4.51393700	-1.55494000
C	-2.35843000	-2.03803100	-1.48918500	S	4.37137100	0.67080300	1.15839500
H	-2.99822100	-1.95391800	-2.36822100	O	5.44773100	1.65505800	0.97872800
H	-1.65933300	-1.19608200	-1.50100600	O	3.89514800	0.30581500	2.49596300
H	-1.77021800	-2.95758300	-1.58697500	H	1.99898400	-0.50273500	0.70654200
C	-2.12813000	-2.44835400	0.93679800	H	1.26096200	1.01405300	1.22915700
H	-1.59269000	-3.35448500	0.63226700	H	4.14126200	2.89455900	-0.39710600
H	-1.37616800	-1.66134100	1.06064000	H	2.60711400	2.65995700	-1.22454100
H	-2.59013500	-2.64665900	1.90699000	H	2.44480200	0.22839400	-2.39428900

H	1.80396700	-1.28269600	-1.73640200
H	0.82719900	-0.33154800	-2.87046900
H	3.12551900	5.34110500	-0.36610100
H	1.41256400	4.95638200	-0.56486500
H	1.97891200	5.66003600	0.97351600
H	4.13548500	-2.09291400	1.94941200
H	4.84312300	-4.21160100	0.84561700
H	6.44609300	-1.95354700	-2.44109800
H	5.73340800	0.15173800	-1.34499400
H	5.88171400	-5.39236200	-0.95051700
H	5.64449600	-4.63386500	-2.53280500
H	7.21044000	-4.51820400	-1.72905600
C	0.13304200	1.61860300	-1.13278000
C	-0.83216500	2.39276300	-1.26169600
C	-1.62039300	3.55035200	-1.52236200
H	-1.93258600	4.11924600	-0.64590200
C	-2.01302200	3.96743400	-2.74042500
H	-1.74020300	3.43171400	-3.64488100
H	-2.61812000	4.86168700	-2.85237400
Pd	-1.15008700	-0.05194700	-0.33317700
H	-0.65776600	-1.50432900	-0.00410000
P	-3.36869700	-0.72590600	0.23793400
C	-3.45135600	-1.58557000	1.98588800
C	-3.93276800	-2.00391400	-1.11846700
C	-4.61437700	0.77805100	0.24357700
C	-3.22270100	-3.35776900	-0.89243000
H	-3.42068000	-3.99734600	-1.76262600
H	-2.13892000	-3.23764500	-0.80806300
H	-3.58904600	-3.89233200	-0.01317800
C	-3.43013900	-1.49094800	-2.49026800
H	-2.34468700	-1.34712600	-2.47847700
H	-3.66821500	-2.24351800	-3.25415500
H	-3.89247800	-0.55312700	-2.79943000
C	-5.45143700	-2.26175800	-1.20078300
H	-6.01342300	-1.37451500	-1.50212900
H	-5.63707100	-3.03164800	-1.96184600
H	-5.86977400	-2.62774700	-0.25978900
C	-4.72245000	-2.42750100	2.22974100
H	-5.64495800	-1.85762000	2.09956600
H	-4.77136500	-3.30681400	1.58266200
H	-4.70775400	-2.79317800	3.26523000
C	-2.21401000	-2.49351000	2.18258200
H	-1.28810800	-1.91577500	2.13993400
H	-2.28640400	-2.95654200	3.17593100
H	-2.13946000	-3.29707700	1.45007900
C	-3.35408300	-0.51217800	3.09340100

H	-3.19775300	-1.02093400	4.05324700
H	-2.50426200	0.16025000	2.93821300
H	-4.26365800	0.08408300	3.19309200
C	-4.80856400	1.27221600	-1.20734800
H	-5.36781500	2.21639500	-1.17898900
H	-3.85428100	1.47507100	-1.70228600
H	-5.38626300	0.57743400	-1.82079400
C	-6.00255600	0.50359400	0.85817000
H	-6.62095500	1.40456400	0.74572800
H	-6.53199600	-0.31674100	0.36784500
H	-5.95023000	0.28607900	1.92769200
C	-3.96022400	1.95257800	1.01037800
H	-2.95829400	2.16828200	0.63041300
H	-4.57788300	2.84897400	0.86609900
H	-3.88609200	1.78028400	2.08374000

## 2-Int5''

Zero-point correction= 0.718211 (Hartree/Particle)

Thermal correction to Energy= 0.764406

Thermal correction to Enthalpy= 0.765351

Thermal correction to Gibbs Free Energy= 0.633705

Sum of electronic and zero-point Energies= -2279.812637

Sum of electronic and thermal Energies= -2279.766442

Sum of electronic and thermal Enthalpies= -2279.765498

Sum of electronic and thermal Free Energies= -2279.897144

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.046233

C	-5.77219200	-0.59675500	-0.24811800
C	-5.75278600	-1.17319000	1.02588500
C	-6.68837900	-0.76158500	1.96889600
C	-7.65037700	0.21589400	1.66064900
C	-7.65487700	0.76451300	0.37284800
C	-6.72330200	0.36373400	-0.58703500
C	-8.64790400	0.66220000	2.70291200
S	-4.60256800	-1.15462800	-1.48545700
O	-4.98276600	-0.54550700	-2.76767800
O	-4.45575600	-2.61202100	-1.37166700
H	-5.02467500	-1.94167700	1.26360700
H	-6.67967500	-1.20914100	2.95987800
H	-8.39937900	1.51228800	0.11202100
H	-6.73602800	0.77671500	-1.59001500
H	-8.16018800	1.25674400	3.48617400
H	-9.43883600	1.27756600	2.26374500
H	-9.11958100	-0.19533000	3.19649300
C	-2.98935100	0.98388100	-1.06561300
C	-0.76520000	-0.97849800	-0.40525100
C	-2.14221000	1.58441400	0.04218300

H	-3.99613100	1.41432700	-1.03325800	H	5.75171900	-2.57188700	-1.23731500
H	-2.56477400	1.20196300	-2.05286200	C	3.10735000	-2.14376800	-1.87256400
N	-3.13393300	-0.49469200	-0.89634300	H	2.14989800	-1.61896400	-1.88010100
C	-1.94769500	-1.24620500	-1.32944700	H	3.76006800	-1.67593000	-2.60886900
H	-1.63851300	-0.99001700	-2.35169100	H	2.92854100	-3.17437400	-2.20868700
H	-2.19260900	-2.31353000	-1.28673400	C	5.39262700	0.21641900	-2.10634500
O	0.30568800	-0.63787200	-0.90521400	H	4.42774400	0.49177200	-2.54423300
C	-0.92296500	-1.26820500	1.06551900	H	6.15699500	0.85474300	-2.56820600
H	-0.60702100	-2.30679900	1.24185300	H	5.62600600	-0.81326900	-2.38504600
H	-0.27804800	-0.60901300	1.64994000	C	5.34347300	1.98827000	-0.40324700
H	-1.96128700	-1.17184800	1.38579200	H	6.23061200	2.43271400	-0.87433200
C	-2.81641700	1.73980100	1.39303600	H	4.45752900	2.39477200	-0.89520900
H	-2.10555700	2.07641800	2.15271900	H	5.32742600	2.31233700	0.63709000
H	-3.63265000	2.47535000	1.34340600	C	6.77968100	-0.03459800	-0.03287700
H	-3.26643700	0.79638800	1.72993700	H	6.90898000	-1.11611000	-0.11050000
C	-0.90866600	2.01147400	-0.19282600	H	7.58261600	0.43337000	-0.61835800
C	0.31958600	2.38821200	-0.43608100	H	6.93773400	0.25317800	1.00946200
C	0.55897900	3.75555400	-0.93039500	H	2.58119900	2.14209400	0.39774200
H	-0.34203000	4.35443400	-1.08725200				
C	1.73754800	4.32558000	-1.21734800	<b>2-Ts3''</b>			
H	2.67393000	3.79101400	-1.09525800	Zero-point correction= 0.7209381 (Hartree/Particle)			
H	1.79034000	5.34781800	-1.58266200	Thermal correction to Energy= 0.764569			
Pd	1.81944300	0.93212700	-0.15267500	Thermal correction to Enthalpy= 0.765513			
P	3.85602100	-0.37603200	0.23822200	Thermal correction to Gibbs Free Energy= 0.642832			
C	5.42080600	0.45338000	-0.57950900	Sum of electronic and zero-point Energies= -2279.797576			
C	4.14062500	-0.45806700	2.16448700	Sum of electronic and thermal Energies= -2279.753945			
C	3.72442800	-2.19807900	-0.45262700	Sum of electronic and thermal Enthalpies= -2279.753001			
C	4.63161000	0.91404700	2.67908700	Sum of electronic and thermal Free Energies= -2279.875682			
H	3.98153500	1.72890100	2.34712400	HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2281.024128			
H	4.60786300	0.89783300	3.77667800	C	5.83276300	-0.64181100	0.35825300
H	5.65921500	1.13907500	2.38532800	C	6.24674500	-0.86409100	-0.95900300
C	5.12213700	-1.54042500	2.65901700	C	7.36283300	-0.18902400	-1.44132900
H	6.11972100	-1.43731300	2.22497300	C	8.08070900	0.70412000	-0.62721200
H	5.22931600	-1.44888700	3.74846000	C	7.64850100	0.90107000	0.68935700
H	4.76684500	-2.55423800	2.45868100	C	6.52978900	0.23168800	1.19053700
C	2.76220300	-0.68228000	2.83199600	C	9.29849900	1.41800000	-1.16476200
H	2.88890700	-0.64570200	3.92248600	S	4.41308000	-1.53325900	0.99572700
H	2.05937100	0.10644600	2.54351600	O	4.34350700	-1.27712600	2.44282800
H	2.31458500	-1.64651500	2.58787400	O	4.44804700	-2.90931900	0.48731700
C	2.72407400	-2.99588800	0.41283100	H	5.70343500	-1.56265200	-1.58674400
H	2.52234700	-3.95356600	-0.08476400	H	7.68840900	-0.35868300	-2.46504800
H	3.10764700	-3.22717500	1.40901200	H	8.19464800	1.58380600	1.33547200
H	1.77129700	-2.47001700	0.51377600	H	6.20164500	0.37257200	2.21487500
C	5.04441300	-2.99415900	-0.51955900	H	9.07688000	1.92889700	-2.10933800
H	5.54523100	-3.07221900	0.44831700	H	9.67114700	2.16430700	-0.45661300
H	4.82149900	-4.01604500	-0.85586600	H	10.11440500	0.71185500	-1.36499400

C	2.76450900	0.57615000	0.64904200	C	-4.80525700	-3.04811500	0.56575200
C	0.79476800	-0.67326600	-0.54536500	H	-5.53823600	-2.98423300	-0.24187200
C	1.78440500	1.08704500	-0.40373000	H	-4.52057800	-4.10401700	0.66471600
H	3.66651800	1.19595800	0.70883700	H	-5.29683400	-2.76514300	1.49964900
H	2.29873400	0.53675500	1.64231000	C	-2.57239800	-2.38125100	1.50976500
N	3.14161700	-0.77028100	0.17172100	H	-1.62274600	-1.86959000	1.34023000
C	1.91748000	-1.58126400	0.02226200	H	-3.00273000	-2.03160800	2.44756200
H	1.55510800	-1.95477400	0.98814900	H	-2.36167700	-3.45241600	1.63311900
H	2.13000600	-2.42820300	-0.63474500	C	-4.67513300	-0.13194100	2.68078600
O	-0.25116100	-0.63118300	0.21958700	H	-3.62530800	0.09456700	2.89184700
C	0.56703700	-0.78723700	-2.04947000	H	-5.28351300	0.41098000	3.41556300
H	0.05637300	-1.74048500	-2.24227100	H	-4.84716900	-1.19699100	2.84759600
H	-0.08157400	0.01846100	-2.40587900	C	-5.05179400	1.88264400	1.32341100
H	1.49698100	-0.78653900	-2.62286600	H	-5.80654300	2.21677400	2.04783100
C	2.46834800	1.49840800	-1.71326900	H	-4.07656000	2.23823700	1.66276000
H	1.74020900	1.71368500	-2.50026400	H	-5.27639900	2.36322200	0.37107600
H	3.07326100	2.40318200	-1.56491100	C	-6.55146000	-0.10346000	1.01487000
H	3.14131000	0.70817200	-2.05890000	H	-6.66654600	-1.18683600	0.94675400
C	0.76068000	1.92138800	0.02292800	H	-7.17002400	0.23792700	1.85538300
C	-0.29889900	2.51182700	0.37697900	H	-6.97135800	0.34205300	0.10969600
C	-0.60099500	3.81327500	0.95737300	H	-2.76362000	2.04041900	-0.13377700
H	0.27234000	4.35371400	1.32542000				
C	-1.79557400	4.40844500	1.06583100	<b>1a</b>			
H	-2.70720700	3.93608400	0.71683900	Zero-point correction=	0.354079	(Hartree/Particle)	
H	-1.87923700	5.40015500	1.50113800	Thermal correction to Energy=	0.377436		
Pd	-1.78323700	0.86140300	0.01878500	Thermal correction to Enthalpy=	0.378380		
P	-3.81940600	-0.32955600	-0.04971700	Thermal correction to Gibbs Free Energy=	0.297580		
C	-5.09288300	0.33773700	1.26911100	Sum of electronic and zero-point Energies=	-1338.242270		
C	-4.57843100	-0.10855900	-1.82913500	Sum of electronic and thermal Energies=	-1338.218913		
C	-3.52559900	-2.22729200	0.29829700	Sum of electronic and thermal Enthalpies=	-1338.217969		
C	-5.18052200	1.30580900	-1.98284900	Sum of electronic and thermal Free Energies=	-1338.298770		
H	-4.46240300	2.08551900	-1.71320100	HF( $\omega$ b97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])=	-1338.621892		
H	-5.44448600	1.45098400	-3.03840900	N	0.31363100	-0.64162900	0.08843700
H	-6.09423400	1.44969400	-1.40211900	C	0.69171600	-0.17791300	-1.23917100
C	-5.66039300	-1.13892000	-2.21503500	H	-0.03331500	-0.54997600	-1.97111900
H	-6.51274900	-1.13441900	-1.53118000	H	0.68956200	0.91700000	-1.28618500
H	-6.04214500	-0.88835200	-3.21370500	C	2.05534900	-0.67410700	-1.72890100
H	-5.27031100	-2.15774000	-2.26918700	C	0.71442900	0.22077600	1.20893600
C	-3.41813100	-0.18581700	-2.85011400	H	0.12844200	-0.06899600	2.08420700
H	-3.82418400	-0.00742600	-3.85486900	H	0.49021700	1.26690900	0.96582900
H	-2.66654200	0.58261000	-2.64352800	C	2.18731000	0.03636100	1.50829200
H	-2.91668900	-1.15376300	-2.86485100	C	3.06813100	0.85969600	0.99000400
C	-2.78249800	-2.85145800	-0.90268200	C	3.90900400	1.65362800	0.42238700
H	-2.49347700	-3.87449700	-0.62973800	C	4.72494000	1.95482700	-0.76978700
H	-3.39658300	-2.92174900	-1.80343100	C	4.71694500	2.88918100	0.43366800
H	-1.86609300	-2.30114900	-1.12785600	H	4.19938900	2.25411400	-1.67212000

H	5.61188700	1.35070800	-0.94274900	H	6.48440700	1.84916300	0.62782200
H	5.60063300	2.91572700	1.06693300	H	5.37814600	2.06462100	-0.73728900
H	4.19636500	3.83973000	0.34372300	C	6.25335200	0.13321100	-0.64923900
S	-1.06622600	-1.56089900	0.24306100	C	5.67274000	-1.06379500	-0.49777800
O	-1.09691500	-2.43978000	-0.91624600	C	5.90216000	-2.33238000	-1.20360900
O	-1.06377900	-2.07887900	1.60116100	C	7.02468800	-2.83336300	-1.72278000
C	-2.42913200	-0.42366100	0.09501900	C	4.56106300	-3.04941100	-1.19030500
C	-2.88642100	0.24933800	1.22556800	S	3.93931600	2.30866600	1.79664400
C	-2.98367800	-0.17332300	-1.15693000	O	3.06988400	1.73129400	2.80692500
C	-3.89940100	1.18971200	1.09071300	O	5.05016100	3.17719000	2.14915300
H	-2.47139900	0.01617500	2.20046200	C	2.92138300	3.15341000	0.60673200
C	-3.99686200	0.77081900	-1.27306200	C	3.45662500	4.21553400	-0.11616700
H	-2.64376000	-0.73351300	-2.02151400	C	1.63016500	2.68974100	0.35213500
C	-4.46381200	1.47019900	-0.15733900	C	2.68763500	4.81828900	-1.10734000
H	-4.26549500	1.70879300	1.97248300	H	4.45383500	4.57589000	0.11401700
H	-4.43849900	0.96059400	-2.24758300	C	0.88363400	3.30008800	-0.64495800
C	-5.54153600	2.51437200	-0.29581200	H	1.20759900	1.87528300	0.93200700
H	-6.17591100	2.55302100	0.59468200	C	1.39703500	4.36730300	-1.38945900
H	-5.10029600	3.50918500	-0.42955400	H	3.09863200	5.65467100	-1.66621800
H	-6.18002400	2.31732400	-1.16172300	H	-0.12040600	2.94173100	-0.84834900
C	2.46993800	-2.06600600	-1.32806400	C	0.56140400	5.00366200	-2.47013700
H	2.82812600	-2.05124000	-0.29381400	H	1.06010500	5.87378800	-2.90628800
H	1.61737000	-2.75147100	-1.36444700	H	0.36082900	4.28956600	-3.27724300
H	3.27474400	-2.40665400	-1.98152700	H	-0.40756700	5.33009500	-2.07619500
C	2.54559600	-1.16641000	2.34445800	C	4.64081600	-1.90590600	1.67229000
H	2.21855400	-1.02621200	3.38225600	H	5.27993300	-2.79091900	1.58748500
H	2.02623800	-2.05472100	1.96518200	H	5.12184100	-1.19076200	2.34445200
H	3.62204700	-1.35301800	2.34362800	H	3.67673900	-2.20623800	2.09656100
O	2.70747000	0.02958000	-2.46928500	C	7.42631700	0.40312500	-1.54816800
<b>PdL</b>				H	7.40962100	-0.24636200	-2.42910000
Zero-point correction= 0.682662 (Hartree/Particle)				H	7.42643300	1.44508800	-1.88660600
Thermal correction to Energy= 0.718445				H	8.37507400	0.23227200	-1.02438000
Thermal correction to Enthalpy= 0.719389				Pd	1.42390300	-2.15809900	-0.46331400
Thermal correction to Gibbs Free Energy= 0.619109				P	-0.83025400	-1.84871400	-0.34991400
Sum of electronic and zero-point Energies= -1599.317596				C	-1.71111300	-3.42457600	0.23693300
Sum of electronic and thermal Energies= -1599.281812				C	-1.44309800	-1.32762900	-2.07382400
Sum of electronic and thermal Enthalpies= -1599.280868				C	-0.65100800	-0.04390600	-2.38586500
Sum of electronic and thermal Free Energies= -1599.381149				H	-0.86161400	0.75181400	-1.66702900
HF(6-311+G(d,p)/Lanl2dz, SMD[toluene])= -1600.333256				H	0.42644800	-0.23891900	-2.35993100
N	4.60091700	1.02803000	0.94934400	H	-0.91977000	0.32195300	-3.38527500
C	3.64969600	0.05016500	0.42489500	C	-0.97941500	-2.40955000	-3.06751000
H	2.81609100	-0.04680700	1.12156300	H	-1.08068200	-2.01799700	-4.08820100
H	3.25664700	0.34001900	-0.56078400	H	0.06816000	-2.68769800	-2.90424200
C	4.40768300	-1.26395400	0.30790200	H	-1.59750800	-3.31066800	-3.00300400
C	5.70101600	1.35399300	0.04687200	C	-2.93801000	-1.09116400	-2.31490900
				H	-3.07202600	-0.69701300	-3.33178000



H	-3.51665100	-2.01416000	-2.25219000	H	-7.62963000	3.09392900	-1.28207000
H	-3.37379800	-0.37676600	-1.62232600	C	-2.84102800	2.39510800	-0.67952200
C	-1.01016900	-4.64074800	-0.39670900	H	-1.88654500	1.93861600	-0.40207700
H	-1.47203200	-5.55904500	-0.00958200	C	-2.95334500	3.71720200	0.09380100
H	-1.10166800	-4.65776800	-1.48551900	H	-2.15254500	4.40493800	-0.20475400
H	0.05657900	-4.65033700	-0.14994000	H	-3.91418100	4.20354900	-0.11143900
C	-3.20579600	-3.49336200	-0.08896000	H	-2.87416300	3.56009500	1.17268400
H	-3.36534800	-3.75899700	-1.13873000	C	-2.81604800	2.67533300	-2.18829000
H	-3.68300800	-4.27280400	0.51883200	H	-3.64799200	3.32150900	-2.49031400
H	-3.72112100	-2.54951300	0.09826900	H	-1.89050800	3.19567100	-2.46115800
C	-1.47823700	-3.52426800	1.75473200	H	-2.87192500	1.75404800	-2.77361600
H	-0.40804100	-3.47714900	1.98689900	C	-4.67001800	-1.37150800	2.26585600
H	-1.97476900	-2.72960400	2.31591700	H	-3.64417400	-1.74673700	2.28547700
H	-1.86342600	-4.48670500	2.11461000	C	-5.61633200	-2.57797900	2.18932900
C	-1.23255700	-0.53551700	0.97313900	H	-5.30132100	-3.33830600	2.91202600
C	-2.35315400	0.27250000	1.31175000	H	-6.64413300	-2.29577700	2.44592500
C	-0.09780600	-0.39979200	1.80144000	H	-5.63127900	-3.03716300	1.19752600
C	-2.23857000	1.16098200	2.39687000	C	-4.91679000	-0.63517400	3.59381400
C	-0.01183600	0.46839400	2.88074600	H	-5.91245000	-0.17608300	3.59526600
H	0.76707500	-1.01601900	1.56339000	H	-4.86512500	-1.33984600	4.43179200
C	-1.09907100	1.27623400	3.17664500	H	-4.17685200	0.14886200	3.76822600
H	-3.09773500	1.78622500	2.62198600				
H	0.91041300	0.53347300	3.44833000	<b>3-Int1-a</b>			
O	3.66103200	-2.15957000	-0.53308800	Zero-point correction=	1.038966	(Hartree/Particle)	
H	7.03076900	-3.80201100	-2.21585700	Thermal correction to Energy=	1.099692		
H	7.97440600	-2.31553200	-1.65120500	Thermal correction to Enthalpy=	1.100636		
H	4.16660400	-3.23511700	-2.19239600	Thermal correction to Gibbs Free Energy=	0.940254		
H	4.61083300	-4.00154000	-0.64694900	Sum of electronic and zero-point Energies=	-2937.565478		
H	-1.06506100	1.98701000	3.99673600	Sum of electronic and thermal Energies=	-2937.504751		
C	-3.70504400	0.37866900	0.65236500	Sum of electronic and thermal Enthalpies=	-2937.503807		
C	-3.93852500	1.42258500	-0.26998600	Sum of electronic and thermal Free Energies=	-2937.664189		
C	-4.79098200	-0.40605500	1.09194400	HF( $\omega$ b97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])=	-2939.237560		
C	-5.21122200	1.58697600	-0.81053300	N	-5.52814400	0.78657100	0.13428400
C	-6.04250500	-0.21855600	0.50045500	C	-4.70097200	0.15699200	1.15813000
C	-6.27277500	0.75677400	-0.46236900	H	-5.33809100	-0.18600600	1.98060300
H	-5.37687600	2.38233300	-1.53266400	H	-4.17031900	-0.71200800	0.75308700
H	-6.87470200	-0.84296400	0.81398000	C	-3.67317700	1.09672300	1.79354400
C	-7.63882600	0.91751900	-1.10273800	C	-5.04444400	0.63790500	-1.24695100
H	-8.30337900	0.17159500	-0.64739200	H	-5.83186300	0.99582800	-1.91419600
C	-7.57894300	0.62988700	-2.60926000	H	-4.84777600	-0.42090300	-1.46318500
H	-6.94092100	1.35915200	-3.12219200	C	-3.79333200	1.46900500	-1.44419400
H	-7.16920900	-0.36683400	-2.80244100	C	-2.61741900	0.90737900	-1.28585300
H	-8.57846000	0.68590000	-3.05516900	C	-1.49976900	0.30104800	-1.07742600
C	-8.23774800	2.30302100	-0.82768300	C	-0.49130700	-0.10827600	-0.08753400
H	-9.24734100	2.37725800	-1.24724400	C	-0.34137900	-0.42029400	-1.61971900
H	-8.29573000	2.50045700	0.24758900	H	-0.77307300	-0.91777300	0.58155200

