

# **Asymmetric Synthesis of Azepine-Fused Cyclobutanes from Yne-Methylenecyclopropanes Involving Cyclopropanation/C-C Cleavage/Wagner-Meerwein Rearrangement and Reaction Mechanism**

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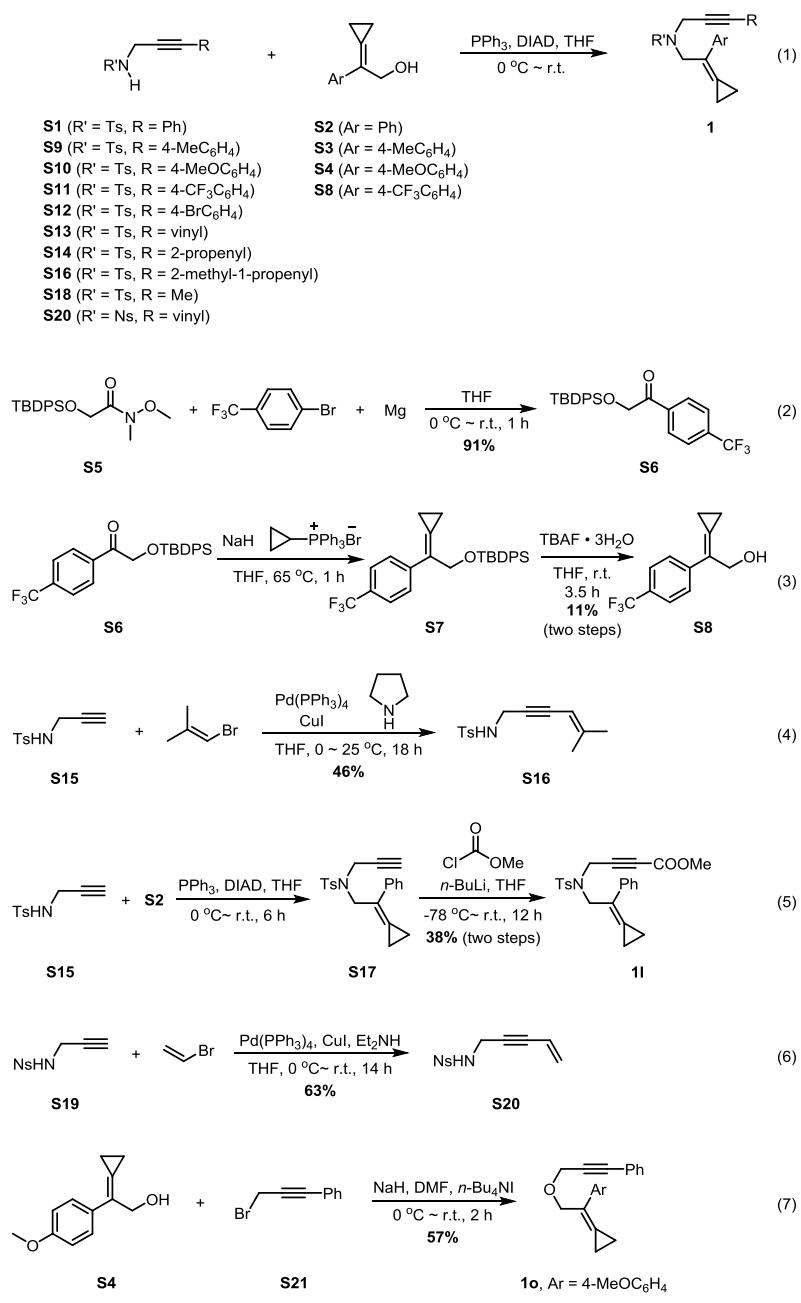
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## I. Scheme for Synthesis of Substrates

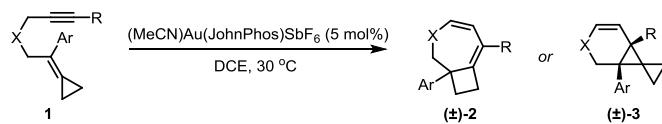


r.t. = room temperature; TBDPS = *t*-butyldiphenylsilyl.

**Scheme S1** Synthesis of substrates

## II. Racemic Product Synthesis

### Racemic product synthesis



#### General procedure A: (5 mol % catalyst)

**General procedure of Au(I)-catalyzed cyclization/rearrangement reaction:** Under nitrogen, the commercially available  $(\text{MeCN})\text{Au}(\text{JohnPhos})\text{SbF}_6$  (7.8 mg, 10.1  $\mu\text{mol}$ ) was added to a flame-dried glassware containing **1** (0.2 mmol). Anhydrous DCE (4.0 ml) was added and the glassware was then immersed into an oil bath at 30 °C. The reaction was monitored by TLC. Upon completion, the reaction mixture was purified by flash column chromatography on silica gel to afford  $(\pm)\text{-2}$  or  $(\pm)\text{-3}$ .

Entry	Substrate	Product <sup>b</sup>	Entry	Substrate	Product <sup>b</sup>
1	<b>1a</b> , Ar = Ph	$(\pm)\text{-2a}$ , 96 %	9 <sup>c</sup>	<b>1i</b> , R <sup>1</sup> = R <sup>2</sup> = H	$(\pm)\text{-2i}$ , 68 %
2	<b>1b</b> , Ar = 4-MeC <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2b}$ , 94 %	10	<b>1j</b> , R <sup>1</sup> = Me, R <sup>2</sup> = H	$(\pm)\text{-2j}$ , 90 %
3	<b>1c</b> , Ar = 4-MeOC <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2c}$ , 99 %	11 <sup>c</sup>	<b>1k</b> , R <sup>1</sup> = H, R <sup>2</sup> = Me	$(\pm)\text{-2k}$ , 94 %
4	<b>1d</b> , Ar = 4-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-3d}$ , 89 %	12	<b>1l</b> , R = CO <sub>2</sub> Me	N. R.
5	<b>1e</b> , R = 4-MeC <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2e}$ , 99 %	13 <sup>c</sup>	<b>1m</b> , R = Me	$(\pm)\text{-2m}$ + $(\pm)\text{-3m}$ : 82 % $(\pm)\text{-2m}$ / $(\pm)\text{-3m}$ = 1.3 / 1
6	<b>1f</b> , R = 4-MeOC <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2f}$ , 97 %	14	<b>1n</b>	$(\pm)\text{-2n}$ , 81 %
7	<b>1g</b> , R = 4-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2g}$ , 93 %	15	<b>1o</b> , Ar = 4-MeOC <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2o}$ , 60 %
8	<b>1h</b> , R = 4-BrC <sub>6</sub> H <sub>4</sub>	$(\pm)\text{-2h}$ , 97 %			

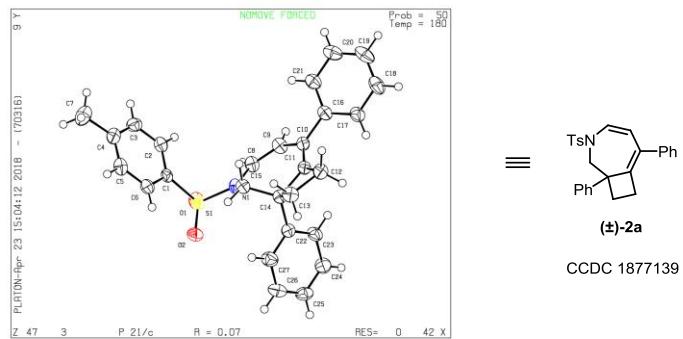
<sup>a</sup> Reaction conditions: 0.2 mmol **1**, 5 mol%  $(\text{MeCN})\text{Au}(\text{JohnPhos})\text{SbF}_6$ , DCE (0.05 M), 30 °C, 12 h; <sup>b</sup> isolated yields; <sup>c</sup> 1 h; N. R. = no reaction.

**Table S1** <sup>a</sup> Racemic product synthesis

### III. X-ray Crystal Analysis

Crystal compound ( $\pm$ )-**2a** was obtained by adding *n*-hexane to its dichloromethane solution and then stilling for several days.

#### Crystalllographic Data of Compound ( $\pm$ )-**2a**



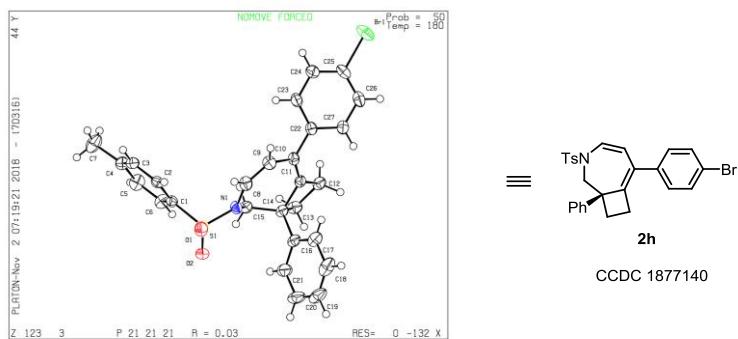
**Table S2** Crystal data and structure refinement for Compound ( $\pm$ )-**2a**.

Identification code	3
Empirical formula	C <sub>27</sub> H <sub>25</sub> NO <sub>2</sub> S
Formula weight	427.54
Temperature/K	179.99(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c
a/Å	12.7314(8)
b/Å	23.7964(15)
c/Å	7.2381(4)
α/°	90
β/°	90.855(5)
γ/°	90
Volume/Å <sup>3</sup>	2192.6(2)
Z	4
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.295
μ/mm <sup>-1</sup>	0.172
F(000)	904.0
Crystal size/mm <sup>3</sup>	0.2 × 0.1 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.884 to 54.968
Index ranges	-16 ≤ h ≤ 16, -30 ≤ k ≤ 29, -9 ≤ l ≤ 9
Reflections collected	21099
Independent reflections	4899 [R <sub>int</sub> = 0.0776, R <sub>sigma</sub> = 0.0626]
Data/restraints/parameters	4899/0/281
Goodness-of-fit on F <sup>2</sup>	1.007

Final R indexes [ $I \geq 2\sigma(I)$ ]       $R_1 = 0.0718$ ,  $wR_2 = 0.1452$   
 Final R indexes [all data]       $R_1 = 0.0993$ ,  $wR_2 = 0.1552$   
 Largest diff. peak/hole / e Å<sup>-3</sup>      0.50/-0.39

Crystal compound **2h** was obtained by adding *n*-hexane to its ether solution and then stilling for several days.

### Crystallographic Data of Compound **2h**



**Table S3** Crystal data and structure refinement for Compound **2h**.

Identification code	3
Empirical formula	C <sub>27</sub> H <sub>24</sub> BrNO <sub>2</sub> S
Formula weight	506.44
Temperature/K	180.00(10)
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	7.05990(10)
b/Å	15.7538(2)
c/Å	20.8421(3)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/Å <sup>3</sup>	2318.06(6)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.451
$\mu/\text{mm}^{-1}$	1.888
F(000)	1040.0
Crystal size/mm <sup>3</sup>	0.25 × 0.12 × 0.1
Radiation	Mo Kα ( $\lambda = 0.71073$ )
2Θ range for data collection/°	4.686 to 54.966
Index ranges	-9 ≤ h ≤ 9, -20 ≤ k ≤ 20, -27 ≤ l ≤ 27
Reflections collected	53482
Independent reflections	5320 [ $R_{\text{int}} = 0.0287$ , $R_{\text{sigma}} = 0.0136$ ]

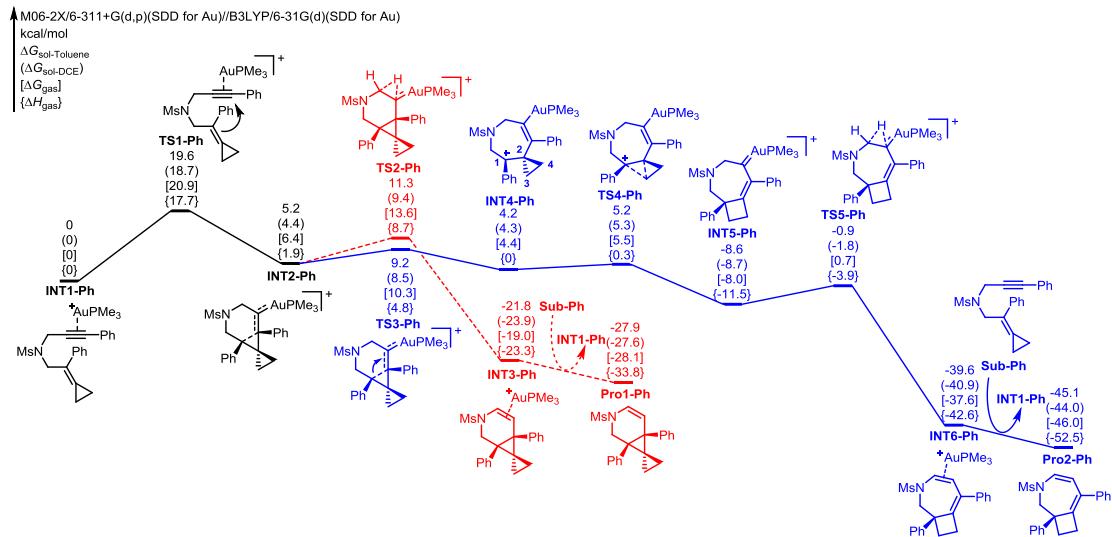
Data/restraints/parameters 5320/0/290  
Goodness-of-fit on  $F^2$  1.032  
Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0253$ ,  $wR_2 = 0.0659$   
Final R indexes [all data]  $R_1 = 0.0273$ ,  $wR_2 = 0.0669$   
Largest diff. peak/hole / e Å<sup>-3</sup> 0.77/-0.61  
Flack parameter -0.0053(16)

#### IV. DFT Calculations

1. The computed energy surface for the reaction of **1a**
2. Study of the rearrangement of the homoallylic cation
3. The computed energy surface for the reaction of the substrate used in Shi's work
4. The chemoselectivity of **1m**
5. Discussion of DFT functionals
6. The chemoselectivity of **1d**
7. Energy data
8. Cartesian coordinates of all stationary points

##### 1. The computed energy surface for the reaction of **1a**

Here we give all data from different calculation methods for reaction of **1a** in order to better understand factors affecting the reaction outcomes. As shown in **Figure S1**, the ring expansion (through **TS3-Ph**) has a lower activation energy than the direct [1,2]-hydride shift of **INT2-Ph** (through **TS2-Ph**) in  $\Delta G_{\text{sol-DCE}}$ ,  $\Delta G_{\text{gas}}$  and  $\Delta H_{\text{gas}}$ . These data are consistent with the experiment observation that only 3-azabicyclo[5.2.0]nonadiene product (**Pro2-Ph**) is found.

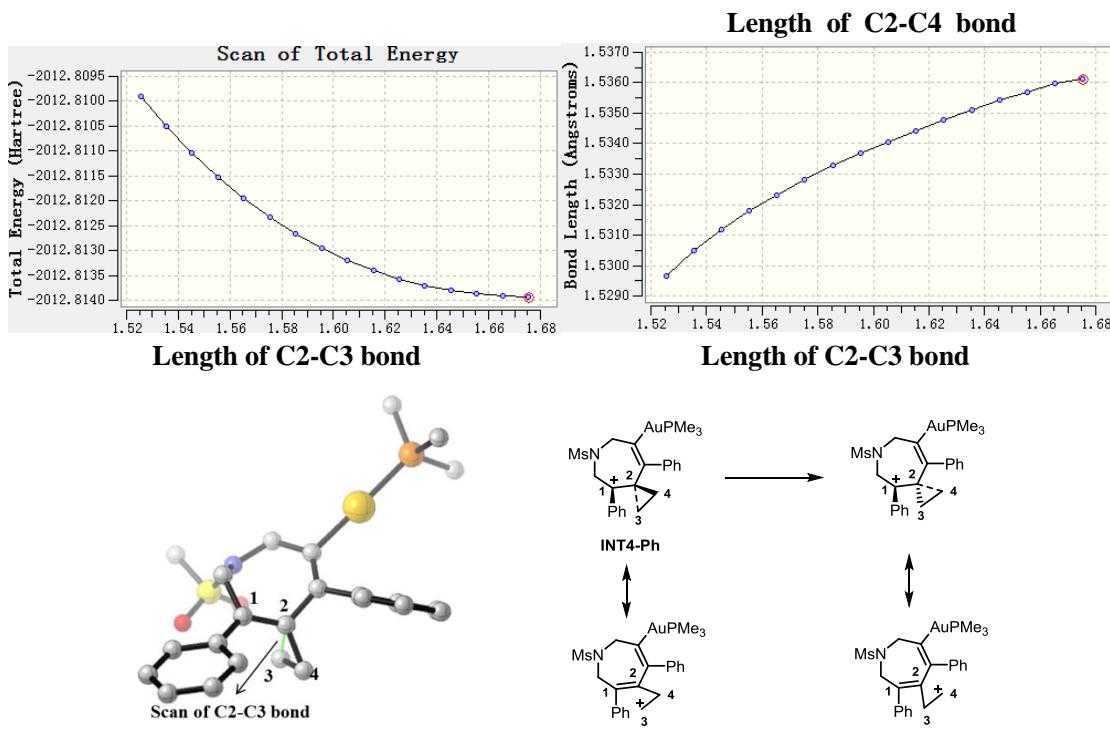


**Figure S1** Energy surface for the reaction of **1a**

##### 2. Study of the rearrangement of the homoallylic cation

Relaxed scans of potential energy surfaces at B3LYP/6-31G(d) (SDD for Au) level were then performed to locate another homoallylic cation at C4 (**Figure S2**). During the scan of the potential energy surface, only the single-point energy of each structure could be obtained. Due to this, we give single-point energies in the gas phase ( $\Delta E_{\text{gas}}$ ) to discuss processes.

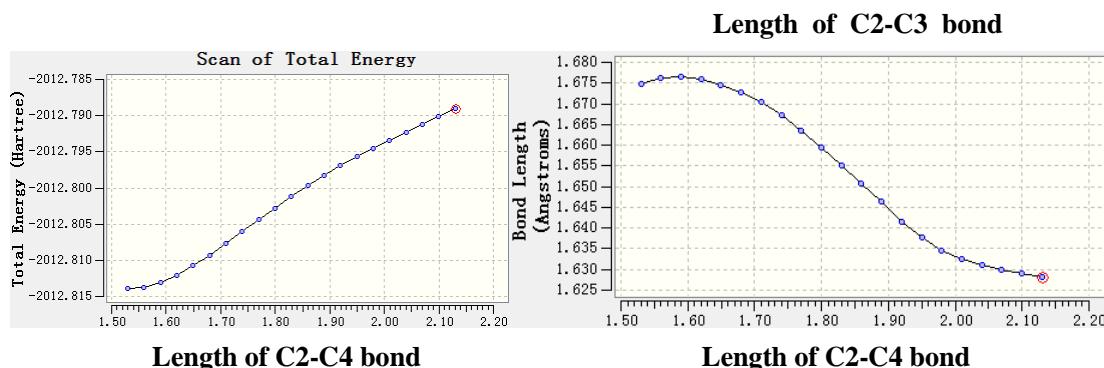
As shown in **Figure S2**, with the length of C2-C3 bond in **INT4-Ph** decrease (from 1.68 Å to 1.53 Å), the  $\Delta E_{\text{gas}}$  has an increase of 2.5 kcal/mol. Although C2-C3 bond becomes shorter, the C2-C4 bond is the same (from 1.54 Å to 1.53 Å). This can be attributed to the steric repulsion between the methylene group at C4 and phenyl group adjacent to C2.

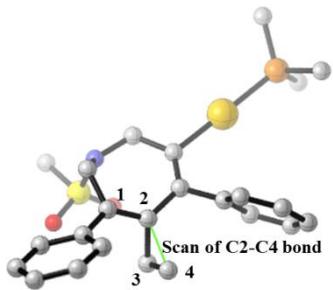


**Figure S2** The rearrangement of the homoallylic cation and scan of C2-C3 bond

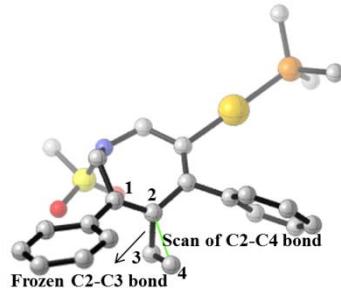
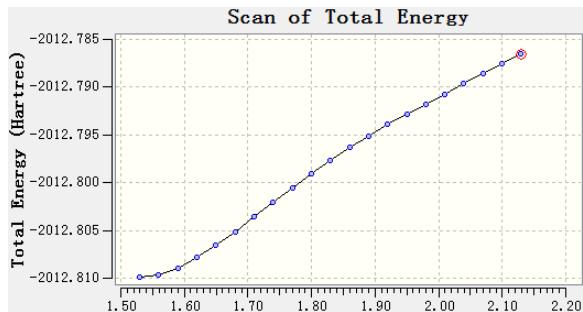
Based on the final structure in **Figure S2**, we sequentially scanned the length of C2-C4 bond. With its increase to 2.13 Å, the  $\Delta E_{\text{gas}}$  is an increase of 15.7 kcal/mol (**Figure S3**). During the scan, the C2-C3 bond will change from 1.67 Å to 1.63 Å, which is just a slight decrease. If we freeze the C2-C3 bond to 1.53 Å at this scan, a similar result of 14.4 kcal/mol in  $\Delta E_{\text{gas}}$  can be found (**Figure S4**).

From these two calculations, we can conclude that the formation of another homoallylic cation at C4 with the C2-C3 bond formation and the C2-C4 bond breaking in **INT4-Ph** has a rearrangement energy of 18.2 kcal/mol (2.5 kcal/mol + 15.7 kcal/mol). This process can be excluded because the Wagner-Meerwein rearrangement of **INT4-Ph** is faster, which has an activation energy of 1.0 kcal/mol. Therefore, there is no rearrangement of the homoallylic cation here.





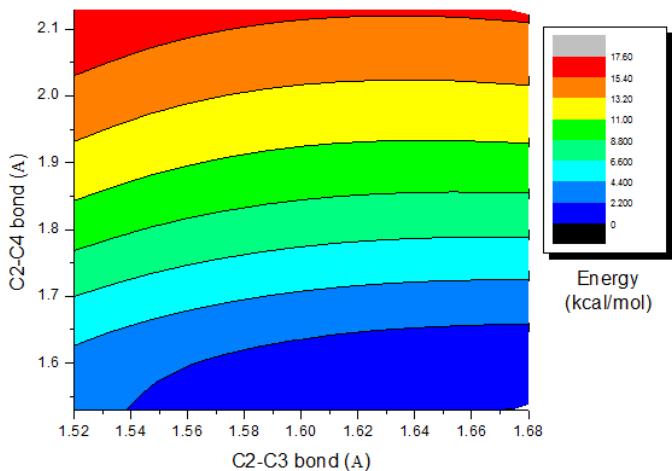
**Figure S3** Scan of C2-C4 bond



#### Length of C2-C4 bond

**Figure S4** Scan of C2-C4 bond with a fixed C2-C3 bond

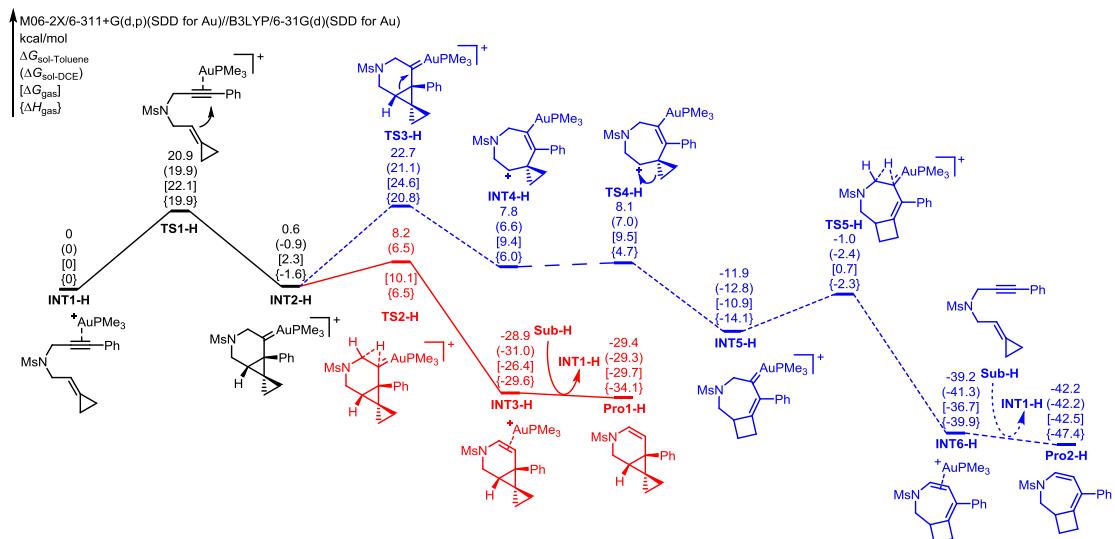
We also scanned the energy surface given in **Figure S5**. The energy rises to 17.6 kcal/mol with the C2-C3 bond decreasing and the C2-C4 bond increasing, which is also consistent with previous results.



**Figure S5** The scanned energy surface

### 3. The computed energy surface for the reaction of the substrate used in Shi's work

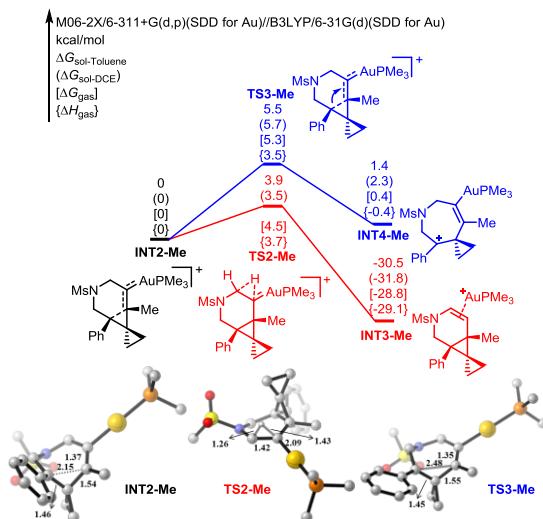
The full energy surface for MCP substrate without the aromatic group is given in **Figure S6**. Here we give all data from different calculation methods in order to better understand factors affecting the reaction outcomes. The ring expansion via **TS3-H** is disfavored compared to the direct [1,2]-hydride shift via **TS2-H**. The calculation results show that only cyclopropanation product (**Pro1-H**) will be observed in Shi's work, which is consistent with experiments.



**Figure S6** Energy surface for the reaction of the substrate used in Shi's work

#### 4. The chemoselectivity of **1m**

We also studied the reaction of substrate **1m**, which gave a mixture of two products **2m** and **3m** with a ratio of 1.3/1. Because both two chemoselectivity determination steps (through **TS2-Me** and **TS3-Me**) come from a same **INT2-Me**, we just discuss these two transition states here. The computed energy differences of **TS2-Me** and **TS3-Me** in  $\Delta G_{\text{gas}}$  and  $\Delta H_{\text{gas}}$  are only 0.7 kcal/mol and -0.2 kcal/mol respectively, which is consistent with the observed ratio of 1.3/1 for two products. However, the energy differences of them in  $\Delta G_{\text{sol-Toluene}}$  and  $\Delta G_{\text{sol-DCE}}$  are a little bigger, 1.6 kcal/mol and 2.3 kcal/mol respectively. It could be attributed to some errors in the solvation calculations.