H	0.10946300	0.68415400	0.35726300	H	2.90227200	-4.52238500	-1.01086800
H	0.36744100	0.16770100	-2.19810700	H	2.54609100	-3.18822700	-2.11102000
H	-0.48659700	-1.44487600	-1.95385900	C	5.63894600	-4.06829200	-0.84609200
S	-7.17808500	0.81750200	0.38147700	H	5.31466700	-4.76887800	-0.07255000
O	-7.36906800	1.12171200	1.79128900	H	5.89409900	-4.66385000	-1.73240500
O	-7.73479200	1.65455000	-0.66762200	H	6.56243200	-3.58721600	-0.51402500
C	-7.73105300	-0.85222000	0.10712400	C	5.06159800	-2.19452300	-2.38496400
C	-8.00020400	-1.27912900	-1.19186400	H	4.28966800	-1.50195100	-2.72877400
C	-7.82855200	-1.73148400	1.18194100	H	5.94867900	-1.61703900	-2.10763400
C	-8.35721200	-2.60359400	-1.40918000	H	5.32947800	-2.84038700	-3.23106500
H	-7.95580200	-0.57380000	-2.01513200	C	5.16316800	-0.56035600	0.28438000
C	-8.18826600	-3.05352600	0.94570200	C	4.85978800	0.81787100	0.17274800
H	-7.65216300	-1.37414400	2.19094700	C	6.50973700	-0.91692700	0.46243000
C	-8.44959800	-3.51076900	-0.34849000	C	5.90894600	1.74813000	0.23770900
H	-8.57731400	-2.93757600	-2.41964800	C	7.53478100	0.01701300	0.52937300
H	-8.27499800	-3.73962000	1.78386400	H	6.77167400	-1.96303200	0.54856300
C	-8.80873800	-4.95245100	-0.60152000	C	7.23119700	1.36754400	0.41356500
H	-9.52072900	-5.04663500	-1.42711000	H	5.66241400	2.80181100	0.14028000
H	-7.91639300	-5.53123200	-0.86842400	H	8.56045900	-0.31233600	0.66650900
H	-9.25054800	-5.41609900	0.28521800	O	-2.60028400	0.65798200	2.14993400
C	-4.10070000	2.52331600	2.01713800	H	8.01388600	2.11912000	0.45678100
H	-4.08812200	3.05793400	1.06247700	C	3.50412600	1.44802800	-0.02123300
H	-5.12883500	2.56420600	2.39163400	C	3.02861200	1.71378700	-1.32276000
H	-3.40912900	3.00774400	2.70845000	C	2.81434800	1.97444400	1.08601200
C	-4.00159700	2.92800300	-1.76106300	C	1.85221000	2.44417100	-1.47880800
H	-4.41082200	3.04430300	-2.77254000	C	1.64471200	2.70861000	0.87866500
H	-4.73202900	3.36789900	-1.07121800	C	1.13349800	2.94226800	-0.39317600
H	-3.06821900	3.49252400	-1.70123600	H	1.48034000	2.64395800	-2.48240800
Pd	1.82191700	-1.04865400	-0.32660700	H	1.11654400	3.09697600	1.74344100
P	3.86335100	-1.88886600	0.12913800	C	-0.13814700	3.73895000	-0.63552400
C	4.54148000	-3.06449700	-1.23077000	H	-0.65813700	3.25295000	-1.47288400
C	3.91239400	-2.79897300	1.80784200	C	-1.09852800	3.74602700	0.55546100
C	3.20790500	-1.86970000	2.80732700	H	-1.33395100	2.73250400	0.89662000
H	3.76291300	-0.93761500	2.94424200	H	-0.68396100	4.30416600	1.40334300
H	2.19704400	-1.62137000	2.46931800	H	-2.03579400	4.24049300	0.27750900
H	3.14072000	-2.36447600	3.78522500	C	0.20536900	5.17397900	-1.06312500
C	3.06432100	-4.07538200	1.68281800	H	0.85212700	5.18198800	-1.94674000
H	2.88981500	-4.49105700	2.68359700	H	-0.70402000	5.73968600	-1.29771600
H	2.09084300	-3.85660700	1.22971000	H	0.73337400	5.69579000	-0.25624300
H	3.55721900	-4.85167100	1.09020700	C	3.32268000	1.80468000	2.50861300
C	5.28619600	-3.14656300	2.39948500	H	4.08769400	1.02301100	2.49807400
H	5.13497800	-3.68885200	3.34200700	C	3.99711500	3.09217500	3.00435700
H	5.88983200	-3.78630300	1.75192800	H	3.28833200	3.92874400	2.99666000
H	5.86187700	-2.24615400	2.63254100	H	4.36198800	2.96544400	4.03022200
C	3.33652800	-3.86280500	-1.76698100	H	4.84801600	3.36397300	2.37175300
H	3.66254200	-4.48661400	-2.61015400	C	2.21628300	1.36867300	3.47821300

H	1.63460200	0.53822900	3.06840500	C	9.07950500	1.81701400	1.34271900
H	2.65234600	1.04849200	4.43115400	C	9.37624100	3.16461400	-1.07574600
H	1.52290400	2.18873600	3.69637800	H	9.22126200	1.22514600	-2.00494900
C	3.81055500	1.29406600	-2.55727900	C	9.24685800	3.19676400	1.32388300
H	4.58320600	0.58953200	-2.23944000	H	8.98993500	1.28050800	2.28131900
C	2.94378700	0.58098800	-3.60034600	C	9.39440800	3.89017600	0.11951700
H	2.18386700	1.24630800	-4.02680200	H	9.49999000	3.68684500	-2.02072800
H	3.56497000	0.22189100	-4.42896700	H	9.26857300	3.74360900	2.26271300
H	2.43541900	-0.28057600	-3.15200400	C	9.60708800	5.38224900	0.10977100
C	4.52497700	2.50728200	-3.16960300	H	10.67749000	5.61913300	0.13256300
H	5.12144800	2.20713400	-4.03885900	H	9.18788700	5.83910600	-0.79175800
H	3.80164100	3.26345200	-3.49727100	H	9.14533400	5.85729200	0.98037300
H	5.19527700	2.97592500	-2.44136500	C	5.98320300	-3.04750100	1.50906000
				H	5.88007600	-3.39301100	0.47525900
<b>3-Ts1-a</b>				H	7.05262200	-3.04037900	1.74239400
Zero-point correction= 1.036522 (Hartree/Particle)				H	5.44175500	-3.72696300	2.16958700
Thermal correction to Energy= 1.097045				C	6.08517200	-2.87940600	-2.24815200
Thermal correction to Enthalpy= 1.097990				H	6.46501200	-2.71361500	-3.26410700
Thermal correction to Gibbs Free Energy= 0.934402				H	6.93912200	-3.19714600	-1.63764900
Sum of electronic and zero-point Energies= -2937.527589				H	5.34836400	-3.68560100	-2.28193400
Sum of electronic and thermal Energies= -2937.467066				Pd	-0.00760100	-0.64471600	-0.38940000
Sum of electronic and thermal Enthalpies= -2937.466122				P	-2.22495400	-0.11587600	0.30266300
Sum of electronic and thermal Free Energies= -2937.629710				C	-2.51689000	1.72270200	-0.06764600
HF( $\omega$ b97xd/6-311+G(d,p)/LanL2dz, SMD[ <i>toluene</i> ])= -2939.200523				C	-2.37325800	-0.48004900	2.15883600
N	7.08891100	-0.79212100	-0.02216500	C	-2.54697700	-2.00186600	2.30641600
C	6.25311700	-0.49358400	1.13272900	H	-3.48931500	-2.36690300	1.89250000
H	6.89119600	-0.22314800	1.98108000	H	-1.73386100	-2.53883000	1.80456400
H	5.58791500	0.35290900	0.92665500	H	-2.51844200	-2.26266600	3.37171800
C	5.39858100	-1.66415300	1.62615500	C	-1.04310300	-0.11907600	2.84713100
C	6.48692200	-0.51948800	-1.33476200	H	-1.12302800	-0.35688800	3.91615300
H	7.28886800	-0.50585100	-2.07665200	H	-0.20954500	-0.69029800	2.42637100
H	6.00127900	0.46459600	-1.32120200	H	-0.79769700	0.94193800	2.76114900
C	5.49498900	-1.60808400	-1.69007100	C	-3.50787900	0.26903600	2.86341400
C	4.21662700	-1.43148700	-1.45407900	H	-3.70546100	-0.19056700	3.84022500
C	2.96900200	-1.23649000	-1.17072800	H	-3.23263700	1.31267500	3.04571700
C	2.02660400	-1.38434900	-0.05251200	H	-4.43472500	0.26365700	2.28749800
C	1.71917200	-0.70741100	-1.73759300	C	-1.37428300	2.50816700	0.60390600
H	2.21808000	-0.74735500	0.81164500	H	-1.35836200	3.52559600	0.19242800
H	1.72739600	-2.40753900	0.17962900	H	-1.52469600	2.59750900	1.68443900
H	1.23895000	-1.32896400	-2.49535700	H	-0.39719400	2.04616900	0.42113600
H	1.70177900	0.36653400	-1.93394200	C	-3.83734200	2.38353900	0.34203600
S	8.73954900	-0.63286200	0.14097500	H	-3.95722900	2.43450900	1.42549700
O	9.06440300	-1.13935000	1.46560000	H	-3.84217000	3.41619200	-0.03273800
O	9.32729500	-1.19589400	-1.06301100	H	-4.70795600	1.87932400	-0.06703300
C	9.05680800	1.11916900	0.13798700	C	-2.32851600	1.83347900	-1.59230500
C	9.21049500	1.78539000	-1.07593400	H	-1.32527300	1.50527400	-1.88525600

H	-3.05319100	1.22702400	-2.14201400
H	-2.45701900	2.87804500	-1.90335000
C	-3.49048300	-1.25030600	-0.53356300
C	-4.90745200	-1.27428400	-0.65805300
C	-2.79172700	-2.33954400	-1.09415000
C	-5.50492700	-2.36183400	-1.31688200
C	-3.40653000	-3.41243200	-1.72460300
H	-1.70591000	-2.33253600	-1.02752400
C	-4.78700600	-3.42663100	-1.83983100
H	-6.58549200	-2.34952900	-1.42394500
H	-2.80133900	-4.21863300	-2.12791000
O	4.32994800	-1.43446400	2.15020600
H	-5.30358000	-4.24267200	-2.33643800
C	-5.92159600	-0.23901300	-0.24563900
C	-6.59690000	-0.32171200	0.98943700
C	-6.34146100	0.71274300	-1.20165700
C	-7.57220500	0.63226100	1.28939800
C	-7.33879900	1.62418000	-0.86296900
C	-7.94580500	1.62310500	0.38949700
H	-8.07295800	0.59300800	2.25291400
H	-7.64501800	2.36445900	-1.59728600
C	-8.98872000	2.66161300	0.75805500
H	-9.33210300	2.43364400	1.77567000
C	-8.37982800	4.07050500	0.77661500
H	-7.52022500	4.11752200	1.45310200
H	-8.03547900	4.36147000	-0.22272700
H	-9.11990500	4.80894600	1.10519200
C	-10.20934900	2.59879000	-0.16931200
H	-10.65276800	1.59781900	-0.16930000
H	-10.97425400	3.31512300	0.15095400
H	-9.93480500	2.84455900	-1.20173600
C	-5.76493600	0.75543500	-2.61174700
H	-4.81848600	0.20667900	-2.60762900
C	-6.70178800	0.03973600	-3.59735100
H	-7.68679700	0.52126800	-3.60998700
H	-6.29053300	0.07781700	-4.61255800
H	-6.84124700	-1.01083900	-3.32766400
C	-5.48148800	2.18101300	-3.10659200
H	-4.94116000	2.77064300	-2.36084500
H	-4.87518300	2.14593700	-4.01832200
H	-6.40684100	2.71387500	-3.35349400
C	-6.37751500	-1.47612200	1.96175600
H	-5.34640100	-1.81906500	1.84773600
C	-6.59564500	-1.10705300	3.43637600
H	-7.66305000	-1.03018800	3.67395000
H	-6.17909000	-1.89154000	4.07722800

H	-6.12259900	-0.15967000	3.70722200
C	-7.29804600	-2.65816900	1.61227500
H	-7.16864800	-3.46611300	2.34163600
H	-8.34778100	-2.34284000	1.63568800
H	-7.08383700	-3.06345200	0.62124200

### 3-Int2-a

Zero-point correction= 1.040011 (Hartree/Particle)

Thermal correction to Energy= 1.099376

Thermal correction to Enthalpy= 1.100320

Thermal correction to Gibbs Free Energy= 0.947979

Sum of electronic and zero-point Energies= -2937.592882

Sum of electronic and thermal Energies= -2937.533517

Sum of electronic and thermal Enthalpies= -2937.532573

Sum of electronic and thermal Free Energies= -2937.684914

HF(ωb97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])= -2939.262838

C	3.95509900	-1.31145300	0.42721200
H	4.67505500	-1.48335800	1.23525800
H	3.20151700	-0.60826400	0.80007900
C	3.26778400	-2.66962100	0.21775700
C	3.88125300	0.17745500	-1.59337700
H	4.60112000	0.83911100	-2.08390900
H	3.23098900	0.78705300	-0.95453800
C	3.05666200	-0.53187400	-2.65913200
C	1.74300300	-0.59108900	-2.57845300
C	0.43251600	-0.62760500	-2.48469300
C	-0.44855800	-1.56663300	-1.71649600
C	-0.55910200	0.44559400	-2.80880300
H	0.00553900	-2.09409800	-0.87734200
H	-1.04646400	-2.22614500	-2.35538200
H	-1.20256500	0.20867000	-3.66292700
H	-0.18988200	1.47148000	-2.84751500
S	6.32463100	-0.57463600	-0.62843100
O	6.80791200	-1.75545200	0.09775400
O	6.78839600	-0.24860100	-1.97903100
C	6.65601100	0.85497100	0.40972600
C	6.72665600	2.12662900	-0.16634200
C	6.82429100	0.68793900	1.78679000
C	6.94680000	3.23382700	0.65034800
H	6.64277700	2.23912100	-1.24189400
C	7.04390300	1.80728900	2.58809700
H	6.81730700	-0.30840100	2.21550600
C	7.10012700	3.09556300	2.03778900
H	7.01289600	4.22167700	0.20075000
H	7.18585900	1.67591700	3.65806000
C	7.31085000	4.30547600	2.91689500

H	7.85921300	5.09339000	2.39001100	H	-4.50711300	-0.96914700	3.14369300
H	6.35041800	4.73362800	3.23390200	H	-6.10139700	3.01532500	3.22694200
H	7.86851400	4.05017500	3.82379400	O	2.32123500	-2.95358200	0.93239200
C	3.85198600	-3.61934800	-0.79684100	H	-5.94534400	0.72205100	4.21904400
H	3.61048000	-3.26320600	-1.80445600	C	-3.02754400	-0.89014200	1.04394500
H	4.94425900	-3.64238200	-0.71782400	C	-3.69741800	-1.84035600	0.21347900
H	3.42910500	-4.61570500	-0.65264000	C	-1.83151900	-1.30128900	1.71286700
C	3.84764200	-1.10372400	-3.82155500	C	-3.17107100	-3.13149300	0.08427900
H	4.33977600	-0.30279300	-4.39113600	C	-1.35447400	-2.60491800	1.53860600
H	4.64856600	-1.76591300	-3.46989900	C	-2.02080600	-3.54938600	0.75176700
H	3.19863400	-1.66156800	-4.50173000	H	-3.70644200	-3.85360600	-0.52719000
Pd	-1.71684600	-0.00605900	-1.11711600	H	-0.44415700	-2.89705400	2.05301400
P	-2.91212100	2.04636200	-0.51844000	C	-1.55103000	-4.99492400	0.64443500
C	-4.19583200	2.75509500	-1.79110500	H	-2.33709800	-5.54191800	0.10511600
C	-1.71079500	3.47095300	0.01456600	C	-0.25000600	-5.13192000	-0.17026600
C	-0.58120800	2.79962100	0.81881800	H	-0.37222500	-4.72245400	-1.17870600
H	-0.95192100	2.35935700	1.74850300	H	0.58059100	-4.60209100	0.30810100
H	-0.08895700	2.01382500	0.23897300	H	0.02633900	-6.18989800	-0.26297100
H	0.16955100	3.55510100	1.08788100	C	-1.40291800	-5.65433200	2.02908500
C	-1.07634200	4.09655500	-1.24569500	H	-2.33019200	-5.58110100	2.60876900
H	-0.26086200	4.76337000	-0.93568300	H	-1.15187400	-6.71601800	1.91981900
H	-0.64818700	3.33704600	-1.90597300	H	-0.60199700	-5.18547400	2.61214400
H	-1.78223700	4.69894900	-1.82353200	C	-1.10320200	-0.40269200	2.71196500
C	-2.30698400	4.58847500	0.89246900	H	-1.55662200	0.59165000	2.66100900
H	-1.51815900	5.32263100	1.10597500	C	-1.28976500	-0.90927000	4.15779600
H	-3.12718700	5.12724000	0.41215100	H	-0.85981100	-1.90934600	4.28484500
H	-2.66053000	4.20484300	1.85339800	H	-0.78899700	-0.23660200	4.86479200
C	-3.54724900	2.64768500	-3.19035200	H	-2.34842900	-0.96069600	4.43362100
H	-4.28151900	2.94954200	-3.94937300	C	0.39512200	-0.25639100	2.38506700
H	-2.67356100	3.29441600	-3.30362900	H	0.53788900	0.10988800	1.36425800
H	-3.23502700	1.62185000	-3.40395700	H	0.86358700	0.45327800	3.07872200
C	-4.67374000	4.20472600	-1.57606400	H	0.92991300	-1.20805400	2.46404500
H	-3.86191500	4.93373000	-1.62821800	C	-5.05709500	-1.55982600	-0.42282200
H	-5.38511600	4.45907600	-2.37352000	H	-5.26497600	-0.49373400	-0.31294100
H	-5.20051700	4.34071300	-0.62709700	C	-5.08347800	-1.88983700	-1.92715200
C	-5.43445300	1.83914200	-1.78631100	H	-4.97212000	-2.96475900	-2.10945800
H	-5.16915900	0.80631400	-2.02155100	H	-6.04008300	-1.58261500	-2.36708000
H	-5.96358900	1.85545800	-0.82874900	H	-4.27317800	-1.37748300	-2.45717500
H	-6.13313200	2.18290300	-2.56062300	C	-6.18078400	-2.31554400	0.31737900
C	-3.88076100	1.61539000	1.01437300	H	-7.15586400	-2.08018400	-0.12639800
C	-3.80635800	0.30834600	1.56529700	H	-6.03677700	-3.40057100	0.25653200
C	-4.72238600	2.55803200	1.63873500	H	-6.21665400	-2.04001100	1.37673300
C	-4.56246500	0.03059700	2.72272600				
C	-5.46434300	2.25816300	2.77791200				
H	-4.80091100	3.55518500	1.22493500				
C	-5.37798700	0.98130400	3.32921500				

**3-Ts2-a**

Zero-point correction= 1.038940 (Hartree/Particle)

Thermal correction to Energy= 1.098007

Thermal correction to Enthalpy= 1.098951				P	-2.71334800	-1.89332500	0.30912000
Thermal correction to Gibbs Free Energy= 0.945520				C	-3.09313700	-3.08378400	1.80678500
Sum of electronic and zero-point Energies= -2937.542371				C	-2.20712000	-2.93084100	-1.24966400
Sum of electronic and thermal Energies= -2937.483303				C	-1.49847000	-1.95645800	-2.21601900
Sum of electronic and thermal Enthalpies= -2937.482359				H	-2.11365200	-1.08978900	-2.46360800
Sum of electronic and thermal Free Energies= -2937.635790				H	-0.55965600	-1.58270000	-1.80355100
HF(ωb97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.214588				H	-1.27265800	-2.48802200	-3.14979300
N	4.40476200	-0.08797000	-1.27863500	C	-1.18613400	-4.02761900	-0.87898200
C	3.94544400	-1.45325100	-1.00724800	H	-0.80367000	-4.46786600	-1.80808200
H	4.80205500	-2.13754100	-1.02036200	H	-0.32077600	-3.62937500	-0.34621900
H	3.48219200	-1.51410400	-0.01709500	H	-1.62237100	-4.83826900	-0.28982700
C	2.95949300	-2.02571000	-2.03581800	C	-3.39672300	-3.58130800	-1.98198500
C	3.69440000	0.99052000	-0.53358100	H	-3.01381400	-4.12401800	-2.85596000
H	4.25160000	1.91259000	-0.72175000	H	-3.93225500	-4.30681700	-1.36185500
H	3.72602200	0.76942100	0.54224400	H	-4.11570500	-2.84109600	-2.34382600
C	2.24989400	1.14373100	-1.00230800	C	-1.74818500	-3.44660200	2.47340000
C	1.20814700	0.73366500	-0.27520900	H	-1.94713000	-4.07898200	3.34865700
C	1.07323200	0.12580100	1.00584200	H	-1.07716200	-4.00012200	1.81250200
C	0.88833300	0.77808300	2.23874200	H	-1.22904100	-2.54859800	2.81617200
C	0.61050500	-1.26287400	0.99214500	C	-3.84569900	-4.39363100	1.48680100
S	6.04918300	0.12071300	-1.59395500	H	-3.33819000	-5.01210700	0.74385200
O	6.45041800	-1.02585400	-2.42099900	H	-3.91104600	-4.98680500	2.40860400
O	6.21361000	1.50009400	-2.05830500	H	-4.87173300	-4.22402800	1.15311500
C	6.92544800	-0.02861500	-0.03112000	C	-3.91467400	-2.29453100	2.84634100
C	7.03712900	1.08399000	0.80857700	H	-3.39046400	-1.38948200	3.16459000
C	7.46020300	-1.26179900	0.34854400	H	-4.90434900	-2.01351600	2.47555900
C	7.67604300	0.94834500	2.03874200	H	-4.05667200	-2.92328400	3.73524700
H	6.64677500	2.04460800	0.49023500	C	-4.37146100	-1.10304700	-0.07316400
C	8.09808500	-1.37845500	1.58317900	C	-4.53573000	0.30565400	-0.14309300
H	7.39728000	-2.10765600	-0.32749200	C	-5.52279500	-1.90487100	-0.20145700
C	8.21461000	-0.28127800	2.44717100	C	-5.83756800	0.82991800	-0.24959000
H	7.76409700	1.81396700	2.69104500	C	-6.80107500	-1.36695600	-0.33139300
H	8.51806400	-2.33745700	1.87692000	C	-6.96368100	0.01666200	-0.33147600
C	8.93229000	-0.40672400	3.77035400	H	-5.95465300	1.90880800	-0.28625100
H	8.45023200	0.19777900	4.54635000	H	-7.65900000	-2.02741700	-0.42265100
H	8.95900700	-1.44526100	4.11537400	O	2.08172300	-2.78735400	-1.66411700
H	9.97145000	-0.06108200	3.68916800	H	0.66025700	0.20412700	3.13024600
C	3.18523100	-1.69305900	-3.49099400	H	1.04163300	1.84538800	2.34702200
H	2.84231100	-0.67131600	-3.68755500	H	0.83926100	-1.87296900	0.12336900
H	4.25186300	-1.72044500	-3.73690700	H	0.62834900	-1.79857100	1.93999800
H	2.61885100	-2.38832600	-4.11469000	C	-3.42028700	1.31853500	-0.14577100
C	2.10188000	1.84145000	-2.34159700	C	-2.89109900	1.78700100	1.10244600
H	2.36594300	2.90735300	-2.26040600	C	-3.04829300	1.97502800	-1.35195000
H	2.77363000	1.42329400	-3.10310000	C	-1.92486900	2.81149900	1.09316100
H	1.07090800	1.77199600	-2.69889800	C	-2.08510400	2.99004500	-1.27628100
Pd	-1.17039100	-0.19647600	0.76503400	C	-1.50133000	3.42411900	-0.08662700