**Figure S7** Chemoselectivity of **1m**

#### 5. Discussion of DFT functionals

Although it had been proved that the M06-2X functional was reliable in the study of late-transition-metal-catalyzed reactions (Au, Pt, and Ir)<sup>1</sup>. We still test several widely used functionals to validate this conclusion. The computed energy differences of **TS2-Me** and **TS3-Me** of substrate **1m** (Figure S7) in  $\Delta G_{\text{gas}}$  and  $\Delta H_{\text{gas}}$  are used to evaluate different functionals. The

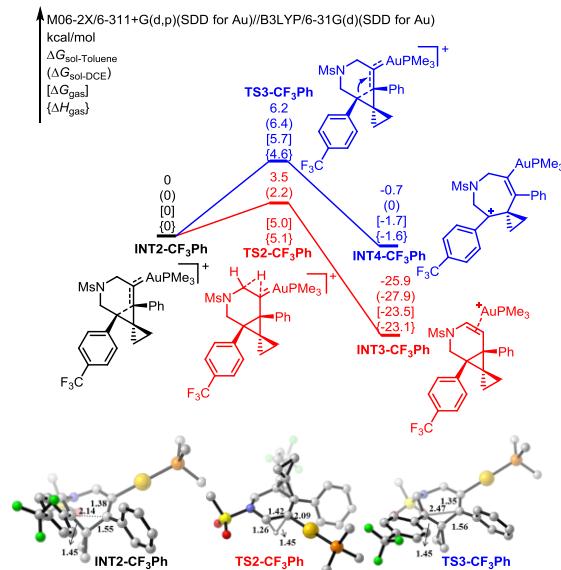
smaller the difference is, the more accurate the functional is. The results of single-point energy calculations in the gas phase are given in **Table S4**, in which the M06-2X functional performs best.

functional	$\Delta\Delta H_{\text{gas}}^{\ddagger}$ (TS3-Me – TS2-Me)	$\Delta\Delta G_{\text{gas}}^{\ddagger}$ (TS3-Me – TS2-Me)
M06-2X/6-311+G(d,p)	-0.2	0.7
M06-2X/6-311G(d,p) <sup>2</sup>	0.1	1.1
M06 <sup>3</sup> /6-311+G(d,p)	-3.1	-2.1
M06-L <sup>4</sup> /6-311+G(d,p)	-3.8	-2.9
B3LYP/6-311+G(d,p)	-8.0	-6.6
B3LYP-D3 <sup>5</sup> /6-311+G(d,p)	-9.8	-8.5
BMK <sup>6</sup> /6-311+G(d,p)	-5.0	-3.7

**Table S4** Results of single-point energy calculations in the gas phase

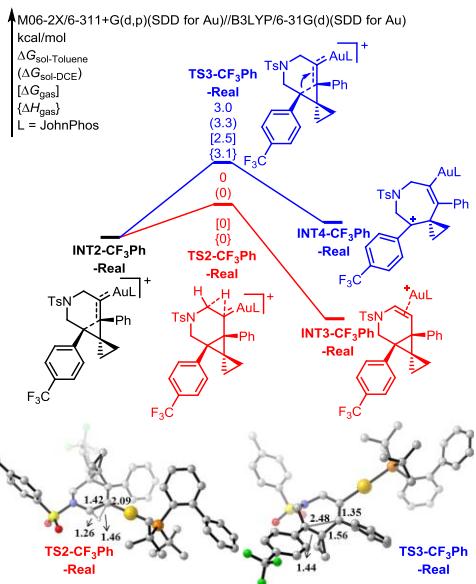
## 6. The chemoselectivity of **1d**

As shown in **Figure S8**, substrate **1d** also gives a non-classical cation intermediate **INT2-CF<sub>3</sub>Ph**. The electron-withdrawing CF<sub>3</sub> group in the aryl ring has an influence on this non-classical cation intermediate, in which a shorter elongated C-C bond of 2.14 Å is found in **INT2-CF<sub>3</sub>Ph** comparing to **INT2-Ph**. Comparing to a phenyl group in **INT4-Ph**, this electron-withdrawing CF<sub>3</sub> group also has less stabilization on the cation intermediate **INT4-CF<sub>3</sub>Ph** (-0.7 kcal/mol of **INT4-CF<sub>3</sub>Ph** from **INT2-CF<sub>3</sub>Ph** vs. -1.0 kcal/mol of **INT4-Ph** from **INT2-Ph** in  $\Delta G_{\text{sol-Toluene}}^{\ddagger}$ ). These make the expansion step become more difficult than the direct [1,2]-hydride shift (6.2 kcal/mol of **TS3-CF<sub>3</sub>Ph** vs. 3.5 kcal/mol of **TS2-CF<sub>3</sub>Ph** in  $\Delta G_{\text{sol-Toluene}}^{\ddagger}$ ), which can explain that only product **3d** was obtained experimentally.



**Figure S8** Chemoselectivity of **1d**

Because of small energy differences of **TS2-CF<sub>3</sub>Ph** and **TS3-CF<sub>3</sub>Ph** in  $\Delta G_{\text{gas}}$  and  $\Delta H_{\text{gas}}$  in **Figure S8**, we performed calculations using a real model of **1d**. In **Figure S9**, it gives results consistent with the experimental observation that only product **3d** was found.



**Figure S9** Chemoselectivity of 1d with a real model

7. Energy data <sup>a</sup>

	E <sup>b</sup>	H <sup>c</sup>	G <sup>d</sup>	E <sup>e</sup>	$\Delta E_{\text{sol-Toluene}}$	$\Delta E_{\text{sol-DCE}}$
<b>INT1-Ph</b>	-2012.811279	-2012.288116	-2012.395264	-2012.460546	-0.032500	-0.052238
<b>TS1-Ph</b>	-2012.785894	-2012.263684	-2012.365861	-2012.431314	-0.034456	-0.055750
<b>INT2-Ph</b>	-2012.813621	-2012.289670	-2012.389798	-2012.458282	-0.034265	-0.055397
<b>TS2-Ph</b>	-2012.785877	-2012.266080	-2012.365643	-2012.443264	-0.035964	-0.058787
<b>INT3-Ph</b>	-2012.838817	-2012.314256	-2012.414706	-2012.499084	-0.036755	-0.059906
<b>Sub-Ph</b>	-1416.052425	-1415.656317	-1415.740067	-1415.911617	-0.006933	-0.013240
<b>Pro1-Ph</b>	-1416.090738	-1415.693730	-1415.768485	-1415.966383	-0.006441	-0.012357
<b>TS3-Ph</b>	-2012.808021	-2012.285257	-2012.383643	-2012.452545	-0.034118	-0.055211
<b>INT4-Ph</b>	-2012.813928	-2012.289615	-2012.389676	-2012.461812	-0.032631	-0.052470
<b>TS4-Ph</b>	-2012.810217	-2012.287076	-2012.385808	-2012.460152	-0.032912	-0.052692
<b>INT5-Ph</b>	-2012.836267	-2012.311852	-2012.413396	-2012.480205	-0.033345	-0.053468
<b>TS5-Ph</b>	-2012.816469	-2012.295795	-2012.395559	-2012.464343	-0.035012	-0.056448
<b>INT6-Ph</b>	-2012.878479	-2012.352572	-2012.451669	-2012.531313	-0.035661	-0.057618
<b>Pro2-Ph</b>	-1416.132478	-1415.734084	-1415.807460	-1415.997669	-0.005474	-0.010149
<b>INT1-H</b>	-1781.762040	-1781.324642	-1781.419910	-1781.441852	-0.033051	-0.052646
<b>TS1-H</b>	-1781.733027	-1781.297178	-1781.388876	-1781.408623	-0.034972	-0.056108
<b>INT2-H</b>	-1781.761588	-1781.324071	-1781.413119	-1781.444546	-0.035717	-0.057599
<b>TS2-H</b>	-1781.741307	-1781.306813	-1781.396337	-1781.428611	-0.036084	-0.058174
<b>INT3-H</b>	-1781.804347	-1781.365444	-1781.455586	-1781.490629	-0.037039	-0.059729
<b>Sub-H</b>	-1185.004887	-1184.694606	-1184.766560	-1184.896016	-0.006145	-0.011614
<b>Pro1-H</b>	-1185.049798	-1184.738359	-1184.803336	-1184.951556	-0.005679	-0.010693
<b>TS3-H</b>	-1781.729284	-1781.294092	-1781.383329	-1781.406561	-0.035939	-0.058024
<b>INT4-H</b>	-1781.754136	-1781.315955	-1781.405899	-1781.433082	-0.035405	-0.056921
<b>TS4-H</b>	-1781.753607	-1781.316348	-1781.404018	-1781.434237	-0.035194	-0.056405
<b>INT5-H</b>	-1781.793214	-1781.354370	-1781.444580	-1781.465757	-0.034567	-0.055457

<b>TS5-H</b>	-1781.768954	-1781.333682	-1781.424221	-1781.443402	-0.035695	-0.057323
<b>INT6-H</b>	-1781.832427	-1781.392408	-1781.482745	-1781.508000	-0.036984	-0.059603
<b>Pro2-H</b>	-1185.084920	-1184.772043	-1184.836365	-1184.974026	-0.005714	-0.010789
<b>INT2-Me</b>	-1821.080334	-1820.612533	-1820.705470	-1820.746679	-0.034664	-0.055955
<b>TS2-Me</b>	-1821.055927	-1820.591910	-1820.683513	-1820.737012	-0.035624	-0.057670
<b>TS3-Me</b>	-1821.073098	-1820.606395	-1820.696499	-1820.740038	-0.034283	-0.055196
<b>INT3-Me</b>	-1821.114056	-1820.645762	-1820.738237	-1820.793553	-0.037264	-0.060833
<b>INT4-Me</b>	-1821.077443	-1820.609171	-1820.700941	-1820.747776	-0.032967	-0.052839
<b>INT2-CF<sub>3</sub>Ph</b>	-2349.840753	-2349.308513	-2349.418660	-2349.502938	-0.035549	-0.057781
<b>TS2-CF<sub>3</sub>Ph</b>	-2349.816170	-2349.287974	-2349.398311	-2349.490694	-0.037904	-0.062215
<b>TS3-CF<sub>3</sub>Ph</b>	-2349.833534	-2349.302717	-2349.411085	-2349.494236	-0.034767	-0.056653
<b>INT3-CF<sub>3</sub>Ph</b>	-2349.866249	-2349.333552	-2349.444364	-2349.540098	-0.039307	-0.064806
<b>INT4-CF<sub>3</sub>Ph</b>	-2349.840764	-2349.308300	-2349.418711	-2349.505698	-0.033945	-0.054958
<b>TS2-CF<sub>3</sub>Ph-Real</b>	-3239.488987	-3238.553705	-3238.710447	-3239.036451	-0.031570	-0.052392
<b>TS3-CF<sub>3</sub>Ph-Real</b>	-3239.500293	-3238.562770	-3238.720578	-3239.033691	-0.030801	-0.051038

<sup>a</sup> in a.u.

<sup>b</sup> single-point energies at the level of B3LYP/6-31G(d) (SDD for Au)

<sup>c</sup> enthalpies at the level of B3LYP/6-31G(d) (SDD for Au)

<sup>d</sup> Gibbs free energies at the level of B3LYP/6-31G(d) (SDD for Au)

<sup>e</sup> single-point energies at the level of M06-2X/6-311+G(d,p) (SDD for Au)

### The single-point energies for Figure S5

<b>2.13</b>	-2012.788649	-2012.788881	-2012.788997	-2012.788975	-2012.788793	-2012.788425	-2012.787843	-2012.787012	-2012.785895
<b>2.07</b>	-2012.790841	-2012.791065	-2012.7911701	-2012.791136	-2012.790941	-2012.790558	-2012.789958	-2012.789110	-2012.787977
<b>2.01</b>	-2012.793106	-2012.793313	-2012.793400	-2012.793346	-2012.793131	-2012.792727	-2012.792107	-2012.791239	-2012.790095
<b>1.95</b>	-2012.795486	-2012.795662	-2012.795716	-2012.795629	-2012.795379	-2012.794940	-2012.794281	-2012.793390	-2012.792220
<b>1.89</b>	-2012.798161	-2012.798273	-2012.798265	-2012.798119	-2012.797812	-2012.797319	-2012.796612	-2012.795660	-2012.794426
<b>1.83</b>	-2012.801152	-2012.801211	-2012.801149	-2012.800946	-2012.800582	-2012.800033	-2012.799271	-2012.798265	-2012.796982
<b>1.77</b>	-2012.804389	-2012.804399	-2012.804286	-2012.804032	-2012.803616	-2012.803015	-2012.802203	-2012.801148	-2012.799818
<b>1.71</b>	-2012.807704	-2012.807675	-2012.807524	-2012.807233	-2012.806782	-2012.806149	-2012.805307	-2012.804227	-2012.802876
<b>1.65</b>	-2012.810768	-2012.810718	-2012.810547	-2012.810240	-2012.809775	-2012.809131	-2012.808282	-2012.807198	-2012.805850
<b>1.59</b>	-2012.813105	-2012.813044	-2012.812864	-2012.812549	-2012.812080	-2012.811436	-2012.810595	-2012.809531	-2012.808216
<b>1.53</b>	-2012.813913	-2012.813861	-2012.813693	-2012.813393	-2012.812945	-2012.812328	-2012.811522	-2012.810505	-2012.809256
	<b>1.68</b>	<b>1.66</b>	<b>1.64</b>	<b>1.62</b>	<b>1.60</b>	<b>1.58</b>	<b>1.56</b>	<b>1.54</b>	<b>1.52</b>

Energy surface calculated at the level of B3LYP/6-31G(d) (SDD for Au) (a.u.)

The first column in red C2-C3 bond distances

The last row in blue is C2-C4 bond distance

Others in black are single-point energies

### 8. Cartesian coordinates of all stationary points

<b>INT1-Ph</b>	C	-0.28302300	0.27618700	-1.03007000
	C	-0.21267200	1.51307200	-0.93636800
C	C	-0.79681300	-1.81615700	0.68981700

C	-3.23055700	-1.43277500	0.33036400	C	3.66303500	-1.11192600	2.37604900
C	-3.99607100	-2.31689000	-0.31275400	H	2.96886600	-1.95195900	2.28471800
C	-5.30594700	-2.68719600	-0.86036300	H	4.64194100	-1.46867400	2.71419300
C	-4.12449400	-3.66933400	-0.87361000	H	3.26374900	-0.40634300	3.11070200
C	-0.23903600	2.93530300	-0.82471400	C	4.64301500	-1.49897600	-0.35781900
C	0.56011100	3.73277300	-1.67167400	H	4.90203500	-1.01680900	-1.30505400
C	0.49420100	5.11848100	-1.57732800	H	5.55383700	-1.88542600	0.11186500
C	-0.36254900	5.71708200	-0.64716700	H	3.95375000	-2.32131500	-0.56817200
C	-1.15875100	4.93049000	0.19120500	C	5.01395900	1.08360600	0.98019100
C	-1.10276100	3.54236700	0.11140600	H	5.95685100	0.69670800	1.38169900
N	-0.98324400	-2.09504100	-0.52389600	H	5.20728700	1.57783600	0.02377000
S	0.42291000	-3.01517500	-0.25870100	H	4.60422500	1.82101300	1.67650100
O	0.93978100	-2.78649500	1.10204900				
O	1.31144000	-2.78971000	-1.40976400				
C	-3.74135000	-0.09547200	0.73933800	C	2.64189700	1.34222500	-0.90142000
C	-4.65179300	0.60670800	-0.07148200	C	-0.17342200	0.59027100	-0.00711400
C	-5.16260300	1.84164000	0.32398200	C	2.55795900	0.00965900	1.20522600
C	-4.77782600	2.40636300	1.54276400	C	2.44050500	0.82008100	2.43314300
C	-3.87476900	1.72340200	2.36044700	C	2.94403100	-0.62206500	2.48016700
C	-3.35808700	0.48908800	1.96084800	N	1.70262800	2.23766800	-0.24926700
H	-1.89752300	-0.79751000	-1.84011400	S	2.22911800	3.67030900	0.46234900
H	-0.30439300	-1.37708200	-2.36002100	O	1.23276300	4.02441000	1.47396100
H	-1.78821900	-2.72245900	1.30135500	O	3.64101300	3.46586000	0.79067100
H	-1.31841600	-1.02745800	1.27992400	H	2.25381400	1.09915900	-1.89938400
H	-6.12566800	-2.87479300	-0.16799400	H	3.59751700	1.85918600	-1.04107400
H	-5.62508900	-2.26873800	-1.81385300	H	3.14822200	1.63533800	2.56173100
H	-3.66223300	-3.89498300	-1.83405600	H	1.45606000	1.01955400	2.84878300
H	-4.16370900	-4.51999500	-0.19338600	H	2.29061200	-1.36795100	2.92857000
H	1.21584500	3.25679400	-2.39439000	H	4.00439600	-0.80696900	2.64798800
H	1.10610800	5.73379800	-2.22960900	C	2.15296700	4.92058200	-0.83826400
H	-0.41152200	6.79985200	-0.57833400	H	2.48931800	5.86200300	-0.39698600
H	-1.82651100	5.40057700	0.90651600	H	2.81842800	4.63000500	-1.65364300
H	-1.72477700	2.92395200	0.75093100	H	1.12190300	5.01740100	-1.18497600
H	-4.95383400	0.17946700	-1.02247100	C	2.91037200	0.05981600	-0.11534600
H	-5.86326800	2.36428000	-0.32126100	C	0.41873500	-0.46349700	0.44639600
H	-5.18487200	3.36374100	1.85546700	C	0.32826800	-1.84815600	0.81858700
H	-3.58365300	2.14102600	3.32062600	C	-0.06038100	-2.20647100	2.12965500
H	-2.68394300	-0.03833200	2.63023600	C	0.58174500	-2.86439000	-0.12805800
C	-0.19949600	-4.70157500	-0.33896700	C	-0.20700800	-3.54668400	2.47415400
H	-0.58513700	-4.87803300	-1.34373700	H	-0.26759100	-1.42509600	2.85479900
H	0.64606500	-5.35933100	-0.12421500	C	0.43537100	-4.20284200	0.22876500
H	-0.98082200	-4.83694000	0.41084300	H	0.87624100	-2.59215400	-1.13564400
Au	1.74740200	0.32674700	-0.12857900	C	0.04359900	-4.54556100	1.52620100
P	3.81476000	-0.28875700	0.74465000	H	-0.51760200	-3.81513500	3.47945900

### TS1-Ph

H	0.62435000	-4.97948500	-0.50619200	H	-1.88354900	-1.13856900	2.90995700
H	-0.07007300	-5.59064000	1.79928200	H	-2.11546700	1.39100400	3.15836200
C	3.59686400	-1.04125600	-0.80860400	H	-3.76152400	1.30432700	2.38528900
C	3.83198900	-2.28232500	-0.17333900	C	-2.78097300	-4.61435500	-1.05412900
C	4.07963100	-0.87839200	-2.12714000	H	-3.26630800	-5.52689400	-0.69929600
C	4.51549500	-3.30414500	-0.82475100	H	-3.31669100	-4.21414500	-1.91720600
H	3.47529000	-2.44520300	0.83508900	H	-1.73546200	-4.81728400	-1.29587700
C	4.77115500	-1.90004100	-2.77166000	C	-2.71142200	0.34263100	-0.13364400
H	3.93876600	0.05714700	-2.65639700	C	-0.70414900	0.40732100	0.74469800
C	4.99107300	-3.11857300	-2.12509400	C	-0.05954300	1.74452100	0.92908600
H	4.68384700	-4.24698200	-0.31254800	C	0.27034800	2.21214900	2.21390900
H	5.14173500	-1.74299300	-3.78024800	C	0.26743500	2.54660700	-0.17891200
H	5.53180600	-3.91430000	-2.62897500	C	0.91201500	3.43980900	2.38323000
C	0.27792500	1.97703100	-0.39671500	H	0.06594500	1.59350500	3.08271700
H	-0.03647200	2.13642000	-1.44120200	C	0.89648300	3.78099100	-0.00818900
H	-0.26088000	2.70253600	0.21769900	H	0.02464200	2.19583800	-1.17789600
Au	-2.25771600	0.21776500	-0.22818600	C	1.22007100	4.23130300	1.27363100
P	-4.56912500	-0.07959500	-0.48060900	H	1.17377400	3.77606500	3.38245000
C	-5.03989200	-1.09773400	-1.93861000	H	1.13334200	4.38952800	-0.87664400
H	-4.59290400	-2.09275700	-1.85583200	H	1.71053700	5.19113900	1.40816300
H	-6.12891000	-1.19713800	-2.00241300	C	-3.15927000	1.56636500	-0.75506300
H	-4.66894400	-0.62786800	-2.85422400	C	-3.08806500	2.80971700	-0.07094800
C	-5.37071600	-0.91115500	0.95135100	C	-3.73451000	1.55513100	-2.05564200
H	-5.20606900	-0.32447500	1.85985500	C	-3.56635700	3.97317100	-0.65842700
H	-6.44790300	-1.01579100	0.78212200	H	-2.64756700	2.85448000	0.91523800
H	-4.93241500	-1.90291900	1.09627000	C	-4.22695600	2.71852100	-2.62688300
C	-5.49518200	1.49527300	-0.68831600	H	-3.81671000	0.63025600	-2.61400600
H	-6.56689400	1.29835700	-0.79930200	C	-4.14158900	3.93196000	-1.93217200
H	-5.33705600	2.13657700	0.18372700	H	-3.49877000	4.91394800	-0.12134500
H	-5.13456700	2.02395800	-1.57552800	H	-4.67712500	2.68665400	-3.61403300
				H	-4.52561300	4.84189600	-2.38409400
<b>INT2-Ph</b>				C	-0.61401400	-1.94248400	-0.26532700
C	-2.81941200	-0.97011400	-0.89346200	H	-0.21771200	-2.18366500	-1.26612800
C	-0.01632000	-0.61850000	0.14472000	H	-0.23092900	-2.71335200	0.41426700
C	-2.17409000	0.26902500	1.21909200	Au	2.03441700	-0.48036300	-0.17670600
C	-2.64823200	-0.62596100	2.33424000	P	4.37586200	-0.37808200	-0.48946800
C	-2.76867700	0.86978500	2.46752200	C	4.94341800	1.04501400	-1.51094100
N	-2.07444700	-2.03790700	-0.26975400	H	4.62801300	1.98254800	-1.04356100
S	-2.85440000	-3.41855200	0.29499400	H	6.03418700	1.04239900	-1.61018200
O	-2.04057100	-3.94116500	1.39169800	H	4.49326800	0.98859000	-2.50654400
O	-4.25930700	-3.03781700	0.47419100	C	5.33003800	-0.22342200	1.07741500
H	-2.51160600	-0.84242100	-1.94060300	H	5.12443700	-1.08306700	1.72215700
H	-3.88217900	-1.24804000	-0.89119700	H	6.40536500	-0.17635200	0.87453500
H	-3.55365400	-1.20378100	2.17684800	H	5.02428500	0.68358500	1.60717600

C	5.09752000	-1.85388200	-1.32081900	H	2.82536300	-1.57949400	-1.94384100
H	6.18280900	-1.74998200	-1.42620400	C	5.52132400	-3.02572500	-0.45959600
H	4.87951100	-2.75146400	-0.73451200	H	6.16620500	-2.65450100	1.56473000
H	4.65190800	-1.97461800	-2.31273000	H	4.64513900	-3.17770900	-2.42528500
				H	6.32021700	-3.73017600	-0.67188300

### TS2-Ph

C	2.83550500	1.18819500	-0.22322300	H	0.16825000	1.24816200	-1.33642300
C	-0.05714800	0.57556500	-0.06991700	H	-0.21093000	2.73018500	-0.32721900
C	1.56630700	-0.20089300	1.57602800	Au	-2.12815500	0.27755600	-0.03167200
C	1.25665600	0.70916600	2.71954800	P	-4.45382600	-0.05869600	0.09988300
C	1.53754600	-0.76312800	2.95603400	C	-5.16257500	-0.89247800	-1.37886500
N	1.79736700	2.23006100	-0.10878100	H	-4.69165700	-1.87079200	-1.51227600
S	2.24878100	3.82951200	-0.66240200	H	-6.24343600	-1.02713800	-1.26373400
O	3.23776700	3.66411400	-1.72223700	H	-4.97055200	-0.29115900	-2.27240000
O	0.98696600	4.53589100	-0.87736900	C	-4.96377800	-1.11003700	1.52060500
H	3.10631100	1.04801600	-1.27621000	H	-4.65494400	-0.64117100	2.45957600
H	3.73437300	1.53696500	0.29584900	H	-6.05077600	-1.24410100	1.52859900
H	2.02000900	1.42723000	3.00928300	H	-4.48178000	-2.08946900	1.44844500
H	0.23685700	1.05936300	2.85948200	C	-5.43049100	1.48851400	0.28252900
H	0.69505800	-1.39113000	3.23227800	H	-6.50066200	1.26272000	0.33945400
H	2.47673800	-1.04812700	3.42208000	H	-5.12633800	2.01437100	1.19228900
C	3.05665000	4.50174900	0.79717000	H	-5.24848700	2.14576800	-0.57291100
H	3.40026700	5.50167200	0.51995900				
H	2.32947800	4.55589100	1.60839000				
H	3.91108600	3.87646700	1.06243900				
C	2.40330500	-0.15941900	0.36369400	C	0.12570500	-0.42264300	-0.94041800
C	0.87690500	-0.52419900	0.24513100	C	1.13951600	-0.91213900	1.46681300
C	0.45809800	-1.91884600	-0.14361900	C	0.05022300	-1.10937700	2.46587000
C	0.71225800	-3.04160900	0.65645600	C	1.35630700	-1.88221100	2.57488500
C	-0.17458000	-2.11686700	-1.38364200	N	0.45500100	1.91976000	-0.43488100
C	0.32222800	-4.31643000	0.24169600	S	-0.24412000	3.53050700	-0.61991100
H	1.23366600	-2.93060900	1.59890800	O	-1.07243100	3.46094700	-1.82066300
C	-0.56186000	-3.39150100	-1.80055900	O	-0.79417600	3.88290200	0.68474100
H	-0.35205000	-1.27086800	-2.04292500	H	-0.14441800	-0.33140600	3.20188500
C	-0.32053500	-4.49748800	-0.98386800	H	-0.83543200	-1.66235400	2.15658300
H	0.52987400	-5.17133200	0.87886800	H	1.34737000	-2.94644500	2.35753400
H	-1.03953900	-3.51865400	-2.76816700	H	2.02965900	-1.59909300	3.37938500
H	-0.61726100	-5.49147100	-1.30556300	C	1.20359700	4.54147800	-0.95579900
C	3.45071200	-1.21006000	0.09022300	H	0.83660900	5.56617200	-1.05908100
C	4.40581300	-1.51922600	1.06804200	H	1.89792800	4.47634800	-0.11635200
C	3.55571700	-1.80999200	-1.17329000	H	1.66048900	4.20171600	-1.88651800
C	5.43385600	-2.42392100	0.79641500	C	1.83453700	0.28224300	0.88833600
H	4.35588500	-1.04383900	2.04347100	C	1.25284400	-0.86578300	-0.01965200
C	4.58071800	-2.71534400	-1.44464000	C	2.16996100	-1.83125600	-0.73512700

### INT3-Ph

C	0.12570500	-0.42264300	-0.94041800
C	1.13951600	-0.91213900	1.46681300
C	0.05022300	-1.10937700	2.46587000
C	1.35630700	-1.88221100	2.57488500
N	0.45500100	1.91976000	-0.43488100
S	-0.24412000	3.53050700	-0.61991100
O	-1.07243100	3.46094700	-1.82066300
O	-0.79417600	3.88290200	0.68474100
H	-0.14441800	-0.33140600	3.20188500
H	-0.83543200	-1.66235400	2.15658300
H	1.34737000	-2.94644500	2.35753400
H	2.02965900	-1.59909300	3.37938500
C	1.20359700	4.54147800	-0.95579900
H	0.83660900	5.56617200	-1.05908100
H	1.89792800	4.47634800	-0.11635200
H	1.66048900	4.20171600	-1.88651800
C	1.83453700	0.28224300	0.88833600
C	1.25284400	-0.86578300	-0.01965200
C	2.16996100	-1.83125600	-0.73512700
C	2.00480900	-3.21219300	-0.55796500

C	3.11967600	-1.37905900	-1.66277900	C	2.47731300	-0.15740500	-0.85237200
C	2.78263100	-4.12151000	-1.27743700	C	-1.10124900	-0.43178900	0.52512000
H	1.25945900	-3.58141800	0.14103500	C	-2.22378100	0.34320000	-0.16064300
C	3.90018800	-2.28639600	-2.37916300	C	-3.01539100	-0.22086100	-1.07492600
H	3.26224400	-0.31288100	-1.81241000	C	-4.18926400	-0.10097300	-1.95413000
C	3.73468900	-3.66003100	-2.18771800	C	-3.40663500	-1.41524100	-1.83289300
H	2.64374100	-5.18830000	-1.12636400	C	3.71527900	0.49148600	-0.55309400
H	4.63915800	-1.91997400	-3.08604700	C	4.07691500	1.68556700	-1.20610700
H	4.34277500	-4.36583500	-2.74608000	C	5.28595500	2.31058700	-0.90969900
C	3.32562100	0.50143600	0.97505900	C	6.14871200	1.75954100	0.04127800
C	4.18418600	-0.41972500	1.59282500	C	5.79703700	0.57611700	0.69591600
C	3.90093100	1.64556700	0.39598400	C	4.59168200	-0.05759100	0.40327700
C	5.55968100	-0.19157600	1.65197100	N	-0.69365400	-1.64492800	-0.19875000
H	3.78494600	-1.32946800	2.02210100	S	-0.26023300	-2.97582700	0.77347500
C	5.27555700	1.87515600	0.45201000	O	0.26377900	-2.53652000	2.07228300
H	3.27496300	2.36220400	-0.12912000	O	0.51022100	-3.88722300	-0.07779500
C	6.11286100	0.95814100	1.08832400	C	-2.41404500	1.75074300	0.28476500
H	6.19959700	-0.91969800	2.14224900	C	-3.03169900	2.70372300	-0.54688900
H	5.69110000	2.76895400	-0.00511100	C	-3.22174200	4.01589800	-0.12156200
H	7.18320300	1.13457400	1.13759200	C	-2.79757100	4.41585100	1.14839600
C	-0.04558800	0.94099400	-1.21906600	C	-2.17712500	3.48738300	1.98382600
H	-0.02571300	-1.06766700	-1.80714300	C	-1.98398600	2.17300500	1.55657500
H	-0.56629900	1.27640600	-2.11119000	H	-0.43211900	-0.81715300	-2.07751100
C	0.97452400	1.55336400	0.90803700	H	0.35658700	-2.38181200	-1.84600700
H	0.10629000	1.41869100	1.56184200	H	-1.41365900	-0.72304800	1.53358100
H	1.54867400	2.39537800	1.29401300	H	-0.23087700	0.22396300	0.66347800
Au	-2.01185000	-0.47894200	-0.23037100	H	-5.17972600	-0.03990600	-1.50317000
P	-4.26260200	-0.69976100	0.38779200	H	-4.10217000	0.45058700	-2.89008200
C	-5.06707500	-2.19479300	-0.31643800	H	-2.80591800	-1.73184900	-2.68535000
H	-4.55059700	-3.09502000	0.02938200	H	-3.87541600	-2.24354900	-1.30239200
H	-6.11733000	-2.24415300	-0.00956900	H	3.40238700	2.11183900	-1.94243900
H	-5.01467800	-2.16402800	-1.40868800	H	5.55505700	3.23100700	-1.42090200
C	-4.53850500	-0.81162500	2.20164900	H	7.09060600	2.25016400	0.27130400
H	-4.14378500	0.08221100	2.69352900	H	6.46472700	0.14414000	1.43642400
H	-5.60883500	-0.89590700	2.41846600	H	4.31297700	-0.97744200	0.90783300
H	-4.02261900	-1.68762600	2.60564600	H	-3.34962100	2.41235200	-1.54167700
C	-5.29666300	0.71399300	-0.16879900	H	-3.69603000	4.73191900	-0.78788300
H	-6.33727200	0.56885600	0.14121600	H	-2.94441400	5.44041600	1.47908800
H	-4.91882700	1.64481800	0.26393300	H	-1.84000900	3.78282600	2.97387400
H	-5.25477400	0.79826200	-1.25857200	H	-1.50364400	1.47238100	2.23253400
				C	-1.87462900	-3.72397200	1.07417400
<b>Sub-Ph</b>							
C	0.16804600	-1.41184000	-1.37964400	H	-2.29028700	-4.04927600	0.11990100
C	1.43429000	-0.72607400	-1.09720300	H	-1.70883900	-4.57657500	1.73702200
				H	-2.53098700	-2.99743800	1.55712200

<b>Pro1-Ph</b>				<b>TS3-Ph</b>			
C	-1.36632200	0.74377000	-0.30709000	H	3.48587200	4.62104600	-0.12991300
C	-0.51098900	-1.94991700	-0.54432400	C	-1.81586500	-1.65581300	-0.61005800
C	0.12955200	-0.47938700	1.42616100	H	-0.17119700	-2.92030800	-0.89026100
C	-0.76417600	-0.88382900	2.54053700	H	-2.56792600	-2.35716600	-0.95092900
C	0.65588000	-0.41319100	2.81911500	C	-2.59917500	-1.07064400	-0.98597500
N	-2.28675800	-0.39561100	-0.18918900	C	0.19314800	-0.58417100	0.11493900
S	-3.94510700	-0.09144800	-0.17419200	C	-2.03636000	0.42639800	0.96666700
O	-4.60156700	-1.37447000	0.07237300	C	-2.48090000	-0.31718500	2.26303300
O	-4.15574200	1.07015500	0.68937200	C	-2.53388400	1.17054000	2.18894800
H	-1.25424800	1.00538500	-1.37088600	N	-1.83756600	-2.06988100	-0.27785300
H	-1.82032800	1.58851500	0.21562000	S	-2.65393300	-3.28184000	0.55718500
H	-1.58679000	-0.22401200	2.80533600	O	-1.90472500	-3.56335900	1.78144800
H	-0.98706100	-1.94260900	2.65260600	O	-4.05998000	-2.85622600	0.58888800
H	1.38942700	-1.14883200	3.14061100	H	-2.07214300	-0.79148900	-1.91174100
H	0.79117400	0.57033800	3.26422700	H	-3.55502000	-1.49604100	-1.29932500
C	-4.35469300	0.41064700	-1.86358900	H	-3.41222100	-0.87367700	2.22996300
H	-5.42682200	0.61971400	-1.88519300	H	-1.67164600	-0.81608500	2.78597300
H	-3.79322900	1.31160100	-2.11990400	H	-1.79312600	1.74404400	2.73657900
H	-4.11591700	-0.40733700	-2.54655500	H	-3.51753900	1.62882700	2.15701900
C	0.02510400	0.45207700	0.26829400	C	-2.54090500	-4.74338600	-0.49312100
C	0.50032200	-1.03997700	0.08005600	H	-3.04928900	-5.55562200	0.03218300
C	1.92021300	-1.37882200	-0.29170200	H	-3.03417400	-4.53991600	-1.44541300
C	2.69480700	-2.21626000	0.52239900	H	-1.48832500	-4.99382100	-0.64055100
C	2.45953900	-0.94590700	-1.51161500	C	-2.86255100	0.20409300	-0.20511600
C	3.98182000	-2.59869400	0.13666200	C	-0.52560700	0.45225400	0.59661100
H	2.28393100	-2.57924300	1.46024700	C	0.08967300	1.80959200	0.79152200
C	3.74426100	-1.32531000	-1.89964400	C	0.78808200	2.11192000	1.97280500
H	1.86803300	-0.29962600	-2.15423100	C	-0.02854200	2.80722300	-0.18990200
C	4.51115400	-2.15203000	-1.07491300	C	1.36272900	3.37114100	2.16019100
H	4.56771500	-3.24826600	0.78189000	H	0.89315600	1.34797000	2.73886400
H	4.14780700	-0.97416100	-2.84581600	C	0.54394500	4.06753400	-0.00214700
H	5.51277300	-2.44720200	-1.37607400	H	-0.54955300	2.58556600	-1.11830500
C	0.99358700	1.60321500	0.14435200	C	1.23987200	4.35363500	1.17474000
C	2.25390000	1.57307900	0.77112900	H	1.90305400	3.58473100	3.07844600
C	0.66385700	2.76331200	-0.57964700	H	0.45237200	4.82287600	-0.77803900
C	3.13980700	2.64366300	0.67076600	H	1.68238000	5.33449900	1.32298700
H	2.55195200	0.69968700	1.33710900	C	-3.84466300	1.13039800	-0.68796800
C	1.55058100	3.83800600	-0.67843100	C	-3.72291400	2.51693200	-0.38348700
H	-0.29717900	2.85337500	-1.07337900	C	-4.93072400	0.71329200	-1.51011600
C	2.79531600	3.78549100	-0.05491100	C	-4.62672100	3.43398300	-0.89692500
H	4.10540700	2.58258000	1.16602100	H	-2.87978100	2.85932500	0.20420700
H	1.25817100	4.71874200	-1.24439100	C	-5.85041400	1.63480700	-1.98458800

H	-5.08613000	-0.33741100	-1.72443500	C	-0.44270000	0.63420500	0.38152600
C	-5.69723000	2.99553400	-1.68651700	C	0.29979500	1.92037000	0.63112700
H	-4.50625600	4.49083500	-0.68130500	C	1.18071800	2.05076800	1.71780100
H	-6.69168700	1.30037600	-2.58299400	C	0.10956200	3.02944900	-0.20994100
H	-6.41637700	3.71454000	-2.06821800	C	1.86231000	3.24912900	1.94614100
C	-0.36805100	-1.95011000	-0.21459100	H	1.32516000	1.20652500	2.38649200
H	0.04887700	-2.26873100	-1.18171300	C	0.79672500	4.22397500	0.01107200
H	-0.01163200	-2.66687900	0.53272400	H	-0.56476600	2.94779200	-1.05993200
Au	2.24151000	-0.39712300	-0.22431600	C	1.67486600	4.33812300	1.09201400
P	4.56593300	-0.20125400	-0.59821300	H	2.53266000	3.33338600	2.79736600
C	5.04972500	1.25270400	-1.62101100	H	0.64754300	5.06519100	-0.66034400
H	4.71036900	2.17287000	-1.13597000	H	2.20241300	5.27066500	1.27073200
H	6.13650800	1.29500900	-1.75168400	C	-4.19154400	0.86084200	-0.67166200
H	4.57281500	1.18789200	-2.60356400	C	-4.27833500	2.26168300	-0.87300500
C	5.56739300	-0.02202000	0.93724600	C	-5.34780200	0.06728700	-0.87468000
H	5.41520100	-0.89330100	1.58124700	C	-5.47401300	2.84051600	-1.27793800
H	6.63315800	0.06753500	0.70068100	H	-3.38947300	2.87470700	-0.76624400
H	5.24483200	0.86877500	1.48438000	C	-6.54890800	0.66407600	-1.23874100
C	5.32852900	-1.63575700	-1.46656900	H	-5.30631400	-0.99730600	-0.67329400
H	6.40386300	-1.48146100	-1.60714100	C	-6.61335500	2.04565600	-1.44951100
H	5.17132000	-2.54679900	-0.88147500	H	-5.52184200	3.90932500	-1.46161200
H	4.85547800	-1.76988400	-2.44394600	H	-7.43800600	0.05321700	-1.35961200
				H	-7.55116200	2.50403600	-1.74945000
				C	-0.31960900	-1.84527100	-0.25296300

#### INT4-Ph

C	-2.50872000	-0.98583500	-1.13752600	H	0.11143700	-2.22264100	-1.18996900
C	0.25133700	-0.47410100	0.02271000	H	0.01803300	-2.52429000	0.53667400
C	-1.95087500	0.81070800	0.53498200	Au	2.32433000	-0.41514800	-0.23413500
C	-2.62726900	0.35555700	1.99862100	P	4.66263000	-0.37881200	-0.56563300
C	-2.43813400	1.76265000	1.63770600	C	5.25794700	1.02117400	-1.60468200
N	-1.78805100	-1.97548600	-0.35624200	H	4.97172100	1.97060600	-1.14241800
S	-2.64372000	-2.87513700	0.78002900	H	6.34707300	0.98990100	-1.71721800
O	-1.92148400	-2.84766200	2.05462000	H	4.79373700	0.96927300	-2.59406300
O	-4.03454300	-2.40062400	0.69435000	C	5.65168700	-0.23935000	0.98239800
H	-1.83729100	-0.65856800	-1.94679000	H	5.43353000	-1.08781800	1.63786000
H	-3.38524300	-1.42329400	-1.61747700	H	6.72450400	-0.22317700	0.76180600
H	-3.61750700	-0.08646800	1.97533900	H	5.38011800	0.67984400	1.50986700
H	-1.88582500	-0.19850800	2.56388600	C	5.34277900	-1.87517400	-1.39766200
H	-1.63191500	2.30243400	2.12110200	H	6.42836100	-1.79598900	-1.52057900
H	-3.32862200	2.35386500	1.46533400	H	5.11399400	-2.76426500	-0.80247400
C	-2.58652600	-4.56242800	0.15489200	H	4.87912000	-1.99263300	-2.38168600
H	-3.12103000	-5.18792400	0.87409200				
H	-3.07422800	-4.59533600	-0.82073400				
H	-1.54383300	-4.87856200	0.08404500				
C	-2.90156900	0.26294600	-0.37568500				

#### TS4-Ph

C	-2.71154400	-1.08299900	-1.03883400
C	0.20891500	-0.42620300	-0.13200600

C	-1.93769900	0.91796900	0.35449500		Au	2.28620800	-0.36877000	-0.32926700
C	-2.96571500	0.32480600	1.70350200		P	4.63307600	-0.30752700	-0.59877900
C	-2.49379800	1.73418200	1.49111600		C	5.25118500	1.23459100	-1.39300600
N	-1.80829100	-2.00748200	-0.38540600		H	4.94996200	2.10143200	-0.79737200
S	-2.40825300	-2.93705400	0.88890500		H	6.34292500	1.21918800	-1.48053400
O	-1.53996100	-2.75593500	2.05828600		H	4.81348800	1.33594100	-2.39063100
O	-3.84281500	-2.62812500	0.96539200		C	5.57811000	-0.41704200	0.97827500
H	-2.26942300	-0.81168900	-2.00903800		H	5.33604700	-1.35330300	1.48992600
H	-3.65997800	-1.57475200	-1.25514000		H	6.65649500	-0.37950000	0.79024100
H	-4.02878100	0.11485800	1.73724400		H	5.29917100	0.41394400	1.63298200
H	-2.33125700	-0.38834300	2.22050400		C	5.32597700	-1.66146900	-1.63687400
H	-1.73986200	2.11685700	2.17156100		H	6.41395300	-1.56884000	-1.72315800
H	-3.28333000	2.44710500	1.27536900		H	5.08363300	-2.63075200	-1.19096300
C	-2.22133500	-4.63545700	0.32358800		H	4.88339300	-1.62349200	-2.63672000
H	-2.57671700	-5.27997900	1.13130700					
H	-2.82586500	-4.77437700	-0.57402700					
H	-1.16655600	-4.83352000	0.12267100					
C	-2.98734500	0.21792300	-0.29875200					
C	-0.47521300	0.67735300	0.29534500					
C	0.30879700	1.89216400	0.72968400					
C	1.10501300	1.85823600	1.88679300					
C	0.24047000	3.08760000	-0.00278400					
C	1.82250400	2.98661600	2.29163700					
H	1.15534900	0.94273600	2.47026000					
C	0.96332700	4.21355200	0.39688800					
H	-0.36640400	3.13114200	-0.90459500					
C	1.75554000	4.16630900	1.54647900					
H	2.42639800	2.94533600	3.19413000					
H	0.90702900	5.12678700	-0.18897400					
H	2.31101500	5.04452000	1.86278400					
C	-4.27736400	0.86930700	-0.67126900					
C	-4.27576200	2.16186700	-1.22351100					
C	-5.49166400	0.16642400	-0.56588000					
C	-5.46746000	2.74120800	-1.65831000					
H	-3.33967600	2.70280700	-1.33102600					
C	-6.68038800	0.75729000	-0.98792000					
H	-5.50422300	-0.83008800	-0.13124400					
C	-6.67051200	2.04292500	-1.53702100					
H	-5.45456400	3.73600400	-2.09337400					
H	-7.61511400	0.21375700	-0.88933700					
H	-7.59813600	2.49762300	-1.87159000					
C	-0.36244300	-1.77151800	-0.50471900					
H	-0.06849800	-1.99002400	-1.54203800					
H	0.14564500	-2.52175400	0.10895200					

### INT5-Ph

C	-3.34553600	-0.78368900	-1.14292600
C	-0.13446700	-0.19469100	-0.37933700
C	-2.10993500	-0.05065000	1.07456700
C	-4.15124900	-0.45112800	1.40219200
C	-2.94541400	-0.10291600	2.31930000
N	-2.07457700	-1.40936900	-1.49717200
S	-1.74931900	-2.96420500	-0.87890300
O	-0.29090200	-3.03754400	-0.70150000
O	-2.66317400	-3.22500700	0.23860800
H	-3.63981300	-0.15169800	-1.98617200
H	-4.09943800	-1.56653300	-1.03970900
H	-5.09021000	0.06407800	1.60797900
H	-4.30657800	-1.52959500	1.34272200
H	-2.61875500	-0.82231900	3.07607900
H	-3.06185600	0.87737200	2.79670500
C	-2.20274200	-4.04947900	-2.24077900
H	-2.02719600	-5.07390000	-1.90334800
H	-3.25942400	-3.90327800	-2.47275200
H	-1.57532500	-3.81401600	-3.10172400
C	-3.31983300	0.07677800	0.16831600
C	-0.74450700	-0.20585400	0.90203800
C	0.12450000	-0.29157100	2.12166400
C	0.92252500	-1.43082800	2.32032500
C	0.14863300	0.73681700	3.07544100
C	1.72885200	-1.53364500	3.45600400
H	0.88641000	-2.24057000	1.59704100
C	0.96314000	0.63421800	4.20449900
H	-0.45956300	1.62574300	2.92847400

C	1. 75304000	-0. 50198300	4. 39762100	H	4. 04362900	0. 16516100	-1. 67513000
H	2. 32970200	-2. 42575900	3. 60912400	C	1. 95332300	3. 45967800	-0. 31036800
H	0. 97612900	1. 43840700	4. 93465800	H	1. 40270800	4. 16347500	-0. 94113600
H	2. 37807100	-0. 58573300	5. 28205900	H	2. 04662500	3. 89196400	0. 69275000
C	-3. 66548400	1. 54328300	-0. 15040600	C	3. 31511900	2. 90092000	-0. 81937400
C	-2. 70622000	2. 56238700	-0. 18278600	H	3. 41933600	2. 98903800	-1. 90452000
C	-4. 99425800	1. 85783400	-0. 47716800	H	4. 21411600	3. 28639300	-0. 33647900
C	-3. 06626300	3. 86794700	-0. 53175700	Au	-1. 90101100	-0. 66899500	0. 03928800
H	-1. 67213900	2. 35171700	0. 07425400	P	-4. 00430600	-1. 45213500	0. 73969200
C	-5. 35084800	3. 15779400	-0. 83243000	C	-4. 25911700	-3. 25579300	0. 48456800
H	-5. 75703200	1. 08340900	-0. 45607800	H	-3. 50096900	-3. 81999200	1. 03559200
C	-4. 38710600	4. 16945800	-0. 85856800	H	-5. 25328000	-3. 55743900	0. 83120700
H	-2. 30961200	4. 64748500	-0. 54250300	H	-4. 16264000	-3. 49668200	-0. 57821900
H	-6. 38351800	3. 38104100	-1. 08452600	C	-4. 33437400	-1. 17731200	2. 52837400
H	-4. 66690500	5. 18339500	-1. 12834200	H	-4. 27751800	-0. 10845500	2. 75431900
C	-0. 90875000	-0. 52985300	-1. 63042700	H	-5. 32867900	-1. 54874300	2. 79847800
H	-1. 25107300	0. 41119400	-2. 08861500	H	-3. 58242500	-1. 69776500	3. 12875700
H	-0. 21399800	-0. 96844800	-2. 35125000	C	-5. 41607200	-0. 65121700	-0. 12556400
Au	1. 85969600	0. 25779900	-0. 58497000	H	-6. 36895900	-1. 03860500	0. 25069800
P	4. 15778100	0. 79584100	-0. 82860700	H	-5. 37968100	0. 43083400	0. 03084400
C	4. 66993700	2. 29034400	0. 11462600	H	-5. 34950700	-0. 84650200	-1. 19998200
H	4. 45370400	2. 14743000	1. 17743500	S	3. 17334100	-2. 37443900	-1. 43354400
H	5. 74114300	2. 48030900	-0. 01181100	O	4. 09077300	-2. 09565400	-2. 53198600
H	4. 10825500	3. 16081600	-0. 23721100	O	2. 13248000	-3. 39729000	-1. 52148600
C	5. 28314700	-0. 53664100	-0. 24226600	C	4. 12006100	-2. 63406700	0. 07378200
H	5. 10057600	-1. 45302300	-0. 81137000	H	4. 71464600	-3. 53626400	-0. 09188600
H	6. 33018400	-0. 24008700	-0. 36627700	H	4. 76617100	-1. 77245500	0. 24850300
H	5. 09042000	-0. 74366200	0. 81449700	H	3. 42706400	-2. 77466200	0. 90439700
C	4. 68731600	1. 12805100	-2. 55896600	C	-0. 97355000	2. 37937500	-0. 57631600
H	5. 75631600	1. 36300700	-2. 59854100	C	-1. 22897500	3. 34680700	0. 40815000
H	4. 49130100	0. 24967500	-3. 18107800	C	-1. 85766800	2. 27663200	-1. 66394000
H	4. 12042200	1. 97114000	-2. 96490800	C	-2. 33870700	4. 18831100	0. 30988600
				H	-0. 56297300	3. 43155500	1. 26244900
<b>TS5-Ph</b>				C	-2. 96398100	3. 12178600	-1. 76539300
C	0. 97222500	-0. 96222200	-0. 85012400	H	-1. 66847900	1. 54636100	-2. 44703600
N	2. 33216300	-0. 86787600	-1. 09807500	C	-3. 20856100	4. 07884800	-0. 77711200
C	0. 00300900	0. 03943300	-0. 51453200	H	-2. 52191700	4. 92962800	1. 08250500
C	0. 22817600	1. 49072600	-0. 48825200	H	-3. 62689000	3. 04043200	-2. 62229500
C	2. 99313400	0. 38582100	-1. 47856500	H	-4. 06732200	4. 73896200	-0. 85757900
C	2. 85946900	1. 45854000	-0. 37889000	C	3. 49134400	0. 99524500	0. 93049500
C	1. 45544000	2. 03521100	-0. 28862100	C	4. 89127100	0. 96023500	1. 04165800
H	0. 66500100	-1. 99175100	-0. 68685600	C	2. 72168300	0. 56891100	2. 01945100
H	0. 17607900	-0. 62831300	-1. 78162900	C	5. 50356000	0. 50157600	2. 20847400
H	2. 56426000	0. 75652100	-2. 41776200	H	5. 51027900	1. 30107600	0. 21467500

C	3. 33418300	0. 11290000	3. 19111800	C	-0. 35546800	0. 13394300	2. 67981100
H	1. 63712800	0. 60838200	1. 96529200	C	-2. 01925200	-1. 53215700	2. 17657700
C	4. 72490600	0. 07471800	3. 28841800	C	-1. 31761200	0. 90043600	3. 34162800
H	6. 58757100	0. 48790000	2. 27806800	H	0. 66893400	0. 49227900	2. 63930500
H	2. 72035700	-0. 20398200	4. 02974700	C	-2. 98594500	-0. 75692800	2. 82233000
H	5. 20076000	-0. 27409600	4. 20016000	H	-2. 32792100	-2. 47510300	1. 74102200
				C	-2. 64065500	0. 45864100	3. 41563500
<b>INT6-Ph</b>				H	-1. 02420000	1. 83158300	3. 82042600
N	-0. 55251400	-2. 28331600	-0. 80893600	H	-4. 00899900	-1. 11867400	2. 87377300
C	0. 07276500	-1. 26712200	-1. 46234400	H	-3. 38805700	1. 04375400	3. 94437000
C	1. 19820500	-0. 51431100	-1. 09886900	Au	-0. 29466000	1. 18126800	-0. 68640200
C	-0. 03321200	-2. 95464000	0. 39924600	P	-1. 60698800	3. 07664900	-0. 37165000
C	0. 41954600	-1. 99188800	1. 52039500	C	-1. 67853100	4. 15551300	-1. 85741800
C	1. 73521200	-1. 29860500	1. 18427200	H	-2. 08826800	3. 59508100	-2. 70275100
C	2. 12656000	-0. 68769900	0. 04753000	H	-2. 31171500	5. 02850600	-1. 66510000
H	-0. 36978000	-1. 04361700	-2. 42823700	H	-0. 67191400	4. 49353300	-2. 12042900
H	1. 62890000	0. 00863300	-1. 95333400	C	-3. 35326600	2. 67357100	0. 02857900
H	-0. 81928900	-3. 62078700	0. 75701300	H	-3. 38964000	2. 07667000	0. 94451000
H	0. 82468600	-3. 57030900	0. 11173500	H	-3. 93424500	3. 59215700	0. 16608100
C	3. 51097900	-0. 16830600	-0. 13404200	H	-3. 79157000	2. 08764500	-0. 78453800
C	4. 20422400	-0. 36277600	-1. 34211300	C	-1. 03048800	4. 16670000	0. 98938200
C	4. 16232000	0. 51936600	0. 90457900	H	-1. 68924400	5. 03639500	1. 08752800
C	5. 50706900	0. 10820800	-1. 50258000	H	-1. 03108700	3. 60501200	1. 92732800
H	3. 73500400	-0. 91119600	-2. 15534000	H	-0. 01157000	4. 50930500	0. 78678300
C	5. 46406000	0. 99251400	0. 74307200				
H	3. 63739800	0. 69985400	1. 83784500	<b>Pro2-Ph</b>			
C	6. 14127200	0. 78815200	-0. 46093200	N	-1. 20390600	-1. 43288300	0. 29874900
H	6. 02882100	-0. 06145700	-2. 44010400	C	-0. 19519800	-1. 87266200	-0. 56188200
H	5. 94727900	1. 52633300	1. 55647200	C	1. 06892800	-1. 40626400	-0. 70137500
H	7. 15503200	1. 15672200	-0. 58697100	C	-0. 92211500	-0. 59026700	1. 46167300
C	2. 44727600	-1. 84211200	2. 40531600	C	-0. 30619700	0. 78094900	1. 08666800
H	3. 41251700	-2. 32686100	2. 22396400	C	1. 14007800	0. 68664300	0. 63017700
H	2. 58712700	-1. 11237000	3. 21153200	C	1. 77172400	-0. 28120900	-0. 07204900
C	1. 21725800	-2. 76654900	2. 64839900	H	-0. 49838300	-2. 72288200	-1. 16281500
H	1. 40561100	-3. 81388400	2. 39305900	H	1. 66397100	-1. 97242800	-1. 41263800
H	0. 76396800	-2. 72048200	3. 64008600	H	-1. 85593300	-0. 46396100	2. 01109100
S	-2. 03810700	-2. 88988500	-1. 53067700	H	-0. 21978600	-1. 12616300	2. 11046500
O	-2. 83992600	-3. 41326700	-0. 43115800	C	0. 22929700	1. 59860700	2. 32071400
O	-2. 51039800	-1. 82585100	-2. 41203900	H	-0. 31346700	2. 51549800	2. 56442700
C	-1. 46601000	-4. 27276600	-2. 53409200	H	0. 30605300	0. 97810400	3. 21946500
H	-2. 35760300	-4. 71224100	-2. 98909700	C	1. 59944800	1. 76009600	1. 59716500
H	-0. 78950800	-3. 90083400	-3. 30568500	H	1. 70279000	2. 75328900	1. 14154700
H	-0. 97487400	-5. 00350800	-1. 88861100	H	2. 50751500	1. 55398900	2. 17412400
C	-0. 68513500	-1. 10246600	2. 09510400	C	3. 25597100	-0. 25789700	-0. 22145200

C	4. 00637400	-1. 44277400	-0. 12069700	N	-0. 56723100	2. 62727300	0. 51259600
C	3. 94583400	0. 94239100	-0. 46324800	S	1. 09567400	2. 83463600	0. 24133800
C	5. 39542300	-1. 42598300	-0. 24481400	O	1. 44257100	2. 47546800	-1. 14297600
H	3. 49534200	-2. 38145300	0. 07513200	O	1. 79369900	2. 16637500	1. 35240100
C	5. 33485300	0. 96026200	-0. 58887800	H	-1. 97589900	1. 81441400	1. 78045600
H	3. 38328200	1. 86410200	-0. 57775500	H	-0. 29761200	1. 62836400	2. 32647400
C	6. 06644200	-0. 22397500	-0. 47919300	H	-0. 98885400	3. 57439300	-1. 30414100
H	5. 95452900	-2. 35378600	-0. 15483000	H	-1. 54824600	1. 90541300	-1. 24535300
H	5. 84508400	1. 90024700	-0. 78304100	H	-5. 90036100	2. 38573000	0. 48534600
H	7. 14840200	-0. 21098200	-0. 57965500	H	-5. 97566500	3. 36333000	-1. 05453200
S	-2. 78684000	-2. 02651200	0. 03543200	H	-4. 65739000	1. 53757800	-2. 27162400
O	-3. 54011400	-1. 76146100	1. 26175100	H	-4. 58930500	0. 56501900	-0. 72660800
O	-2. 66318700	-3. 38074800	-0. 50703500	H	-1. 60691700	-3. 03992900	2. 31313200
C	-3. 45104400	-0. 98283200	-1. 27642900	H	-2. 78923300	-5. 17585000	1. 85576300
H	-2. 78688900	-1. 03979000	-2. 14054200	H	-3. 94087900	-5. 51674100	-0. 31774600
H	-4. 43480200	-1. 38826300	-1. 52596700	H	-3. 91847700	-3. 72757000	-2. 03937500
H	-3. 53209100	0. 04231800	-0. 91394700	H	-2. 73917200	-1. 58735400	-1. 59042200
C	-1. 24513300	1. 58292700	0. 19266900	C	1. 30046900	4. 61334200	0. 42258900
C	-2. 43768900	2. 10536900	0. 72005000	H	1. 02879800	4. 89162500	1. 44161400
C	-0. 96303800	1. 80484800	-1. 16101200	H	2. 35310000	4. 83072400	0. 22627300
C	-3. 32337700	2. 82459500	-0. 08331300	H	0. 67097200	5. 12647200	-0. 30691300
H	-2. 67740900	1. 94893900	1. 76934200	Au	0. 91126800	-0. 74543500	0. 15498600
C	-1. 84692400	2. 52706300	-1. 96788000	P	3. 10371000	-1. 08699800	-0. 54525900
H	-0. 04338100	1. 40953000	-1. 58133100	C	4. 29422900	-0. 40013800	0. 67036700
C	-3. 03011500	3. 03862300	-1. 43356800	H	4. 22730400	-0. 95900600	1. 60845900
H	-4. 23959300	3. 22159100	0. 34602200	H	5. 31641900	-0. 46718400	0. 28254600
H	-1. 60681400	2. 69058200	-3. 01540300	H	4. 04042800	0. 64406000	0. 87228200
H	-3. 71647900	3. 60250800	-2. 05952900	C	3. 59236100	-2. 84089500	-0. 79172500
				H	2. 95778600	-3. 30071500	-1. 55480500
				H	4. 63822100	-2. 90013200	-1. 11184200