H	-1.54206900	3.16593200	2.04436300	C	-5.11744800	-0.71744000	1.05438700
H	-1.78288300	3.47684300	-2.20190400	H	-6.02945900	-1.04415000	1.56713200
C	-3.64921500	1.81342900	-2.76744900	H	-4.95336700	-1.37934100	0.19799500
H	-2.78788700	1.91695000	-3.44122100	C	-3.97738500	-0.94311900	2.06041300
C	-4.58554100	3.00891300	-3.06766900	C	-4.63916000	1.00519000	-0.69537700
H	-4.09095700	3.96895600	-2.89064000	H	-4.99644500	1.99675100	-0.98459000
H	-4.91366000	2.98174700	-4.11391700	H	-4.95936000	0.27869200	-1.44894200
H	-5.48132700	2.97151700	-2.43660100	C	-3.12723700	1.01472400	-0.54247500
C	-4.35914400	0.51719500	-3.19325200	C	-2.37029100	-0.01889300	-0.95449100
H	-3.79382100	-0.37986700	-2.94082000	C	-2.67845300	-1.28346600	-1.62706600
H	-5.35601900	0.41914000	-2.75836400	C	-3.42161200	-1.57065700	-2.71251000
H	-4.47775300	0.53439700	-4.28351300	C	-1.64183900	-2.15476800	-0.98291800
H	-5.42424200	-2.98113500	-0.20428400	S	-6.71851000	1.45890600	1.00510800
H	-7.95245900	0.46007700	-0.41147800	O	-7.04257600	1.03636200	2.37383300
C	-0.53940100	4.60606700	-0.09517500	O	-6.52723600	2.86928600	0.65704100
H	-0.19746300	4.72841600	-1.13171900	C	-8.00596400	0.80803800	-0.06664400
C	-1.27789000	5.90158500	0.30245500	C	-8.19502200	1.36229600	-1.33602700
H	-1.64468500	5.84205700	1.33475000	C	-8.79291000	-0.26187700	0.36677500
H	-0.60686000	6.76638100	0.23412200	C	-9.16745500	0.82484800	-2.17650200
H	-2.14023800	6.08602300	-0.34823100	H	-7.60784600	2.22015700	-1.64575600
C	0.70898300	4.39514300	0.77565900	C	-9.76164600	-0.78611600	-0.48778800
H	0.45188400	4.32014300	1.83962600	H	-8.66638800	-0.65304800	1.37045500
H	1.23741200	3.48261800	0.48450900	C	-9.95928900	-0.26027100	-1.77214200
H	1.39205200	5.24607400	0.66631900	H	-9.32119700	1.26191400	-3.16020300
C	-3.59006700	1.45928000	2.43085400	H	-10.38107900	-1.61210400	-0.14681700
H	-4.12593700	0.51532000	2.30662300	C	-10.98976500	-0.85413300	-2.70298000
C	-2.65437200	1.30647500	3.64114400	H	-11.42438700	-0.09233800	-3.35874000
H	-2.16311200	2.25073000	3.90309900	H	-10.54070800	-1.62099100	-3.34825900
H	-3.23374100	0.99163500	4.51765500	H	-11.80407300	-1.33125400	-2.14812300
H	-1.87154300	0.56645200	3.45111200	C	-3.74449100	0.11874600	3.11124200
C	-4.64800800	2.54576200	2.73062100	H	-3.21126500	0.96450800	2.66318800
H	-5.19182700	2.30476200	3.65211900	H	-4.69370200	0.50967500	3.49199600
H	-4.17265100	3.52476500	2.86431400	H	-3.14011500	-0.29981400	3.91939500
H	-5.37972400	2.63596300	1.92185000	C	-2.57088600	2.24272700	0.14029000
				H	-2.58561100	3.10777900	-0.53929000
<b>3-Int3-a</b>				H	-3.17456000	2.52719300	1.01167300
Zero-point correction= 1.040461 (Hartree/Particle)				H	-1.53486500	2.09123800	0.46155800
Thermal correction to Energy= 1.100040				Pd	-0.42939600	-0.52390200	-0.53322700
Thermal correction to Enthalpy= 1.100985				P	1.86044500	-1.25603700	0.08088500
Thermal correction to Gibbs Free Energy= 0.944751				C	2.85095900	-1.76750700	-1.49175800
Sum of electronic and zero-point Energies= -2937.584042				C	1.89324900	-2.67732100	1.41162100
Sum of electronic and thermal Energies= -2937.524463				C	0.77042600	-2.41898700	2.44220300
Sum of electronic and thermal Enthalpies= -2937.523519				H	0.97959800	-1.54973800	3.07052100
Sum of electronic and thermal Free Energies= -2937.679753				H	-0.20889000	-2.28239300	1.97326000
HF(ob97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.255200				H	0.70667800	-3.28930100	3.10828100
N	-5.28075800	0.67259900	0.60727900	C	1.58739400	-4.03228400	0.74153500

H	1.45441900	-4.78515300	1.52891600	C	2.51066600	2.84656400	-1.00533600
H	0.66312300	-4.00496100	0.15617300	H	2.09312400	1.90897500	-1.37772300
H	2.40212900	-4.37928100	0.10102400	H	2.25005400	2.94272300	0.05080800
C	3.22402400	-2.77584000	2.17241300	H	2.00975900	3.66296200	-1.54006900
H	3.16693000	-3.60167400	2.89473700	H	0.46602800	0.18648300	1.79747100
H	4.07340600	-2.97191100	1.51449700	H	2.88194000	3.15002900	3.71102300
H	3.42607100	-1.86160500	2.73721400	C	8.42459100	0.89209100	-2.35566800
C	1.97827900	-2.77802300	-2.27882700	H	8.21639600	1.58771200	-3.18012200
H	2.46344200	-2.95751800	-3.24709100	C	9.70857800	1.37774000	-1.65627100
H	1.87146700	-3.74460800	-1.78686400	H	9.98758900	0.71479400	-0.82858100
H	0.98034200	-2.37495200	-2.47354400	H	10.54773500	1.39862400	-2.36179100
C	4.24553200	-2.37109000	-1.26466800	H	9.58051300	2.38623200	-1.24796800
H	4.20301900	-3.30662200	-0.69840300	C	8.62544100	-0.50611200	-2.97085300
H	4.69857600	-2.60343200	-2.23816400	H	8.85325700	-1.25093500	-2.19893300
H	4.91408600	-1.67952100	-0.74983000	H	7.72592500	-0.83873500	-3.50047200
C	2.95478700	-0.52374000	-2.39577300	H	9.45877800	-0.49902700	-3.68357300
H	1.96721100	-0.08781000	-2.58578800	C	6.13912100	-0.58887900	1.91092000
H	3.61036900	0.23934400	-1.98179900	H	5.12303600	-0.72358400	2.28795200
H	3.37343300	-0.82797800	-3.36425700	C	6.78549600	-1.98248400	1.79856900
C	2.49848800	0.24970500	1.06454700	H	7.85979800	-1.91852800	1.59056800
C	3.70898100	1.00334300	1.14878300	H	6.67424800	-2.52274000	2.74577600
C	1.43235000	0.67356800	1.89679100	H	6.32937400	-2.58637500	1.00800700
C	3.80066300	2.01530800	2.12712900	C	6.90502200	0.25098100	2.95678500
C	1.54238000	1.69275900	2.83938900	H	6.95405600	-0.28087000	3.91486700
C	2.75575100	2.35704700	2.97910700	H	7.93187400	0.44461400	2.62427400
H	4.73194400	2.57051000	2.18628700	H	6.42189300	1.21703100	3.13230200
H	0.68244900	1.95881800	3.44757600				
O	-3.35049200	-1.98718600	2.03085700	<b>3-Ts3-a</b>			
H	-3.38305800	-2.55660600	-3.17048200	Zero-point correction=	1.041620	(Hartree/Particle)	
H	-4.03318000	-0.82241200	-3.20856600	Thermal correction to Energy=	1.099182		
H	-1.92192000	-2.53674200	0.00160900	Thermal correction to Enthalpy=	1.100126		
H	-1.13805400	-2.89687000	-1.60627000	Thermal correction to Gibbs Free Energy=	0.954979		
C	4.91452500	0.95068500	0.24041500	Sum of electronic and zero-point Energies=	-2937.553940		
C	6.05059600	0.16845700	0.58474700	Sum of electronic and thermal Energies=	-2937.496378		
C	4.99070900	1.82338800	-0.87680800	Sum of electronic and thermal Enthalpies=	-2937.495434		
C	7.16762800	0.16614100	-0.25667400	Sum of electronic and thermal Free Energies=	-2937.640581		
C	6.13194400	1.75618200	-1.69491000	HF( $\omega$ b97xd/6-311+G(d,p)/Lanl2dz, SMD[ <i>toluene</i> ])=	-2939.220274		
C	7.21978800	0.92977500	-1.42521000	N	4.28578600	-1.61552900	-0.33287600
H	8.02415200	-0.444464500	0.01357500	C	3.21199800	-1.01180600	0.46106800
H	6.17354700	2.39982600	-2.57217800	H	3.47002800	-1.13167600	1.51878600
C	4.02360400	2.96568900	-1.26047600	H	3.09676400	0.05924700	0.25464300
H	4.13317400	3.06384700	-2.34898600	C	1.85575100	-1.71199100	0.28189200
C	4.54012200	4.29123000	-0.65222000	C	4.40941600	-1.23543500	-1.74571800
H	5.59317100	4.46343300	-0.89827900	H	5.07125100	-1.96655800	-2.21981000
H	3.95575200	5.13708900	-1.03418700	H	4.90785100	-0.25037600	-1.84116400
H	4.44365700	4.28498800	0.43905000	C	3.09756900	-1.16047400	-2.50891700



C	1.89048700	-1.22156100	-1.95932000	H	-1.26136000	-4.05399100	2.38804200
C	0.59087300	-0.94095300	-2.30787800	H	-1.68834300	-4.17044000	0.68058700
C	0.00389800	0.38936400	-2.22129500	H	-0.73347600	-2.78750500	1.26027200
C	-0.56040800	-1.84275300	-2.22137200	C	-3.93143300	-3.66036600	2.31044500
S	5.72189900	-2.00496000	0.45348400	H	-4.17605400	-4.42004100	1.56515700
O	5.35240800	-2.49810400	1.78396700	H	-3.55373500	-4.19222300	3.19377800
O	6.50199200	-2.82107900	-0.48141900	H	-4.85542100	-3.15938600	2.61497100
C	6.62407100	-0.46701200	0.69054600	C	-2.49736700	-1.75822000	3.02790600
C	7.50478200	-0.02096100	-0.29824600	H	-1.64020500	-1.12484600	2.79916300
C	6.41909300	0.28499900	1.85072300	H	-3.34098000	-1.13240900	3.33526600
C	8.17076200	1.19163900	-0.12369300	H	-2.21751600	-2.38384600	3.88568400
H	7.68605200	-0.63428000	-1.17435400	C	-4.32887600	-0.17620500	0.90221500
C	7.09369400	1.49394100	2.00880800	C	-3.98869700	1.20407800	0.76347800
H	5.76355600	-0.09141400	2.62863800	C	-5.51967700	-0.49906500	1.58415500
C	7.97236000	1.97060200	1.02471200	C	-4.87063000	2.15479800	1.31610200
H	8.86463600	1.53304700	-0.88824200	C	-6.37919900	0.46354400	2.10696800
H	6.94382100	2.07259300	2.91732600	H	-5.78296100	-1.53955900	1.71792100
C	8.67707700	3.29602100	1.19392100	C	-6.05032700	1.80852200	1.96884000
H	9.62313900	3.32054700	0.64329800	H	-4.60186700	3.20294700	1.23883700
H	8.05898500	4.12236900	0.81773600	H	-7.28626600	0.16052000	2.62264600
H	8.89093200	3.50491900	2.24751300	O	0.85306500	-1.15604400	0.77458600
C	1.89964100	-3.22960100	0.13885400	H	-0.73164300	0.64521100	-2.98811600
H	0.93290900	-3.60409900	-0.20304300	H	0.62533100	1.21649500	-1.88913800
H	2.68932300	-3.57085100	-0.52939000	H	-1.28650400	-1.76136000	-3.03212900
H	2.09130700	-3.65370600	1.13607000	H	-0.40025500	-2.85994100	-1.87069000
C	3.33336300	-0.97330200	-4.00017500	H	-6.69346000	2.58410400	2.37581900
H	4.01633500	-0.13297000	-4.19485100	C	-2.73331800	1.82280100	0.15817000
H	3.79958300	-1.86388700	-4.44616000	C	-1.59504500	2.01082600	1.01061900
H	2.39411100	-0.78111500	-4.52508600	C	-2.77395700	2.56260200	-1.07163500
Pd	-1.38329300	-0.44964700	-0.83055400	C	-0.51215200	2.78998800	0.57680400
P	-3.24318100	-1.57641800	0.28519700	C	-1.65613400	3.32705400	-1.43320700
C	-2.83878700	-2.67847700	1.84326900	C	-0.51493700	3.46017700	-0.64174200
C	-4.33354900	-2.65221300	-0.92047200	H	0.33363900	2.90551800	1.24552500
C	-4.49840800	-1.86912100	-2.23495200	H	-1.69521600	3.87325900	-2.37407900
H	-5.16384300	-1.01545000	-2.10341900	C	0.61674400	4.38697600	-1.06958800
H	-3.54305300	-1.50904200	-2.62559400	H	0.51229000	4.54260200	-2.15229100
H	-4.95172300	-2.52714300	-2.98841200	C	2.01982400	3.80892300	-0.81796100
C	-3.55573400	-3.94732600	-1.24225800	H	2.21851600	3.67772200	0.25198500
H	-4.07192200	-4.47171200	-2.05699300	H	2.15057000	2.83640900	-1.30414600
H	-2.53579800	-3.73957100	-1.57706700	H	2.78401000	4.48972200	-1.21083900
H	-3.50571200	-4.63647700	-0.39651400	C	0.46646300	5.76486400	-0.39038800
C	-5.75712200	-3.01903800	-0.45180200	H	1.24144200	6.45723000	-0.74082700
H	-6.22127300	-3.64724000	-1.22415400	H	-0.51156800	6.20942000	-0.60530400
H	-5.78284500	-3.58470500	0.48064100	H	0.56113800	5.67502800	0.69857800
H	-6.38699200	-2.13244900	-0.33933200	C	-3.96747300	2.76317200	-2.02584300
C	-1.55391100	-3.46706300	1.50644600	H	-3.50496200	3.05897400	-2.97641000

C	-4.84508300	3.96507900	-1.60554700	C	-7.13239800	-0.78925700	0.37588700
H	-4.23438400	4.84114000	-1.36131400	C	-5.76785200	1.14303800	0.89066400
H	-5.51556700	4.23825800	-2.42953200	C	-7.69742600	-0.71630600	1.64530400
H	-5.46919800	3.72846600	-0.73924900	H	-7.45054400	-1.54349500	-0.33618200
C	-4.83343100	1.54889400	-2.35750200	C	-6.34057400	1.20081800	2.15402400
H	-4.21737700	0.74262500	-2.75800200	H	-5.03319700	1.87786900	0.57792300
H	-5.38097600	1.17305400	-1.48951200	C	-7.30723900	0.27094700	2.55236000
H	-5.57027700	1.82311800	-3.12271400	H	-8.45907400	-1.43652000	1.93224600
C	-1.59678800	1.60379500	2.48528400	H	-6.03727800	1.98518800	2.84277900
C	-0.24583700	1.06435900	2.99255800	C	-7.89896100	0.33076800	3.93766500
H	-0.37690000	0.63328700	3.99255900	H	-8.83789000	-0.22736100	3.99655700
H	0.17479000	0.30294800	2.32915500	H	-7.20881800	-0.10034500	4.67273300
H	0.49308500	1.86879600	3.09492900	H	-8.09703700	1.36383700	4.24095300
C	-2.03267200	2.80587600	3.35514900	C	-1.22617900	-0.72754900	-2.23358800
H	-1.32796000	3.63923500	3.24898500	H	-0.31032200	-1.26639200	-2.49294000
H	-3.02898500	3.16972300	3.08595200	H	-2.02530200	-1.05120500	-2.90700900
H	-2.05424500	2.51547300	4.41259500	H	-1.03540000	0.34093200	-2.38505900
H	-2.34746500	0.82643900	2.62315700	C	-3.23115400	-4.51505600	-0.39087900
<b>3-Int4</b>				H	-3.78298500	-4.68609100	0.54332100
Zero-point correction= 1.044749 (Hartree/Particle)				H	-3.85618500	-4.90728800	-1.20339000
Thermal correction to Energy= 1.102242				H	-2.31143300	-5.10107900	-0.34750700
Thermal correction to Enthalpy= 1.103186				Pd	1.26634900	-0.81220500	0.09702800
Thermal correction to Gibbs Free Energy= 0.955080				P	3.58557700	-1.15551400	0.12576100
Sum of electronic and zero-point Energies= -2937.608786				C	4.23227100	-1.74943600	-1.57469500
Sum of electronic and thermal Energies= -2937.551293				C	4.37403000	-2.29972900	1.47184200
Sum of electronic and thermal Enthalpies= -2937.550349				C	4.45946700	-1.58024500	2.82746700
Sum of electronic and thermal Free Energies= -2937.698454				H	5.03804100	-0.65395400	2.78521400
HF(ωb97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])= -2939.281386				H	3.47181300	-1.35951900	3.22845100
N	-3.98794000	-0.88446800	-1.28373800	H	4.95630100	-2.25071000	3.53940200
C	-2.94423500	-0.25213200	-0.48105200	C	3.42766100	-3.49771600	1.67161400
H	-2.87219400	0.79330300	-0.77665100	H	3.81465100	-4.12165700	2.48695500
H	-3.15729100	-0.31173200	0.59669400	H	2.42357500	-3.16311400	1.94808600
C	-1.59707400	-0.94051000	-0.75173200	H	3.34985900	-4.13208500	0.78457700
C	-4.19621200	-2.31376400	-1.05552900	C	5.78424200	-2.84327500	1.17228100
H	-4.58873400	-2.75060400	-1.97910600	H	6.06188500	-3.52270600	1.98754600
H	-4.96298100	-2.48070900	-0.27584300	H	5.84896600	-3.41598200	0.24751700
C	-2.95358000	-3.04881300	-0.61092900	H	6.54499400	-2.05915200	1.14712000
C	-1.77800800	-2.42902300	-0.41754600	C	3.97264700	-3.25682300	-1.75166300
C	-0.58426500	-3.06755600	0.18693900	H	4.25298700	-3.53409000	-2.77522000
C	-0.67155700	-3.86393800	1.26455800	H	4.55509000	-3.88832400	-1.07918400
C	0.74791600	-2.74156500	-0.38976700	H	2.91610500	-3.50328300	-1.62701100
S	-5.36004400	-0.00089900	-1.57698400	C	5.70797000	-1.43257200	-1.86347200
O	-4.93989700	1.33460800	-1.97005900	H	6.40385800	-1.91778700	-1.17664500
O	-6.20863600	-0.81542000	-2.43260600	H	5.94742400	-1.78744300	-2.87369800
C	-6.16642400	0.14165300	0.00649600	H	5.89624700	-0.35518700	-1.84288300
				C	3.40177000	-1.02879400	-2.64407900

H	2.32653000	-1.14976700	-2.48431600	C	2.67616000	2.36949600	-2.18064900
H	3.62692200	0.03556600	-2.65968700	C	2.12330800	1.88734900	-3.53063500
H	3.65415800	-1.43297400	-3.63238800	H	2.94073600	1.75144700	-4.24746100
C	4.31267400	0.52700300	0.42218500	H	1.58297200	0.94144500	-3.43460700
C	3.51733100	1.69280200	0.54902700	H	1.43586400	2.62107700	-3.96513300
C	5.69748100	0.64347400	0.62014300	C	3.15009000	3.82690000	-2.31032300
C	4.15811100	2.89525600	0.88538100	H	2.30168700	4.48952200	-2.51597300
C	6.30855300	1.84378900	0.95332100	H	3.63972900	4.17521600	-1.39663000
H	6.32151500	-0.23462500	0.51814700	H	3.86517300	3.92189300	-3.13569000
C	5.52647300	2.98257200	1.09657500	H	3.55703600	1.77352400	-1.92913900
H	3.54664300	3.78834100	0.97081600				
H	7.38324800	1.88351900	1.10114300				
O	-0.68487900	-0.34562000	0.09673200	<b>3-Ts4</b>			
H	0.21532000	-4.31864900	1.70037200	Zero-point correction=	1.042441	(Hartree/Particle)	
H	-1.61745000	-4.06390200	1.75695900	Thermal correction to Energy=	1.100043		
H	1.50003000	-3.43637200	-0.02554200	Thermal correction to Enthalpy=	1.100987		
H	0.74816800	-2.74409000	-1.48435700	Thermal correction to Gibbs Free Energy=	0.953972		
H	5.97590000	3.93530600	1.35972500	Sum of electronic and zero-point Energies=	-2937.584519		
C	2.03637900	1.85239600	0.27129100	Sum of electronic and thermal Energies=	-2937.526917		
C	1.66693700	2.24062500	-1.04750600	Sum of electronic and thermal Enthalpies=	-2937.525973		
C	1.07485100	2.01129800	1.30914800	Sum of electronic and thermal Free Energies=	-2937.672988		
C	0.37171400	2.67706600	-1.30964400	HF( $\omega$ b97xd/6-311+G(d,p)/Lanl2dz, SMD[ <i>toluene</i> ])=	-2939.249158		
C	-0.20544100	2.45037600	0.97590400	N	-4.35952300	-1.73664300	0.20805400
C	-0.58636900	2.79444600	-0.31241700	C	-3.17924800	-0.99735300	-0.25530100
H	0.11739700	2.96652400	-2.32305200	H	-3.06614700	-1.15260100	-1.32869600
H	-0.94000900	2.53803300	1.77356000	H	-3.26566700	0.07960100	-0.05015600
C	-1.96972800	3.36940600	-0.56220100	C	-1.94874100	-1.55004700	0.49260200
H	-2.67827300	2.76284600	0.01785200	C	-4.69833900	-1.54210200	1.62105600
C	-2.41130500	3.33604500	-2.02597100	H	-5.36614800	-2.35559900	1.92276100
H	-1.81815600	4.03037100	-2.63390500	H	-5.25498400	-0.59766800	1.77496800
H	-2.32513700	2.33463500	-2.45760000	C	-3.47476600	-1.51243500	2.51259900
H	-3.46106500	3.62914500	-2.10780200	C	-2.23508700	-1.54462900	1.99400800
C	-2.03995800	4.80522000	-0.01570800	C	-0.94549900	-1.43135500	2.70077400
H	-3.04684400	5.21742500	-0.14563700	C	-0.58318600	-2.12606800	3.79509100
H	-1.78681000	4.84369700	1.04914200	C	-0.00889100	-0.49677900	2.03722900
H	-1.33514300	5.45157100	-0.55219100	S	-5.65440800	-1.91732200	-0.85597400
C	1.30475400	1.86656500	2.81240800	O	-5.07689800	-2.25814100	-2.15741900
H	0.30749200	1.69073200	3.23250500	O	-6.61470100	-2.79085400	-0.17600300
C	1.81834800	3.17686100	3.43181900	C	-6.42043900	-0.29969800	-1.01447300
H	1.20975000	4.03041600	3.11506800	C	-7.46773100	0.05712400	-0.16145600
H	1.78073200	3.11576600	4.52562600	C	-5.94678300	0.59863400	-1.97546300
H	2.85742700	3.36912900	3.14643300	C	-8.03258100	1.32769700	-0.26919700
C	2.16218200	0.68990300	3.24523600	H	-7.85136300	-0.66495000	0.55139500
H	1.80299900	-0.23021900	2.77045900	C	-6.52304600	1.86350700	-2.06821700
H	3.21016300	0.83942500	2.97933500	H	-5.15917900	0.29552100	-2.65699800
H	2.10971100	0.55987900	4.33258600	C	-7.56744300	2.25144300	-1.21520300
				H	-8.85571200	1.60195300	0.38618400