### INT1-H

C	-0. 95561300	1. 58176900	1. 45762600	H	3. 47181300	-3. 39656000	0. 14269900
C	-0. 96895600	0. 17937900	0. 92414300	C	3. 45430100	-0. 23554800	-2. 13165400
C	-1. 45385700	-0. 93372100	0. 66540300	H	4. 51851400	-0. 31426000	-2. 37894300
C	-1. 46370800	2. 82855700	-0. 65816700	H	2. 86445900	-0. 69071200	-2. 93288900
C	-2. 82009900	3. 30766600	-0. 21577300	H	3. 16656100	0. 81595500	-2. 04426100
C	-3. 94977800	2. 67802500	-0. 50966100	H	-2. 84511100	4. 23609800	0. 35447900
C	-5. 41498200	2. 65016000	-0. 45274000				
C	-4. 62182300	1. 55361100	-1. 18338000				
C	-2. 09777200	-2. 17878100	0. 38973000				
C	-2. 11043300	-3. 19836900	1. 36452800				
C	-2. 77503500	-4. 39255800	1. 10431100				
C	-3. 42390800	-4. 58241600	-0. 12012000				
C	-3. 41216200	-3. 57575800	-1. 09114700				
C	-2. 75280300	-2. 37576400	-0. 84434600				

### TS1-H

C	-3. 10401300	-0. 13348200	-1. 66833400
C	-0. 47938700	-0. 23468000	-0. 33162400
C	-3. 15226700	1. 64838800	0. 13751200
C	-3. 69132700	1. 34407700	1. 46494000
C	-3. 33665500	2. 77656100	1. 05323400
N	-2. 75886500	-1. 20772900	-0. 74746400

S	-3.92448700	-1.87098900	0.28314100	
O	-3.32543400	-2.00070600	1.61493500	<b>INT2-H</b>
O	-5.15481200	-1.10933900	0.05867300	C -3.12921200 0.58917200 -1.47550700
H	-2.53650800	-0.27882000	-2.59580500	C -0.60234700 -0.05639200 -0.21503600
H	-4.16600600	-0.21072500	-1.91802800	C -2.24238200 1.70299800 0.66882400
H	-4.73330100	1.03643100	1.51909100	C -2.86202400 1.22016600 1.92757700
H	-3.05110600	0.84297000	2.18806100	C -2.34841200 2.65113300 1.80242600
H	-2.45669200	3.23426800	1.50300100	N -2.99358100 -0.68145400 -0.77344400
H	-4.13697100	3.48172900	0.83220200	S -4.31266900 -1.32159000 0.08745100
C	-4.18044100	-3.53414600	-0.36247800	O -3.75623300 -1.98320400 1.27160000
H	-4.92030000	-4.01541300	0.28186700	O -5.31623900 -0.26019700 0.19714500
H	-4.55567100	-3.46104700	-1.38462500	H -2.75055900 0.49180300 -2.50202700
H	-3.23811000	-4.08473500	-0.32671600	H -4.18935600 0.84931400 -1.52625100
C	-2.82551000	1.25613300	-1.11508900	H -3.93206400 1.03516600 1.90845400
C	-0.71102500	1.03499300	-0.36155400	H -2.30117900 0.54611500 2.56872600
C	-0.19138300	2.37381200	-0.22140000	H -1.44934100 2.91172300 2.35295600
C	0.17431000	2.85216200	1.05541400	H -3.06225100 3.46518000 1.69731400
C	-0.00650200	3.20202600	-1.34671500	C -4.97452900 -2.59224600 -1.00260100
C	0.72596900	4.12420200	1.19459100	H -5.83282600 -3.03425800 -0.49052900
H	0.03595300	2.21217500	1.92191200	H -5.28993400 -2.12673200 -1.93814400
C	0.53853500	4.47375000	-1.19757200	H -4.20597900 -3.34773200 -1.17630100
H	-0.28078100	2.83693100	-2.33189500	C -2.38206200 1.70108700 -0.75532900
C	0.90440000	4.93664600	0.07113000	C -0.92564200 1.31576300 -0.19869800
H	1.01151300	4.48365100	2.17869700	C 0.15900000 2.35897000 -0.23229300
H	0.682222800	5.10484700	-2.06931100	C 0.97140700 2.57652400 0.89195000
H	1.32775300	5.93044700	0.18317100	C 0.38974200 3.11305300 -1.38970400
C	-1.34641700	-1.46172700	-0.50587100	C 1.98821900 3.53210100 0.85921300
H	-0.92585000	-2.03625500	-1.34443300	H 0.80453100 1.99753400 1.79717300
H	-1.25117200	-2.08119700	0.38968300	C 1.40937700 4.06744400 -1.42406500
Au	1.60362600	-0.60344500	-0.09522600	H -0.22227700 2.95287000 -2.27369300
P	3.87058900	-1.12537100	0.18687900	C 2.20853000 4.28103700 -0.29976000
C	4.99220900	-0.20225600	-0.94107200	H 2.59910500 3.70004900 1.74180800
H	4.87273300	0.87367500	-0.78386700	H 1.57559400 4.64414600 -2.32924300
H	6.03583300	-0.47836000	-0.75561600	H 2.99406600 5.03057100 -0.32359400
H	4.74068500	-0.42907600	-1.98125000	C -1.64294900 -1.10726700 -0.42214800
C	4.50288100	-0.77239200	1.87742100	H -1.23440000 -1.78057700 -1.19633700
H	3.93647800	-1.35100300	2.61300600	H -1.69133700 -1.71989900 0.49046500
H	5.56357100	-1.03480500	1.95372000	Au 1.34770000 -0.72067400 -0.05561600
H	4.37952900	0.29052400	2.10491500	P 3.58095300 -1.49587000 0.12054100
C	4.26177200	-2.89838200	-0.10330800	C 4.79275400 -0.44138600 -0.77548400
H	5.33090100	-3.08394700	0.04556500	H 4.74788200 0.58164400 -0.39052800
H	3.69054100	-3.52324900	0.58947600	H 5.80913600 -0.82958400 -0.65017600
H	3.98908600	-3.17664100	-1.12548500	H 4.54762900 -0.41841200 -1.84147100
H	-2.59470500	2.02653400	-1.84987700	C 4.20156800 -1.56183000 1.85152200

H	3. 58088200	-2. 24106000	2. 44334500	H	-1. 38648900	-0. 65874400	0. 93226400
H	5. 23901100	-1. 91192200	1. 87615400	Au	1. 29912900	-0. 74152200	0. 00502000
H	4. 14985200	-0. 56605200	2. 30152100	P	3. 49987300	-1. 57606200	0. 09619100
C	3. 84609500	-3. 19104300	-0. 54166900	C	4. 09381800	-1. 90304200	1. 80611200
H	4. 89552000	-3. 48685500	-0. 43860900	H	3. 44546400	-2. 63912800	2. 29045700
H	3. 21837200	-3. 90376500	0. 00140700	H	5. 11982200	-2. 28601600	1. 78917200
H	3. 56868500	-3. 22289200	-1. 59949200	H	4. 06589700	-0. 97958700	2. 39198900
H	-2. 35657400	2. 66198800	-1. 26776900	C	3. 74291800	-3. 16633900	-0. 79535900
				H	3. 49006300	-3. 04261000	-1. 85250700
<b>TS2-H</b>				H	4. 78360900	-3. 49737800	-0. 71218300
C	-3. 24107200	0. 85571700	-1. 18224900	H	3. 08859200	-3. 93354700	-0. 37094200
C	-0. 64608900	0. 00608600	-0. 11459800	C	4. 74483400	-0. 43191800	-0. 62658500
C	-2. 05387800	1. 89003000	0. 88653700	H	5. 75252200	-0. 85103400	-0. 53461400
C	-2. 66083500	1. 36795500	2. 14191100	H	4. 52231600	-0. 26248600	-1. 68423300
C	-2. 17516200	2. 81312600	2. 03834200	H	4. 70556200	0. 53097300	-0. 10913100
N	-3. 02136200	-0. 48623900	-0. 61568300	H	-2. 37343400	2. 86946700	-1. 04659300
S	-4. 36120400	-1. 41788900	-0. 04318000				
O	-3. 75456600	-2. 48346400	0. 75096400	<b>INT3-H</b>			
O	-5. 32660500	-0. 47508500	0. 51510500	C	-2. 32782500	-0. 34294000	1. 36834700
H	-3. 06177400	0. 82233300	-2. 26467800	C	-0. 66515900	-0. 77988900	-0. 98286900
H	-4. 28810600	1. 12076700	-1. 01189500	C	-2. 09521400	-2. 62038300	0. 04460800
H	-3. 72939600	1. 16854800	2. 14923000	C	-3. 25269900	-2. 85077200	-0. 86149400
H	-2. 07682000	0. 70115500	2. 77532900	C	-2. 60938100	-4. 00453600	-0. 09737700
H	-1. 27805300	3. 07931400	2. 59037700	N	-2. 47262400	0. 41994200	0. 10776300
H	-2. 91635500	3. 60629400	1. 97739200	S	-3. 31576000	1. 96634600	0. 21223900
C	-5. 05458100	-2. 11662900	-1. 54916800	O	-3. 04462500	2. 48466500	1. 54814100
H	-5. 93254800	-2. 69373900	-1. 24778400	O	-2. 94653900	2. 69342400	-0. 99869600
H	-5. 35194800	-1. 30577600	-2. 21716200	H	-1. 70121300	0. 24097100	2. 05311700
H	-4. 31140900	-2. 76581700	-2. 01504700	H	-3. 31874900	-0. 43022900	1. 82609900
C	-2. 33982700	1. 90165900	-0. 54793400	H	-4. 23931000	-2. 51964000	-0. 54369000
C	-0. 92964100	1. 45928000	-0. 06916200	H	-3. 09255000	-2. 80338400	-1. 93672200
C	0. 24420600	2. 38395400	-0. 26724200	H	-2. 01494400	-4. 71804600	-0. 66258900
C	1. 13289100	2. 64343100	0. 78770400	H	-3. 16222100	-4. 43960800	0. 73191000
C	0. 47643700	2. 98553400	-1. 51032800	C	-5. 03761100	1. 45956000	0. 10114900
C	2. 22740200	3. 48984700	0. 60220300	H	-5. 62899600	2. 37391300	0. 19768100
H	0. 96314400	2. 18780100	1. 76019200	H	-5. 20478600	0. 99485200	-0. 87169200
C	1. 57222500	3. 83159600	-1. 69829300	H	-5. 27017400	0. 77693800	0. 92047100
H	-0. 20436400	2. 79604900	-2. 33648700	C	-1. 70937900	-1. 71463900	1. 15196800
C	2. 44890600	4. 08646000	-0. 64227500	C	-0. 74937500	-1. 93479000	-0. 01859700
H	2. 89704600	3. 69630900	1. 43263000	C	0. 51640400	-2. 73223400	0. 16007600
H	1. 73568800	4. 29478700	-2. 66708200	C	0. 96460400	-3. 56485100	-0. 87660400
H	3. 29452900	4. 75310900	-0. 78437900	C	1. 28199000	-2. 64294100	1. 33033600
C	-1. 74194700	-0. 89194200	-0. 24403400	C	2. 15095200	-4. 28809900	-0. 74706700
H	-1. 54828600	-1. 96041600	-0. 29513800	H	0. 37774800	-3. 65504800	-1. 78813500

C	2.46785100	-3.37014300	1.46423800	H	1.33169900	0.94668400	1.96893800
H	0.94480100	-2.00964700	2.14740700	H	1.37484300	-0.79266000	2.28151600
C	2.90599300	-4.19253300	0.42483100	H	2.62550200	0.48944300	-1.48907300
H	2.48029000	-4.93376800	-1.55618600	H	0.92875800	0.76394200	-1.08963200
H	3.04267000	-3.30044400	2.38371700	H	1.05650600	4.98368600	0.96408900
H	3.82416800	-4.76309800	0.52969000	H	1.68501400	5.36521500	-0.70649200
C	-1.60863200	0.25065600	-0.91929200	H	-0.09251600	3.83421500	-1.72628800
H	-0.30152900	-1.00435200	-1.98731300	H	-0.72110000	3.44348400	-0.05803200
H	-1.72478400	0.95686200	-1.73598200	H	-3.58919900	1.03068500	1.76226100
H	-1.43421000	-2.18424500	2.09511100	H	-5.93153200	0.76962000	0.98639300
Au	0.92555700	0.70006200	-0.40466300	H	-6.45933600	-0.78361900	-0.88231900
P	2.71746300	2.09098100	0.17137800	H	-4.63364800	-2.07724000	-1.96839200
C	4.34448500	1.23985400	0.10013900	H	-2.28990600	-1.81840400	-1.18598000
H	4.52898400	0.87567400	-0.91477000	C	4.13261800	-1.81281000	-0.34917100
H	5.14809100	1.92672600	0.38680900	H	4.62187700	-1.60752800	0.60354700
H	4.34359600	0.38229000	0.77913900	H	4.39122900	-2.81061800	-0.71147800
C	2.88391400	3.55844400	-0.92207600	H	4.40266500	-1.06479300	-1.09693000
H	1.97103500	4.15943700	-0.87625400	H	3.29480800	2.31038600	0.20835600
H	3.73489200	4.17235000	-0.60779300				
H	3.03615000	3.23740800	-1.95662700				
C	2.59868800	2.77110900	1.87476300	C	1.13317700	-0.39700900	1.29906300
H	3.45737500	3.41693600	2.08797200	C	-0.26695200	-0.55938900	-1.22157700
H	1.67802200	3.35281200	1.97872100	C	-0.56815400	1.40900300	0.39261700
H	2.57684300	1.95365400	2.60140200	C	0.12844300	2.58911500	-0.17440200
				C	-1.17265900	2.74693700	0.61038200

### Pro1-H

### Sub-H

C	1.13418200	-0.03733100	1.52938000	S	3.49256500	-0.53012100	-0.06125100
C	-0.27593100	-0.13816200	1.13467300	O	3.94379700	-0.90148300	1.28089800
C	-1.43131900	-0.23204200	0.77761800	O	3.86503100	-1.30991400	-1.24333300
C	1.94669900	0.79008500	-0.68312000	H	1.04754000	-1.42062100	1.68869900
C	2.29638600	2.17583200	-0.20853100	H	1.75890800	0.16329300	1.99856100
C	1.46469000	3.20497100	-0.28466100	H	1.04848200	2.92923600	0.29769900
C	1.20860400	4.63290000	-0.05588800	H	0.10006400	2.73726500	-1.25192900
C	0.13920000	3.71157400	-0.66921300	H	-2.07480800	3.00086900	0.05795800
C	-2.78366900	-0.37550600	0.33784600	H	-1.12069600	3.18815700	1.60409700
C	-3.82326100	0.35358900	0.94625900	C	4.00545400	1.17478300	-0.35953800
C	-5.13696200	0.20354400	0.50762600	H	5.09689500	1.18081000	-0.41340200
C	-5.43366800	-0.66939900	-0.54216600	H	3.57384100	1.50927300	-1.30460200
C	-4.40772200	-1.39601200	-1.15249400	H	3.66292100	1.79829400	0.46838700
C	-3.09172400	-1.25504000	-0.71869500	C	-0.25653500	0.21312000	1.20612400
N	2.10330300	-0.19129400	0.41907700	C	-1.04134100	0.05667300	-0.10291600
S	2.34592800	-1.80452200	-0.09345600	C	-2.51490000	-0.25206800	-0.07074000
O	1.71235200	-2.04734100	-1.39533100	C	-3.36881900	0.33708000	-1.01594800
O	2.05235200	-2.66619100	1.05589300	C	-3.06392000	-1.14282600	0.85971500

C	-4.73401900	0.05006400	-1.02529500	H	-1.31657000	4.71568400	2.01577900
H	-2.95690400	1.02598300	-1.75002100	H	-2.57235100	5.20290200	-0.07574800
C	-4.43057900	-1.43056800	0.85548100	C	1.48821700	-1.34879400	0.39131300
H	-2.41585500	-1.62128800	1.58943100	H	1.04851200	-1.96747900	1.18603900
C	-5.27031300	-0.83413800	-0.08618400	H	1.48635800	-1.96531600	-0.51332000
H	-5.37957200	0.51900800	-1.76346600	Au	-1.44182400	-0.67124000	0.05961400
H	-4.83727600	-2.12492400	1.58620900	P	-3.71553100	-1.29811200	-0.06119900
H	-6.33384500	-1.05724300	-0.09014200	C	-4.33435600	-2.19701800	1.42155200
C	1.05800000	-0.75224400	-1.16256300	H	-4.22227000	-1.56720100	2.30910300
H	-0.80169100	-0.85476600	-2.11811700	H	-5.39012700	-2.46293100	1.30195500
H	1.63123000	-1.18118900	-1.97511000	H	-3.75028100	-3.10982900	1.57166800
H	-0.82620600	0.08846300	2.12699700	C	-4.88208200	0.11327100	-0.25512400
				H	-4.65147100	0.65944800	-1.17446600

### TS3-H

C	3.16353700	-0.06435800	1.73756500	H	-4.77268000	0.80101000	0.58862600
C	0.58124900	-0.16161300	0.17008800	C	-4.11213000	-2.41545300	-1.47014100
C	2.43907200	1.68138400	0.00818600	H	-5.17637100	-2.67462000	-1.47472500
C	3.23451100	1.73894100	-1.36102900	H	-3.85922400	-1.92336800	-2.41400100
C	2.78434400	2.98260000	-0.69244100	H	-3.52069900	-3.33259900	-1.39263600
N	2.89737900	-1.09864600	0.76362300	H	3.51849700	2.09888000	1.85052200
S	4.14373500	-1.46088400	-0.33441500				

O	3.56478300	-1.52895800	-1.67709600
O	5.23432800	-0.52781200	-0.01481300
H	2.49673100	-0.18233500	2.60838800
H	4.17920500	-0.16851400	2.14339000
H	4.27596500	1.44043800	-1.31984500
H	2.66305400	1.32621900	-2.18641000
H	1.95631300	3.53066000	-1.12938300
H	3.54206800	3.60178800	-0.21556300
C	4.66953600	-3.11810700	0.13091000
H	5.46961900	-3.40094800	-0.55770900
H	5.03760300	-3.09871800	1.15795600
H	3.82339200	-3.80005400	0.02726100
C	3.06701600	1.32707300	1.21787600
C	0.96761200	1.12817800	0.05823700
C	-0.01289200	2.26585900	0.03161700
C	-0.71591700	2.55625800	-1.14997900
C	-0.23031300	3.06557200	1.16284800
C	-1.64041100	3.60335700	-1.18348500
H	-0.54506700	1.95113000	-2.03616300
C	-1.15232100	4.11166700	1.12801300
H	0.31758500	2.86082600	2.08033000
C	-1.86096500	4.38281400	-0.04610900
H	-2.17959500	3.81449900	-2.10283800

### INT4-H

C	-3.41832400	-0.37629000	-1.73775400
C	-0.63949700	-0.19485900	-0.39085200
C	-2.47087500	1.60819100	-0.45951900
C	-3.04048500	2.57196000	0.74630900
C	-2.74888000	3.23025900	-0.48853800
N	-2.92811900	-1.36542200	-0.77011500
S	-3.88430900	-1.47656700	0.63917400
O	-3.00913300	-1.66599300	1.79377500
O	-4.82624800	-0.33493900	0.57225400
H	-2.68171600	-0.33661000	-2.55150400
H	-4.37609000	-0.68523600	-2.16197200
H	-4.05637400	2.34126900	1.04658400
H	-2.30182000	2.59613200	1.54093200
H	-1.81124300	3.76088700	-0.60392800
H	-3.54912500	3.53600800	-1.15315500
C	-4.83751200	-2.9800900	0.38136900
H	-5.50335800	-3.08552000	1.24134400
H	-5.41501800	-2.88304900	-0.53951100
H	-4.14525000	-3.82171200	0.32625800
C	-3.52793700	0.96663100	-1.09463300
C	-1.06106800	1.09755100	-0.30822200
C	-0.03550500	2.15727400	0.01344900

C	0.38600000	2.35997000	1.33817900	H	-3.47083700	3.65593900	-0.52134300
C	0.52634200	2.95542500	-0.99794600	C	-4.48403900	-3.15621000	0.46631900
C	1.33875800	3.33545500	1.64443800	H	-5.16044000	-3.31697700	1.30939900
H	-0.02088600	1.73216100	2.12740500	H	-4.99698400	-3.33157800	-0.48042800
C	1.48378100	3.92548200	-0.69372200	H	-3.60215500	-3.79267300	0.56064000
H	0.22236700	2.80141700	-2.03095800	C	-3.42984700	1.06045900	-1.20679900
C	1.88862500	4.12137000	0.62968200	C	-1.02016800	1.14044200	-0.28401300
H	1.65002400	3.47957100	2.67542100	C	0.00475400	2.21279700	-0.01971100
H	1.91296000	4.52775200	-1.48967700	C	0.61234700	2.33227900	1.24131300
H	2.62713300	4.88167000	0.86708000	C	0.36151100	3.12644400	-1.02543300
C	-1.45678700	-1.44574100	-0.61983500	C	1.55820700	3.33159800	1.48620800
H	-1.08074100	-1.95443500	-1.51659100	H	0.34132500	1.63541000	2.03018900
H	-1.26877500	-2.12844800	0.21338600	C	1.31206300	4.11987700	-0.78394100
Au	1.38941200	-0.65483700	-0.17026800	H	-0.09935800	3.04934500	-2.00765400
P	3.67451100	-1.20014800	0.06673500	C	1.91203700	4.22610300	0.47387000
C	4.34992400	-0.90921600	1.75586300	H	2.01192700	3.41433400	2.47013300
H	3.79375800	-1.50724000	2.48393200	H	1.58357500	4.81086100	-1.57713400
H	5.41009800	-1.18078300	1.80346600	H	2.64494400	5.00478700	0.66442600
H	4.23741700	0.14612300	2.02127800	C	-1.45969800	-1.39783000	-0.55940900
C	4.08946400	-2.95998500	-0.28301100	H	-1.04380000	-1.94863500	-1.41279300
H	3.80934100	-3.20961600	-1.31070800	H	-1.32506200	-2.04986300	0.30899200
H	5.16149400	-3.14083800	-0.14958200	Au	1.40609400	-0.64801200	-0.13364400
H	3.52977800	-3.61276300	0.39350300	P	3.68597000	-1.23323400	0.05894400
C	4.79650900	-0.24278900	-1.03651900	C	4.32355300	-1.24887500	1.78695800
H	5.84250700	-0.52045000	-0.86747600	H	3.75514400	-1.96834700	2.38387900
H	4.53908800	-0.43585000	-2.08225800	H	5.38377600	-1.52284800	1.80928900
H	4.67363200	0.82745800	-0.84548400	H	4.19992200	-0.25829700	2.23456400
H	-4.48681500	1.47288200	-1.14428500	C	4.10263500	-2.90576800	-0.58991600
				H	3.84002600	-2.96628600	-1.65029700
				H	5.17148000	-3.11502700	-0.47335300

#### TS4-H

C	-3.32738600	-0.30569000	-1.80947700
C	-0.61745800	-0.15960800	-0.34095800
C	-2.41069000	1.66753800	-0.49069300
C	-3.36665900	2.06107700	0.95317300
C	-2.79361000	3.06804800	0.09280400
N	-2.91680700	-1.29035900	-0.80091400
S	-3.96729900	-1.43594100	0.53315700
O	-3.21211100	-1.22282800	1.77237600
O	-5.12910800	-0.58597500	0.21755600
H	-2.55095000	-0.30797600	-2.58660100
H	-4.27311600	-0.59575300	-2.26836000
H	-4.41934500	1.80304700	0.93244200
H	-2.79422700	1.62189500	1.76413800
H	-1.92139100	3.60556000	0.44691500

#### INT5-H

C	-3.74375400	-1.13417300	-1.41256000
C	-0.58275500	-0.35200800	-0.58998200
C	-2.45795500	1.15999500	-1.04178600
C	-4.52446700	1.47188300	-1.40888700
C	-3.32272200	2.39152900	-1.04344300
N	-2.76044400	-1.69647700	-0.48573700

S	-3.05248700	-1.47811600	1.18367000
O	-1.73067300	-1.39083900	1.82215400
O	-4.04516700	-0.41049200	1.35020200
H	-3.72845400	-1.75597200	-2.31359400
H	-4.73687700	-1.23397900	-0.96968500
H	-5.18614100	1.80929100	-2.20825800
H	-5.10430300	1.20199700	-0.52431400
H	-3.34546500	2.94554100	-0.09936800
H	-3.06482300	3.09573500	-1.84402800
C	-3.81168900	-3.03567600	1.66700300
H	-4.04199000	-2.95959600	2.73250600
H	-4.72835700	-3.17526800	1.09089800
H	-3.10351000	-3.84445600	1.48120200
C	-3.49651600	0.35069000	-1.77731900
C	-1.21918300	0.91147300	-0.47841800
C	-0.49364600	2.04277100	0.18681900
C	-0.16520900	1.93912900	1.54889700
C	-0.14850500	3.20699800	-0.51518500
C	0.49762800	2.98603100	2.19291400
H	-0.45299100	1.04896300	2.10131800
C	0.52165700	4.24786100	0.13037100
H	-0.38839400	3.29402700	-1.57196000
C	0.84401300	4.13985200	1.48553700
H	0.73310500	2.90327600	3.25025700
H	0.78766200	5.14338000	-0.42394500
H	1.35593700	4.95488400	1.98905700
C	-1.34881100	-1.61959700	-0.88191100
H	-1.29540300	-1.81269700	-1.96526700
H	-0.81086400	-2.44985400	-0.41739800
Au	1.45236600	-0.51467700	-0.34298700
P	3.79984100	-0.70774600	-0.05874000
C	4.34168000	-0.40922400	1.67420200
H	3.87394700	-1.14028700	2.34034700
H	5.43049800	-0.49118600	1.75900300
H	4.03094900	0.59134100	1.98896300
C	4.48838100	-2.35790300	-0.49175900
H	4.27096200	-2.58642500	-1.53938900
H	5.57267800	-2.37819600	-0.33896400
H	4.02496200	-3.12778800	0.13233900
C	4.77355900	0.48610300	-1.06473900
H	5.84568100	0.36384500	-0.87705200
H	4.57571600	0.32395300	-2.12842900
H	4.47933300	1.50881500	-0.81130000
H	-3.26906200	0.42779400	-2.85179600

### TS5-H

C	-1.72042000	-0.80218200	0.12339400
N	-3.07285900	-0.61982800	0.39481600
C	-0.63982600	0.13979000	0.05031700
C	-0.76402800	1.60263800	-0.05004300
C	-3.66409100	0.67001300	0.77117900
C	-3.37026400	1.76612300	-0.25622300
C	-1.93934500	2.24208400	-0.26630400
H	-1.27931800	-0.52192000	-1.02876900
H	-1.42826800	-1.84726100	0.16561300
H	-4.74293300	0.52972700	0.86519800
H	-3.27020100	0.95688300	1.75188900
H	-3.73637000	1.44015700	-1.23782500
C	-2.34587200	3.69797900	-0.29617400
H	-1.82105200	4.36818000	0.39158200
H	-2.29378500	4.13250000	-1.30172000
C	-3.79237900	3.23414600	0.06871100
H	-4.01872300	3.37774200	1.12942000
H	-4.60801600	3.64401100	-0.52945200
Au	1.28931500	-0.70612300	0.00113000
P	3.43824800	-1.65753100	-0.07459600
C	4.42937000	-1.37687400	1.44962300
H	3.92182600	-1.82266800	2.31019300
H	5.42445600	-1.82349900	1.35009300
H	4.53485200	-0.30291000	1.62867400
C	4.48145500	-0.99968100	-1.43925600
H	5.47420000	-1.46205200	-1.42229300
H	4.00604500	-1.20803100	-2.40230200
H	4.58702700	0.08410000	-1.33445100
C	3.44828000	-3.48138900	-0.31293300
H	4.47540600	-3.86020600	-0.34486600
H	2.91306100	-3.96615300	0.50888800
H	2.94405500	-3.73559200	-1.24993900
S	-4.14989600	-1.85586500	-0.21489900
O	-3.28330400	-2.84596700	-0.84874700
O	-5.20572700	-1.15955000	-0.94329400
C	-4.84299300	-2.55605700	1.29141300
H	-4.03864200	-3.00899800	1.87310000
H	-5.35197100	-1.77323300	1.85673000
H	-5.56209400	-3.31571000	0.97396300
C	0.49822000	2.40721300	0.03476000
C	0.93052600	3.17544000	-1.05658900
C	1.25295000	2.43049000	1.21999700

C	2.09519200	3.94141700	-0.97029000	H	5.94807900	-1.19032400	-0.89033200
H	0.35676100	3.16535800	-1.97951000	H	4.93563200	-2.38741900	-0.02804500
C	2.41370000	3.20165200	1.30812300	Au	-0.27844500	1.06196800	-0.24955200
H	0.91648400	1.86176400	2.08359100	P	-0.72012500	3.19210700	0.59764400
C	2.83884700	3.95647600	0.21167500	C	0.69687600	3.91512900	1.51710100
H	2.41720400	4.52998000	-1.82463400	H	1.57407200	3.96888400	0.86582100
H	2.97637400	3.22488400	2.23736800	H	0.44754100	4.92167600	1.87013700
H	3.73871800	4.56073900	0.28184300	H	0.94351700	3.28432500	2.37602100
				C	-1.12584400	4.41054400	-0.71565000
<b>INT6-H</b>				H	-2.01248500	4.08237200	-1.26583800
N	2.28551000	-1.14914900	-0.25575700	H	-1.32052400	5.39375900	-0.27385100
C	1.30306200	-0.77854000	-1.12160500	H	-0.29124800	4.49149600	-1.41805200
C	-0.07553200	-1.04544400	-1.10346300	C	-2.14031300	3.24269500	1.76249500
C	2.03169200	-1.80947200	1.04270700	H	-2.31134700	4.26722800	2.11015200
C	1.20693100	-3.08273300	0.87023700	H	-3.04258800	2.87735600	1.26352100
C	-0.25546100	-2.90090800	0.51894100	H	-1.93707600	2.60119000	2.62488700
C	-0.85746800	-1.99780500	-0.27225900				
H	1.68231300	-0.21807900	-1.97104400	<b>Pro2-H</b>			
H	-0.54748300	-0.79529200	-2.05514200	N	-1.95996700	-0.15109400	-0.10746000
H	2.99897200	-2.02891900	1.50084700	C	-1.04389800	-1.13474700	-0.50732000
H	1.51511500	-1.10416500	1.70525200	C	0.30754100	-1.08791200	-0.55462900
H	1.72119700	-3.75991200	0.17575100	C	-1.55756000	1.07296600	0.59527100
C	0.73799100	-3.84055000	2.15320300	C	-0.52184200	1.87597900	-0.20143100
H	1.24731200	-4.78073700	2.37572700	C	0.87244900	1.29080200	-0.23642800
H	0.76481000	-3.20304600	3.04276700	C	1.26315700	0.00038200	-0.30624300
C	-0.69576600	-3.93295500	1.53985400	H	-1.53376800	-2.04128500	-0.84234900
H	-0.89024400	-4.91260000	1.08579100	H	0.75781700	-2.01791600	-0.89161600
H	-1.54070600	-3.68697600	2.18772200	H	-2.45560400	1.67426100	0.74951700
C	-2.34585100	-1.90638600	-0.39585900	H	-1.13316100	0.81366700	1.57456300
C	-3.14380900	-1.63426000	0.72687800	H	-0.93592900	2.10927100	-1.19019100
C	-2.97300100	-2.08405400	-1.63975100	C	2.69160500	-0.38579300	-0.13513300
C	-4.53249900	-1.54739800	0.61021500	C	3.03702100	-1.55511900	0.56589500
H	-2.67227600	-1.48662600	1.69503700	C	3.73265400	0.40085700	-0.65797200
C	-4.36076100	-1.99701700	-1.75631200	C	4.37127400	-1.91658100	0.74969200
H	-2.37599200	-2.31754800	-2.51844300	H	2.24925500	-2.17523100	0.98506500
C	-5.14437000	-1.72771900	-0.63178800	C	5.06740600	0.04020000	-0.47530000
H	-5.13557000	-1.34084500	1.49009400	H	3.49021200	1.28732900	-1.23555500
H	-4.83026700	-2.14900400	-2.72401600	C	5.39366200	-1.11946600	0.23092000
H	-6.22473400	-1.66355300	-0.72268200	H	4.61239600	-2.82145700	1.30174400
S	3.82592700	-0.29811000	-0.41310500	H	5.85414200	0.66130400	-0.89593000
O	4.14374100	0.21763900	0.91406200	H	6.43366900	-1.40195200	0.37054400
O	3.68187700	0.57916900	-1.57217000	C	1.51515900	2.60271700	0.17719600
C	4.95357600	-1.63911700	-0.82242800	H	2.24285800	2.56467400	0.99642000
H	4.65792900	-2.06503900	-1.78242700	H	1.97563100	3.15274900	-0.65390500

C	0.08333200	3.13052600	0.50601800	C	0.39577600	1.50768300	-0.42123100
H	-0.12155100	3.14178700	1.58185400	H	-0.04294800	1.52015200	-1.43324900
H	-0.19241200	4.10194600	0.08678700	H	-0.04220800	2.35720900	0.11704800
S	-3.61790800	-0.53675400	-0.15986800	Au	-2.11134500	-0.09061300	0.01932100
O	-4.34851900	0.72800000	-0.23602400	P	-4.44885900	-0.38086300	-0.23420900
O	-3.78992000	-1.58715500	-1.16199900	C	-4.93127300	-1.84756600	-1.23756400
C	-3.95318600	-1.26633300	1.45960600	H	-4.54618800	-2.75929400	-0.77116700
H	-5.01315000	-1.53091000	1.48091600	H	-6.02126600	-1.92015200	-1.31751900
H	-3.33630200	-2.15920000	1.57940400	H	-4.50328700	-1.76723400	-2.24121200
H	-3.73293900	-0.53095400	2.23618100	C	-5.35668300	-0.59325600	1.35318400
				H	-5.20081000	0.28331300	1.98902200

### INT2-Me

C	2.66655500	0.62649400	-0.93422200	H	-6.42963300	-0.71838500	1.17211800
C	-0.06763000	0.23750000	0.25317900	C	-4.97843700	-1.47296000	1.88237400
C	2.18082800	-0.22263600	1.39257000	C	-5.29082700	1.03380500	-1.05827900
C	2.56375400	0.91783300	2.29415500	H	-6.36750500	0.85006400	-1.14020900
C	2.77839300	-0.50291600	2.74946300	H	-5.12724600	1.94894200	-0.48147200
N	1.83955700	1.72851000	-0.50197400	H	-4.87561700	1.17935800	-2.05996200
S	2.50416600	3.24686800	-0.20460900	C	0.26967400	-1.93869700	1.49888500
O	1.66004900	3.88359300	0.80603200	H	0.28549900	-1.97942100	2.59461800
O	3.93857600	3.02324400	0.00186400	H	-0.74588200	-2.15035500	1.15734400
H	2.36584800	0.29204900	-1.93522200	H	0.91714700	-2.74925600	1.14106000
H	3.70400600	0.98092100	-1.00167300				

### TS2-Me

H	3.43700800	1.50423600	2.02568500	C	2.70414200	0.63264800	-0.74293600
H	1.75752800	1.49249900	2.73904100	C	-0.07183000	0.23004800	0.05151700
H	2.12604300	-0.90167100	3.52122400	C	1.93819000	-0.34214500	1.51352900
H	3.80135700	-0.86607400	2.79771200	C	2.00472300	0.72428700	2.55128600
C	2.31182200	4.17559200	-1.73912500	C	2.24516500	-0.73883100	2.91075600
H	2.72064100	5.17348500	-1.56230700	N	1.77529800	1.75477500	-0.53930200
H	2.87011100	3.67480100	-2.53253300	S	2.37555300	3.34886000	-0.24315600
H	1.24996400	4.24490700	-1.98465100	O	1.21046000	4.09895500	0.22074100
C	2.67113900	-0.52853800	0.05553600	O	3.58745500	3.20629900	0.55879100
C	0.73576500	-0.59217600	0.99685800	H	2.67375800	0.32656300	-1.79562700
C	3.17968700	-1.82119400	-0.35666000	H	3.71276600	0.98886500	-0.51756900
C	3.43626800	-2.84588000	0.59310200	H	2.85078900	1.40636000	2.52958900
C	3.48950200	-2.09270500	-1.71693000	H	1.08018000	1.17521800	2.91166400
C	3.96951900	-4.06789000	0.20306700	H	1.46989600	-1.24607600	3.47990300
H	3.23176700	-2.66928500	1.63965200	H	3.25493300	-1.05319100	3.15861000
C	4.02787500	-3.31283500	-2.09831000	C	2.84574300	3.92674400	-1.88126100
H	3.30957000	-1.34974500	-2.48398800	H	3.26816000	4.92601800	-1.74805900
C	4.26825900	-4.30613100	-1.14135000	H	3.60006900	3.25481900	-2.29572300
H	4.16213500	-4.83324700	0.94835500	H	1.95726300	3.96854700	-2.51347100
H	4.25911700	-3.49626600	-3.14285900	C	2.40010200	-0.58552600	0.13861600
H	4.68945300	-5.26029600	-1.44404500	C	0.88472200	-0.80113500	0.50284900

C	3. 25946000	-1. 76515000	-0. 23193000	H	3. 28625000	1. 02731700	-1. 50622900
C	4. 42565400	-2. 05470800	0. 48969900	H	3. 25228300	1. 04128000	2. 15644600
C	2. 95335000	-2. 53774000	-1. 36304800	H	1. 52109500	0. 93425200	2. 73679600
C	5. 25758000	-3. 10628000	0. 10096100	H	1. 86704100	-1. 56402100	3. 14142400
H	4. 69183300	-1. 45092100	1. 35218100	H	3. 57119000	-1. 41654900	2. 51683000
C	3. 78219200	-3. 59015800	-1. 75026900	C	2. 13115200	4. 30170600	-1. 15307700
H	2. 05683100	-2. 31909000	-1. 93903200	H	2. 61676400	5. 21187600	-0. 79260800
C	4. 93586900	-3. 87785500	-1. 01675600	H	2. 59316100	3. 96785300	-2. 08399500
H	6. 15726500	-3. 31982700	0. 67071400	H	1. 06102400	4. 47468600	-1. 28443200
H	3. 52867300	-4. 18467900	-2. 62329500	C	2. 80013100	-0. 46831300	-0. 04931400
H	5. 58210300	-4. 69729500	-1. 31741800	C	0. 50069100	-0. 79918700	0. 80674400
C	0. 42752100	1. 51199400	-0. 31045200	C	3. 88384800	-1. 34725100	-0. 37575400
H	-0. 26171500	2. 28396200	-0. 64301900	C	3. 90957700	-2. 67165700	0. 14797300
H	0. 05864200	1. 39012400	0. 88421900	C	4. 93435000	-0. 94870200	-1. 25182500
Au	-2. 13530700	-0. 09604000	-0. 03414500	C	4. 91224000	-3. 55635500	-0. 21566100
P	-4. 46209000	-0. 46688900	-0. 15273000	H	3. 10728400	-3. 00149700	0. 79616900
C	-4. 94620100	-2. 22193800	0. 10863600	C	5. 95523900	-1. 82880200	-1. 57426000
H	-4. 60462000	-2. 55871400	1. 09188400	H	4. 98437100	0. 06910400	-1. 61981400
H	-6. 03415400	-2. 33360200	0. 05069600	C	5. 94146900	-3. 13496100	-1. 06760300
H	-4. 48095000	-2. 85374700	-0. 65377200	H	4. 90292500	-4. 57243500	0. 16559900
C	-5. 42271300	0. 47939900	1. 09823500	H	6. 76760800	-1. 50267600	-2. 21562100
H	-5. 25506600	1. 55194100	0. 96285000	H	6. 73830200	-3. 82389600	-1. 33248300
H	-6. 49291500	0. 26878400	0. 99933200	C	0. 13999000	1. 46587000	-0. 29137600
H	-5. 09576000	0. 20351600	2. 10508500	H	-0. 35930900	1. 65585100	-1. 25266900
C	-5. 20727200	-0. 00446500	-1. 76944600	H	-0. 21000600	2. 23773800	0. 40275000
H	-6. 28637500	-0. 19151100	-1. 76403200	Au	-2. 35643000	-0. 19488700	-0. 04451700
H	-5. 02982600	1. 05634300	-1. 96967100	P	-4. 69350100	-0. 45730600	-0. 31489000
H	-4. 74722600	-0. 58906200	-2. 57159900	C	-5. 21026500	-2. 06098900	-1. 05992700
C	0. 34123700	-2. 21232500	0. 66995600	H	-4. 87561300	-2. 88868800	-0. 42739600
H	-0. 47087300	-2. 22073200	1. 40677600	H	-6. 29943900	-2. 10979800	-1. 16521000
H	-0. 05054600	-2. 61007700	-0. 27263400	H	-4. 75016100	-2. 17466800	-2. 04606500
H	1. 12239000	-2. 89045000	1. 01955000	C	-5. 65097200	-0. 35860600	1. 25581500
				H	-5. 47787700	0. 61105900	1. 73203600
<b>TS3-Me</b>							
C	2. 39322700	0. 60762400	-1. 04039700	H	-6. 72335400	-0. 48004500	1. 06869600
C	-0. 30678300	0. 10736100	0. 21258200	H	-5. 31627400	-1. 14160400	1. 94278500
C	1. 99231500	-0. 56625000	1. 15359000	C	-5. 47414000	0. 81146000	-1. 39835700
C	2. 37045400	0. 42400500	2. 29469900	H	-6. 55339700	0. 64372500	-1. 48082400
C	2. 55219500	-1. 04367200	2. 47992800	H	-5. 29812400	1. 80926400	-0. 98546000
N	1. 59191600	1. 66815900	-0. 47990600	H	-5. 02845800	0. 76944200	-2. 39671000
S	2. 36833400	3. 03929500	0. 11209200	C	0. 04580600	-2. 20413300	1. 15861100
O	1. 65354200	3. 47972000	1. 31024600	H	0. 04177300	-2. 38163500	2. 24137100
O	3. 79728100	2. 69681400	0. 14619900	H	-0. 96502300	-2. 38207400	0. 78523700
H	1. 83622300	0. 11278400	-1. 85066100	H	0. 70375600	-2. 96397700	0. 71419400

**INT3-Me**

C	1. 94883600	0. 59504700	-0. 76701300	H	-6. 23464400	-0. 20529500	-0. 09609700
C	0. 10357000	0. 45596800	1. 46329200	H	-5. 28716700	-0. 01429100	1. 40268600
C	2. 56857900	-0. 15011000	1. 64410600	C	-4. 07497900	-0. 43200600	-2. 26242900
C	3. 21961000	0. 99983400	2. 33088800	H	-5. 05661200	-0. 79100200	-2. 59001200
C	3. 65016200	-0. 43242100	2. 62375900	H	-3. 99155100	0. 63426900	-2. 49220500
N	1. 23158800	1. 76560400	-0. 22635700	H	-3. 29662000	-0. 96919700	-2. 81226500
S	1. 60803300	3. 37204000	-0. 86170800	C	0. 74528500	-1. 97505700	1. 97856500
O	0. 80074300	4. 28979000	-0. 06699000	H	0. 39084900	-1. 85790200	3. 01066300
O	3. 06091800	3. 43360700	-0. 91849700	H	-0. 06494600	-2. 43184700	1. 39726200
H	1. 36030800	0. 19254000	-1. 60218700	H	1. 58561900	-2. 67276600	1. 99055700
H	2. 90832000	0. 94521400	-1. 15682000				
H	3. 89505600	1. 63174400	1. 75798900	<b>INT4-Me</b>			
H	2. 66425000	1. 52906100	3. 10328700	C	2. 31686100	0. 48945100	-1. 16888400
H	3. 36871200	-0. 85684600	3. 58478000	C	-0. 38489600	-0. 01592900	0. 10018500
H	4. 62013300	-0. 76264200	2. 26222600	C	1. 90106900	-0. 99364800	0. 81635400
C	0. 95432000	3. 29647200	-2. 53673600	C	2. 51911400	-0. 19719900	2. 14051100
H	1. 18337100	4. 26297500	-2. 99382400	C	2. 46286400	-1. 66352700	2. 07486800
H	1. 45507500	2. 49675500	-3. 08568500	N	1. 53666400	1. 54633200	-0. 55356100
H	-0. 12528300	3. 14349500	-2. 49073700	S	2. 34441100	2. 73876100	0. 31351200
C	2. 17430800	-0. 52681800	0. 25882700	O	1. 63728500	2. 96400900	1. 57603800
C	1. 15762200	-0. 62768700	1. 41319700	O	3. 76238600	2. 34294700	0. 30306800
C	2. 72234800	-1. 75254200	-0. 42768700	H	1. 66344100	-0. 02921600	-1. 88768900
C	4. 10576000	-1. 96265300	-0. 51138400	H	3. 15292800	0. 89283300	-1. 74176300
C	1. 86391300	-2. 65726800	-1. 07130500	H	3. 46870100	0. 31445600	2. 02679300
C	4. 61888300	-3. 06087800	-1. 20384100	H	1. 72923800	0. 38849100	2. 59833900
H	4. 78625600	-1. 26205300	-0. 03629600	H	1. 71629200	-2. 16369800	2. 68039500
C	2. 37433300	-3. 75656700	-1. 76206500	H	3. 40684800	-2. 19104100	2. 01561800
H	0. 78797500	-2. 50377500	-1. 02205300	C	2. 17433900	4. 22897900	-0. 68288100
C	3. 75436600	-3. 96162700	-1. 82813400	H	2. 68118900	5. 03387600	-0. 14487800
H	5. 69332100	-3. 21157600	-1. 25515500	H	2. 64327600	4. 06180200	-1. 65402400
H	1. 69677500	-4. 45376500	-2. 24722900	H	1. 11306400	4. 46059500	-0. 79338100
H	4. 15306600	-4. 81784200	-2. 36434600	C	2. 80869900	-0. 56515600	-0. 19960000
C	0. 34156800	1. 65645200	0. 76715400	C	0. 38737800	-0. 99759200	0. 62308900
H	-0. 15830000	2. 58061300	1. 04471600	C	4. 13649300	-1. 11256600	-0. 39853000
H	-0. 33032800	0. 63135000	2. 45316700	C	4. 32689700	-2. 51616600	-0. 32500800
Au	-1. 79389300	-0. 02223900	0. 42030500	C	5. 22927600	-0. 29141700	-0. 77409200
P	-3. 86632700	-0. 70084000	-0. 45502400	C	5. 55972300	-3. 07461300	-0. 63492000
C	-4. 19453700	-2. 49161600	-0. 19900000	H	3. 48661200	-3. 15924400	-0. 08521300
H	-4. 15775300	-2. 72621400	0. 86884500	C	6. 46959300	-0. 85914300	-1. 03826800
H	-5. 18186100	-2. 75937800	-0. 59038000	H	5. 10875600	0. 78610900	-0. 77975700
H	-3. 43330800	-3. 08778000	-0. 71073800	C	6. 63527400	-2. 24731800	-0. 97932500
C	-5. 29143500	0. 16146300	0. 32295500	H	5. 68667100	-4. 15235900	-0. 60994700
H	-5. 21629500	1. 23870500	0. 14794000	H	7. 31038800	-0. 22115500	-1. 29168700
				H	7. 60307200	-2. 68627900	-1. 20354400

C	0.08267200	1.34051100	-0.38240900	C	0.14462700	-1.03311300	1.37897500
H	-0.39649800	1.55081600	-1.34830700	C	-0.09199600	-1.42872100	2.70783600
H	-0.27588800	2.10391700	0.31556800	C	0.47959900	-2.02136800	0.43587700
Au	-2.46337900	-0.18413800	-0.07361800	C	0.00247600	-2.77038800	3.07990800
P	-4.81847300	-0.32045700	-0.27258900	H	-0.39467300	-0.69181800	3.44567400
C	-5.42876900	-1.88473500	-1.03131600	C	0.58850200	-3.36112100	0.81173300
H	-5.10642600	-2.73875800	-0.42802800	H	0.65757700	-1.73351100	-0.59621800
H	-6.52207200	-1.88716300	-1.09887100	C	0.35218200	-3.73895500	2.13543300
H	-5.00802000	-1.99594900	-2.03519400	H	-0.19911300	-3.05840700	4.10765900
C	-5.72793600	-0.21065800	1.32562900	H	0.85939600	-4.10814300	0.07080100
H	-5.49779900	0.73979800	1.81619700	H	0.43698500	-4.78113600	2.42949400
H	-6.80931900	-0.27922200	1.16559900	C	2.85892800	0.56042400	-0.06285800
H	-5.41172100	-1.02252500	1.98741600	C	3.34975300	-0.38964200	0.86830400
C	-5.57227100	1.00197500	-1.31022500	C	3.53166300	0.67492100	-1.30737100
H	-6.65967100	0.88281900	-1.36626800	C	4.44501900	-1.18727900	0.56523100
H	-5.34158600	1.98305900	-0.88436500	H	2.86581000	-0.50550400	1.82777500
H	-5.15558900	0.96019900	-2.32104500	C	4.63477900	-0.11213100	-1.60010100
C	-0.22682000	-2.32474300	1.05951600	H	3.20822900	1.39580900	-2.04822400
H	-0.34418300	-2.39977200	2.14920600	C	5.08980600	-1.05138100	-0.66698500
H	-1.22097200	-2.43714200	0.62223100	H	4.80834500	-1.90805700	1.28928600
H	0.38135600	-3.18065300	0.73898200	H	5.14899400	0.00128200	-2.54811900
				C	-1.16498000	2.14728600	-0.49237000

### INT2-CF<sub>3</sub>Ph

C	1.28628500	2.46978900	-0.74892200	H	-2.00385000	2.65593300	-0.00094100
C	-1.02210500	0.78265900	0.13217100	Au	-2.58759500	-0.51545500	-0.30264100
C	1.04158900	1.39985900	1.53594000	P	-4.40812600	-1.94978100	-0.77516600
C	0.76302400	2.54783200	2.46763900	C	-3.92829800	-3.51587100	-1.61550000
C	1.63719400	1.40660200	2.92008700	H	-3.21864800	-4.06610000	-0.99053300
N	-0.00313500	3.03202800	-0.42633000	H	-4.80592100	-4.14432100	-1.80111000
S	-0.17568700	4.66980600	-0.07059600	H	-3.44299300	-3.28932900	-2.56954200
O	-1.31594200	4.78159200	0.83836400	C	-5.33910200	-2.49336800	0.71683300
O	1.16426500	5.14324800	0.29095900	H	-5.73470100	-1.62014200	1.24397800
H	1.28355000	2.05699100	-1.76679600	H	-6.16987100	-3.15028700	0.43775300
H	2.02955100	3.27805500	-0.71866300	H	-4.66968700	-3.02988000	1.39577600
H	1.23230500	3.50324200	2.25557400	C	-5.68810800	-1.21106200	-1.87207500
H	-0.24225800	2.62130600	2.87125800	H	-6.50067100	-1.92226800	-2.05540500
H	1.25424100	0.71214700	3.65926600	H	-6.09925000	-0.31078500	-1.40579300
H	2.70568600	1.59030100	2.99796300	H	-5.23771900	-0.92814300	-2.82818100
C	-0.63662700	5.46296800	-1.62359100	C	6.24934100	-1.95793000	-1.01928500
H	-0.77143500	6.52646500	-1.41138400	F	5.80317100	-3.06180600	-1.65320700
H	0.16616900	5.32216100	-2.34993800	F	6.91279500	-2.35749500	0.08029700
H	-1.57419600	5.03120200	-1.98005200	F	7.12147500	-1.34155100	-1.83753100
C	1.73906100	1.42604900	0.26022900				
C	-0.00163400	0.39949000	0.97461100				

### TS2-CF<sub>3</sub>Ph

C	1. 50785200	2. 25041300	-0. 12255100	H	-1. 87380000	2. 63793600	-0. 40272600
C	-1. 00336000	0. 67972800	-0. 02908000	Au	-2. 84278600	-0. 31705500	-0. 07124400
C	0. 71783900	0. 57201200	1. 70393200	P	-4. 91709700	-1. 42981300	-0. 05080400
C	0. 06984800	1. 36954300	2. 78850000	C	-4. 90898300	-3. 01537800	-0. 98236100
C	0. 82438900	0. 09449700	3. 11285800	H	-4. 15353900	-3. 68725500	-0. 56456800
N	0. 17066600	2. 87076000	-0. 08982700	H	-5. 89028800	-3. 49892600	-0. 92932900
S	0. 07182100	4. 50696900	-0. 71334300	H	-4. 66040500	-2. 82623300	-2. 03085500
O	1. 11843200	4. 65304800	-1. 71912000	C	-5. 50274100	-1. 87495800	1. 63528500
O	-1. 34142100	4. 71893500	-1. 02093600	H	-5. 61464900	-0. 97079500	2. 24087500
H	1. 85900400	2. 17945200	-1. 15871800	H	-6. 46706000	-2. 39153500	1. 58274000
H	2. 20627900	2. 90620000	0. 40803000	H	-4. 77283200	-2. 52904300	2. 12133200
H	0. 53093000	2. 31702900	3. 05678500	C	-6. 29279400	-0. 45578200	-0. 78604700
H	-1. 01304500	1. 35577200	2. 88407700	H	-7. 22728500	-1. 02595500	-0. 75235200
H	0. 23502000	-0. 77051200	3. 40371000	H	-6. 42355800	0. 47895900	-0. 23294900
H	1. 78282000	0. 16900800	3. 61922900	H	-6. 06070800	-0. 21115700	-1. 82680600
C	0. 50889200	5. 47459900	0. 73814500	C	6. 84574800	-1. 37072200	-0. 35132800
H	0. 50040400	6. 52001400	0. 41888200	F	7. 38540000	-1. 87279500	0. 77855500
H	-0. 23902500	5. 30321700	1. 51344000	F	7. 66737400	-0. 39237900	-0. 78750300
H	1. 50989400	5. 19816700	1. 07461800	F	6. 85366600	-2. 34606900	-1. 28266000
C	1. 53828900	0. 85677500	0. 51287900				
C	0. 23598400	-0. 01670100	0. 37382300	<b>TS3-CF<sub>3</sub>Ph</b>			
C	0. 34359200	-1. 48211300	0. 03629100	C	1. 11358500	2. 05412800	0. 01387600
C	0. 89037600	-2. 42950900	0. 91265700	C	-0. 81332200	0. 05195600	-0. 99334400
C	-0. 08220100	-1. 91770800	-1. 23114200	C	0. 43042900	-0. 10245000	1. 25441500
C	0. 98725800	-3. 77229100	0. 54181600	C	-0. 53281600	0. 40106800	2. 27666600
H	1. 25904400	-2. 12444400	1. 88392300	C	0. 41652200	-0. 73843300	2. 60297400
C	0. 01827400	-3. 25885200	-1. 60429300	N	-0. 26212500	2. 34887600	-0. 47403300
H	-0. 48148500	-1. 20129000	-1. 94504800	S	-0. 64939300	4. 05616600	-0. 74862800
C	0. 54885500	-4. 19421500	-0. 71409700	O	0. 59192700	4. 69038700	-1. 16786400
H	1. 41436500	-4. 48840800	1. 23800000	O	-1. 85546800	4. 04885200	-1. 57060400
H	-0. 30794100	-3. 56757000	-2. 59358900	H	1. 81093300	2. 39740500	-0. 75514600
H	0. 63196400	-5. 23829000	-1. 00116600	H	1. 29235900	2. 66026500	0. 90912500
C	2. 88757300	0. 21316700	0. 30858400	H	-0. 33962900	1. 37138600	2. 73109000
C	3. 84446300	0. 23382200	1. 33155400	H	-1. 59062900	0. 16200100	2. 17009600
C	3. 24034000	-0. 33162000	-0. 93481900	H	-0. 02102400	-1. 72850600	2. 69860900
C	5. 11838000	-0. 29434300	1. 12677900	H	1. 23775900	-0. 55241900	3. 28931800
H	3. 60049600	0. 66910400	2. 29545500	C	-1. 07030900	4. 60681300	0. 91152000
C	4. 51074600	-0. 86084800	-1. 14490300	H	-1. 30894500	5. 67022100	0. 82361200
H	2. 51274900	-0. 36088400	-1. 74038500	H	-1. 93883100	4. 04648100	1. 26084400
C	5. 45171100	-0. 84459000	-0. 11197800	H	-0. 20966500	4. 47293000	1. 56918100
H	5. 84903500	-0. 28377000	1. 92862400	C	1. 37385300	0. 57877600	0. 33292300
H	4. 76932300	-1. 29374600	-2. 10524300	C	0. 35390300	-0. 49226800	-0. 20227800
C	-0. 95014700	2. 07550500	-0. 29174000	C	0. 87833000	-1. 82071700	-0. 70301300
H	-0. 95808000	1. 34545500	-1. 32103200	C	1. 30106400	-2. 83983400	0. 16193300