H	-6.16288500	2.55849100	-2.82300400	H	6.10902000	-1.18826700	-1.40201900
C	-8.16538700	3.63535200	-1.30818600	C	6.33379200	2.16858900	-1.28392200
H	-8.20301200	3.98669300	-2.34487900	H	4.75418500	3.47045700	-0.65186400
H	-9.18179700	3.66168300	-0.90259100	H	7.70178200	0.59698300	-1.85972100
H	-7.56726600	4.36139600	-0.74139900	O	-0.90929500	-0.60937200	0.29503900
C	-1.58849900	-2.95551200	-0.01060500	H	0.40329100	-2.01106400	4.23735800
H	-0.75163900	-3.36266400	0.56513900	H	-1.25813000	-2.82555300	4.27824900
H	-2.44534800	-3.63162200	0.07537900	H	-0.26797600	0.55581600	2.02607400
H	-1.28517000	-2.90067900	-1.06191500	H	1.03448900	-0.65570000	2.30707600
C	-3.80281500	-1.38836400	3.97904900	H	7.02304900	2.98335200	-1.48922100
H	-2.93821300	-1.06516600	4.56369200	C	2.79106900	1.96296700	-0.01519400
H	-4.61584200	-0.66631000	4.13364300	C	2.65596400	2.32236600	1.34845300
H	-4.15114300	-2.34498300	4.39326800	C	1.76981100	2.32322400	-0.93111700
Pd	1.12228400	-0.98932100	-0.09467300	C	1.48316100	2.96431800	1.76892200
P	3.34171100	-1.40416500	-0.52056200	C	0.62555300	2.97275900	-0.45836900
C	3.44308900	-2.37541500	-2.21630200	C	0.45070900	3.29316900	0.88978300
C	4.19728300	-2.46469100	0.86156600	H	1.37857800	3.23877300	2.81618400
C	3.96580900	-1.71271700	2.18547400	H	-0.14963300	3.24304200	-1.16966800
H	4.44161100	-0.72809600	2.18247700	C	-0.79126700	4.02283900	1.38603500
H	2.90006400	-1.58119600	2.38789400	H	-0.74375700	4.02835000	2.48410300
H	4.40022900	-2.28965500	3.01312800	C	-2.09655100	3.31188700	0.98322600
C	3.46077100	-3.81748300	0.95035800	H	-2.96134300	3.80961200	1.43883500
H	3.77749900	-4.34128600	1.86237600	H	-2.24079800	3.32771300	-0.10345300
H	2.37524900	-3.67715300	0.99804700	H	-2.09467300	2.26290100	1.29813200
H	3.68639300	-4.47451900	0.10527000	C	-0.80110000	5.49224000	0.91921700
C	5.71376000	-2.71283900	0.74049000	H	-1.67165400	6.02392200	1.32285700
H	6.03161400	-3.34573500	1.58033200	H	0.10263000	6.01801600	1.24678600
H	5.99757600	-3.23135900	-0.17770100	H	-0.84628400	5.55645300	-0.17469800
H	6.28496900	-1.78245900	0.80344200	C	1.91443600	2.10881400	-2.43707300
C	2.19704800	-3.28944300	-2.28500500	H	2.75463900	1.42886500	-2.59959200
H	2.16653200	-3.77859900	-3.26857600	C	2.26171400	3.43468600	-3.14605200
H	2.20886600	-4.07446400	-1.52424600	H	2.39172100	3.27331000	-4.22337400
H	1.27450000	-2.71506600	-2.15383500	H	1.46360300	4.17460600	-3.01026900
C	4.67963500	-3.25734900	-2.48238100	H	3.18899400	3.86727300	-2.75467800
H	4.79012000	-4.05989600	-1.74842800	C	0.67092200	1.46355500	-3.07624500
H	4.55755600	-3.73680700	-3.46318900	H	-0.19431300	2.13669700	-3.05833000
H	5.61518900	-2.69380000	-2.52474600	H	0.86955800	1.21985800	-4.12728200
C	3.32328900	-1.34264300	-3.35462600	H	0.39152600	0.54455500	-2.54914600
H	3.24176500	-1.87407700	-4.31229300	C	3.77685800	2.11702800	2.36964700
H	2.42610300	-0.72780100	-3.24207700	H	4.49920700	1.41529900	1.94100300
H	4.14568800	1.27514300	4.34273400	C	4.53000900	3.43857100	2.63428000
C	4.48819800	0.07264900	-0.74949400	H	3.85378900	4.19636200	3.04791200
C	4.11131600	1.42846600	-0.52694800	H	5.34271800	3.28206800	3.35451000
C	5.79371700	-0.16965000	-1.22611000	H	4.96629000	3.84434600	1.71635700
C	5.05427300	2.43870100	-0.80990600	C	3.28887200	1.52457700	3.70539100
C	6.70993300	0.84457200	-1.49097400	H	2.66821800	2.23519000	4.26312300

H	2.70089200	0.61422600	3.55521800	H	-0.53456700	1.63482900	1.59979400
H	4.19244900	-0.68090000	-3.41278700	C	-4.56595200	4.24117600	-1.73098200
<b>3a+PdL</b>				H	-4.03863500	4.42674800	-2.67178100
Zero-point correction= 1.044112 (Hartree/Particle)				H	-5.57892800	3.89267700	-1.96566000
Thermal correction to Energy= 1.102730				H	-4.67202500	5.20531100	-1.21462000
Thermal correction to Enthalpy= 1.103675				Pd	0.48810100	-0.36221300	-0.62555500
Thermal correction to Gibbs Free Energy= 0.950154				P	1.52851700	-2.32878200	-0.33456300
Sum of electronic and zero-point Energies= -2937.646110				C	1.50410900	-3.38289000	-1.98604800
Sum of electronic and thermal Energies= -2937.587491				C	0.67421200	-3.36159100	1.07516100
Sum of electronic and thermal Enthalpies= -2937.586547				C	0.58202600	-2.41875900	2.29045800
Sum of electronic and thermal Free Energies= -2937.740068				H	1.57238900	-2.16833400	2.68131300
HF(ob97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.315106				H	0.07049200	-1.48708900	2.03044300
N	-3.99590100	1.42344700	0.81209900	H	0.02196100	-2.91291800	3.09627100
C	-2.82796900	0.80318800	0.17477400	C	-0.76506300	-3.68621400	0.62319900
H	-2.39756300	0.06753000	0.85502600	H	-1.33326000	-4.06915400	1.48199700
H	-3.08492900	0.31067100	-0.77460500	H	-1.27023400	-2.78863600	0.24929700
C	-1.83424600	1.93492900	-0.09699700	H	-0.79909400	-4.45268200	-0.15725200
C	-4.73881200	2.38044600	-0.01507100	C	1.36342300	-4.65655000	1.54715100
H	-5.33860000	3.00812800	0.65234600	H	0.74533400	-5.11689500	2.33036800
H	-5.44856900	1.86350000	-0.68871400	H	1.48335200	-5.39921700	0.75454000
C	-3.83674300	3.23632000	-0.87842000	H	2.34482100	-4.45827100	1.98684600
C	-2.50538500	3.03951200	-0.89505300	C	0.16960400	-3.06301600	-2.69896400
C	-1.46429800	3.60580300	-1.76547000	H	0.16717100	-3.54173800	-3.68871800
C	-1.38944600	4.80744900	-2.35457400	H	-0.69830500	-3.43561000	-2.14773100
C	-0.37745800	2.54267600	-1.85334900	H	0.04199700	-1.98321300	-2.82470100
S	-4.90814000	0.48276100	1.87689400	C	1.62056000	-4.91691500	-1.87963300
O	-3.94803600	-0.23847900	2.71341800	H	0.81068400	-5.36153700	-1.29532200
O	-5.91400100	1.38584100	2.44165100	H	1.55651500	-5.34283800	-2.89065300
C	-5.77060800	-0.72854500	0.87116900	H	2.57328800	-5.25081900	-1.46034500
C	-7.05440700	-0.44581000	0.39853900	C	2.64288600	-2.86845400	-2.88806700
C	-5.14047300	-1.93478800	0.54856400	H	2.56986900	-1.78811700	-3.03934500
C	-7.70195200	-1.37681000	-0.41346400	H	3.63305800	-3.09583600	-2.48212600
H	-7.54573300	0.47586800	0.69153700	H	2.56650400	-3.34803000	-3.87358000
C	-5.80286900	-2.85157700	-0.26429500	C	3.34847300	-2.28923700	0.15746500
H	-4.15941000	-2.16011300	0.95316200	C	4.07996700	-1.09656400	0.42452000
C	-7.08754000	-2.58675000	-0.76366500	C	4.05301500	-3.51001500	0.21921900
H	-8.70574600	-1.16319000	-0.77242000	C	5.45556000	-1.20875900	0.72055100
H	-5.31794600	-3.79391400	-0.50732100	C	5.40990100	-3.59638200	0.51861900
C	-7.78288200	-3.57970100	-1.66449600	H	3.52352100	-4.43180000	0.02433700
H	-8.86551300	-3.41947100	-1.67851900	C	6.12315500	-2.42796600	0.77013500
H	-7.42357200	-3.49133200	-2.69837200	H	6.00867500	-0.29386400	0.91286600
H	-7.59506100	-4.61034800	-1.34452700	H	5.89855400	-4.56675300	0.54969000
C	-1.16161400	2.43174500	1.18614600	O	-0.82964300	1.45134500	-1.02730200
H	-0.52580600	3.29997100	0.98447000	H	-0.53780300	5.07636100	-2.97472000
H	-1.91627400	2.71607100	1.92468500	H	-2.14952700	5.56872100	-2.22144900
				H	-0.25015800	2.15102000	-2.86769200

H	0.59306700	2.90190600	-1.49372900	Sum of electronic and zero-point Energies=	-2937.532226
H	7.18473100	-2.45989600	1.00097000	Sum of electronic and thermal Energies=	-2937.4703753
C	3.59848600	0.34127800	0.43940500	Sum of electronic and thermal Enthalpies=	-2937.469431
C	3.72582400	1.14126100	-0.72428800	Sum of electronic and thermal Free Energies=	-2937.639441
C	3.29848500	0.96731800	1.67433400	HF( $\omega$ b97xd/6-311+G(d,p)/Lanl2dz, SMD[ <i>toluene</i> ])=	-2939.206013
C	3.53502100	2.52541400	-0.63208900	N	7.21945000 -0.82069100 0.32959700
C	3.10674400	2.35461500	1.70822200	C	6.25881300 -0.23114100 1.25213900
C	3.23084300	3.15995800	0.57566800	H	6.79760000 0.22653600 2.08893000
H	3.66665000	3.12737300	-1.52798400	H	5.66927500 0.55059100 0.75919500
H	2.88848100	2.83137200	2.66111400	C	5.29076000 -1.23169100 1.88957500
C	3.13828800	4.67725200	0.69447300	C	6.79701900 -0.88978600 -1.07572100
H	2.73168200	4.89698400	1.69136100	H	7.68531500 -1.06238500 -1.68781800
C	2.19626800	5.32208700	-0.33683400	H	6.34374200 0.06444500 -1.37287100
H	2.54905100	5.15854400	-1.36240700	C	5.82574400 -2.03579600 -1.27053500
H	1.17941000	4.92134200	-0.26264400	C	4.53390500 -1.80860300 -1.23937800
H	2.14136300	6.40606900	-0.17970800	C	3.27346400 -1.55626400 -1.14865700
C	4.54084000	5.31571400	0.62012900	C	2.12865500 -1.40094700 -0.24043100
H	4.48499200	6.40080700	0.77180500	C	2.01290400 -1.19051500 -1.80789500
H	5.20569500	4.89705200	1.38345700	H	2.14924200 -0.53875700 0.42402000
H	5.00213800	5.13564000	-0.35852800	H	1.71377900 -2.31016300 0.18941900
C	4.15541300	0.55818000	-2.06944600	H	1.51390100 -1.95870900 -2.39515600
H	4.14043500	-0.53078900	-1.98134900	H	1.93455500 -0.17811700 -2.20221800
C	5.60209600	0.96479900	-2.41683500	S	8.84283000 -0.64051500 0.66289000
H	5.91209500	0.51271500	-3.36719200	O	8.97751700 -0.79864000 2.10276300
H	5.69719200	2.05291500	-2.51607300	O	9.55048500 -1.49600800 -0.27472700
H	6.30388100	0.63742700	-1.64193000	C	9.22985100 1.05069300 0.26398700
C	3.19183100	0.93598700	-3.20943900	C	9.56754700 1.38615700 -1.04555600
H	3.19822000	2.01444800	-3.40912100	C	9.13185600 2.02985500 1.24889900
H	3.48289400	0.43109100	-4.13901900	C	9.79426500 2.71842300 -1.36647600
H	2.16668700	0.63886300	-2.95829500	H	9.67803200 0.60839700 -1.79384400
C	3.25690100	0.20126700	2.99657900	C	9.36255600 3.35808800 0.90958900
H	3.24545800	-0.86748000	2.76375700	H	8.90626800 1.74852900 2.27202400
C	1.99765300	0.50942400	3.82816700	C	9.68827100 3.72317400 -0.39933700
H	1.94941400	-0.15171800	4.70174700	H	10.06778900 2.98239200 -2.38455400
H	1.99872000	1.53996100	4.20171600	H	9.29630100 4.12318000 1.67833800
H	1.08610200	0.36489300	3.24110400	C	9.90677000 5.16838000 -0.76685700
C	4.52456300	0.46914200	3.83508300	H	10.66825300 5.27076800 -1.54593900
H	4.61011600	1.53255600	4.08931700	H	8.98075400 5.61304100 -1.15064900
H	4.49277000	-0.09925900	4.77290600	H	10.22230300 5.75780300 0.09891500
H	5.43185100	0.17919000	3.29523400	C	5.83359200 -2.59548900 2.23055600
				H	5.87090100 -3.20517700 1.32192900
				H	6.85669500 -2.52399300 2.61316300
				H	5.17588100 -3.07633100 2.95677500
				C	6.43918200 -3.40573400 -1.41550500
				H	6.94791000 -3.49942100 -2.38304300
				H	7.19944200 -3.55877500 -0.63998600
<b>3-Int1'</b>					
Zero-point correction=	1.036507	(Hartree/Particle)			
Thermal correction to Energy=	1.098358				
Thermal correction to Enthalpy=	1.099302				
Thermal correction to Gibbs Free Energy=	0.929291				

H	5.68758400	-4.19535200	-1.34181400	H	-7.39709000	1.69450400	2.68581400
Pd	-0.17003600	-0.61821100	-0.73688100	H	-8.33072500	1.15132600	-1.43718500
P	-2.33297500	0.13045900	-0.48650000	C	-8.94007600	2.73089500	0.70489900
C	-2.93997400	0.84452700	-2.14019800	H	-8.94368900	3.08769400	1.74321500
C	-2.34648800	1.44780500	0.88410500	C	-8.53740700	3.90983700	-0.19153900
C	-2.05788300	0.67122800	2.18107900	H	-7.53446700	4.26945200	0.06055000
H	-2.85408900	-0.03529600	2.42556900	H	-8.53147900	3.61424100	-1.24725000
H	-1.12161000	0.10826600	2.09655600	H	-9.24200400	4.74166200	-0.07906500
H	-1.96230300	1.37635900	3.01648000	C	-10.35785300	2.24491600	0.37650700
C	-1.15538600	2.39299100	0.63791000	H	-10.64838400	1.41195600	1.02486500
H	-1.04180100	3.05187500	1.50884000	H	-11.08355700	3.05517500	0.50947300
H	-0.22218700	1.83709500	0.49438500	H	-10.42862900	1.90258700	-0.66244300
H	-1.31384900	3.03238700	-0.23596900	C	-6.74525000	-0.95940700	-1.93803600
C	-3.59771200	2.31710600	1.04910400	H	-5.80157800	-1.50998400	-1.96328400
H	-3.52174300	2.87513100	1.99172800	C	-7.87195700	-2.00180300	-1.82940800
H	-3.68098100	3.05930800	0.25327700	H	-8.84905900	-1.50668500	-1.78320900
H	-4.52178700	1.74256800	1.06928400	H	-7.86529100	-2.66466500	-2.70222500
C	-1.76649800	1.60007900	-2.79249200	H	-7.76593000	-2.61941700	-0.93338400
H	-2.07489500	1.93872900	-3.79071500	C	-6.88703500	-0.19765500	-3.26015300
H	-1.47106900	2.48434900	-2.22114400	H	-6.14527200	0.59645500	-3.35822600
H	-0.88760500	0.95484000	-2.89461000	H	-6.75576800	-0.88968700	-4.09925100
C	-4.13904500	1.79663100	-2.08942700	H	-7.88159600	0.25102100	-3.36411000
H	-3.85172500	2.77114800	-1.68762300	C	-5.57049400	-0.27027800	2.95658600
H	-4.50072700	1.97407700	-3.11074400	H	-4.66305600	-0.82187200	2.69629200
H	-4.96944600	1.41475000	-1.49320700	C	-5.18425400	0.83769500	3.94323600
C	-3.24596200	-0.36843700	-3.03401300	H	-6.06807700	1.32196400	4.37394700
H	-2.37983000	-1.03784700	-3.09083000	H	-4.61300100	0.40872600	4.77373400
H	-4.09502500	-0.94862900	-2.66994800	H	-4.57010800	1.60837700	3.47349100
H	-3.48067100	-0.02361800	-4.04912500	C	-6.52058700	-1.26265900	3.64832500
C	-3.48881700	-1.30840500	-0.00801000	H	-6.06765200	-1.64679900	4.56944400
C	-4.86833500	-1.43954200	0.32171700	H	-7.46456600	-0.77080800	3.91110400
C	-2.73655900	-2.50047200	-0.01524300	H	-6.75260500	-2.11488400	3.00365300
C	-5.37635100	-2.71582400	0.61243700				
C	-3.26132100	-3.75364300	0.27141300	<b>3-Ts1'</b>			
H	-1.67907900	-2.42494900	-0.26126000	Zero-point correction=	1.036522	(Hartree/Particle)	
C	-4.60389500	-3.86707700	0.59189200	Thermal correction to Energy=	1.097045		
H	-6.42960300	-2.79097900	0.86489700	Thermal correction to Enthalpy=	1.097990		
H	-2.61569500	-4.62629400	0.24397800	Thermal correction to Gibbs Free Energy=	0.934402		
O	4.16382400	-0.87601200	2.15878600	Sum of electronic and zero-point Energies=	-2937.527589		
H	-5.05000900	-4.82953400	0.82459200	Sum of electronic and thermal Energies=	-2937.467066		
C	-5.91824900	-0.36489300	0.41747500	Sum of electronic and thermal Enthalpies=	-2937.466122		
C	-6.20938900	0.22544000	1.66425600	Sum of electronic and thermal Free Energies=	-2937.629710		
C	-6.75261400	-0.08660000	-0.68762100	HF( $\omega$ b97xd/6-311+G(d,p)/Lanl2dz, SMD[ <i>toluene</i> ])=	-2939.200523		
C	-7.19091600	1.21612800	1.73147800	N	-7.21782000	-0.83445200	-0.03478600
C	-7.71251600	0.91736500	-0.57425400	C	-6.47912800	-0.55561900	-1.26835700
C	-7.92166200	1.60968000	0.61638400	H	-7.19631300	-0.38290700	-2.07828300

H	-5.85880300	0.34238200	-1.16192900	H	2.61103800	-2.12796700	-3.34459000
C	-5.57568800	-1.70021200	-1.75851500	C	1.22894500	0.12306800	-2.87734800
C	-6.53343800	-0.47936600	1.22846700	H	1.29311100	-0.19410100	-3.92729900
H	-7.29458600	-0.40885300	2.00933800	H	0.33450400	-0.32582800	-2.43348200
H	-6.05154300	0.50024000	1.11799700	H	1.10050900	1.20865400	-2.87109000
C	-5.50976300	-1.53284200	1.62660400	C	3.71864100	0.34094100	-2.82135400
C	-4.23112400	-1.33534700	1.38670700	H	3.86210900	-0.09561500	-3.81905800
C	-2.98005100	-1.13029400	1.11484900	H	3.55226700	1.41228100	-2.96498100
C	-2.00487900	-1.32523500	0.02647800	H	4.64641100	0.21779700	-2.25982600
C	-1.75359200	-0.52901900	1.66978300	C	1.37594700	2.68132700	-0.46197200
H	-2.18319000	-0.74736300	-0.88056000	H	1.37834400	3.69876700	-0.04770800
H	-1.65943600	-2.34871400	-0.12648900	H	1.45672800	2.77478800	-1.54916100
H	-1.26266800	-1.08466300	2.47024700	H	0.41441100	2.21223000	-0.22464800
H	-1.75756900	0.55623300	1.78423600	C	3.86338500	2.56692600	-0.31758500
S	-8.90564600	-0.76237600	-0.08314600	H	3.90261100	2.67478500	-1.40371200
O	-9.28833700	-1.33615300	-1.37800000	H	3.91224400	3.58028600	0.10529600
O	-9.36983900	-1.32649500	1.18678600	H	4.75668500	2.03031000	-0.00230000
C	-9.37444000	0.97109600	-0.10720000	C	2.43126200	1.98183400	1.68253300
C	-9.55372900	1.65561800	1.09849400	H	1.46466600	1.58764900	2.01496400
C	-9.52790200	1.62952000	-1.32993800	H	3.21673700	1.42469800	2.19903700
C	-9.87236300	3.01146600	1.07082700	H	2.50014200	3.03194100	1.99581600
H	-9.46845300	1.12527700	2.04087200	C	3.54296600	-1.07802400	0.69016600
C	-9.84691600	2.98650900	-1.33753700	C	4.96730200	-1.14102800	0.85174100
H	-9.42374200	1.07907600	-2.25870400	C	2.79005900	-2.07046700	1.36205900
C	-10.02171400	3.69907500	-0.14292100	C	5.49908600	-2.16637500	1.66257200
H	-10.01518100	3.54364700	2.00820300	C	3.34585200	-3.07846300	2.14544100
H	-9.96947700	3.49869000	-2.28867300	H	1.70706100	-2.03590100	1.25949900
C	-10.39845700	5.16146800	-0.15998900	C	4.72410600	-3.12772500	2.30304700
H	-11.48662900	5.28733800	-0.08365500	H	6.57664700	-2.19534500	1.78926900
H	-9.95014900	5.70070600	0.68122200	H	2.69792100	-3.80589500	2.62719300
H	-10.07769700	5.64762700	-1.08680900	O	-4.50298200	-1.43385800	-2.26613800
C	-6.11934400	-3.10817300	-1.66431100	H	5.19726300	-3.89274500	2.91318200
H	-6.04716300	-3.46053200	-0.62941200	C	6.05594200	-0.24071900	0.29846700
H	-7.17989800	-3.13856100	-1.93638000	C	6.73937500	-0.58094700	-0.89932000
H	-5.53223600	-3.76715100	-2.30764900	C	6.56048500	0.82390200	1.09551300
C	-6.05609800	-2.78302800	2.28301900	C	7.78353300	0.24236800	-1.34320400
H	-6.47155300	-2.55003000	3.27310300	C	7.61589000	1.60321500	0.60818200
H	-6.87790700	-3.20281600	1.69005800	C	8.22389000	1.35281600	-0.62398400
H	-5.28095900	-3.54383500	2.40668600	H	8.28829200	-0.00322900	-2.27354200
Pd	0.03733800	-0.51323600	0.35188400	H	7.98155200	2.42454700	1.21783000
P	2.29514400	0.03400700	-0.26363300	C	9.35163800	2.22907700	-1.15298000
C	2.56041300	1.89597200	0.14553000	H	9.66305100	1.80506100	-2.11756900
C	2.51194800	-0.32682100	-2.14290100	C	8.87686000	3.67126700	-1.41498800
C	2.59495500	-1.86234000	-2.27943900	H	8.02676700	3.68881500	-2.10577600
H	3.49095400	-2.27956500	-1.81463500	H	8.56149000	4.16034800	-0.48556500
H	1.72355400	-2.34652200	-1.82456200	H	9.68449000	4.27176200	-1.85079600