C	0.97549700	-2.05131700	-2.08753900	C	1.16428400	0.53438700	1.28201500
C	1.78484100	-4.05121200	-0.33673000	C	1.21274600	1.51465400	2.49516500
H	1.26878100	-2.69053400	1.23300500	C	1.71197400	0.11757000	2.63138300
C	1.45824400	-3.26056300	-2.58719000	N	0.40344800	2.69245800	-0.35012800
H	0.69402000	-1.27316900	-2.79282800	S	0.75969200	4.16311300	0.39165100
C	1.86131100	-4.27025600	-1.71170700	O	-0.15281700	4.33143300	1.52268000
H	2.10485800	-4.82369200	0.35684100	O	2.21886400	4.16569400	0.56741500
H	1.52532300	-3.40869700	-3.66127300	H	1.17159200	1.33334700	-1.73565000
H	2.23825400	-5.21267800	-2.09779400	H	2.31646500	2.51934700	-1.14867800
C	2.85619200	0.29754900	0.35164300	H	1.93317900	2.32533200	2.45852500
C	3.57279900	0.33785700	1.55437900	H	0.23462600	1.79127000	2.87445800
C	3.55885400	0.08001300	-0.84340600	H	1.11651300	-0.59382000	3.19410400
C	4.95432400	0.14607000	1.57068100	H	2.78413400	-0.01627000	2.73801600
H	3.05431000	0.52500000	2.48937900	C	0.34330600	5.42049500	-0.83084300
C	4.93681200	-0.11466600	-0.83358200	H	0.54849300	6.39133500	-0.37308000
H	3.02344900	0.04536300	-1.78724900	H	0.96467000	5.27898500	-1.71697000
C	5.63710400	-0.08405400	0.37605400	H	-0.71758500	5.33881300	-1.07602100
H	5.49803400	0.16993400	2.50896700	C	2.01608600	0.85673700	0.15759300
H	5.46773700	-0.29912300	-1.76159400	C	-0.21601800	0.00615800	0.79001800
C	-1.00353800	1.43321300	-1.11758200	C	-0.41508900	-1.44959400	1.10528000
H	-1.08816300	-0.50556500	-1.89191500	C	-1.07456300	-1.83946300	2.28365000
H	-1.77516200	1.83585100	-1.76775900	C	0.06088400	-2.44993800	0.24184300
Au	-2.84286200	-0.40406000	-0.13726400	C	-1.26323900	-3.19056300	2.58233900
P	-4.95320900	-1.12439500	0.57456300	H	-1.45745100	-1.07696600	2.95717500
C	-5.94975400	-1.85366500	-0.78618900	C	-0.12432500	-3.80166100	0.54209900
H	-5.42739500	-2.71817900	-1.20616600	H	0.55653800	-2.16710500	-0.68387000
H	-6.92950000	-2.17187400	-0.41384700	C	-0.78521100	-4.17556800	1.71459300
H	-6.09078700	-1.11468200	-1.58028600	H	-1.78090100	-3.47268700	3.49503000
C	-4.89178800	-2.42025800	1.87651200	H	0.24158500	-4.56157700	-0.14306500
H	-4.38132800	-2.03424000	2.76376900	H	-0.92658500	-5.22641900	1.95017700
H	-5.90445900	-2.73153400	2.15432400	C	3.28102300	0.22122500	-0.10142200
H	-4.33893800	-3.28982300	1.50905800	C	3.51387200	-1.10349600	0.36018900
C	-6.00163600	0.21439100	1.27383800	C	4.30494300	0.86529600	-0.84808800
H	-6.98027400	-0.18074200	1.56714600	C	4.69906300	-1.75700500	0.06216800
H	-5.51445300	0.64925900	2.15147100	H	2.73153400	-1.62759100	0.89607000
H	-6.14321100	1.00227400	0.52825600	C	5.50434200	0.21963100	-1.10498300
C	7.13700700	-0.24486700	0.37554800	H	4.18830800	1.89224900	-1.17324300
F	7.59023100	-0.69907700	1.56206900	C	5.69965000	-1.09303800	-0.65846800
F	7.75440500	0.93187200	0.13381600	H	4.85388400	-2.78081200	0.38458000
F	7.53972800	-1.10886500	-0.57934800	H	6.28987500	0.72619000	-1.65444400
				C	-0.96870900	2.14681400	-0.35535100
<b>INT3-CF<sub>3</sub>Ph</b>							
C	1.49066100	1.87781100	-0.83327100	H	-1.36566500	2.22043700	-1.37848200
C	-1.14342700	0.71967700	0.11556200	H	-1.58640100	2.80167400	0.26871900
				Au	-2.99830500	-0.11333800	-0.34619700

P	-5.10630800	-1.04419500	-0.86595300	H	-2.09369500	-1.05698100	2.50123800
C	-5.03268400	-2.50043100	-1.99219300	C	-1.00638300	-4.14452300	0.42416300
H	-4.42103600	-3.28600800	-1.53848300	H	0.20465900	-2.76922400	-0.70405100
H	-6.03624700	-2.89378700	-2.18756900	C	-1.91048500	-4.30095500	1.47803500
H	-4.57063200	-2.21127400	-2.94086300	H	-2.99217800	-3.30071100	3.05407400
C	-6.04594700	-1.65583900	0.59543000	H	-0.70187800	-5.00566300	-0.16433000
H	-6.22460000	-0.83132800	1.29204800	H	-2.30337200	-5.28456500	1.71872900
H	-7.00759000	-2.08181200	0.28959400	C	3.50997000	-0.03717500	-0.19105300
H	-5.46228800	-2.42245200	1.11367100	C	3.84534400	-1.40342400	-0.33923200
C	-6.27318500	0.11180400	-1.69909400	C	4.53431400	0.93207400	-0.28338800
H	-7.22594500	-0.38397500	-1.91408700	C	5.15910200	-1.78459000	-0.57892600
H	-6.45754000	0.97725400	-1.05559100	H	3.06414200	-2.15632900	-0.31793400
H	-5.83560300	0.46810200	-2.63641700	C	5.85249600	0.53981400	-0.48519700
C	7.02462500	-1.78627000	-0.90992500	H	4.29635200	1.97943600	-0.13481500
F	6.85370100	-3.11123200	-1.06574600	C	6.16539400	-0.81426400	-0.63883700
F	7.85333000	-1.59528100	0.13259400	H	5.40497600	-2.83051200	-0.72710400
F	7.62490300	-1.30506800	-2.01208800	H	6.63908500	1.28479400	-0.53279200
				C	-0.78266800	1.96944300	-0.36950800

### INT4-CF<sub>3</sub>Ph

C	1.59993800	1.45265700	-0.96518400	H	-1.16027700	2.16670900	-1.38179400
C	-1.14945700	0.55571400	0.01219600	H	-1.32024600	2.65355400	0.29483600
C	1.17507100	-0.31958000	0.77987100	Au	-3.16440400	0.14354200	-0.35947500
C	1.68909000	0.33775600	2.26240500	P	-5.43708400	-0.29794800	-0.82927300
C	1.71853900	-1.09931800	1.98730800	C	-5.71879000	-1.84144300	-1.79478800
N	0.64315800	2.35455900	-0.34790300	H	-5.32243700	-2.69869300	-1.24251000
S	1.20339800	3.43831300	0.81477800	H	-6.78665500	-1.99728800	-1.98256600
O	0.37985900	3.31956300	2.02153900	H	-5.19238400	-1.77844200	-2.75187500
O	2.65882600	3.22863700	0.87956900	C	-6.50335700	-0.49826100	0.65932700
H	1.08897800	0.96634100	-1.81089600	H	-6.46662500	0.41168600	1.26571600
H	2.44398800	2.00280200	-1.38331900	H	-7.54170300	-0.69625800	0.37238900
H	2.60633500	0.91629700	2.26915900	H	-6.13451500	-1.33019600	1.26658500
H	0.83135500	0.82282000	2.71601600	C	-6.28321100	1.00896800	-1.81372900
H	0.96473600	-1.71599200	2.46302100	H	-7.32689200	0.73863300	-2.00734400
H	2.69219500	-1.56719200	1.91089100	H	-6.25469400	1.95769100	-1.26943000
C	0.89742200	5.05867100	0.09467600	H	-5.76588600	1.14530400	-2.76809800
H	1.23182700	5.80046100	0.82412500	C	7.60673900	-1.24025700	-0.82117200
H	1.46674300	5.14511100	-0.83213700	F	7.69478600	-2.35342200	-1.57323200
H	-0.17312200	5.16869600	-0.08942500	F	8.33243600	-0.27436800	-1.41287300
C	2.10367300	0.34225200	-0.06561300	F	8.17234900	-1.50689700	0.37233400
C	-0.32333200	-0.39146100	0.52401600				
C	-0.88391400	-1.75019900	0.85764700				
C	-1.79073900	-1.92183400	1.91700800				
C	-0.49195500	-2.88205700	0.12414900				
C	-2.29892500	-3.18654400	2.22502400				

### TS2-CF<sub>3</sub>Ph-Real

C	-3.65796000	-0.72054300	-0.65187100
C	-0.70769600	-0.48111500	-0.44465100
C	-2.24099000	0.16440500	1.34227900
C	-2.05003100	-0.97848400	2.28461100

C	-2.16060300	0.44224600	2.80533800	C	5.67283700	1.51326600	2.90799300
N	-2.74954200	-1.87185800	-0.74027200	C	4.59038100	1.66596100	3.76835000
S	-3.39527000	-3.29092800	-1.54720600	H	2.48805200	1.25178900	4.03849400
O	-4.16264300	-2.82108600	-2.69943100	H	6.64426500	1.90211000	3.19790000
O	-2.23829800	-4.17544700	-1.69257300	H	4.71703500	2.17669500	4.71844600
H	-3.90749100	-0.36288500	-1.65887800	C	6.87315400	0.78305900	0.92451700
H	-4.58862200	-1.05892500	-0.18333300	C	7.40218900	1.94489300	0.33793700
H	-2.89277200	-1.64864900	2.43488900	C	7.66515700	-0.37397900	0.95178000
H	-1.07792500	-1.46295500	2.33623000	C	8.66427300	1.93228700	-0.25733700
H	-1.25493000	0.90609700	3.18617600	H	6.81935300	2.86202700	0.35049200
H	-3.06451200	0.73644600	3.33185200	C	8.92892000	-0.38769900	0.35597400
C	-3.07163900	0.44078500	0.15678000	H	7.30600100	-1.25720600	1.47169700
C	-1.51223500	0.64276800	0.08258700	C	9.42743200	0.76235500	-0.25835700
C	-0.94283000	2.03118000	-0.05601400	H	9.05397800	2.83815700	-0.71302900
C	-1.05238200	3.00424500	0.94701100	H	9.52954900	-1.29238300	0.38871000
C	-0.31742200	2.38990800	-1.26257800	H	10.41158900	0.75273000	-0.71760700
C	-0.53164300	4.28607700	0.75859600	C	4.36414200	0.37191800	-1.89948500
H	-1.55971300	2.77393100	1.87571800	C	4.32307000	-2.39947600	-0.20269500
C	0.19937100	3.67199400	-1.45376700	C	3.25453600	-3.25103700	-0.92509500
H	-0.24162100	1.66448600	-2.06859800	H	2.27277400	-3.17015900	-0.44709300
C	0.09964000	4.62509700	-0.43865300	H	3.14370000	-2.97933500	-1.97963800
H	-0.62771800	5.02291900	1.55100500	H	3.56114100	-4.30387700	-0.88803400
H	0.67063200	3.92637500	-2.39910600	C	5.69123300	-2.72224200	-0.83229000
H	0.49885800	5.62456600	-0.58408600	H	5.96952700	-3.74603300	-0.55191200
C	-3.98351700	1.64073000	0.09235400	H	5.64997300	-2.68980800	-1.92433000
C	-4.88454400	1.89968100	1.13336900	H	6.48843400	-2.05698300	-0.49939800
C	-4.02026400	2.45473800	-1.04926000	C	4.32958200	-2.78849400	1.29029000
C	-5.78947800	2.95689200	1.04767900	H	5.11738600	-2.27797200	1.85104800
H	-4.88738000	1.26943100	2.01708100	H	3.37358100	-2.57033000	1.77930000
C	-4.92094500	3.51254000	-1.14026700	H	4.50380300	-3.86840800	1.36993000
H	-3.32907400	2.27353500	-1.86683800	C	3.48335100	-0.13473800	-3.06479200
C	-5.80648600	3.76626700	-0.08946000	H	3.76133800	0.41369200	-3.97332100
H	-6.47623700	3.15523600	1.86374700	H	3.63607300	-1.19943500	-3.26949400
H	-4.93140600	4.14532100	-2.02125700	H	2.41594600	0.03274000	-2.88562500
C	-1.38645300	-1.65314700	-0.88171000	C	4.05692700	1.86457300	-1.65057700
H	-1.02047600	-0.88911500	-1.81317100	H	3.01523500	2.03137300	-1.35374800
H	-0.81846200	-2.55811300	-1.08316900	H	4.70478500	2.29245400	-0.88105000
Au	1.38290800	-0.48156200	-0.39359100	H	4.23195500	2.41835000	-2.58122000
P	3.79244900	-0.54569400	-0.30637100	C	5.83580100	0.20730300	-2.32586900
C	4.30839000	0.34426300	1.26546900	H	6.54437200	0.42983500	-1.53161900
C	3.22799800	0.51488900	2.16016800	H	6.04175500	-0.79397100	-2.70780600
C	5.57444000	0.85376700	1.66800300	H	6.02803800	0.91035100	-3.14621300
C	3.35434700	1.15258200	3.39092300	C	-4.51266400	-3.93962000	-0.32549400
H	2.24743900	0.14231400	1.88086000	C	-3.99916600	-4.67032400	0.75176200

C	-5.88674800	-3.74422100	-0.48510400	H	0.71988900	-4.99204000	-1.04078500
C	-4.88500900	-5.19684300	1.68591700	H	-0.70396700	-5.79509400	0.83475700
H	-2.93101600	-4.83785900	0.84276300	C	4.85486300	-1.34624600	-0.01009600
C	-6.75498600	-4.28189700	0.46404300	C	4.72604200	-2.75671400	0.11420600
H	-6.26396700	-3.19957700	-1.34401300	C	6.03663900	-0.82549600	-0.60108000
C	-6.27317500	-5.01420500	1.55864700	C	5.71994500	-3.59948000	-0.35595000
H	-4.49639300	-5.76995500	2.52347900	H	3.81525300	-3.17500200	0.52598000
H	-7.82528600	-4.13746100	0.34546200	C	7.04598500	-1.67494800	-1.02988300
C	-7.22281100	-5.62475600	2.55927200	H	6.19423000	0.24447500	-0.66622900
H	-8.17164200	-5.08138800	2.59695200	C	6.88571700	-3.06014100	-0.91580300
H	-7.45065600	-6.66422500	2.28967100	H	5.59881000	-4.67551100	-0.29140800
H	-6.79239100	-5.63774900	3.56570800	H	7.95680300	-1.26992200	-1.45581500
C	-6.81991500	4.87718300	-0.20761400	C	1.29168900	1.66513100	0.41565700
F	-7.13293000	5.39319600	0.99941600	H	0.96824600	2.09113900	-0.54669100
F	-7.96897300	4.43321600	-0.76203300	H	0.86677000	2.29987600	1.19990800
F	-6.36566900	5.88365300	-0.98225200	Au	-1.31324100	0.17748600	0.01991200
				P	-3.65752200	0.11555800	-0.60224400

### TS3-CF<sub>3</sub>Ph-Real

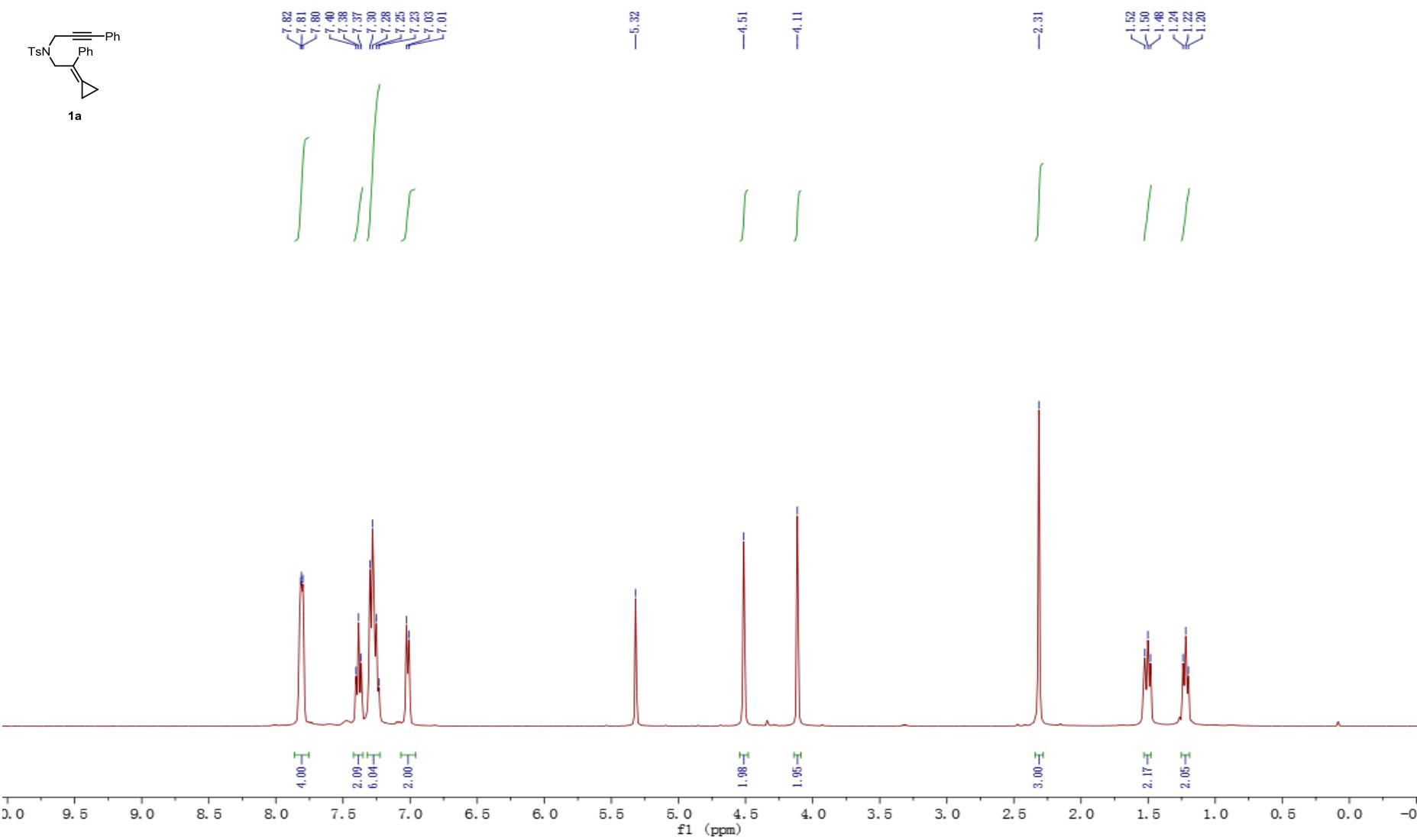
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C	0.70415400	0.27560200	0.54015500	C	-6.00551100	-0.54824900	1.17856400
C	2.85625700	-0.82470700	1.48387900	C	-4.36705900	-0.03346400	3.42227000
C	3.16138800	-0.19954700	2.88100700	H	-2.83258300	0.37587300	2.00590300
C	3.23326700	-1.67504500	2.67838900	C	-6.47925300	-0.68057100	2.49801500
N	2.75740400	1.75973400	0.51421200	C	-5.68681100	-0.42753000	3.61304700
S	3.50755100	2.97623400	1.41215400	H	-3.71834100	0.17532000	4.26819700
O	2.65503600	3.20346700	2.57993200	H	-7.51294100	-0.98336300	2.63590500
O	4.90356100	2.52935400	1.53469700	H	-6.09986800	-0.53651400	4.61173600
H	3.10281100	0.64595400	-1.22717600	C	-7.04987100	-0.85094600	0.14575000
H	4.53697300	1.30544900	-0.47171100	C	-7.39909200	-2.18290400	-0.13068800
H	4.08469500	0.36101700	2.99057100	C	-7.82626200	0.17346400	-0.41562000
H	2.29605700	0.25084900	3.35615900	C	-8.45352500	-2.48022700	-0.99536800
H	2.44329200	-2.29236500	3.09401500	H	-6.84314400	-2.98934800	0.33956600
H	4.21741500	-2.13315100	2.70485200	C	-8.88082100	-0.12227700	-1.28305000
C	3.79084200	-0.48474700	0.43623300	H	-7.62303600	1.20611000	-0.14683300
C	1.38713300	-0.81106600	0.95852000	C	-9.19070800	-1.44983700	-1.58303600
C	0.79711200	-2.19213400	0.91640900	H	-8.70406800	-3.51688600	-1.20257000
C	-0.00932600	-2.65831400	1.96788000	H	-9.46975200	0.68514400	-1.70920100
C	1.05554400	-3.05430400	-0.16143100	H	-10.01325900	-1.68040500	-2.25386800
C	-0.55197000	-3.94477600	1.93513200	C	-3.84054700	-1.33430000	-1.84866300
H	-0.22433900	-1.99954000	2.80512900	C	-4.11319100	1.84747900	-1.32014800
C	0.51763000	-4.34311400	-0.19288300	C	-2.89568400	2.38197000	-2.10732900
H	1.66169900	-2.70301900	-0.99331700	H	-2.00274700	2.46310100	-1.47918900
C	-0.28643600	-4.79262700	0.85712600	H	-2.64830400	1.75528400	-2.96984500
H	-1.18052600	-4.28437300	2.75372800	H	-3.13680200	3.38266200	-2.48855800

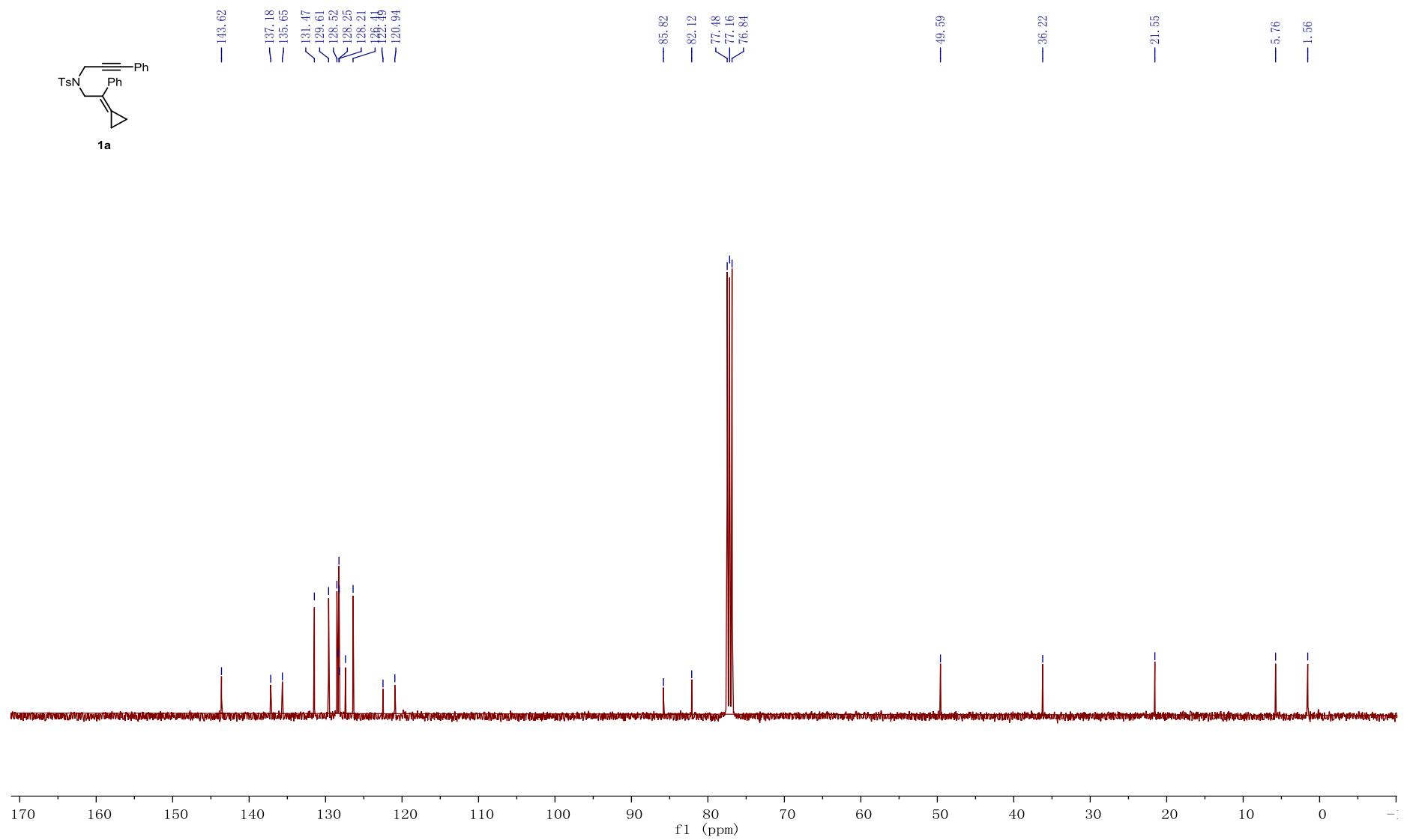
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H	-5.61545700	2.93591700	-2.41942900
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H	-6.20723900	1.37097200	-1.84942300
C	-4.35680000	2.77452600	-0.11020700
H	-5.25753500	2.50197700	0.44743800
H	-3.51300100	2.77104700	0.58902500
H	-4.48297800	3.80179600	-0.47404200
C	-2.63820000	-1.26609600	-2.81905000
H	-2.68782500	-2.13081700	-3.49301000
H	-2.65993600	-0.36704600	-3.44321700
H	-1.67722100	-1.29844200	-2.29579500
C	-3.71920600	-2.62521400	-1.00932700
H	-2.80544900	-2.64037900	-0.40520200
H	-4.57378100	-2.76375800	-0.34250500
H	-3.68293700	-3.48500100	-1.68995600
C	-5.12210300	-1.37901200	-2.70310100
H	-6.03716400	-1.29829400	-2.12057100
H	-5.12578700	-0.59899100	-3.46726600
H	-5.14851600	-2.34275500	-3.22766800
C	3.48433900	4.46090500	0.41705400
C	2.38052100	5.31562700	0.48451200
C	4.56322900	4.74427500	-0.42502300
C	2.35872000	6.45560200	-0.31606800
H	1.56765200	5.10477100	1.17114000
C	4.52212900	5.89026200	-1.21559400
H	5.43136500	4.09403300	-0.43625500
C	3.42334600	6.76238700	-1.17701100
H	1.50482800	7.12581200	-0.26205000
H	5.36306700	6.11811800	-1.86541900
C	3.40626400	8.02036600	-2.01074200
H	3.87931100	8.85057400	-1.47021100
H	3.95516200	7.88844900	-2.94850200
H	2.38421400	8.32880900	-2.25165300
C	7.99405700	-3.99695600	-1.35290700
F	8.83958400	-3.39718800	-2.20833400
F	7.48671200	-5.08834700	-1.95534400
F	8.70287300	-4.40915700	-0.28570900