C	10.58121500	2.21258000	-0.22480800	C	1.94473100	-3.25328900	0.60672500
H	10.94297500	1.19098400	-0.06436200	C	1.46247100	-3.01302200	-1.61503700
H	11.39935200	2.80110200	-0.65718100	H	2.30684300	-2.69416900	1.47317300
H	10.34659000	2.64189500	0.75654200	H	1.81080500	-4.32022700	0.82055500
C	6.06597900	1.08774400	2.52185000	H	1.16665800	-4.01169000	-1.95119500
H	5.09578500	0.59653500	2.64022100	H	1.43158700	-2.27376800	-2.41807600
C	7.02720500	0.44803700	3.54841200	S	7.34390400	0.84917700	0.09346200
H	8.02945700	0.88555300	3.46645500	O	7.93742800	0.88115500	1.43546200
H	6.66554600	0.62026000	4.56955800	O	8.11731600	0.45937600	-1.08811700
H	7.11914300	-0.63191500	3.40173200	C	6.66676400	2.48400700	-0.22279600
C	5.88244500	2.57908600	2.86269000	C	6.41725600	2.88704000	-1.53788500
H	5.26033800	3.09709000	2.12838300	C	6.37753700	3.33326300	0.84830000
H	5.40308000	2.67851500	3.84359700	C	5.85778100	4.14132000	-1.77201100
H	6.84285200	3.10428300	2.92104500	H	6.68785800	2.23827900	-2.36403600
C	6.47885300	-1.88953600	-1.65340100	C	5.81829400	4.58487800	0.59474500
H	5.45920600	-2.21308800	-1.42717800	H	6.61983600	3.02772900	1.86041600
C	6.61584500	-1.78884100	-3.18504300	C	5.54183000	5.00599500	-0.71351400
H	7.66240300	-1.67366800	-3.49045600	H	5.67395500	4.45931000	-2.79546700
H	6.24889100	-2.71197500	-3.64840200	H	5.60358400	5.25011200	1.42756900
H	6.05041000	-0.95271800	-3.60297600	C	4.90998800	6.35221000	-0.97748400
C	7.43263900	-2.99667700	-1.14864900	H	5.24432700	6.77185400	-1.93209600
H	7.24638900	-3.93355500	-1.68798400	H	3.81565100	6.27106400	-1.02322400
H	8.47768400	-2.71083800	-1.31847800	H	5.15045900	7.07020200	-0.18674000
H	7.30492600	-3.19318000	-0.08131600	C	6.55324200	-2.26557300	2.32080400
<b>3-Int2'</b>				H	6.69184900	-2.81758100	1.38458600
Zero-point correction= 1.039925 (Hartree/Particle)				H	7.41168700	-1.59300000	2.42289200
Thermal correction to Energy= 1.099245				H	6.50860900	-2.97240300	3.15211500
Thermal correction to Enthalpy= 1.100190				C	6.25737200	-2.94571600	-1.53590000
Thermal correction to Gibbs Free Energy= 0.948625				H	6.55968100	-2.75140900	-2.57479400
Sum of electronic and zero-point Energies= -2937.555703				H	7.12916100	-2.71425700	-0.91117500
Sum of electronic and thermal Energies= -2937.496383				H	6.02440800	-4.00946200	-1.44049500
Sum of electronic and thermal Enthalpies= -2937.495439				H	6.02440800	-4.00946200	-1.44049500
Sum of electronic and thermal Free Energies= -2937.647003				Pd	0.11529700	-2.54948200	-0.09696100
HF(ob97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.229597				P	-2.12224700	-1.64251200	-0.77527500
N	6.04938000	-0.22905300	0.18959500	C	-3.32355300	-2.99473200	-1.46274700
C	5.23112400	-0.20458600	1.40555600	C	-1.94962800	-0.17569800	-1.99695700
H	5.58965300	0.59130800	2.06819900	C	-0.84157800	0.70856100	-1.38529800
H	4.18461600	0.00960100	1.16129200	H	-1.12369800	1.09906200	-0.40518500
C	5.26240400	-1.48323900	2.25974700	H	0.09267400	0.15017100	-1.26592700
C	5.34180600	-0.58947800	-1.06309400	H	-0.65255400	1.56391900	-2.04763100
H	5.98528700	-0.29037300	-1.89465300	C	-1.40438200	-0.76064400	-3.32078100
H	4.40072600	-0.02753100	-1.12385300	H	-1.06420800	0.07013900	-3.95276800
C	5.06931300	-2.08437700	-1.15310700	H	-0.55304600	-1.42839700	-3.16031500
C	3.86351300	-2.56302100	-0.92952900	H	-2.17110400	-1.30086700	-3.88406300
C	2.64320500	-2.98643800	-0.69712600	C	-3.18104800	0.68739200	-2.32211000
				H	-2.88571200	1.44900600	-3.05740200
				H	-3.99408500	0.10907500	-2.76492500

H	-3.56901700	1.20648700	-1.44793400	H	-7.63741100	-1.76661400	2.07631400
C	-2.48851300	-3.92796900	-2.36910100	H	-6.43055700	-0.68554800	2.78996700
H	-3.13107300	-4.74224400	-2.73053400	C	-7.45726600	-1.04491600	-0.51327700
H	-2.08434300	-3.41505000	-3.24553100	H	-7.06490800	-0.86565600	-1.51907200
H	-1.64993700	-4.36725600	-1.82052600	H	-7.74991900	-2.09878000	-0.44509000
C	-4.52062100	-2.45473200	-2.26143600	H	-8.37238700	-0.45166100	-0.40324800
H	-4.21070600	-1.99886700	-3.20603500	C	-2.56018300	2.57830100	1.49360500
H	-5.19694300	-3.28418900	-2.50973600	H	-1.95496600	1.66904700	1.57288400
H	-5.09351400	-1.71661700	-1.69848400	C	-1.76056700	3.60486800	0.66552800
C	-3.84113800	-3.84510500	-0.28480400	H	-2.20739200	4.60429300	0.71916600
H	-3.02206200	-4.27944200	0.29736900	H	-0.74151000	3.68740500	1.06083400
H	-4.47844000	-3.27814600	0.39909700	H	-1.69405000	3.32482800	-0.38947200
H	-4.43520200	-4.67582200	-0.68735100	C	-2.75019600	3.12872100	2.92443700
C	-2.73699300	-1.18595100	0.96930900	H	-1.78082500	3.39793700	3.36104800
C	-3.62139000	-0.22289100	1.54367700	H	-3.37703000	4.02851700	2.91218200
C	-2.09088700	-2.06800000	1.87306800	H	-3.22378500	2.39758400	3.58509700
C	-3.79594600	-0.23243300	2.94486900				
C	-2.27752600	-2.05352300	3.25123800				
H	-1.42610400	-2.84362000	1.48164000	<b>3-Ts2'</b>			
C	-3.14911900	-1.11946200	3.79834800	Zero-point correction= 1.038458 (Hartree/Particle)			
H	-4.47399800	0.50197000	3.36812000	Thermal correction to Energy= 1.097202			
H	-1.74266600	-2.76240500	3.87641000	Thermal correction to Enthalpy= 1.098146			
O	4.27790500	-1.77514900	2.91238900	Thermal correction to Gibbs Free Energy= 0.942541			
H	-3.32245400	-1.07248000	4.86984700	Sum of electronic and zero-point Energies= -2937.505357			
C	-4.41385400	0.87529900	0.86877200	Sum of electronic and thermal Energies= -2937.446613			
C	-3.90743100	2.20158400	0.86850200	Sum of electronic and thermal Enthalpies= -2937.445669			
C	-5.73930700	0.63946400	0.41515600	Sum of electronic and thermal Free Energies= -2937.601274			
C	-4.69304100	3.22722800	0.32556800	HF(ωb97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.181286			
C	-6.47322900	1.70244700	-0.12247200	N	-5.77244900	0.93890500	-0.12886700
C	-5.96724100	3.00288000	-0.19342200	C	-5.10445200	0.76914000	1.16467100
H	-4.30033800	4.24038400	0.31147700	H	-5.85551000	0.75770400	1.96329500
H	-7.47936800	1.51276500	-0.48305100	H	-4.56389700	-0.18255200	1.19872100
C	-6.77926700	4.14418500	-0.79152200	C	-4.12990900	1.89305000	1.54896300
H	-6.16401900	5.05119800	-0.71485900	C	-5.15372600	0.21664900	-1.27627400
C	-7.07479600	3.91240100	-2.28577300	H	-5.84537200	0.32088000	-2.11672500
H	-6.14992200	3.76641900	-2.85455400	H	-5.05498900	-0.84884300	-1.02651000
H	-7.70164200	3.02496100	-2.43408400	C	-3.79372500	0.81003000	-1.63049700
H	-7.60691900	4.77107300	-2.71241400	C	-2.64539700	0.20229900	-1.33228500
C	-8.07872500	4.40174000	-0.00479400	C	-2.29247200	-1.03970500	-0.72050400
H	-7.86951700	4.60264000	1.05165300	C	-1.95685800	-2.23124500	-1.39216000
H	-8.61474100	5.26489200	-0.41718500	C	-1.70265900	-0.93182100	0.61850500
H	-8.75279300	3.53824100	-0.05372000	S	-7.45256800	1.10379400	-0.11071800
C	-6.43204400	-0.71482400	0.58915900	O	-7.76174500	1.94646100	1.05262500
H	-5.66079000	-1.49153900	0.57339800	O	-7.84799600	1.48783900	-1.46751000
C	-7.13569200	-0.79782100	1.96248100	C	-8.14985100	-0.52042800	0.21606600
H	-7.89431900	-0.01113600	2.05277400	C	-8.34201400	-1.41600300	-0.84040000
				C	-8.47197100	-0.88584700	1.52526700

C	-8.84309500	-2.68796500	-0.57313400	H	2.90415200	-2.50921900	2.30030400
H	-8.12797400	-1.10781900	-1.85812600	C	2.78221400	0.65286800	-1.13309800
C	-8.97421000	-2.16276000	1.77351300	C	4.14386400	0.37418800	-1.45961800
H	-8.35947500	-0.16612600	2.32890400	C	1.95153400	1.08108000	-2.20174100
C	-9.15958700	-3.08529900	0.73472700	C	4.58751400	0.65084800	-2.76961600
H	-9.00078200	-3.38136000	-1.39577100	C	2.40898800	1.31119400	-3.49673200
H	-9.23554100	-2.44334400	2.79100500	C	3.75672100	1.12274900	-3.78047300
C	-9.67599300	-4.47672300	1.01501200	H	5.63022700	0.44941100	-2.99583200
H	-8.84757700	-5.18968300	1.12239600	H	1.71106600	1.63799300	-4.26211000
H	-10.25755100	-4.50979400	1.94191900	O	-3.12042300	1.62181800	2.17853600
H	-10.31190300	-4.83989700	0.20058100	H	-1.57013600	-3.08137500	-0.84148200
C	-4.52261200	3.31149900	1.21317000	H	-2.14913600	-2.35277900	-2.45339600
H	-4.33006700	3.49887700	0.15109500	H	-1.97534400	-0.09993200	1.26272300
H	-5.59398800	3.47010600	1.37336100	H	-1.46407200	-1.86330800	1.13166000
H	-3.92732300	4.00441700	1.81213200	C	5.19949900	-0.28558900	-0.60519800
C	-3.86499000	2.12972100	-2.37406500	C	6.10916100	0.49898500	0.15554600
H	-4.22483900	1.97776400	-3.40294800	C	5.40333200	-1.68725500	-0.69498200
H	-4.57017300	2.82993600	-1.90724200	C	7.10216800	-0.13396500	0.90952100
H	-2.87780900	2.59702200	-2.42694300	C	6.40513400	-2.26418400	0.10514700
Pd	-0.17468900	-0.37761400	-0.66965400	C	7.25096500	-1.52304200	0.92609200
P	1.68033500	0.55215900	0.42269500	H	7.78371600	0.47694300	1.49416100
C	2.32989300	-0.46445200	1.92691000	H	6.53643600	-3.34430600	0.06373900
C	1.43620300	2.42615700	0.91693800	C	4.73933100	-2.68652900	-1.66849900
C	0.54123500	3.11193900	-0.13889800	H	4.74973200	-3.64315400	-1.12857900
H	1.04883300	3.23071900	-1.09966700	C	5.65526300	-2.87513300	-2.90123400
H	-0.39547700	2.56861600	-0.29940000	H	6.68163500	-3.11939200	-2.60793000
H	0.29595800	4.11913500	0.22187300	H	5.27685100	-3.68694500	-3.53412500
C	0.69747500	2.53897800	2.26636300	H	5.68490700	-1.96447800	-3.50986600
H	0.47046200	3.59842900	2.44095600	C	3.28771500	-2.49079100	-2.14049500
H	-0.25720200	2.00347000	2.26910000	H	2.59357600	-2.29928000	-1.32008100
H	1.30440700	2.20248700	3.11046800	H	3.18452000	-1.68275400	-2.86818800
C	2.76348600	3.19745500	0.99133200	H	2.96286500	-3.41489700	-2.63446100
H	2.55756100	4.23715500	1.27942300	H	0.89263700	1.26199900	-2.01744000
H	3.45596100	2.78422400	1.72769500	H	4.15396200	1.31017500	-4.77411200
H	3.26381100	3.22150100	0.01924200	C	8.31097500	-2.20631600	1.77951000
C	1.14750600	-0.65519100	2.90918600	H	8.22530400	-3.28604600	1.59571300
H	1.48058900	-1.33705700	3.70226100	C	9.73651200	-1.78225900	1.37746600
H	0.81601800	0.26422300	3.38927500	H	9.89947900	-0.71216900	1.55287300
H	0.28808500	-1.11337800	2.41503300	H	10.48207600	-2.33173400	1.96442900
C	3.52155100	0.14611100	2.68260700	H	9.92448700	-1.97935700	0.31634300
H	3.27181800	1.10788400	3.14017400	C	8.06843500	-1.97322100	3.28307300
H	3.81141200	-0.53249600	3.49602600	H	8.15399700	-0.91046100	3.53940200
H	4.39369200	0.27660500	2.04001900	H	7.06859800	-2.30871700	3.57981100
C	2.68966400	-1.87672500	1.42877500	H	8.80477800	-2.52116700	3.88305000
H	1.85406900	-2.32786600	0.88330800	C	6.11156000	2.02717500	0.08700500
H	3.57390800	-1.88234600	0.79508800	H	5.13098200	2.34813200	-0.27133400

C	6.36386600	2.71842100	1.44004700	H	-11.42438700	-0.09233800	-3.35874000
H	7.39710900	2.58441100	1.78051800	H	-10.54070800	-1.62099100	-3.34825900
H	6.19545800	3.79724500	1.34476900	H	-11.80407300	-1.33125400	-2.14812300
H	5.70307600	2.34021500	2.22627300	C	-3.74449100	0.11874600	3.11124200
C	7.15426100	2.51466200	-0.94303000	H	-3.21126500	0.96450800	2.66318800
H	7.14687700	3.60957800	-1.00793200	H	-4.69370200	0.50967500	3.49199600
H	8.16382800	2.19937300	-0.65352200	H	-3.14011500	-0.29981400	3.91939500
H	6.95243700	2.11680200	-1.94227500	C	-2.57088600	2.24272700	0.14029000
				H	-2.58561100	3.10777900	-0.53929000
<b>3-Int3'</b>				H	-3.17456000	2.52719300	1.01167300
Zero-point correction= 1.039726 (Hartree/Particle)				H	-1.53486500	2.09123800	0.46155800
Thermal correction to Energy= 1.099652				Pd	-0.42939600	-0.52390200	-0.53322700
Thermal correction to Enthalpy= 1.100597				P	1.86044500	-1.25603700	0.08088500
Thermal correction to Gibbs Free Energy= 0.941944				C	2.85095900	-1.76750700	-1.49175800
Sum of electronic and zero-point Energies= -2937.560457				C	1.89324900	-2.67732100	1.41162100
Sum of electronic and thermal Energies= -2937.500531				C	0.77042600	-2.41898700	2.44220300
Sum of electronic and thermal Enthalpies= -2937.499586				H	0.97959800	-1.54973800	3.07052100
Sum of electronic and thermal Free Energies= -2937.658239				H	-0.20889000	-2.28239300	1.97326000
HF( $\omega$ b97xd/6-311+G(d,p)/LanL2dz, SMD[ <i>toluene</i> ])= -2939.234523				H	0.70667800	-3.28930100	3.10828100
N	-5.28075800	0.67259900	0.60727900	C	1.58739400	-4.03228400	0.74153500
C	-5.11744800	-0.71744000	1.05438700	H	1.45441900	-4.78515300	1.52891600
H	-6.02945900	-1.04415000	1.56713200	H	0.66312300	-4.00496100	0.15617300
H	-4.95336700	-1.37934100	0.19799500	H	2.40212900	-4.37928100	0.10102400
C	-3.97738500	-0.94311900	2.06041300	C	3.22402400	-2.77584000	2.17241300
C	-4.63916000	1.00519000	-0.69537700	H	3.16693000	-3.60167400	2.89473700
H	-4.99644500	1.99675100	-0.98459000	H	4.07340600	-2.97191100	1.51449700
H	-4.95936000	0.27869200	-1.44894200	H	3.42607100	-1.86160500	2.73721400
C	-3.12723700	1.01472400	-0.54247500	C	1.97827900	-2.77802300	-2.27882700
C	-2.37029100	-0.01889300	-0.95449100	H	2.46344200	-2.95751800	-3.24709100
C	-2.67845300	-1.28346600	-1.62706600	H	1.87146700	-3.74460800	-1.78686400
C	-3.42161200	-1.57065700	-2.71251000	H	0.98034200	-2.37495200	-2.47354400
C	-1.64183900	-2.15476800	-0.98291800	C	4.24553200	-2.37109000	-1.26466800
S	-6.71851000	1.45890600	1.00510800	H	4.20301900	-3.30662200	-0.69840300
O	-7.04257600	1.03636200	2.37383300	H	4.69857600	-2.60343200	-2.23816400
O	-6.52723600	2.86928600	0.65704100	H	4.91408600	-1.67952100	-0.74983000
C	-8.00596400	0.80803800	-0.06664400	C	2.95478700	-0.52374000	-2.39577300
C	-8.19502200	1.36229600	-1.33602700	H	1.96721100	-0.08781000	-2.58578800
C	-8.79291000	-0.26187700	0.36677500	H	3.61036900	0.23934400	-1.98179900
C	-9.16745500	0.82484800	-2.17650200	H	3.37343300	-0.82797800	-3.36425700
H	-7.60784600	2.22015700	-1.64575600	C	2.49848800	0.24970500	1.06454700
C	-9.76164600	-0.78611600	-0.48778800	C	3.70898100	1.00334300	1.14878300
H	-8.66638800	-0.65304800	1.37045500	C	1.43235000	0.67356800	1.89679100
C	-9.95928900	-0.26027100	-1.77214200	C	3.80066300	2.01530800	2.12712900
H	-9.32119700	1.26191400	-3.16020300	C	1.54238000	1.69275900	2.83938900
H	-10.38107900	-1.61210400	-0.14681700	C	2.75575100	2.35704700	2.97910700
C	-10.98976500	-0.85413300	-2.70298000	H	4.73194400	2.57051000	2.18628700

H	0.68244900	1.95881800	3.44757600
O	-3.35049200	-1.98718600	2.03085700
H	-3.38305800	-2.55660600	-3.17048200
H	-4.03318000	-0.82241200	-3.20856600
H	-1.92192000	-2.53674200	0.00160900
H	-1.13805400	-2.89687000	-1.60627000
C	4.91452500	0.95068500	0.24041500
C	6.05059600	0.16845700	0.58474700
C	4.99070900	1.82338800	-0.87680800
C	7.16762800	0.16614100	-0.25667400
C	6.13194400	1.75618200	-1.69491000
C	7.21978800	0.92977500	-1.42521000
H	8.02415200	-0.44464500	0.01357500
H	6.17354700	2.39982600	-2.57217800
C	4.02360400	2.96568900	-1.26047600
H	4.13317400	3.06384700	-2.34898600
C	4.54012200	4.29123000	-0.65222000
H	5.59317100	4.46343300	-0.89827900
H	3.95575200	5.13708900	-1.03418700
H	4.44365700	4.28498800	0.43905000
C	2.51066600	2.84656400	-1.00533600
H	2.09312400	1.90897500	-1.37772300
H	2.25005400	2.94272300	0.05080800
H	2.00975900	3.66296200	-1.54006900
H	0.46602800	0.18648300	1.79747100
H	2.88194000	3.15002900	3.71102300
C	8.42459100	0.89209100	-2.35566800
H	8.21639600	1.58771200	-3.18012200
C	9.70857800	1.37774000	-1.65627100
H	9.98758900	0.71479400	-0.82858100
H	10.54773500	1.39862400	-2.36179100
H	9.58051300	2.38623200	-1.24796800
C	8.62544100	-0.50611200	-2.97085300
H	8.85325700	-1.25093500	-2.19893300
H	7.72592500	-0.83873500	-3.50047200
H	9.45877800	-0.49902700	-3.68357300
C	6.13912100	-0.58887900	1.91092000
H	5.12303600	-0.72358400	2.28795200
C	6.78549600	-1.98248400	1.79856900
H	7.85979800	-1.91852800	1.59056800
H	6.67424800	-2.52274000	2.74577600
H	6.32937400	-2.58637500	1.00800700
C	6.90502200	0.25098100	2.95678500
H	6.95405600	-0.28087000	3.91486700
H	7.93187400	0.44461400	2.62427400
H	6.42189300	1.21703100	3.13230200

### 3-Ts3'

Zero-point correction= 1.038793 (Hartree/Particle)

Thermal correction to Energy= 1.096858

Thermal correction to Enthalpy= 1.097802

Thermal correction to Gibbs Free Energy= 0.945948

Sum of electronic and zero-point Energies= -2937.526812

Sum of electronic and thermal Energies= -2937.468747

Sum of electronic and thermal Enthalpies= -2937.467803

Sum of electronic and thermal Free Energies= -2937.619657

HF(ωb97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.198639

N	5.01468900	-0.08898000	-0.99635600
C	3.95658800	-0.42192100	-0.03757300
H	3.85071300	-1.51200100	-0.01479300
H	4.19910800	-0.08113700	0.97578600
C	2.58032900	0.12513600	-0.44194600
C	5.69243100	1.20546200	-0.85552700
H	6.26479400	1.37479500	-1.77302600
H	6.42586700	1.16933200	-0.02644000
C	4.76759300	2.38261100	-0.60058600
C	3.45257500	2.29657200	-0.45491500
C	2.39523100	3.06034500	-0.01859000
C	1.90571000	2.98245200	1.35353100
C	1.24170100	3.51900400	-0.79414500
S	5.94489200	-1.35023200	-1.61043000
O	5.03622200	-2.48575300	-1.79821700
O	6.72154300	-0.79288000	-2.72153300
C	7.11559100	-1.81418900	-0.32655900
C	8.35490000	-1.17279800	-0.25502600
C	6.76809700	-2.79457200	0.60702800
C	9.24070600	-1.51024700	0.76752200
H	8.62866200	-0.44365200	-1.01001600
C	7.66600300	-3.11953300	1.62178600
H	5.81984800	-3.31346100	0.51702800
C	8.91022500	-2.48000600	1.72434600
H	10.20942400	-1.01866500	0.81670400
H	7.40025500	-3.89056700	2.34114500
C	9.86369900	-2.81948800	2.84567200
H	10.90329800	-2.62868700	2.55999200
H	9.65391300	-2.21447900	3.73800100
H	9.77879200	-3.87099400	3.13981500
C	2.24258600	0.07160100	-1.92357900
H	1.39995500	0.73189400	-2.13383000
H	3.08891700	0.33172800	-2.55837200
H	1.93659100	-0.95700100	-2.16614300
C	5.54140600	3.68795100	-0.48791000

H	6.32391600	3.62473800	0.28274200	C	-4.17406800	-1.26080400	0.76366400
H	6.05023500	3.93436100	-1.43126600	C	-5.48079700	-1.18246700	0.20869600
H	4.87595000	4.51668100	-0.23357200	C	-3.43462600	-2.46463100	0.62286500
Pd	0.13622000	2.19195700	0.45277800	C	-5.95788900	-2.23092200	-0.58409700
P	-2.16107500	1.74413700	-0.30866300	C	-3.95998400	-3.47021700	-0.20762300
C	-2.28321200	0.70029900	-1.92145300	C	-5.19859300	-3.37602400	-0.83662400
C	-3.24892100	3.35442900	-0.45322300	H	-6.95384300	-2.15298700	-1.01039500
C	-2.81649400	4.35394300	0.64258200	H	-3.37462100	-4.37763700	-0.34659700
H	-3.08278200	4.01120100	1.64538700	C	-5.70879300	-4.49577000	-1.73362500
H	-1.73926800	4.54794600	0.61608400	H	-4.93339900	-5.27376400	-1.74966700
H	-3.34095100	5.30367100	0.47431500	C	-5.91177700	-4.01639400	-3.18370000
C	-2.99473300	4.03975500	-1.81097200	H	-6.68768800	-3.24360400	-3.24187400
H	-3.47520800	5.02652700	-1.79879800	H	-4.98805500	-3.59390200	-3.59406800
H	-1.92815800	4.19547000	-2.00300300	H	-6.22159700	-4.84904200	-3.82649400
H	-3.42519000	3.48492800	-2.64785700	C	-6.99459000	-5.13817700	-1.17890000
C	-4.75385000	3.09381700	-0.28818600	H	-7.30815000	-5.97927700	-1.80868400
H	-5.30074400	4.03984700	-0.40249300	H	-6.84340600	-5.51205800	-0.16029000
H	-5.14448000	2.39582400	-1.03117400	H	-7.82118900	-4.41808400	-1.15161900
H	-4.98071900	2.70272900	0.70734100	C	-2.15970400	-2.89605300	1.38233900
C	-1.44631300	1.42678700	-3.00458900	H	-1.65841400	-3.59613000	0.70037000
H	-1.30277300	0.73353000	-3.84278000	C	-2.57574700	-3.72411100	2.62208900
H	-1.93139100	2.31823800	-3.40238300	H	-3.26704000	-4.53095400	2.35639100
H	-0.45776200	1.70865000	-2.63400900	H	-1.69131700	-4.17060500	3.09227000
C	-3.69194600	0.43807600	-2.47677600	H	-3.06612800	-3.09072400	3.36985200
H	-4.20236600	1.36197200	-2.76722200	C	-1.08481700	-1.87428300	1.79096600
H	-3.60682300	-0.18011900	-3.38081900	H	-0.74443200	-1.24801800	0.96528500
H	-4.32077400	-0.10394600	-1.76931100	H	-1.40627800	-1.22471900	2.60823700
C	-1.56865200	-0.63717800	-1.64263600	H	-0.20837900	-2.42924700	2.14660200
H	-0.57057100	-0.48571500	-1.22089200	C	-6.43468800	-0.03403300	0.54258600
H	-2.14324600	-1.27403200	-0.97327700	C	-7.26409500	0.46440300	-0.65590000
H	-1.45419500	-1.17663300	-2.59209300	H	-7.80154000	1.38014000	-0.38346400
C	-2.81269100	0.94681300	1.29894200	H	-6.63943800	0.68345400	-1.52746200
C	-3.64649200	-0.15842700	1.65129500	H	-8.01772200	-0.26958600	-0.96367600
C	-2.27074000	1.69403700	2.37451200	C	-7.38398700	-0.44270300	1.69045600
C	-3.96805500	-0.34555700	3.01179700	H	-7.99827900	-1.30310700	1.39937200
C	-2.58058900	1.46889100	3.71319600	H	-6.83127500	-0.71648800	2.59437100
H	-1.56814200	2.49651400	2.15585000	H	-8.05834200	0.38440700	1.94446500
C	-3.46958200	0.45075300	4.03742300	H	-5.83576200	0.80481200	0.90390000
H	-4.61411300	-1.18171600	3.26117300				
H	-2.12531000	2.08559100	4.48302300				
O	1.67717700	0.10649100	0.42067400	<b>3-Int4'</b>			
H	1.48690600	3.89722200	1.77914500	Zero-point correction=	1.043580	(Hartree/Particle)	
H	2.42761600	2.33398700	2.05418600	Thermal correction to Energy=	1.101772		
H	0.82756700	4.48842500	-0.51459100	Thermal correction to Enthalpy=	1.102717		
H	1.20138900	3.30683300	-1.86119600	Thermal correction to Gibbs Free Energy=	0.950112		
H	-3.74679300	0.25312600	5.06918000	Sum of electronic and zero-point Energies=	-2937.586780		
				Sum of electronic and thermal Energies=	-2937.528588		

Sum of electronic and thermal Enthalpies= -2937.527644				H	-1.31109900	2.43595200	3.11435000
Sum of electronic and thermal Free Energies= -2937.680249				H	-0.23622000	3.17360500	1.91238200
HF(ob97xd/6-311+G(d,p)/LanI2dz, SMD[toluene])= -2939.263453				H	-1.37088300	4.17507500	2.84254200
N	5.47213300	-0.30250500	-1.39843900	C	-2.30725300	4.33452400	0.40436800
C	4.33047700	-0.59889200	-0.52806000	H	-2.40500300	5.20207400	1.06949700
H	4.06426500	-1.64914900	-0.65062800	H	-1.36420000	4.44692900	-0.13848200
H	4.55320600	-0.40289000	0.53127900	H	-3.13095900	4.38574300	-0.31114900
C	3.13029000	0.28231200	-0.94833800	C	-3.70372300	2.98027300	1.98164200
C	5.94410800	1.08612000	-1.39947900	H	-3.85490400	3.89626600	2.56882500
H	6.40817000	1.28463100	-2.37144100	H	-4.53924600	2.89580500	1.28307600
H	6.73617200	1.23681900	-0.64078700	H	-3.74404000	2.13566300	2.67463200
C	4.85969800	2.10679100	-1.11600800	C	-2.15538500	2.59191500	-2.37781000
C	3.58279900	1.75914400	-0.84707600	H	-2.60001600	2.54384900	-3.38002500
C	2.53832800	2.71792600	-0.39190100	H	-2.25140400	3.62072900	-2.03227900
C	2.79970600	3.67112600	0.52878800	H	-1.09367400	2.35470900	-2.47538500
C	1.15551700	2.57994100	-0.91791500	C	-4.38280800	1.91399200	-1.42535000
S	6.63961800	-1.48481500	-1.62839700	H	-4.55591600	2.90920000	-1.00452200
O	5.93114800	-2.75795200	-1.77849500	H	-4.79018400	1.92019300	-2.44527700
O	7.54262000	-0.97238600	-2.66401500	H	-4.95552000	1.18568000	-0.85042700
C	7.58574500	-1.57878000	-0.10192000	C	-2.70178500	0.19956100	-2.19512500
C	8.75433500	-0.82649700	0.03733000	H	-1.64222400	-0.07115400	-2.25880400
C	7.12836200	-2.38249000	0.94702600	H	-3.24766800	-0.60362500	-1.70508200
C	9.45964800	-0.87578800	1.23995200	H	-3.08769000	0.28314900	-3.21959000
H	9.11682300	-0.23841900	-0.79896900	C	-2.44240800	0.05604800	1.39527800
C	7.84487100	-2.41888800	2.14094700	C	-3.51303300	-0.88212300	1.51176100
H	6.23932800	-2.98966900	0.81400600	C	-1.41903800	-0.02855300	2.37272600
C	9.01538700	-1.66353600	2.31021900	C	-3.53777700	-1.73108000	2.63780400
H	10.37573400	-0.29924400	1.34444900	C	-1.45602000	-0.89632200	3.46109600
H	7.49502100	-3.05212400	2.95295300	H	-0.54180500	0.60396300	2.27314700
C	9.76827100	-1.69202100	3.61958600	C	-2.54737700	-1.74310300	3.61414900
H	10.81175400	-1.38775000	3.48921400	H	-4.36385900	-2.43117200	2.71652100
H	9.31578000	-1.00778800	4.34984800	H	-0.63223600	-0.90477200	4.16894400
H	9.75884500	-2.69252900	4.06567100	O	2.11287200	0.00276100	-0.04123600
C	2.72021000	-0.08434800	-2.39511800	H	2.02823400	4.36648700	0.85246700
H	1.87089000	0.52157200	-2.72372400	H	3.77228000	3.77142000	0.99797800
H	3.54283900	0.05058400	-3.10336900	H	0.52980400	3.43484600	-0.66061400
H	2.40933300	-1.13549300	-2.41493300	H	1.10480800	2.37514100	-1.98977700
C	5.41166100	3.51448300	-1.16309000	H	-2.61608700	-2.42620500	4.45618600
H	6.02564300	3.74446900	-0.28026200	C	-4.61352100	-1.18717600	0.52404300
H	6.06805600	3.63273200	-2.03612200	C	-5.89475600	-0.58564500	0.65992200
H	4.62071300	4.26396300	-1.22254500	C	-4.43075900	-2.21608000	-0.43647800
Pd	0.31651300	0.88426800	-0.07384600	C	-6.91083000	-0.91725400	-0.24174300
P	-1.96310500	1.46977800	0.19997400	C	-5.48429300	-2.48485300	-1.32775900
C	-2.88943700	1.55673400	-1.48913500	C	-6.71939200	-1.84437500	-1.26923700
C	-2.34396800	3.05733300	1.26881000	H	-7.88190600	-0.44296300	-0.13303800
C	-1.24203600	3.20612400	2.34275300	H	-5.33064600	-3.24881500	-2.08816300

C	-7.81927000	-2.17131400	-2.27037200	C	6.08014400	-0.58175700	1.83762600
H	-7.41848800	-2.93510500	-2.95063700	H	6.53243500	-0.30140300	2.79451700
C	-8.19513900	-0.94467100	-3.12353400	H	6.90490500	-0.92041700	1.18153000
H	-8.61769100	-0.14426000	-2.50435800	C	5.13147700	-1.74641300	2.02812100
H	-7.31916900	-0.53912600	-3.64169700	C	3.85524600	-1.67925800	1.61213100
H	-8.94417700	-1.21325500	-3.87797000	C	2.83433900	-2.74364800	1.61859800
C	-9.06269000	-2.77062700	-1.58604200	C	2.51645600	-3.53120700	2.66218200
H	-9.81495400	-3.05252600	-2.33230100	C	2.10055600	-2.82796100	0.33459800
H	-8.80475700	-3.66410000	-1.00698500	S	6.35598100	1.99565100	1.15210200
H	-9.52799700	-2.05119100	-0.90164200	O	5.44952400	3.07030700	0.74409100
C	-3.24752200	-3.20162600	-0.56261900	O	7.14690800	2.06765700	2.38366600
H	-3.22883000	-3.47337500	-1.62668800	C	7.49965700	1.71102500	-0.20389000
C	-3.58803700	-4.49852400	0.20975400	C	8.76100700	1.16986300	0.05642300
H	-4.56464400	-4.89787200	-0.08342100	C	7.10935500	2.01128100	-1.51257800
H	-2.83011300	-5.26622900	0.01320500	C	9.62848400	0.91959600	-1.00660400
H	-3.60651500	-4.31725900	1.29020400	H	9.06453000	0.98019600	1.08044200
C	-1.81117500	-2.76982300	-0.21823000	C	7.98883200	1.75374600	-2.56164400
H	-1.52095900	-1.83359500	-0.69953600	H	6.14236600	2.46667900	-1.69768800
H	-1.64496600	-2.66772900	0.85636500	C	9.25656300	1.19898700	-2.32873500
H	-1.12542900	-3.54553700	-0.57956100	H	10.61494100	0.50966000	-0.80383500
C	-6.23682400	0.33595200	1.83270000	H	7.69006600	1.99705900	-3.57846700
C	-7.08937000	1.55902800	1.44499500	C	10.19028100	0.90072200	-3.47788800
H	-7.17061400	2.24263000	2.29803500	H	9.95114000	-0.06717800	-3.93836600
H	-6.65857800	2.11352100	0.60539000	H	10.11389800	1.66002600	-4.26359100
H	-8.10986900	1.27329800	1.16534100	H	11.23277700	0.85688300	-3.14694800
C	-6.95369000	-0.45827700	2.94674600	C	2.43402900	0.41046400	1.81648200
H	-7.89690000	-0.87958100	2.57906200	H	1.66973200	-0.18834800	2.32154500
H	-6.33842000	-1.28525000	3.31419100	H	3.06815300	0.88779000	2.57065700
H	-7.18360100	0.19518700	3.79723500	H	1.92966900	1.18806100	1.23231700
H	-5.29920900	0.70608600	2.25356800	C	5.78005300	-2.95421900	2.65560200
<b>3-Ts4'</b>				H	5.18779600	-3.85966000	2.50323800
Zero-point correction= 1.041509 (Hartree/Particle)				H	6.78063900	-3.11898100	2.23398200
Thermal correction to Energy= 1.099893				H	5.91501400	-2.81798000	3.73780900
Thermal correction to Enthalpy= 1.100837				Pd	0.42218400	-1.13536600	-0.31894700
Thermal correction to Gibbs Free Energy= 0.946763				P	-1.85859000	-1.38868800	-0.54352600
Sum of electronic and zero-point Energies= -2937.554931				C	-2.64940500	-1.63610200	1.19625600
Sum of electronic and thermal Energies= -2937.496548				C	-2.33046800	-2.88322700	-1.70354300
Sum of electronic and thermal Enthalpies= -2937.495604				C	-1.37279300	-2.87423300	-2.91569500
Sum of electronic and thermal Free Energies= -2937.649678				H	-1.54111300	-2.01404300	-3.56852500
HF(ob97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.249158				H	-0.32417600	-2.86534600	-2.59950800
N	5.41457500	0.60348800	1.28846100	H	-1.55061700	-3.77879300	-3.51309800
C	4.42104700	0.33348000	0.24238500	C	-2.10653400	-4.21715400	-0.96411800
H	4.04632500	1.28345800	-0.13987900	H	-2.21619900	-5.04047300	-1.68220300
H	4.84706000	-0.25060900	-0.58650800	H	-1.09953000	-4.28423300	-0.53891200
C	3.27088400	-0.47242000	0.87892700	H	-2.83484600	-4.38679300	-0.16710300
				C	-3.77110600	-2.83330300	-2.23432100



H	-3.95610100	-3.71053400	-2.86983200	H	-8.84070900	3.54776100	1.32289500
H	-4.51533700	-2.84403400	-1.43517400	H	-9.57819000	1.94168000	1.21645200
H	-3.93544800	-1.94393700	-2.84870500	C	-6.45014900	-0.40087200	-1.71663200
C	-1.79617500	-2.67754500	1.96124900	H	-5.54255500	-0.69550900	-2.24773800
H	-2.14609900	-2.70640500	3.00181500	C	-7.33259300	0.37558200	-2.71795700
H	-1.88059700	-3.68949800	1.56225700	H	-7.60709700	-0.26511200	-3.56504100
H	-0.73905500	-2.39212000	1.96495500	H	-8.25827400	0.71855600	-2.24048000
C	-4.12533600	-2.06208700	1.24100600	H	-6.81552600	1.25494900	-3.11450900
H	-4.28706900	-3.04724900	0.79226800	C	-7.17551100	-1.68818200	-1.27971000
H	-4.44864100	-2.12851600	2.28898100	H	-8.16606200	-1.47556400	-0.86109700
H	-4.77656000	-1.34031500	0.74569200	H	-7.32518100	-2.34592500	-2.14399400
C	-2.46909800	-0.30387200	1.94552700	H	-6.60921800	-2.24282800	-0.52514100
H	-2.73209400	-0.44672900	3.00242700	C	-3.24170200	2.94038400	0.55061800
H	-1.43011500	0.04154600	1.89748200	H	-2.44901700	2.38408600	0.04058400
H	-1.74381100	3.75842000	1.88794400	C	-3.46411300	4.25478900	-0.23073300
C	-2.53731500	0.09145500	-1.55299400	H	-4.26234300	4.84808700	0.23190800
C	-3.71482300	0.90323000	-1.55428900	H	-2.54858100	4.85861600	-0.22751500
C	-1.59953300	0.33749300	-2.58552600	H	-3.74038200	4.06805600	-1.27182400
C	-3.91743800	1.77672800	-2.64537800	C	-2.72776600	3.28175400	1.96308800
C	-1.81912900	1.21780400	-3.64063300	H	-3.38738000	3.98970100	2.47861500
H	-0.64559700	-0.18047000	-2.54183000	H	-2.62417400	2.39591200	2.59612600
C	-3.01354400	1.92724600	-3.69108800	H	-3.11952200	0.47064000	1.54710200
H	-4.81905700	2.38192100	-2.63943300	<b>3a+PdL'</b>			
H	-1.05537300	1.34736000	-4.40263300	Zero-point correction= 1.044503 (Hartree/Particle)			
O	2.51465100	-1.00245000	-0.19739500	Thermal correction to Energy= 1.103089			
H	1.72269400	-4.27067300	2.59183900	Thermal correction to Enthalpy= 1.104034			
H	3.03643100	-3.45922900	3.61225100	Thermal correction to Gibbs Free Energy= 0.951275			
H	2.66579600	-3.14135700	-0.53735000	Sum of electronic and zero-point Energies= -2937.622613			
H	1.14187100	-3.34229500	0.41069500	Sum of electronic and thermal Energies= -2937.564026			
H	-3.22636100	2.61693900	-4.50347100	Sum of electronic and thermal Enthalpies= -2937.563082			
C	-4.75561200	1.09957600	-0.47020800	Sum of electronic and thermal Free Energies= -2937.715840			
C	-4.51630200	2.08548900	0.52731400	HF(ωb97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2939.291521			
C	-6.03813100	0.50002500	-0.55130300	N	5.00249200	0.40736500	0.97600600
C	-5.51597900	2.34997500	1.47158400	C	3.86744800	-0.22583400	0.29482300
C	-6.99998400	0.80552200	0.42003700	H	2.95295000	-0.00614200	0.84519700
C	-6.75713400	1.71215900	1.45306500	H	3.75629200	0.12414100	-0.74176100
H	-5.32758400	3.09049200	2.24408300	C	4.15145700	-1.72848400	0.29400100
H	-7.97489300	0.33007200	0.35447200	C	6.29777900	0.27880500	0.29905400
C	-7.80962500	2.02332700	2.50924700	H	7.08457500	0.47055100	1.03614800
H	-7.37417600	2.77063400	3.18669700	H	6.41344100	1.04006300	-0.49571300
C	-8.15538600	0.78190900	3.35369200	C	6.49223400	-1.07932500	-0.34314300
H	-8.86867800	1.03891300	4.14611200	C	5.51216900	-2.00225600	-0.32331100
H	-8.60983900	-0.00349800	2.73791200	C	5.39532800	-3.29565200	-1.01404000
H	-7.25977500	0.36087300	3.82361400	C	6.34246700	-4.16207700	-1.39870200
C	-9.07868800	2.64397100	1.89450300	C	3.89970300	-3.53584800	-1.18965700
H	-9.79554100	2.91452500	2.67910500	S	4.71503300	1.85421100	1.79729100

O	3.47566500	1.65597200	2.55276700	H	-4.04333900	-3.92930800	1.01928300
O	5.97892700	2.19635000	2.45362400	H	-4.13247900	-2.24072100	0.48686400
C	4.39404500	3.09781600	0.54427600	C	-1.73984600	-3.01177100	1.98133500
C	5.44998200	3.87371200	0.05967600	H	-0.65268800	-2.97701900	2.11384400
C	3.09740300	3.26203000	0.04524300	H	-2.16444600	-2.12687400	2.46103000
C	5.20161400	4.81264300	-0.94121700	H	-2.11942100	-3.89707900	2.50872500
H	6.44129300	3.76167700	0.48570200	C	-1.54356800	-0.06983200	0.70377300
C	2.87051600	4.20421000	-0.95522600	C	-2.65575600	0.78003400	1.01764300
H	2.27584100	2.68171400	0.45221000	C	-0.31525500	0.25718100	1.32636400
C	3.91516800	4.98818200	-1.46891900	C	-2.43394700	1.87233300	1.88554700
H	6.01985800	5.42561800	-1.31105000	C	-0.12691000	1.33099700	2.19342700
H	1.86160900	4.33937400	-1.33715600	H	0.53661700	-0.38238000	1.10171900
C	3.65671100	5.98782100	-2.57107200	C	-1.20600200	2.16085400	2.47143300
H	4.44415600	6.74656200	-2.61785200	H	-3.27992300	2.51731500	2.10218300
H	3.61840800	5.49203800	-3.55010500	H	0.85349100	1.50703800	2.62856900
H	2.69829600	6.49927800	-2.43070700	O	3.25491900	-2.36530200	-0.65517600
C	3.97185000	-2.35226400	1.68199800	H	6.08252600	-5.08836600	-1.90561900
H	4.27398000	-3.40502000	1.68118700	H	7.39562500	-3.99990800	-1.20088000
H	4.57923400	-1.81915400	2.41835500	H	3.59888500	-3.62443200	-2.23766000
H	2.91738800	-2.29093100	1.97298000	H	3.55961000	-4.43015200	-0.65166700
C	7.81801300	-1.25264000	-1.03651100	H	-1.10424900	3.01754300	3.13278600
H	7.72944900	-1.90158700	-1.91345200	C	-4.09881400	0.72335300	0.55137600
H	8.21866700	-0.28542700	-1.36243900	C	-4.52179000	1.53455400	-0.53756600
H	8.56662900	-1.69976600	-0.36793700	C	-5.08373700	0.05549200	1.32731200
Pd	1.01664200	-2.05804100	-0.52650200	C	-5.87144800	1.53617000	-0.90811000
P	-1.22814000	-1.63802500	-0.38675700	C	-6.41911700	0.08352500	0.90186000
C	-2.10838700	-3.11550700	0.48588100	C	-6.83579100	0.79372000	-0.22341400
C	-1.89381200	-1.37714100	-2.17753300	H	-6.17915400	2.14658800	-1.75242900
C	-1.16338500	-0.11559600	-2.68828200	H	-7.16740400	-0.45012500	1.48139300
H	-1.42915500	0.77847700	-2.11869600	C	-8.29536700	0.78198500	-0.65824300
H	-0.07759500	-0.24668500	-2.62340600	H	-8.83889700	0.14913400	0.05682300
H	-1.43078200	0.06104400	-3.73883900	C	-8.46805200	0.15322400	-2.05427900
C	-1.40436600	-2.56693300	-3.03387700	H	-7.95697200	0.74607100	-2.82229800
H	-1.56838800	-2.33028500	-4.09432300	H	-8.05371200	-0.86042200	-2.08559200
H	-0.33618600	-2.75843100	-2.88032100	H	-9.52917700	0.09797900	-2.32617300
H	-1.95688200	-3.48666900	-2.81831200	C	-8.92764800	2.18576600	-0.60293600
C	-3.41011100	-1.23442300	-2.38551000	H	-9.99248600	2.14047200	-0.86149800
H	-3.60266500	-0.96430500	-3.43361900	H	-8.83737200	2.62175200	0.39809100
H	-3.93825000	-2.17203800	-2.19879100	H	-8.44361500	2.86992500	-1.31010400
H	-3.85809400	-0.46708000	-1.75637700	C	-3.57356800	2.49351300	-1.26502400
C	-1.48519000	-4.42767800	-0.04039900	H	-2.54738400	2.18496000	-1.04532100
H	-1.87450900	-5.26856400	0.55063000	C	-3.74271800	3.93025200	-0.72310900
H	-1.73597900	-4.61974600	-1.08729300	H	-3.05424500	4.61536700	-1.23338100
H	-0.39351900	-4.40850300	0.04853800	H	-4.76439500	4.29128200	-0.89196600
C	-3.63318000	-3.19539800	0.31212800	H	-3.53959200	3.98635700	0.35011100
H	-3.90323600	-3.53666200	-0.69131700	C	-3.74329400	2.50652300	-2.79643400