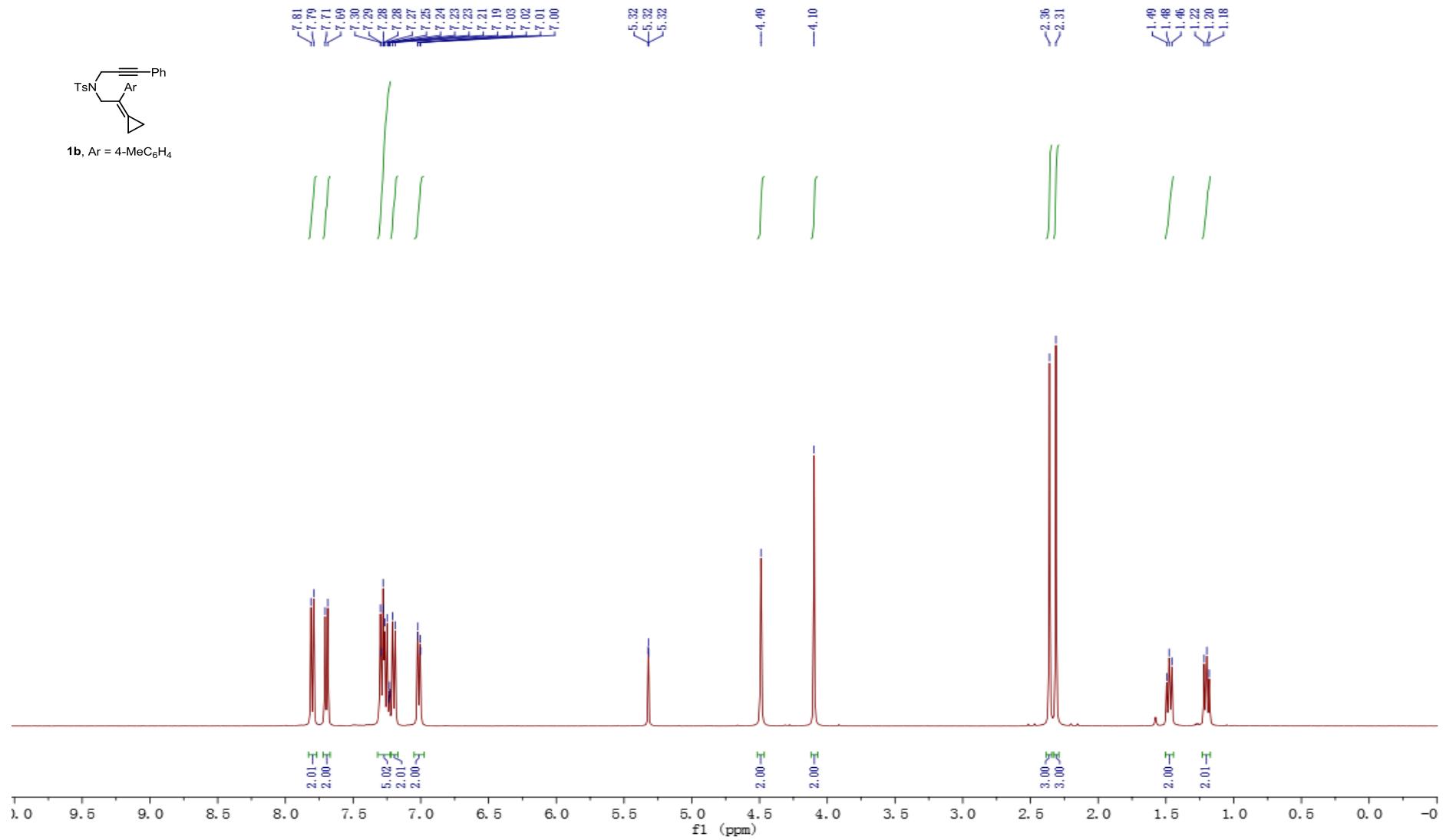
## V. References

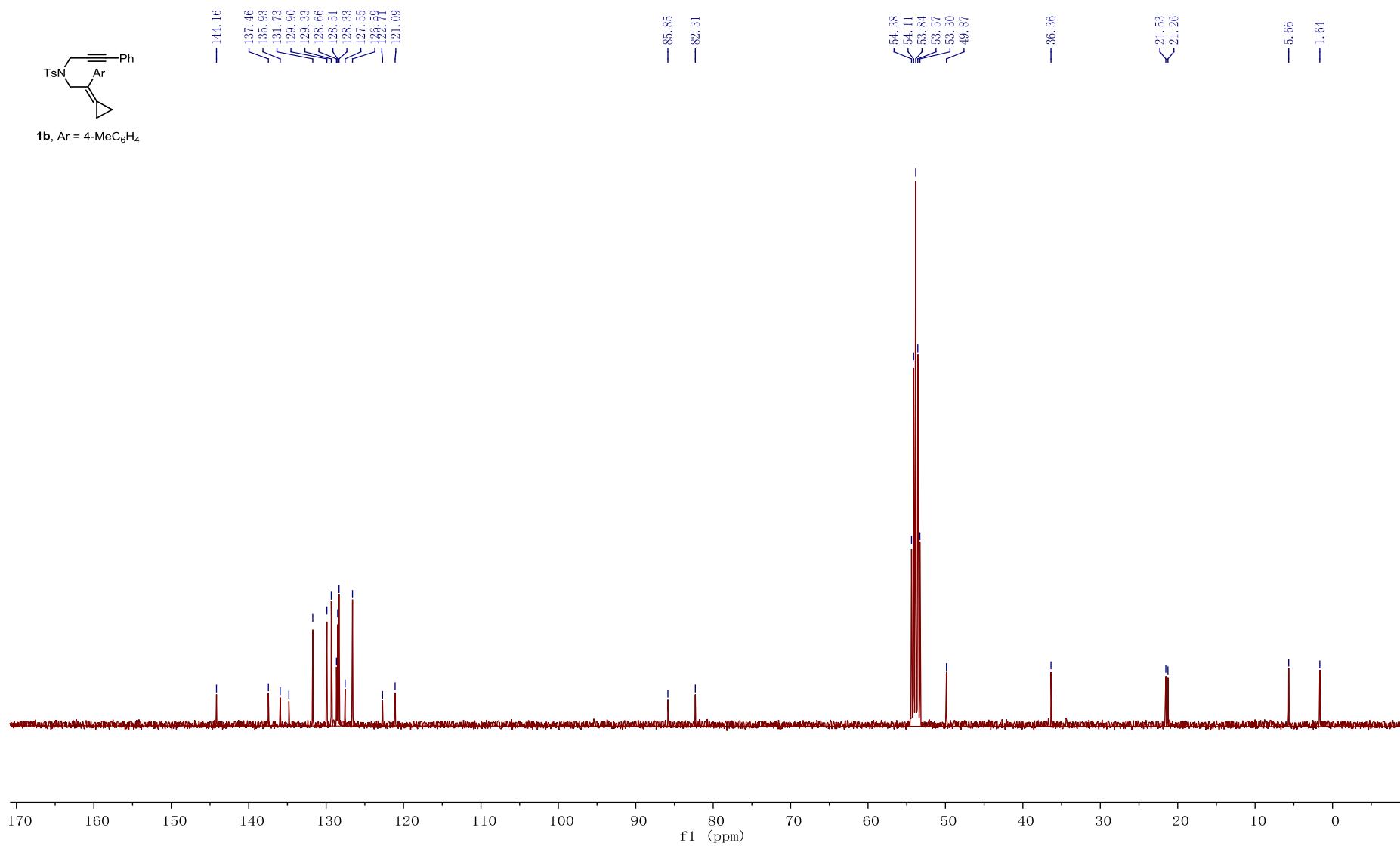
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- (2) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1986**.
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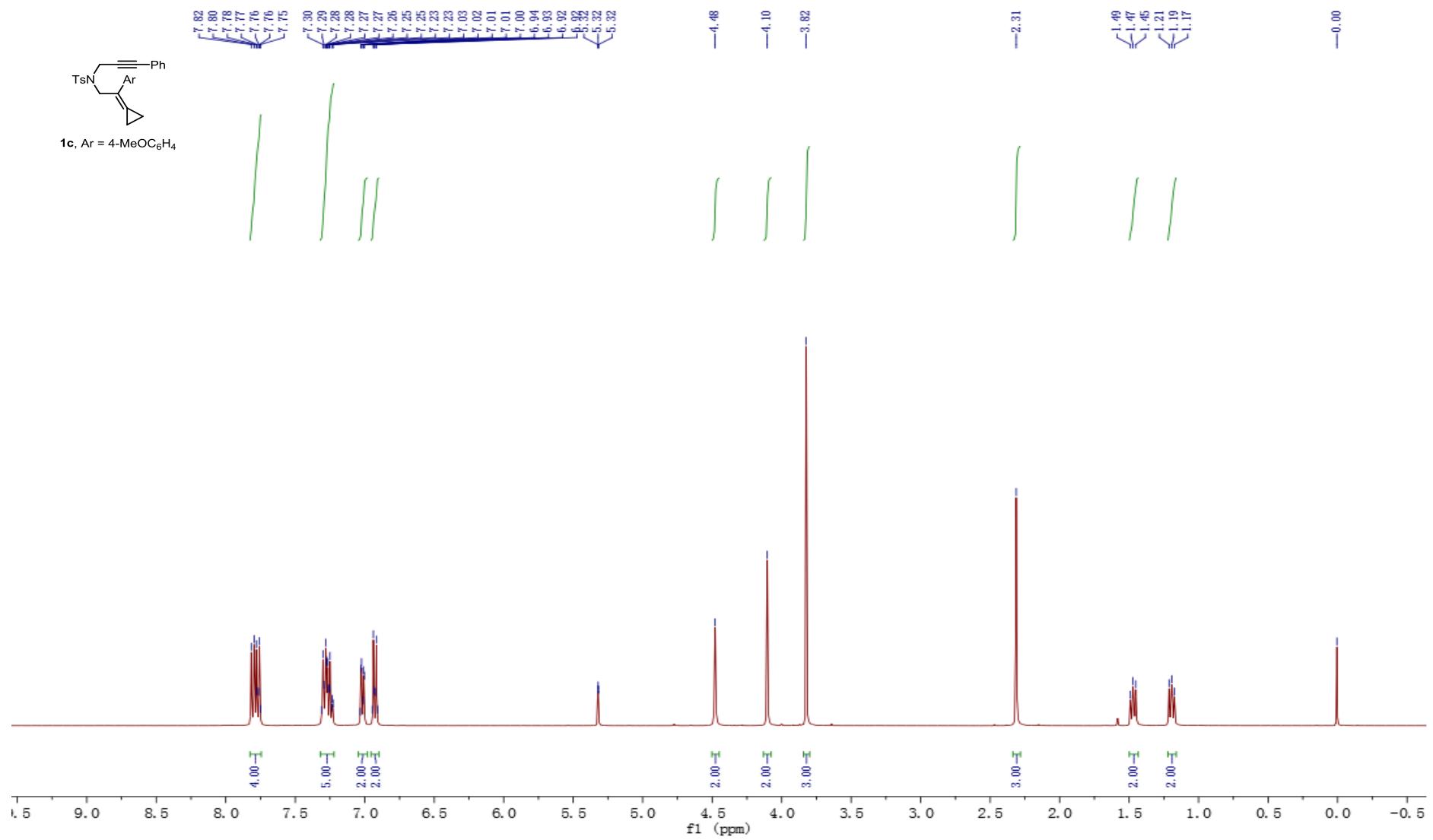
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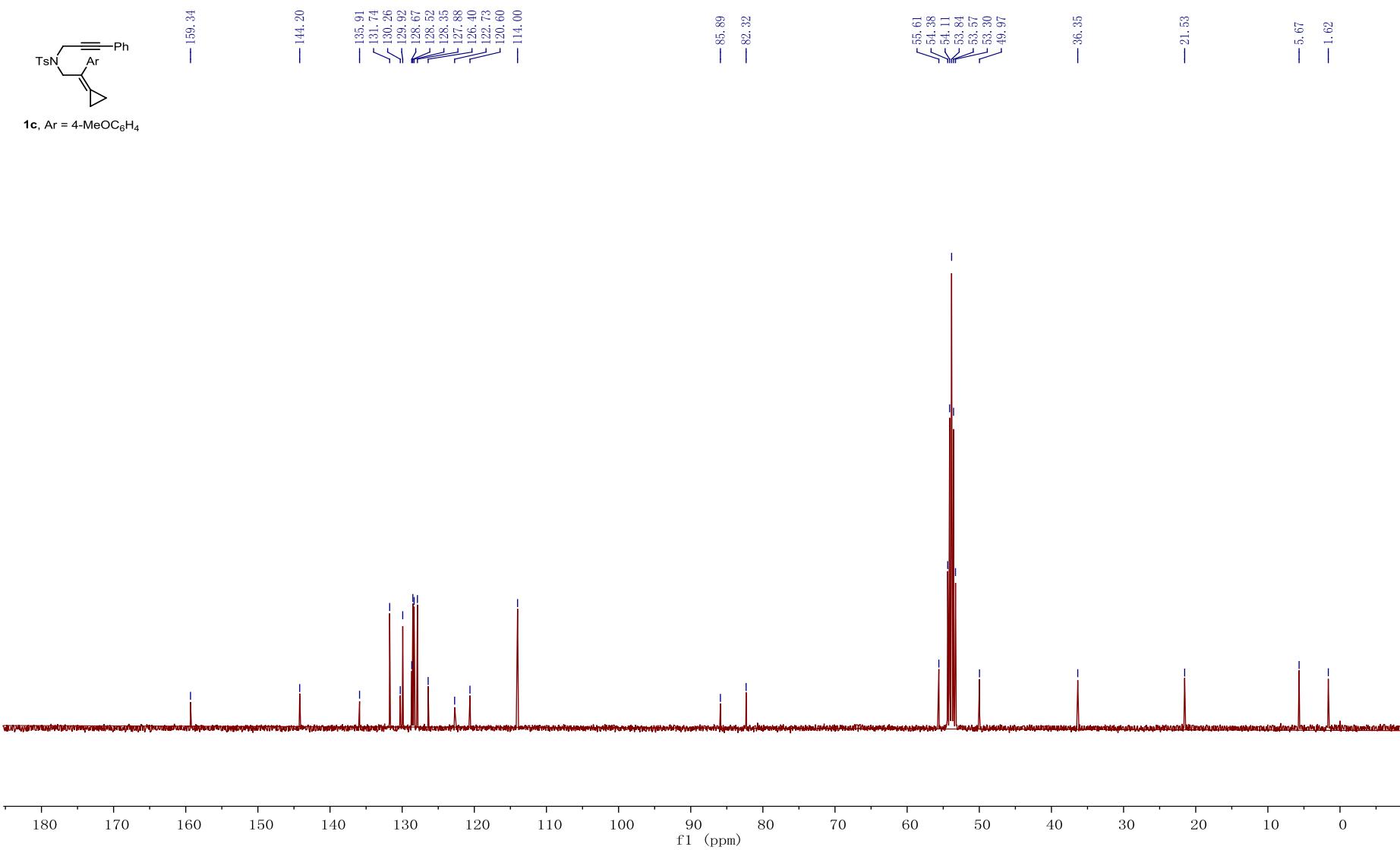