H	-4.69699300	2.95634500	-3.09619300
H	-2.94805100	3.10759300	-3.25315000
H	-3.69594300	1.50213100	-3.22465500
C	-4.76998800	-0.57761600	2.68732100
H	-3.71234100	-0.85455800	2.69519900
C	-5.59276900	-1.83874200	3.01528900
H	-5.18394100	-2.32137700	3.91054000
H	-6.63839900	-1.59330800	3.23540800
H	-5.58309100	-2.56930700	2.20293000
C	-4.98189200	0.45299700	3.81999800
H	-6.02315800	0.79705200	3.83704500
H	-4.75985500	-0.00155300	4.79336600
H	-4.33740000	1.32759400	3.70379900

**1a+ZnCl<sub>2</sub>**

Zero-point correction= 0.358323 (Hartree/Particle)

Thermal correction to Energy= 0.387144

Thermal correction to Enthalpy= 0.388089

Thermal correction to Gibbs Free Energy= 0.294755

Sum of electronic and zero-point Energies= -2324.253744

Sum of electronic and thermal Energies= -2324.224923

Sum of electronic and thermal Enthalpies= -2324.223978

Sum of electronic and thermal Free Energies= -2324.317312

HF(ωb97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -2324.992783

N	-1.62300100	1.17046700	-0.25683200
C	-1.05580200	-0.12756400	-0.59409200
H	-0.36640300	-0.50666800	0.17080800
H	-1.89749800	-0.83089900	-0.64286700
C	-0.40112300	-0.16972000	-1.95929400
C	-2.71220600	1.09973800	0.73740700
H	-2.88409000	2.11557700	1.09967300
H	-2.42124200	0.46238800	1.58319800
C	-3.95913300	0.56251400	0.07134800
C	-4.38270600	-0.64701800	0.36137400
C	-4.77012000	-1.83859200	0.66340400
C	-4.70657000	-3.29069500	0.39714300
C	-5.57897900	-2.73295100	1.51442600
H	-3.79789800	-3.82027500	0.67364100
H	-5.20028000	-3.66838100	-0.49504600
H	-6.65667600	-2.73573700	1.37045600
H	-5.25662000	-2.88867200	2.54104500
S	-0.50303500	2.42380100	-0.13244600
O	0.03255500	2.61374200	-1.47318000
O	-1.16240500	3.50228000	0.57939100
C	0.82317000	1.75633400	0.84657000
C	0.59482900	1.41563200	2.17627100
C	2.05865100	1.51284600	0.24589200

C	1.60337100	0.79071900	2.89997200
H	-0.36085500	1.63451200	2.64304600
C	3.06701000	0.90839100	0.99505400
H	2.23363700	1.81986000	-0.78144800
C	2.84409000	0.51337500	2.32086000
H	1.41911300	0.50323200	3.93081500
H	4.03822400	0.74039700	0.53714700
C	3.89927600	-0.24227400	3.07876800
H	3.83635700	-0.05333300	4.15422300
H	3.75746600	-1.31768000	2.91667900
H	4.90428200	0.01794900	2.73555600
C	-1.19089100	0.27610300	-3.14578000
H	-2.23899600	-0.02188400	-3.04772800
H	-1.15740000	1.37065200	-3.16926500
H	-0.75035900	-0.12043800	-4.06146400
C	-4.62824100	1.46355900	-0.93653600
H	-5.00048500	2.37348200	-0.45018900
H	-3.90826500	1.77881600	-1.70076100
H	-5.46712500	0.96318700	-1.42525600
O	0.73791300	-0.61545100	-2.08960300
Zn	2.23466100	-1.24022200	-0.76914000
Cl	4.17816400	-1.01659800	-1.78322900
Cl	1.33081300	-2.45931200	0.85612900

**3-Int1-b**

Zero-point correction= 1.042039 (Hartree/Particle)

Thermal correction to Energy= 1.108471

Thermal correction to Enthalpy= 1.109415

Thermal correction to Gibbs Free Energy= 0.936339

Sum of electronic and zero-point Energies= -3923.595162

Sum of electronic and thermal Energies= -3923.528731

Sum of electronic and thermal Enthalpies= -3923.527787

Sum of electronic and thermal Free Energies= -3923.700862

HF(ωb97xd/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3925.354956

N	-5.49527900	-0.45432500	0.56910600
C	-4.77036400	-0.11727300	-0.64046700
H	-5.46347500	-0.06719700	-1.48926500
H	-4.26848400	0.85305700	-0.55509000
C	-3.73907700	-1.15615600	-1.03887000
C	-4.92432900	0.09042200	1.81073300
H	-5.65652400	-0.06334800	2.60658900
H	-4.74164800	1.16709900	1.69785000
C	-3.64584900	-0.64773800	2.14892100
C	-2.48546400	-0.16141800	1.76909300
C	-1.36532800	0.33870400	1.37490200
C	-0.33871200	0.42500600	0.31951900

C	-0.18578700	1.15138600	1.69798300	C	3.55670900	4.38086700	0.89938400
H	-0.56380600	1.03193300	-0.55597500	H	3.86404600	5.23482800	1.51815700
H	0.25958200	-0.47229300	0.14385300	H	3.16002400	4.77285800	-0.04111400
H	0.50390300	0.73282500	2.42631800	H	2.74324500	3.85104700	1.40553300
H	-0.29916600	2.23230100	1.71722000	C	5.89416900	4.28146000	0.05831600
S	-7.15586800	-0.63662500	0.45723000	H	5.60767600	4.71906900	-0.90122600
O	-7.38321200	-1.34037300	-0.79564100	H	6.13034000	5.11387100	0.73421000
O	-7.58691500	-1.17095300	1.73564300	H	6.81938500	3.71636800	-0.08038400
C	-7.80262900	1.01006100	0.28769500	C	5.22446400	2.96662100	2.06842200
C	-8.02877800	1.77637800	1.42950200	H	4.42717500	2.41598200	2.57370900
C	-8.01771700	1.53706600	-0.98309600	H	6.11004500	2.32598100	2.01646500
C	-8.46134100	3.08834800	1.28736000	H	5.47253200	3.83706700	2.68952400
H	-7.89391300	1.34021800	2.41376400	C	5.37574600	0.58889100	0.02884800
C	-8.45159600	2.85189300	-1.10509100	C	5.02335700	-0.69280100	0.51477500
H	-7.87572300	0.91444300	-1.86016400	C	6.73969800	0.85688200	-0.16907700
C	-8.67158200	3.64773300	0.02255200	C	6.04369400	-1.61921500	0.78015900
H	-8.64855300	3.68661100	2.17486400	C	7.73629300	-0.07340400	0.09317300
H	-8.63050800	3.26354400	-2.09450500	H	7.03771400	1.82929100	-0.53837000
C	-9.11149300	5.08187400	-0.11914200	C	7.38433400	-1.32750700	0.57572900
H	-9.75219400	5.38652800	0.71368600	H	5.75994200	-2.59517900	1.16402700
H	-8.24300600	5.75121400	-0.12961900	H	8.77745100	0.18478100	-0.07586500
H	-9.66224200	5.24080400	-1.05066500	O	-2.71377100	-0.74084100	-1.57927500
C	-4.05699200	-2.59693400	-0.84212500	H	8.14376000	-2.07232300	0.79437400
H	-3.95585200	-2.82565600	0.22390800	C	3.63925300	-1.21041600	0.81353700
H	-5.10451400	-2.78190100	-1.10254500	C	3.10084000	-1.05860300	2.10823000
H	-3.37703900	-3.23180800	-1.41332100	C	2.98164100	-2.03680800	-0.11786200
C	-3.81167300	-1.95347600	2.88525500	C	1.89961800	-1.69279000	2.42120900
H	-4.16718800	-1.77022600	3.90679200	C	1.77705400	-2.64929400	0.23958100
H	-4.56997100	-2.57695800	2.39507900	C	1.21489400	-2.48655400	1.50347000
H	-2.87334100	-2.50881100	2.94245600	H	1.48869900	-1.58726600	3.42388900
Pd	2.02640900	1.30296400	0.31529800	H	1.28373200	-3.28995800	-0.48719700
P	4.11367300	1.92437000	-0.28627500	C	-0.04808600	-3.21083300	1.93634400
C	4.76536500	3.44828200	0.68400800	H	-0.50640400	-2.60502800	2.73087000
C	4.25657300	2.26824200	-2.15629700	C	-1.08156100	-3.37000300	0.82111200
C	3.59524600	1.06737000	-2.84735200	H	-1.36138800	-2.39705300	0.40058200
H	4.14962200	0.14438400	-2.65447500	H	-0.71940200	-4.00106400	0.00416900
H	2.56275000	0.93283900	-2.51304400	H	-1.98959000	-3.84247000	1.21280600
H	3.58270100	1.22769500	-3.93305500	C	0.31183200	-4.57910200	2.53572300
C	3.41562800	3.51479000	-2.47679200	H	1.01963200	-4.47147500	3.36408100
H	3.30084700	3.60011500	-3.56470300	H	-0.58273100	-5.09110800	2.90934000
H	2.41510200	3.43659500	-2.03708100	H	0.77758600	-5.21669100	1.77541200
H	3.88277700	4.43955400	-2.12386500	C	3.58025600	-2.34523900	-1.48114500
C	5.66321300	2.42173600	-2.75311300	H	4.38651800	-1.62878200	-1.66194700
H	5.56460700	2.64225900	-3.82389200	C	4.20644700	-3.74804800	-1.48990900
H	6.24207600	3.23358700	-2.30742300	H	3.44809500	-4.51205100	-1.28236500
H	6.23873400	1.49558500	-2.66593900	H	4.64543900	-3.96458300	-2.47040600

H	4.99498300	-3.83901600	-0.73620700	S	-5.70597200	0.47583800	0.33590100
C	2.56391200	-2.20881600	-2.62005300	O	-5.71880500	1.50494900	1.36298100
H	2.03176100	-1.25443000	-2.56299400	O	-6.83718500	0.24082600	-0.54193400
H	3.07199200	-2.24627400	-3.58986600	C	-5.23264900	-1.05847700	1.10241800
H	1.82886900	-3.02136400	-2.60985200	C	-5.38654100	-2.24975700	0.39691500
C	3.84958200	-0.30746800	3.19816600	C	-4.58667700	-1.03818500	2.33732400
H	4.65184700	0.26031000	2.72069700	C	-4.84722500	-3.41947800	0.91912800
C	2.96993100	0.69451700	3.95248500	H	-5.92519700	-2.25912300	-0.54521300
H	2.16879900	0.19843500	4.51332900	C	-4.04637400	-2.21616500	2.83932900
H	3.57170700	1.25898800	4.67401600	H	-4.51940600	-0.11134800	2.89822100
H	2.51523500	1.40591800	3.25334300	C	-4.14210400	-3.41537000	2.12652900
C	4.50798000	-1.30133300	4.16589000	H	-4.95885300	-4.34911900	0.36866600
H	5.08380800	-0.77046400	4.93268900	H	-3.53374900	-2.19983300	3.79722300
H	3.75286500	-1.91552500	4.67090900	C	-3.46455700	-4.66129100	2.63127000
H	5.18836800	-1.97403000	3.63336600	H	-3.48859500	-4.71748000	3.72366700
Zn	-1.03983300	-1.38264700	-2.61057900	H	-3.93030500	-5.56508900	2.22815800
Cl	-0.18238900	0.46588700	-3.43214900	H	-2.41090800	-4.66327800	2.32404500
Cl	-1.03693000	-3.57449100	-2.87332300	C	-3.46647600	3.59899900	-0.50096800
				H	-3.56496500	3.44197700	-1.58079500
<b>3-Ts1-b</b>				H	-4.47415200	3.54561300	-0.07585700
Zero-point correction= 1.041507 (Hartree/Particle)				H	-3.00756400	4.57111400	-0.31330600
Thermal correction to Energy= 1.106690				C	-4.30948700	1.88319700	-3.80061100
Thermal correction to Enthalpy= 1.107634				H	-4.91391000	1.32028100	-4.52250200
Thermal correction to Gibbs Free Energy= 0.940603				H	-5.00819200	2.46591400	-3.18687900
Sum of electronic and zero-point Energies= -3923.595189				H	-3.66440300	2.57040800	-4.35320300
Sum of electronic and thermal Energies= -3923.530005				Pd	1.94811100	0.14160100	-1.60058600
Sum of electronic and thermal Enthalpies= -3923.529061				P	3.70076200	0.30958600	-0.08177300
Sum of electronic and thermal Free Energies= -3923.696093				C	3.50684700	1.89094400	0.96938000
HF(ωb97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])= -3925.351407				C	5.40392900	0.33875400	-0.95912300
N	-4.39779500	0.84781900	-0.65288300	C	5.78048500	-1.11374300	-1.29190800
C	-3.15137700	1.07394800	0.06055900	H	5.97954100	-1.71172200	-0.39736200
H	-3.24168500	0.81518600	1.12093200	H	4.98973700	-1.60248700	-1.86796500
H	-2.35592800	0.42842300	-0.33047800	H	6.68784400	-1.11683400	-1.90908500
C	-2.63937100	2.49714000	0.05552600	C	5.19020500	1.07648300	-2.29690900
C	-4.27641800	0.11088800	-1.92751100	H	6.12196600	1.04661500	-2.87699400
H	-5.28954700	-0.07891100	-2.28696900	H	4.39652000	0.60421000	-2.88532600
H	-3.77254000	-0.84915200	-1.75904900	H	4.91624700	2.12528600	-2.15715700
C	-3.50707400	0.94724200	-2.93310400	C	6.58856600	1.00376100	-0.24199700
C	-2.19589600	0.85811800	-2.94160700	H	7.46682900	0.95128200	-0.89824000
C	-0.91962800	0.76296600	-2.74769700	H	6.40908300	2.06098000	-0.03176400
C	0.07050600	1.28364000	-1.79829200	H	6.86344200	0.50574400	0.69105100
C	0.29345100	-0.00811400	-3.05880600	C	3.65054300	3.11560400	0.05289300
H	-0.14733500	1.07890200	-0.75005100	H	3.32390000	4.01309900	0.59395000
H	0.48328000	2.26863800	-2.01412400	H	4.68532700	3.28655800	-0.25758600
H	0.83006600	0.30256800	-3.95617100	H	3.02753300	3.02321900	-0.84338800
H	0.23091100	-1.08451500	-2.88181000	C	4.43313200	2.03746500	2.18546700



C	2.07372300	3.32496800	2.24569700	H	-6.20654800	-0.72155100	-0.10319700
C	0.18677100	5.30817000	1.72667000	H	-6.85203100	-0.31794500	-1.70354000
H	1.26474400	5.64408100	-0.11221300	C	-3.81947300	-0.33145800	1.23329500
C	1.06294500	3.58902800	3.16096700	C	-3.06782600	-1.49160200	1.51300400
H	2.82478700	2.56853700	2.44900300	C	-4.86201100	0.01915400	2.10400200
C	0.10300300	4.57559900	2.91441500	C	-3.42721400	-2.27170500	2.62156100
H	-0.54140900	6.08954600	1.52631600	C	-5.18893300	-0.75294000	3.21007500
H	1.01773800	3.01577000	4.08292900	H	-5.43733100	0.91665100	1.91101000
C	-1.00777600	4.81493600	3.90342100	C	-4.47122800	-1.91688200	3.46353000
H	-1.59564000	5.69956200	3.64276800	H	-2.86449400	-3.17938400	2.81721600
H	-1.68770800	3.95519800	3.93139100	H	-6.00359600	-0.45191500	3.86146800
H	-0.61332300	4.95386400	4.91528900	O	3.62307600	-0.47259600	0.26924200
C	4.49517600	0.42450200	-1.78595200	H	-4.72053400	-2.54548100	4.31289100
H	3.93105700	0.57395100	-2.71305300	C	-1.88042400	-2.00285800	0.73132600
H	5.12478400	1.31096900	-1.64875200	C	-2.08269000	-2.90901100	-0.34159400
H	5.12206200	-0.46782300	-1.83604400	C	-0.57789300	-1.87631800	1.29408200
C	2.52071600	2.74515900	-4.46500100	C	-0.98757200	-3.62787600	-0.84270800
H	2.24941400	3.74007800	-4.84080100	C	0.47206400	-2.59863200	0.73882900
H	3.53848200	2.82467600	-4.06090800	C	0.28914300	-3.48930100	-0.32316000
H	2.52999600	2.04834800	-5.30627900	H	-1.15330100	-4.33820000	-1.64878500
Pd	-1.75001800	-0.52955600	-1.49705800	H	1.45512200	-2.51442500	1.19571700
P	-3.47612800	0.62337300	-0.30685100	C	1.44522500	-4.32411800	-0.84426600
C	-5.15255800	0.89823900	-1.16274600	H	1.05774200	-4.95915400	-1.65136100
C	-2.74879000	2.26751100	0.30382600	C	2.55437000	-3.44837600	-1.44032800
C	-1.34905600	1.91100300	0.82402300	H	2.22319300	-2.93720000	-2.34929800
H	-1.41100000	1.25164700	1.69352500	H	2.83553200	-2.66185600	-0.72735900
H	-0.75117400	1.40979900	0.05348100	H	3.44796200	-4.03525600	-1.67625600
H	-0.82536100	2.82297600	1.13068900	C	1.99920600	-5.24477200	0.25280300
C	-2.58268200	3.23649300	-0.87586100	H	1.20722900	-5.87486100	0.67052100
H	-2.00396500	4.10608900	-0.53829600	H	2.77961400	-5.89702000	-0.15413400
H	-2.03268200	2.77180000	-1.69985400	H	2.43877000	-4.66994800	1.07571400
H	-3.53853900	3.60739500	-1.25800900	C	-0.32156100	-1.11502200	2.59101000
C	-3.50572600	2.95964700	1.44556000	H	-1.21908500	-0.53655800	2.83395100
H	-2.96756700	3.87860600	1.71284900	C	-0.07988700	-2.10311700	3.74505900
H	-4.52581300	3.24428800	1.17813600	H	0.83513700	-2.67982000	3.57257800
H	-3.54499500	2.33015600	2.33988900	H	0.03816900	-1.55970000	4.68918200
C	-4.85194400	1.20667500	-2.64158300	H	-0.91016100	-2.80591900	3.86028200
H	-5.79924100	1.33632200	-3.17991400	C	0.85749300	-0.14098600	2.50455800
H	-4.26949400	2.12317500	-2.77026100	H	0.70457600	0.58954400	1.70889900
H	-4.29923300	0.38878100	-3.11054600	H	0.95468200	0.40602000	3.44947600
C	-6.04315700	2.02115700	-0.61125300	H	1.80519000	-0.65733200	2.32531500
H	-5.57254100	3.00392700	-0.70010200	C	-3.48405300	-3.29409400	-0.80014300
H	-6.96962000	2.05310200	-1.19837100	H	-4.17971000	-2.55101500	-0.40287200
H	-6.33206300	1.86869200	0.43161200	C	-3.64984700	-3.31643100	-2.32318000
C	-5.92975000	-0.42772900	-1.11977400	H	-3.02993000	-4.08958700	-2.79044200
H	-5.35169900	-1.23976000	-1.57077000	H	-4.69269700	-3.53155800	-2.58324400

H	-3.37112800	-2.35162300	-2.76115300	H	-9.09324600	-1.71070300	3.65489200
C	-3.87270500	-4.64747600	-0.18611100	H	-8.05177800	-0.33978300	4.05551100
H	-4.89816100	-4.91409600	-0.46531600	H	-9.50013700	-0.08495900	3.07599100
H	-3.20606400	-5.44324100	-0.53762900	C	-2.17414100	0.14576900	-3.05506900
H	-3.81457600	-4.61631200	0.90676300	H	-1.41164200	-0.58520900	-2.76031500
Zn	4.71965800	-2.13008400	0.78880800	H	-3.00316100	-0.41065700	-3.50064400
Cl	6.31946100	-2.66548500	-0.62471700	H	-1.75517100	0.87155700	-3.75234100
Cl	3.89243100	-2.78558900	2.72644200	C	-1.20812300	-3.04144000	-1.96428000
<b>3-Ts2-b</b>				H	-1.24971100	-4.12609300	-1.78730600
Zero-point correction= 1.042570 (Hartree/Particle)				H	-1.96264400	-2.82700500	-2.73285700
Thermal correction to Energy= 1.107325				H	-0.21444100	-2.79963200	-2.35360600
Thermal correction to Enthalpy= 1.108269				Pd	1.53253500	-0.26690500	0.90334700
Thermal correction to Gibbs Free Energy= 0.940217				P	2.62710000	1.68766500	0.35678900
Sum of electronic and zero-point Energies= -3923.569677				C	2.88518200	2.88977400	1.81982500
Sum of electronic and thermal Energies=-3923.504922				C	1.78089500	2.57345800	-1.10196100
Sum of electronic and thermal Enthalpies= -3923.503978				C	1.19149000	1.47370500	-2.00703800
Sum of electronic and thermal Free Energies= -3923.672031				H	1.93143800	0.72830800	-2.30263500
HF(ωb97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])= -3925.329990				H	0.38899800	0.92619200	-1.50866600
N	-3.67295900	-1.30561100	-1.03962300	H	0.78692600	1.93755500	-2.91517900
C	-3.40602600	0.08724300	-0.75368700	C	0.60696600	3.44111300	-0.61576800
H	-4.32580600	0.65691700	-0.56810000	H	0.03200100	3.76723200	-1.49079600
H	-2.83308400	0.16752300	0.17711300	H	-0.05459500	2.87596500	0.05013500
C	-2.63072900	0.83258300	-1.82107000	H	0.92034300	4.34344800	-0.08721200
C	-2.92517000	-2.30696200	-0.24423000	C	2.72634300	3.45230900	-1.93340900
H	-3.38802000	-3.27690500	-0.44464900	H	2.15436200	3.91785700	-2.74492900
H	-3.02771500	-2.07579600	0.82440300	H	3.17080300	4.26061400	-1.34499800
C	-1.46995800	-2.29019000	-0.67761200	H	3.53410800	2.87085700	-2.38665300
C	-0.51727100	-1.64406900	-0.00797100	C	1.57346000	2.95982600	2.62362200
C	-0.53301700	-0.98374600	1.25855200	H	1.72282500	3.62140100	3.48541300
C	-0.12910800	-1.55368200	2.46890400	H	0.73064000	3.35481900	2.05182000
C	-0.36274300	0.46784700	1.21458100	H	1.29833400	1.97164300	3.00087000
S	-5.19022000	-1.65565700	-1.62518300	C	3.32545800	4.32105400	1.46980200
O	-5.47984700	-0.60605000	-2.59422100	H	2.63005300	4.83374700	0.80250200
O	-5.18734700	-3.06010000	-1.99313100	H	3.36939300	4.90501200	2.39717400
C	-6.28802200	-1.43224200	-0.24509500	H	4.32336900	4.36014800	1.02857800
C	-6.38900100	-2.43822500	0.71428800	C	3.94228700	2.26546500	2.74705300
C	-6.97081100	-0.22847800	-0.09450500	H	3.63688900	1.26851200	3.07679200
C	-7.17411000	-2.22224800	1.83865700	H	4.92737600	2.19340800	2.27725600
H	-5.87454800	-3.38260700	0.56962200	H	4.04028700	2.89291200	3.64132800
C	-7.75224300	-0.03019600	1.03836500	C	4.34883300	1.26133900	-0.18796000
H	-6.90634200	0.52908900	-0.86856700	C	4.75743400	-0.08505900	-0.27207700
C	-7.85848400	-1.01577700	2.02251700	C	5.31081100	2.25575000	-0.41733300
H	-7.26121200	-3.00574900	2.58653300	C	6.11083900	-0.37741500	-0.48060100
H	-8.28965400	0.90651700	1.15728200	C	6.64498200	1.95163300	-0.65424900
C	-8.67485500	-0.77733100	3.26644000	C	7.05542000	0.62309300	-0.65763100
				H	6.41163000	-1.41974500	-0.53019400



H	7.35901400	2.75155900	-0.82357600
O	-2.35539100	2.02578700	-1.64662300
H	-0.05170400	-0.94136400	3.36142200
H	-0.01191400	-2.62602400	2.57589100
H	-0.73327700	0.99228000	0.33879800
H	-0.48896900	1.02575900	2.13889900
C	3.82665900	-1.25900500	-0.21568600
C	3.50143200	-1.84076100	1.04359300
C	3.44891800	-1.91091600	-1.41331300
C	2.71230800	-3.00345700	1.06838900
C	2.67171400	-3.06272200	-1.30844600
C	2.27484400	-3.62067500	-0.09700100
H	2.47983000	-3.44775300	2.03090100
H	2.36041500	-3.55919300	-2.22646100
C	3.89063400	-1.58246400	-2.84971200
H	3.00334500	-1.78459000	-3.46411900
C	4.97350700	-2.59147600	-3.27826400
H	4.64659800	-3.62550400	-3.13358200
H	5.22684300	-2.45527400	-4.33577700
H	5.88754600	-2.44160400	-2.69202400
C	4.36260500	-0.17466500	-3.23878500
H	3.72031000	0.61670600	-2.85489700
H	5.38057100	0.03362600	-2.90229700
H	4.35765400	-0.10318500	-4.33224400
H	5.01765100	3.29660200	-0.41407000
H	8.09796900	0.36673700	-0.81903200
C	1.51495800	-4.93460800	-0.08851500
H	1.01744100	-5.02050300	-1.06300200
C	2.50873700	-6.10062200	0.03644900
H	3.03521900	-6.05484700	0.99763600
H	1.98812600	-7.06326900	-0.01966300
H	3.26058100	-6.06826500	-0.75945600
C	0.42939900	-5.02209700	0.98587200
H	0.85483400	-4.99293100	1.99660100
H	-0.28069900	-4.19776800	0.88073400
H	-0.11460200	-5.96849100	0.89143900
C	4.24909800	-1.42737500	2.31151100
H	4.63831800	-0.41742800	2.15783800
C	3.39889700	-1.40876900	3.58498100
H	3.04059900	-2.40881000	3.85348300
H	4.00007700	-1.04079600	4.42418100
H	2.52216900	-0.76429900	3.47014000
C	5.45832200	-2.35850400	2.49852800
H	6.04752700	-2.05178600	3.36988800
H	5.12837600	-3.39207400	2.65566100
H	6.11444100	-2.34508300	1.62293800

Zn	-2.61862300	3.53037300	-0.28250600
Cl	-3.02688100	2.73223800	1.73752000
Cl	-2.49267200	5.48626700	-1.26824300

### 3-Int3-b

Zero-point correction= 1.043305 (Hartree/Particle)

Thermal correction to Energy= 1.108795

Thermal correction to Enthalpy= 1.109739

Thermal correction to Gibbs Free Energy= 0.938941

Sum of electronic and zero-point Energies= -3923.615554

Sum of electronic and thermal Energies=-3923.550064

Sum of electronic and thermal Enthalpies=-3923.549119

Sum of electronic and thermal Free Energies=-3923.719918

HF(ωb97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])=-3924.658858

N	2.62685000	2.59297700	-1.20345000
C	2.36873500	1.29415400	-0.60922400
H	1.99011200	1.34958500	0.41566500
H	1.58977200	0.80511400	-1.20941000
C	3.54848600	0.35783000	-0.64049600
C	1.57477800	3.09928700	-2.10731400
H	1.81361700	4.14391300	-2.32161100
H	0.59767600	3.05224500	-1.60637000
C	1.56136300	2.29027900	-3.39180800
C	0.77836900	1.23616700	-3.47488400
C	-0.12021000	0.29368700	-3.27653300
C	-0.02525100	-1.01078300	-2.56352300
C	-1.59619100	0.45154800	-3.32300200
H	0.83216600	-1.17339600	-1.90444500
H	-0.22372200	-1.88116400	-3.19600300
H	-2.09369200	-0.21289300	-4.03752200
H	-1.99002400	1.46663400	-3.36894400
S	3.36150900	3.67456100	-0.16174300
O	4.41182500	2.90518300	0.49187900
O	3.64219800	4.87718100	-0.92344300
C	2.12849200	4.06207800	1.06357700
C	1.19176900	5.05800800	0.79799000
C	2.07372300	3.32496800	2.24569700
C	0.18677100	5.30817000	1.72667000
H	1.26474400	5.64408100	-0.11221300
C	1.06294500	3.58902800	3.16096700
H	2.82478700	2.56853700	2.44900300
C	0.10300300	4.57559900	2.91441500
H	-0.54140900	6.08954600	1.52631600
H	1.01773800	3.01577000	4.08292900
C	-1.00777600	4.81493600	3.90342100
H	-1.59564000	5.69956200	3.64276800

H	-1.68770800	3.95519800	3.93139100	H	-6.00359600	-0.45191500	3.86146800
H	-0.61332300	4.95386400	4.91528900	O	3.62307600	-0.47259600	0.26924200
C	4.49517600	0.42450200	-1.78595200	H	-4.72053400	-2.54548100	4.31289100
H	3.93105700	0.57395100	-2.71305300	C	-1.88042400	-2.00285800	0.73132600
H	5.12478400	1.31096900	-1.64875200	C	-2.08269000	-2.90901100	-0.34159400
H	5.12206200	-0.46782300	-1.83604400	C	-0.57789300	-1.87631800	1.29408200
C	2.52071600	2.74515900	-4.46500100	C	-0.98757200	-3.62787600	-0.84270800
H	2.24941400	3.74007800	-4.84080100	C	0.47206400	-2.59863200	0.73882900
H	3.53848200	2.82467600	-4.06090800	C	0.28914300	-3.48930100	-0.32316000
H	2.52999600	2.04834800	-5.30627900	H	-1.15330100	-4.33820000	-1.64878500
Pd	-1.75001800	-0.52955600	-1.49705800	H	1.45512200	-2.51442500	1.19571700
P	-3.47612800	0.62337300	-0.30685100	C	1.44522500	-4.32411800	-0.84426600
C	-5.15255800	0.89823900	-1.16274600	H	1.05774200	-4.95915400	-1.65136100
C	-2.74879000	2.26751100	0.30382600	C	2.55437000	-3.44837600	-1.44032800
C	-1.34905600	1.91100300	0.82402300	H	2.22319300	-2.93720000	-2.34929800
H	-1.41100000	1.25164700	1.69352500	H	2.83553200	-2.66185600	-0.72735900
H	-0.75117400	1.40979900	0.05348100	H	3.44796200	-4.03525600	-1.67625600
H	-0.82536100	2.82297600	1.13068900	C	1.99920600	-5.24477200	0.25280300
C	-2.58268200	3.23649300	-0.87586100	H	1.20722900	-5.87486100	0.67052100
H	-2.00396500	4.10608900	-0.53829600	H	2.77961400	-5.89702000	-0.15413400
H	-2.03268200	2.77180000	-1.69985400	H	2.43877000	-4.66994800	1.07571400
H	-3.53853900	3.60739500	-1.25800900	C	-0.32156100	-1.11502200	2.59101000
C	-3.50572600	2.95964700	1.44556000	H	-1.21908500	-0.53655800	2.83395100
H	-2.96756700	3.87860600	1.71284900	C	-0.07988700	-2.10311700	3.74505900
H	-4.52581300	3.24428800	1.17813600	H	0.83513700	-2.67982000	3.57257800
H	-3.54499500	2.33015600	2.33988900	H	0.03816900	-1.55970000	4.68918200
C	-4.85194400	1.20667500	-2.64158300	H	-0.91016100	-2.80591900	3.86028200
H	-5.79924100	1.33632200	-3.17991400	C	0.85749300	-0.14098600	2.50455800
H	-4.26949400	2.12317500	-2.77026100	H	0.70457600	0.58954400	1.70889900
H	-4.29923300	0.38878100	-3.11054600	H	0.95468200	0.40602000	3.44947600
C	-6.04315700	2.02115700	-0.61125300	H	1.80519000	-0.65733200	2.32531500
H	-5.57254100	3.00392700	-0.70010200	C	-3.48405300	-3.29409400	-0.80014300
H	-6.96962000	2.05310200	-1.19837100	H	-4.17971000	-2.55101500	-0.40287200
H	-6.33206300	1.86869200	0.43161200	C	-3.64984700	-3.31643100	-2.32318000
C	-5.92975000	-0.42772900	-1.11977400	H	-3.02993000	-4.08958700	-2.79044200
H	-5.35169900	-1.23976000	-1.57077000	H	-4.69269700	-3.53155800	-2.58324400
H	-6.20654800	-0.72155100	-0.10319700	H	-3.37112800	-2.35162300	-2.76115300
H	-6.85203100	-0.31794500	-1.70354000	C	-3.87270500	-4.64747600	-0.18611100
C	-3.81947300	-0.33145800	1.23329500	H	-4.89816100	-4.91409600	-0.46531600
C	-3.06782600	-1.49160200	1.51300400	H	-3.20606400	-5.44324100	-0.53762900
C	-4.86201100	0.01915400	2.10400200	H	-3.81457600	-4.61631200	0.90676300
C	-3.42721400	-2.27170500	2.62156100	Zn	4.71965800	-2.13008400	0.78880800
C	-5.18893300	-0.75294000	3.21007500	Cl	6.31946100	-2.66548500	-0.62471700
H	-5.43733100	0.91665100	1.91101000	Cl	3.89243100	-2.78558900	2.72644200
C	-4.47122800	-1.91688200	3.46353000				
H	-2.86449400	-3.17938400	2.81721600				

3-Ts3-b

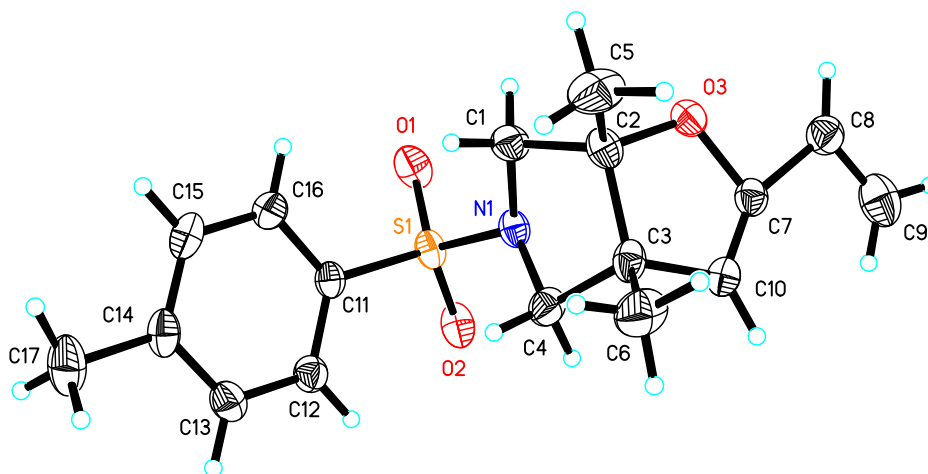
S250

Zero-point correction= 1.044232 (Hartree/Particle)				H	-2.48104200	-1.09585000	4.90255500
Thermal correction to Energy= 1.108023				Pd	1.31109900	0.14721100	1.06769400
Thermal correction to Enthalpy= 1.108967				P	3.44816000	-0.25473400	0.04190400
Thermal correction to Gibbs Free Energy= 0.946707				C	3.70856600	-1.69336200	-1.17326200
Sum of electronic and zero-point Energies= -3923.585970				C	4.70677700	-0.37510600	1.47309400
Sum of electronic and thermal Energies=-3923.522179				C	4.17540200	0.48317600	2.64004700
Sum of electronic and thermal Enthalpies= -3923.521235				H	3.87942500	1.48909100	2.34105100
Sum of electronic and thermal Free Energies= -3923.683495				H	3.30489500	0.01649000	3.10659300
HF(ωb97xd/6-311+G(d,p)/LanL2dz, SMD[toluene])= -3925.337988				H	4.96118400	0.57613100	3.40048000
N	-4.03004900	-1.46875000	0.50391700	C	4.77211600	-1.81831900	2.00150900
C	-2.74042800	-1.37197000	-0.14910100	H	5.34224800	-1.81836000	2.93872300
H	-2.89981900	-1.52530700	-1.22323100	H	3.77653600	-2.21575600	2.22337200
H	-2.24221900	-0.40566300	-0.01308800	H	5.27723400	-2.50397700	1.31734900
C	-1.80580600	-2.48940300	0.25528400	C	6.12017400	0.10185900	1.11188100
C	-4.20920500	-1.11654100	1.91601300	H	6.77229900	-0.02277400	1.98523500
H	-5.00922900	-1.75179900	2.30681800	H	6.56097600	-0.47406000	0.29289300
H	-4.56416300	-0.07481600	2.00938000	H	6.13611100	1.16020600	0.83460800
C	-2.98389400	-1.23174000	2.80871300	C	3.00294900	-2.90937900	-0.55278300
C	-1.72576200	-1.27809400	2.40796200	H	2.91717400	-3.69307900	-1.31648900
C	-0.45350800	-0.88713600	2.57786900	H	3.51999400	-3.34804300	0.30064800
C	-0.06685700	0.53157100	2.57652100	H	2.01419200	-2.59176900	-0.19587300
C	0.84048900	-1.52682100	2.26910900	C	5.14753300	-2.08609800	-1.53828100
S	-5.37196200	-1.31039600	-0.47017100	H	5.76754900	-2.30819800	-0.66694200
O	-5.09010100	-2.04057900	-1.69419300	H	5.11305000	-2.99456900	-2.15208500
O	-6.52238900	-1.61243100	0.36296500	H	5.64687100	-1.32054700	-2.13696500
C	-5.44446200	0.41970100	-0.89309800	C	2.94958500	-1.34564200	-2.46385200
C	-6.26252500	1.27551200	-0.16161700	H	1.88744100	-1.18096600	-2.26553100
C	-4.65030100	0.90531000	-1.93106200	H	3.36123000	-0.46256700	-2.96235800
C	-6.28337500	2.62928100	-0.47850500	H	3.01345200	-2.19199200	-3.15701300
H	-6.88768500	0.87521600	0.62943300	C	3.87656400	1.27010200	-0.91956400
C	-4.67488000	2.26315100	-2.22660500	C	2.96474600	2.34269200	-1.00720100
H	-4.04534000	0.22390700	-2.52059600	C	5.07286800	1.36117800	-1.64646600
C	-5.49557700	3.14256800	-1.51213000	C	3.26166000	3.42060800	-1.85173400
H	-6.92892100	3.29854000	0.08413900	C	5.36068600	2.44357300	-2.46710100
H	-4.06130200	2.64257300	-3.03971800	H	5.80464700	0.56819200	-1.56992800
C	-5.56540900	4.60306500	-1.87622300	C	4.43868300	3.47733400	-2.58368900
H	-5.67296700	5.23083600	-0.98649100	H	2.54912300	4.23869200	-1.91178800
H	-4.66921900	4.92636100	-2.41373000	H	6.29675300	2.47231900	-3.01604900
H	-6.42891200	4.79569000	-2.52374700	O	-0.65443900	-2.46182000	-0.23220400
C	-2.35641200	-3.77685300	0.80014000	H	0.61588400	0.80919900	3.38702400
H	-1.59375100	-4.29602200	1.38616700	H	-0.83347900	1.27459600	2.38086800
H	-3.25770100	-3.63873800	1.39215200	H	1.55794300	-1.46990700	3.09115300
H	-2.61982300	-4.40227400	-0.06659800	H	0.83861900	-2.50427500	1.78952700
C	-3.36628800	-1.21751000	4.27482800	H	4.63857500	4.32688800	-3.22946000
H	-4.06522300	-0.39697700	4.48711600	C	1.66356600	2.47079000	-0.25850600
H	-3.87075900	-2.14971000	4.56071100	C	0.47337900	1.99484000	-0.88277900

C	1.55651000	3.34296000	0.85576400	H	3.18076200	6.25783300	1.79787700
C	-0.77108600	2.34296900	-0.35611600	H	2.51496100	5.87068300	0.20219500
C	0.27847100	3.61685300	1.35700900	C	4.15667400	3.88637700	1.22057700
C	-0.89086700	3.14849400	0.77053000	H	4.42159800	2.83203900	1.19628200
H	-1.66756800	1.99916400	-0.86529600	H	4.45498900	4.31597100	0.26115400
H	0.19427300	4.25141900	2.23717600	H	4.76122700	4.36470400	1.99913900
C	-2.24872800	3.56209900	1.30883100	C	0.51593200	1.30615800	-2.24005600
H	-2.09170100	3.96761000	2.31694700	C	-0.41345500	0.09596500	-2.34457700
C	-3.23446900	2.39367700	1.42078200	H	-0.24535200	-0.43093400	-3.29004800
H	-3.47416800	1.97675800	0.43709900	H	-0.24896500	-0.61226600	-1.52791700
H	-2.83675900	1.58542400	2.04257900	H	-1.46859100	0.39690000	-2.32493300
H	-4.17657300	2.73511300	1.86295000	C	0.19374500	2.32655300	-3.34335900
C	-2.83201800	4.68206900	0.43517300	H	-0.82010700	2.72558700	-3.21722400
H	-3.80259300	5.01228200	0.82289700	H	0.89247600	3.16884900	-3.33105900
H	-2.16025400	5.54602200	0.39815500	H	0.25200700	1.84992900	-4.32790700
H	-2.98175700	4.32369100	-0.58949200	H	1.53573900	0.95713600	-2.41031300
C	2.67708400	4.15500600	1.53203700	Zn	0.41117900	-4.10732000	-0.79160300
H	2.54358900	3.98006200	2.60858300	Cl	0.36416400	-4.21139400	-3.00092100
C	2.42982600	5.65614400	1.27406700	Cl	0.99328500	-5.42841500	0.89767900
H	1.44107000	5.98500600	1.60390300				

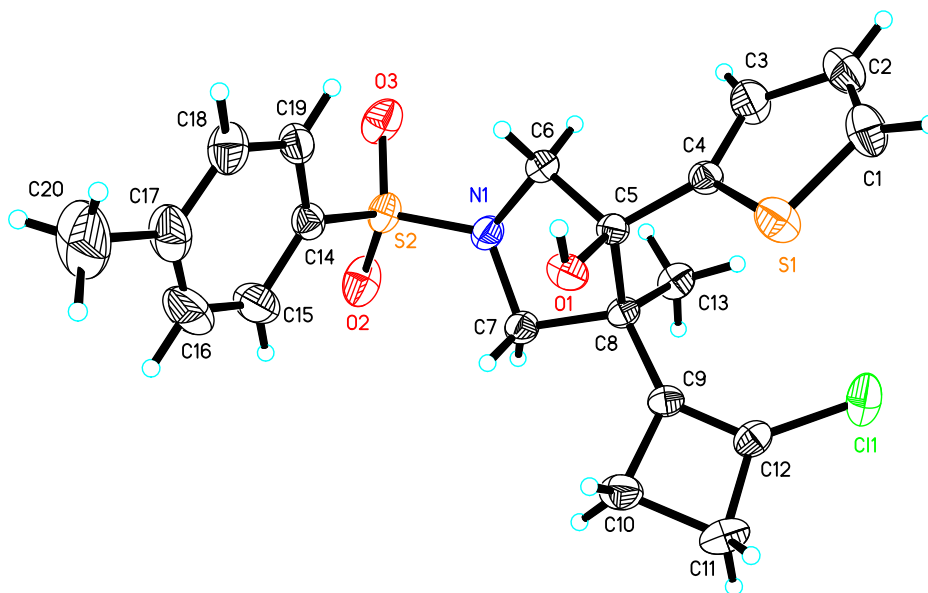
## 11. X-Ray structures

### (a) Product 3a



The crystal data of **3a** have been deposited in CCDC with number 2206931. Empirical Formula:  $C_{17}H_{21}NO_3S$ ; Formula Weight: 319.41; Crystal Color, Habit: colorless; Crystal Dimensions: 0.180 x 0.150 x 0.110 mm<sup>3</sup>; Crystal System: Monoclinic; Lattice Parameters:  $a = 10.3144(3)$  Å,  $\alpha = 90$  deg.  $b = 12.2204(4)$  Å,  $\beta = 92.9460(10)$  deg.  $c = 13.0932(4)$  Å,  $\gamma = 90$  deg.;  $V = 1648.17(9)$  Å<sup>3</sup>; Space group: P 21/c;  $Z = 4$ ;  $D_{calc} = 1.287$  g/cm<sup>3</sup>;  $F_{000} = 680$ ; Diffractometer: Rigaku AFC7R; Residuals: R;  $R_w$ : 0.0479, 0.1211.

**(b) Product 14**



The crystal data of **14** have been deposited in CCDC with number 2246469. Empirical Formula:  $C_{20}H_{22}ClNO_3S_2$ ; Formula Weight: 423.95; Crystal Color, Habit: colorless; Crystal Dimensions: 0.200 x 0.150 x 0.120 mm<sup>3</sup>; Crystal System: Monoclinic; Lattice Parameters:  $a = 19.7752(8)$  Å,  $\alpha = 90$  deg.  $b = 9.1254(3)$  Å,  $\beta = 96.4770(10)$  deg.  $c = 11.5285(4)$  Å,  $\gamma = 90$  deg.;  $V = 2067.12(13)$  Å<sup>3</sup>; Space group: P 21/c;  $Z = 4$ ;  $D_{calc} = 1.362$  g/cm<sup>3</sup>;  $F_{000} = 888$ ; Diffractometer: Rigaku AFC7R; Residuals:  $R$ ;  $R_w$ : 0.0429, 0.1105.

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