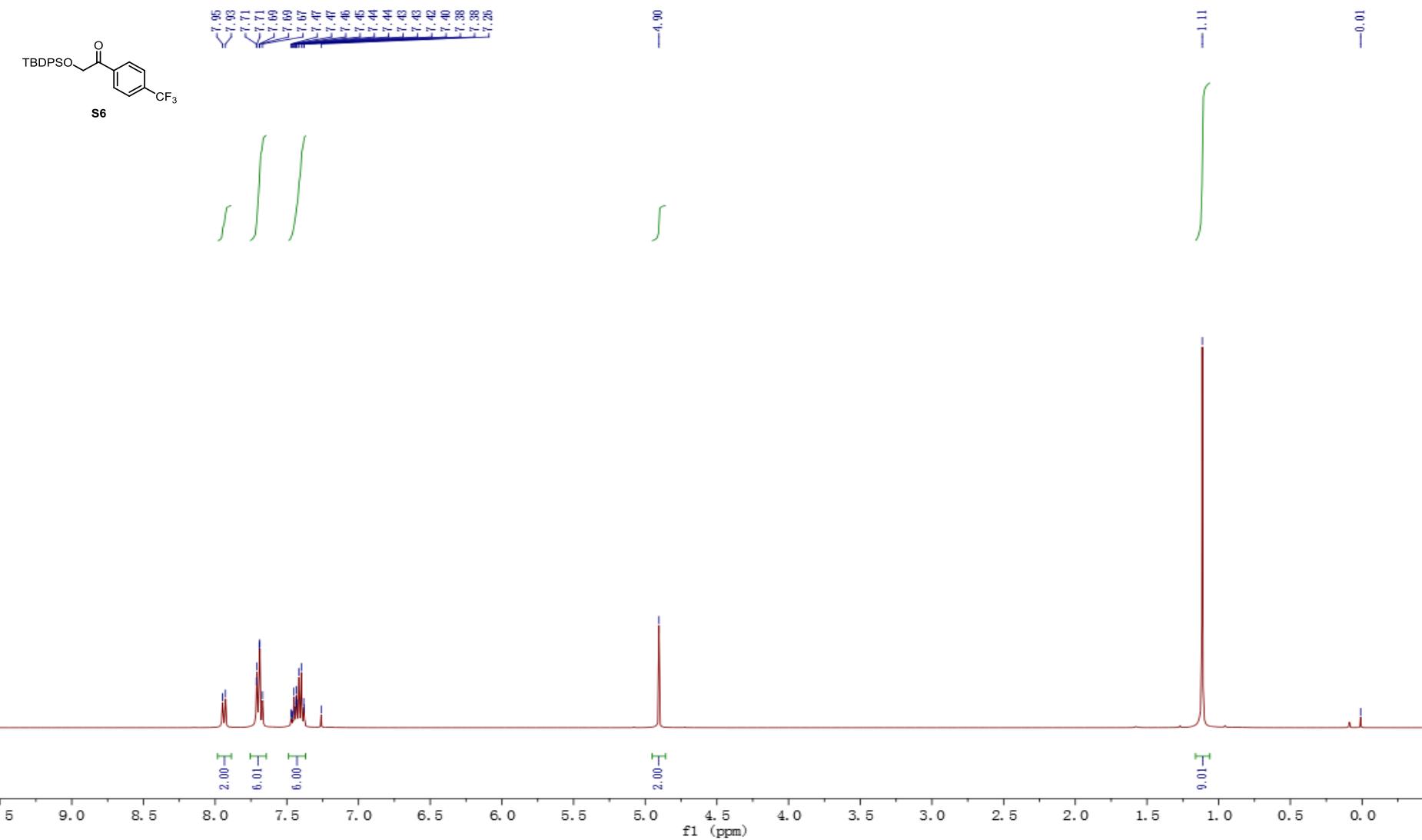


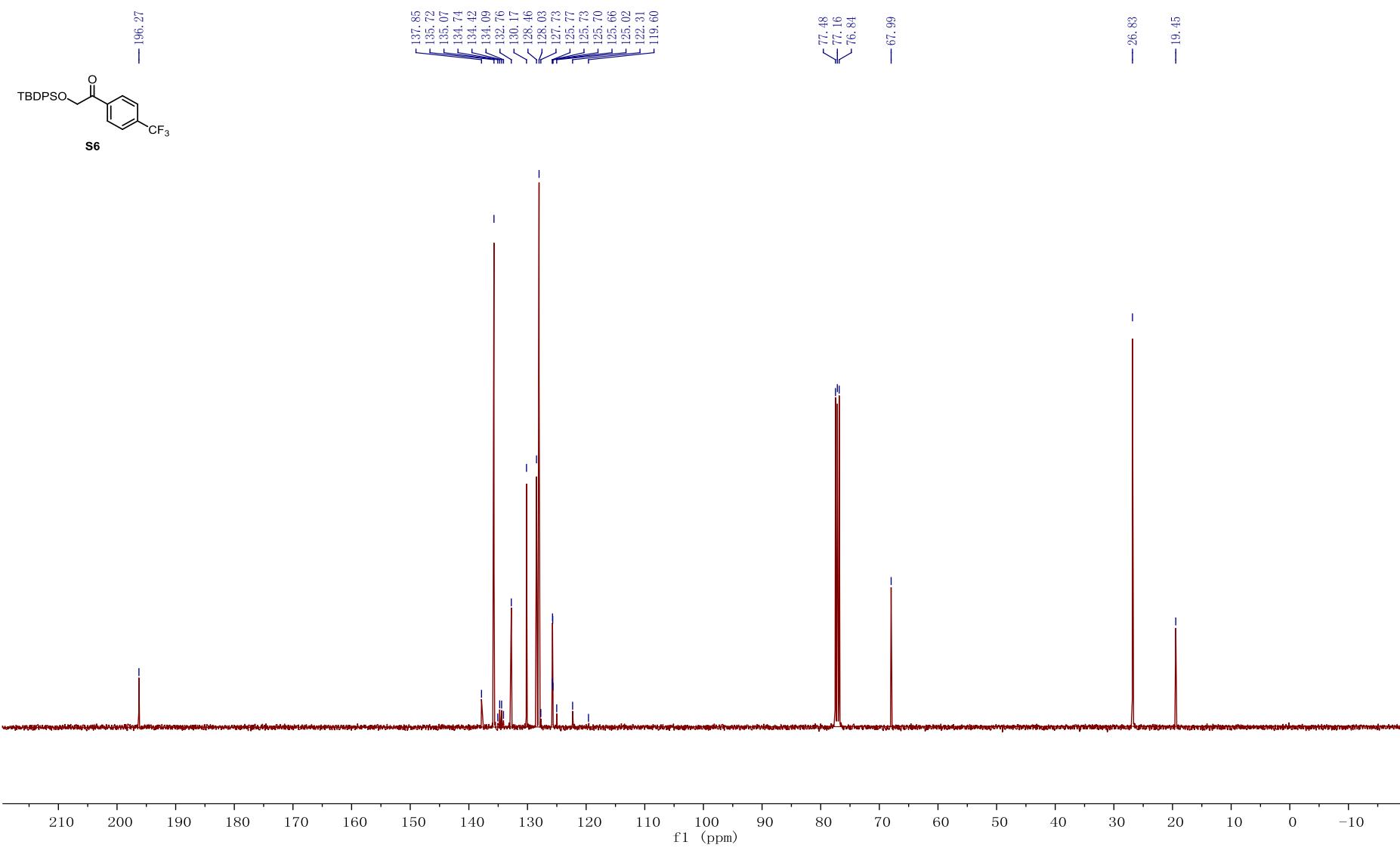


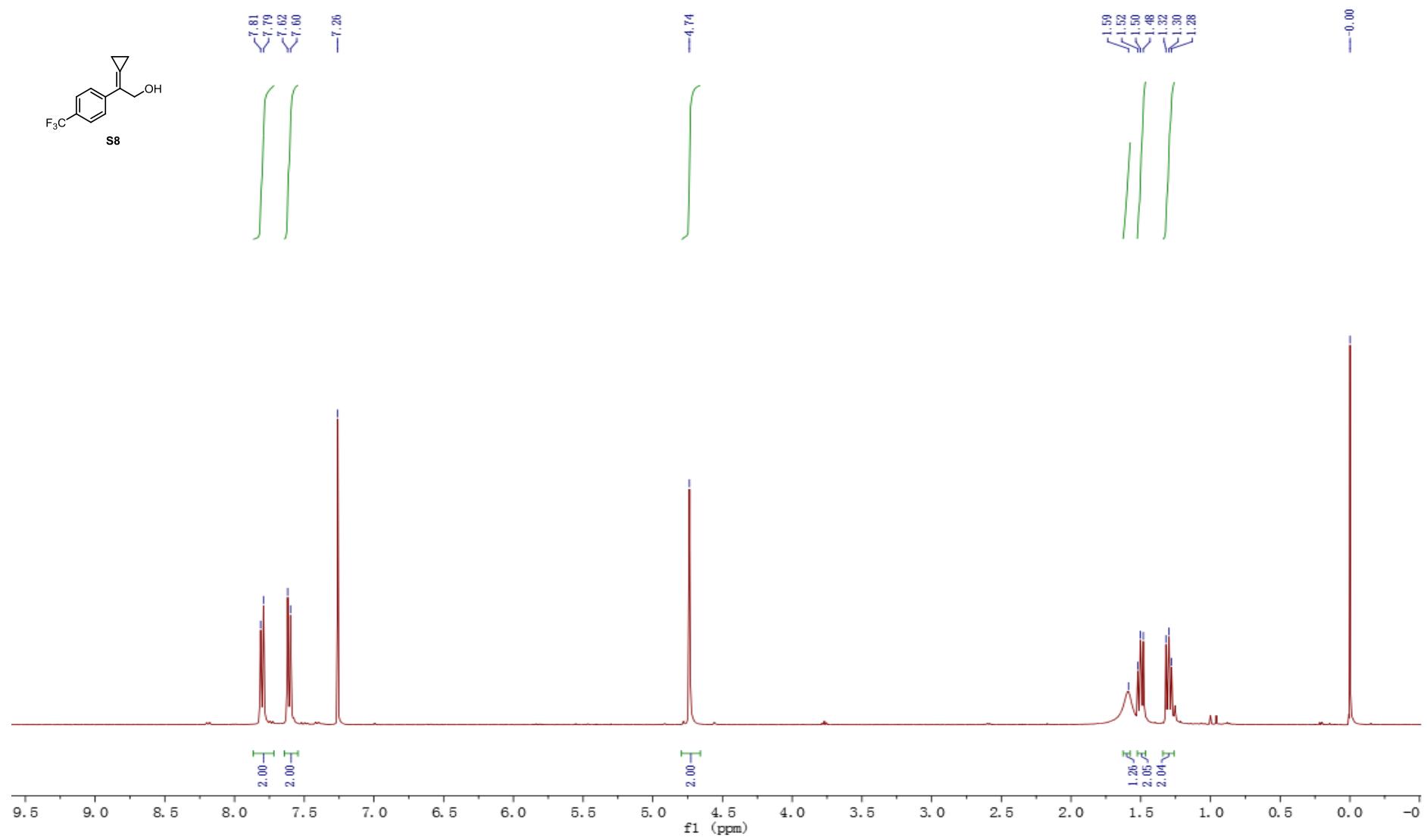


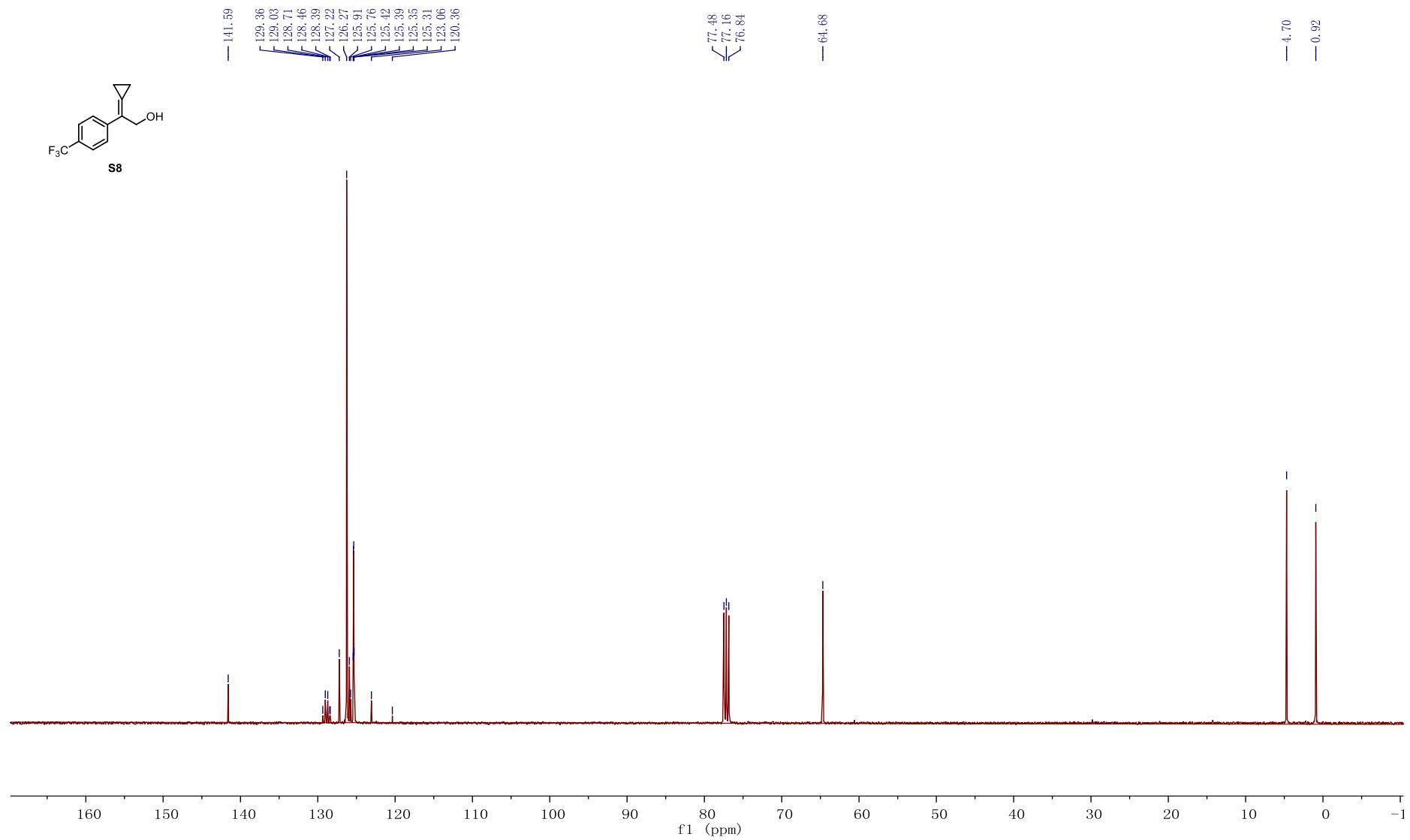


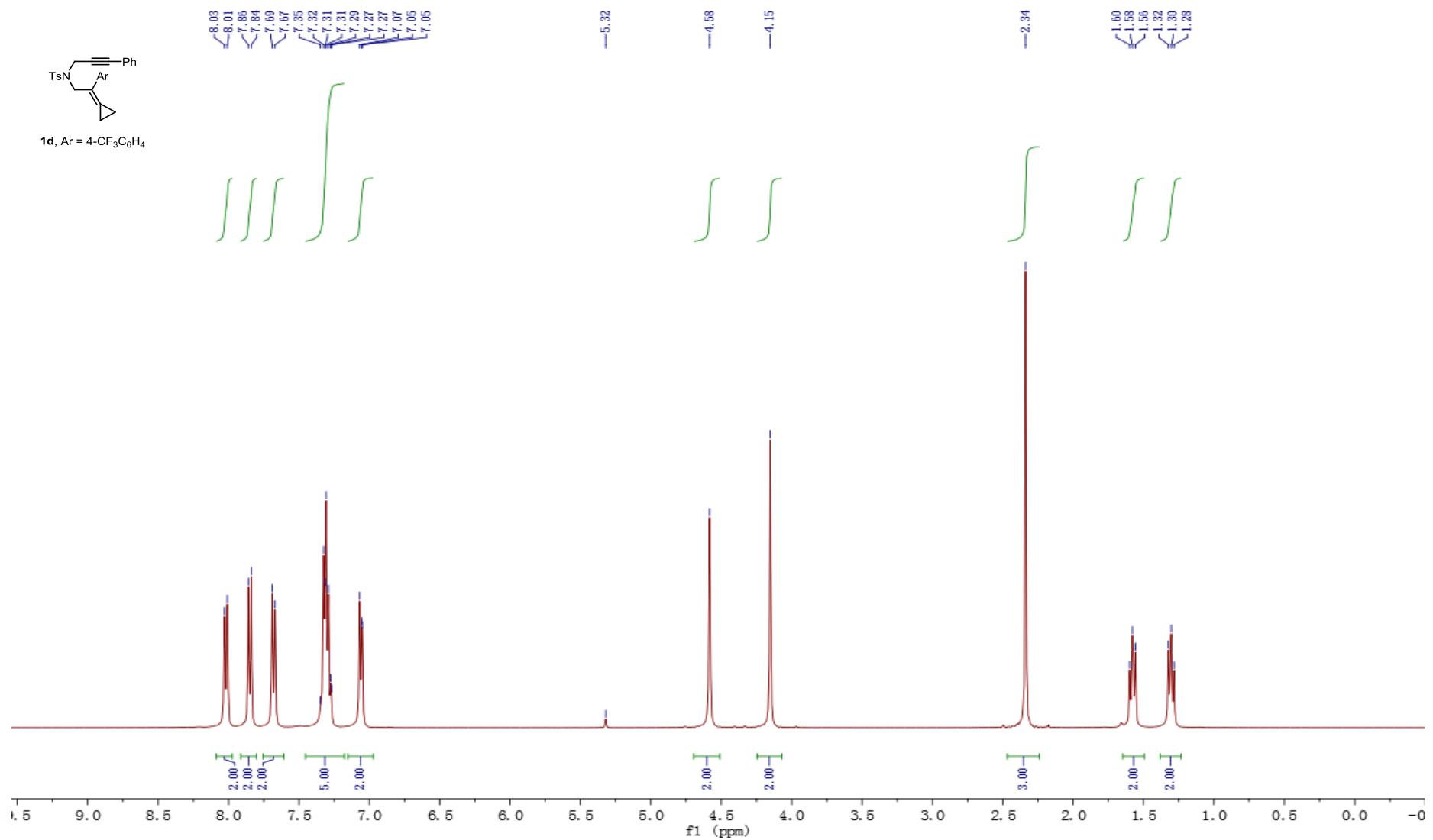


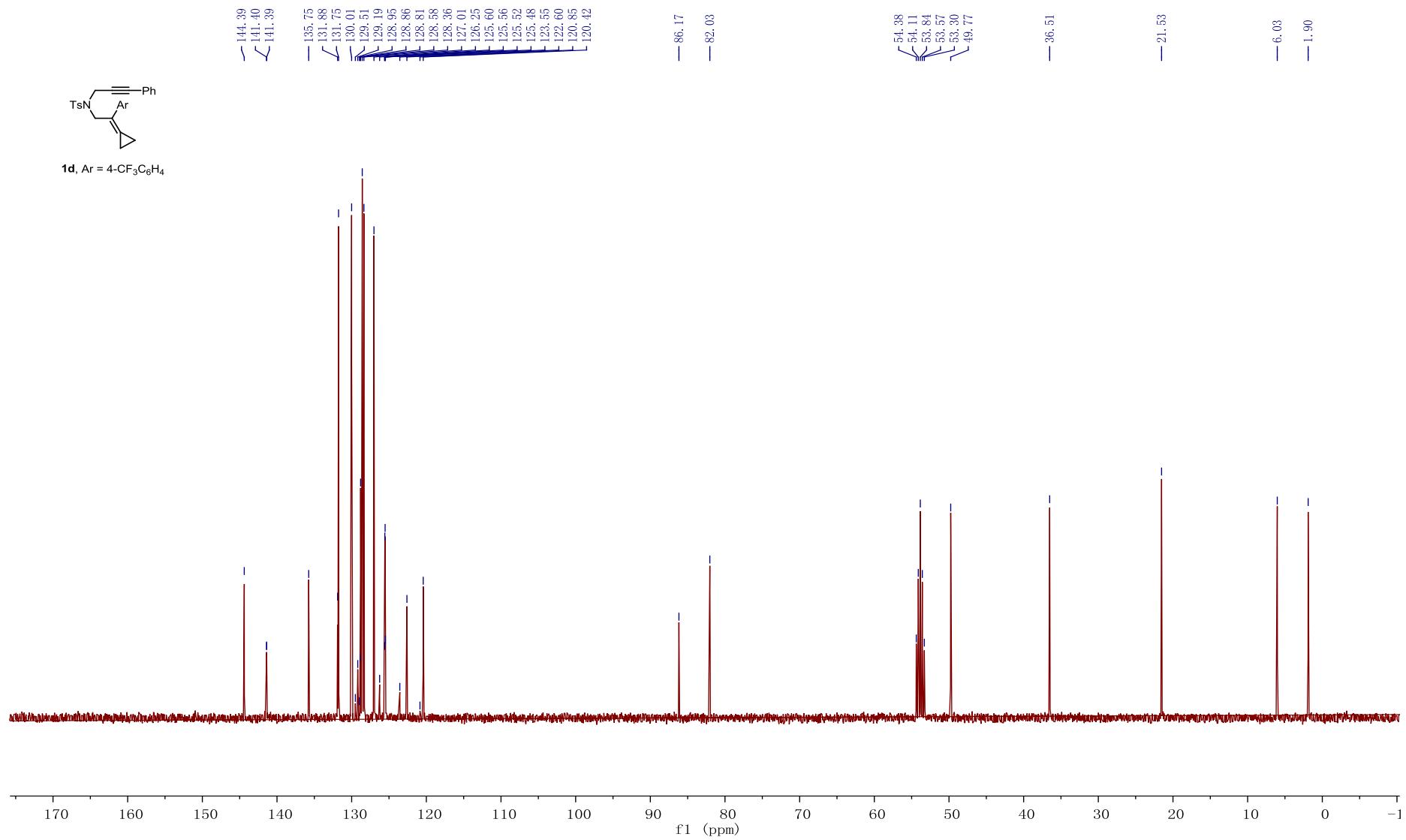


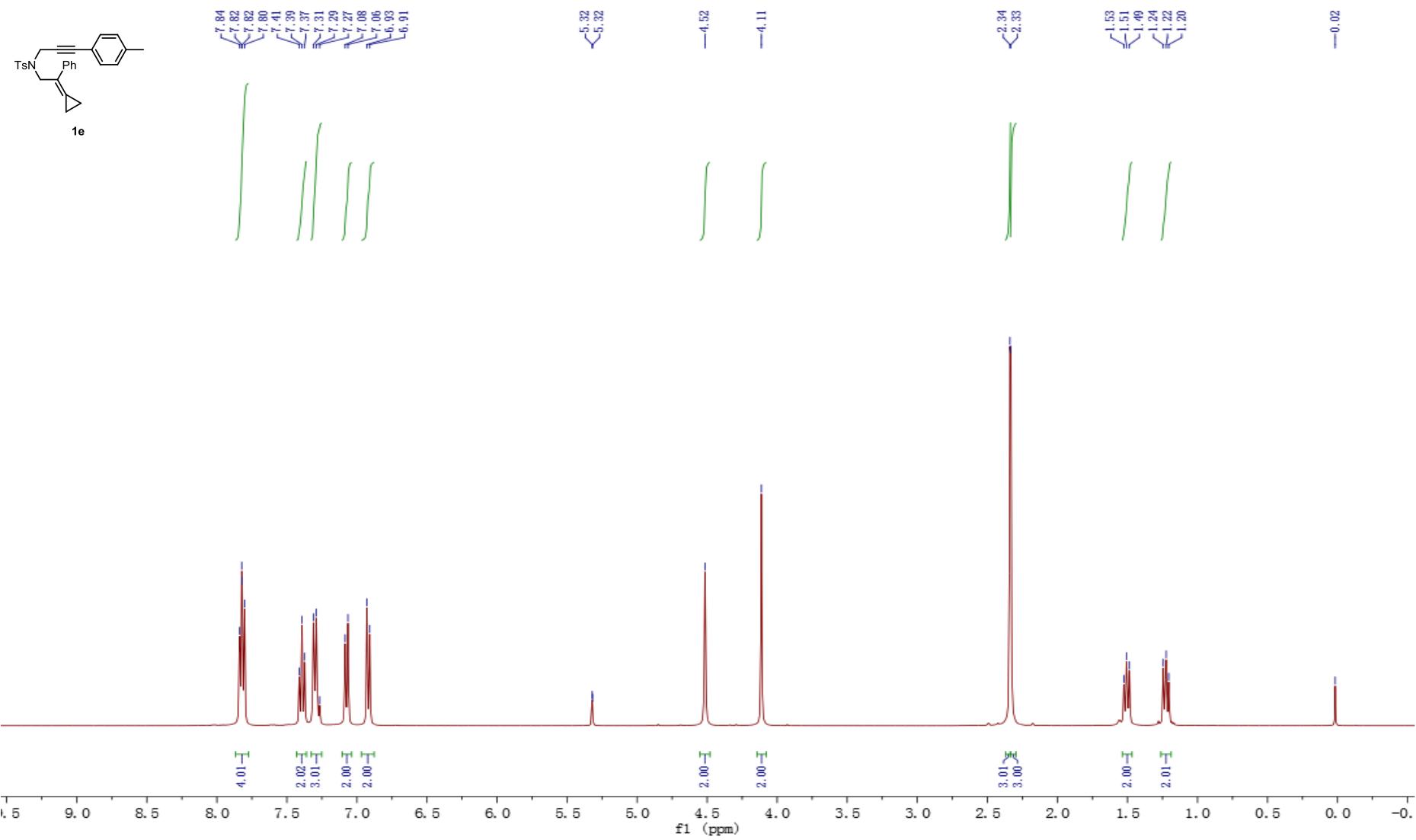


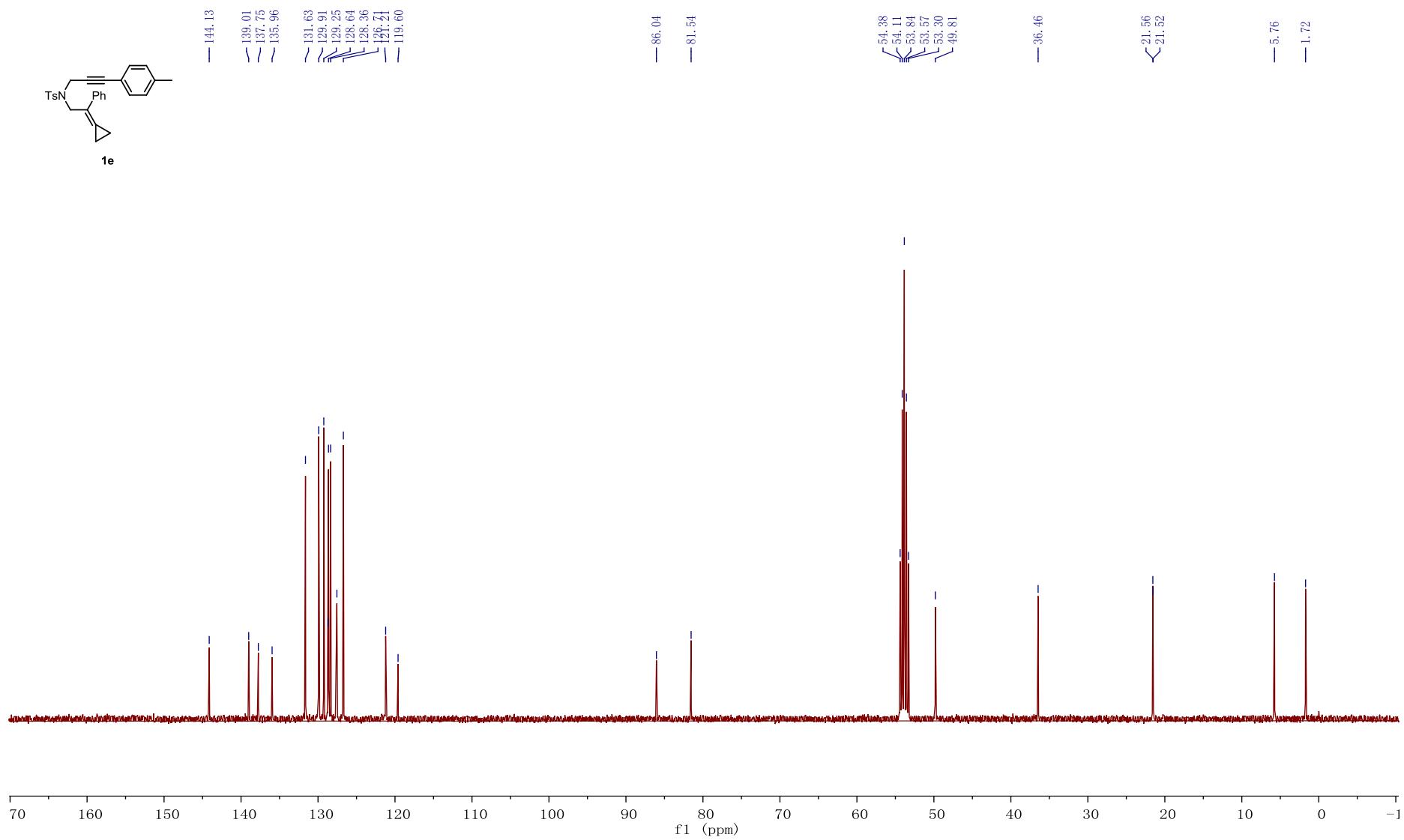


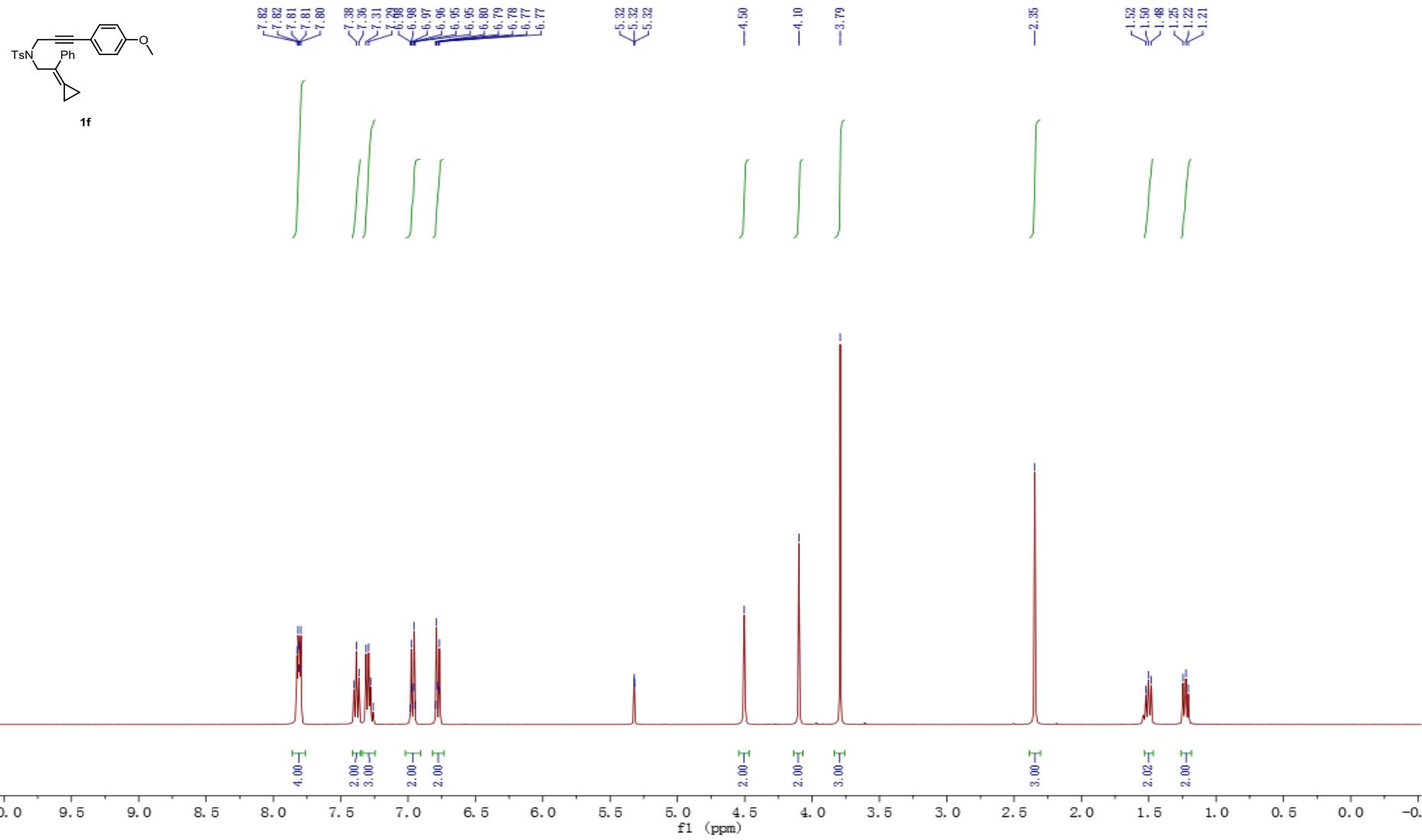


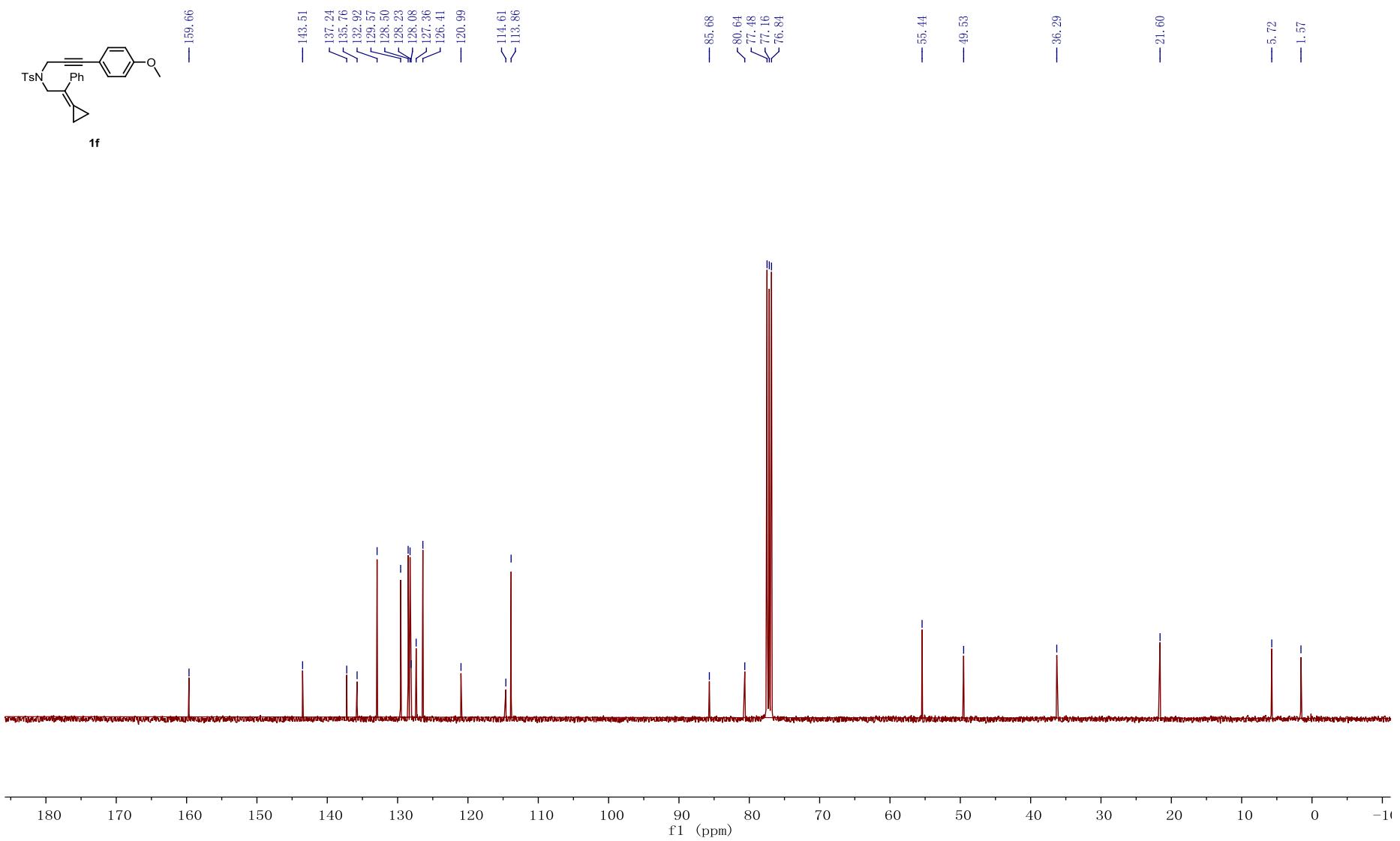


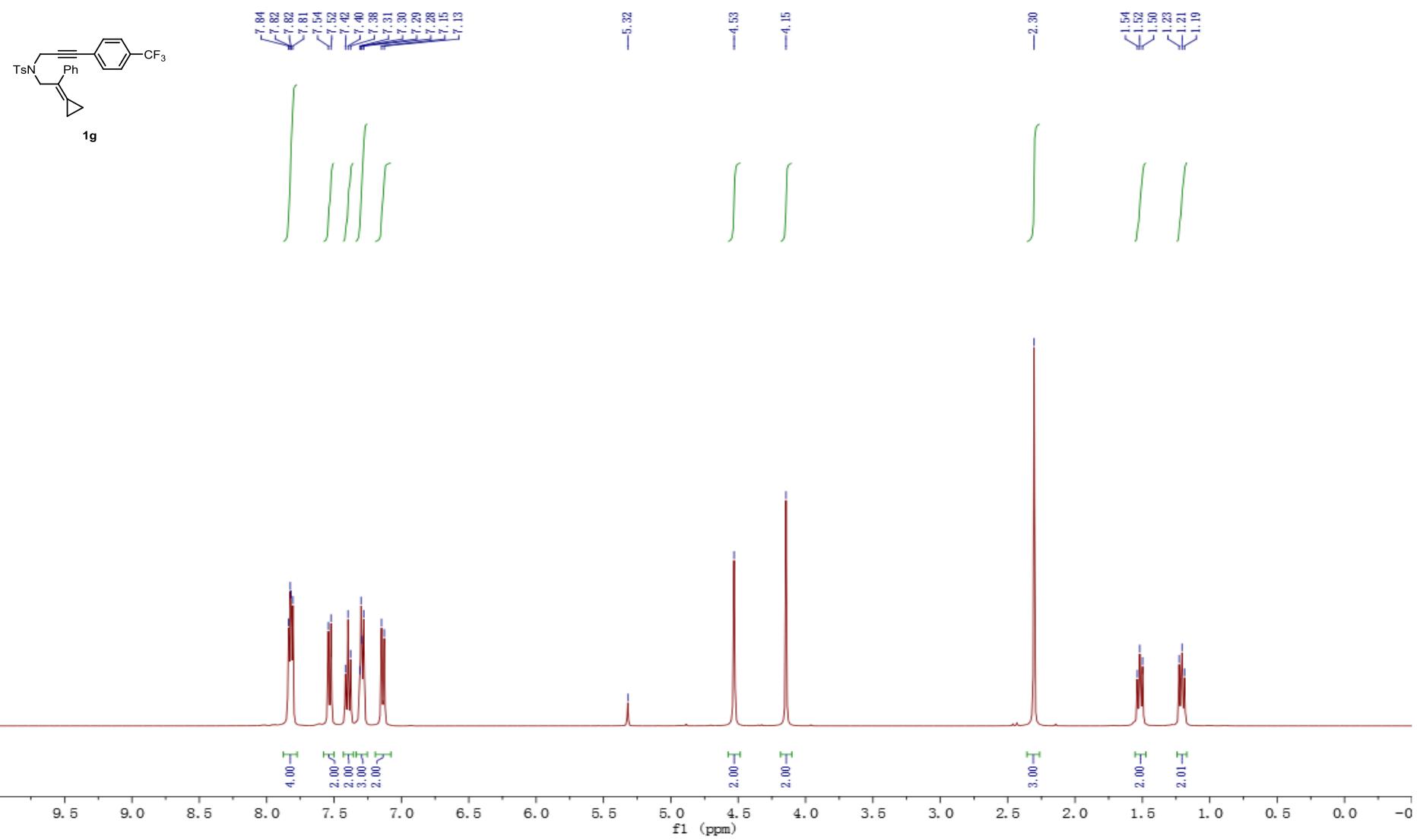


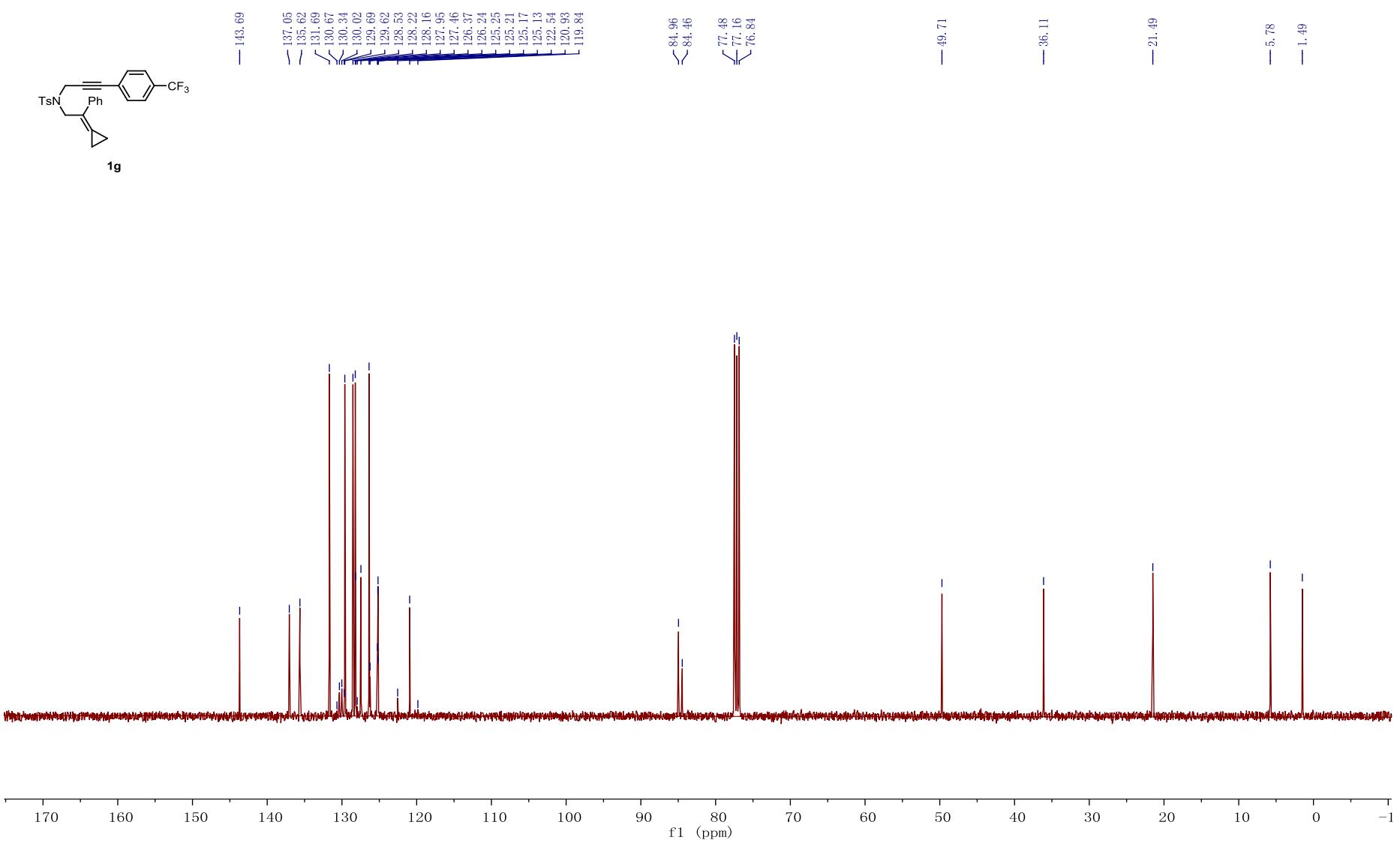


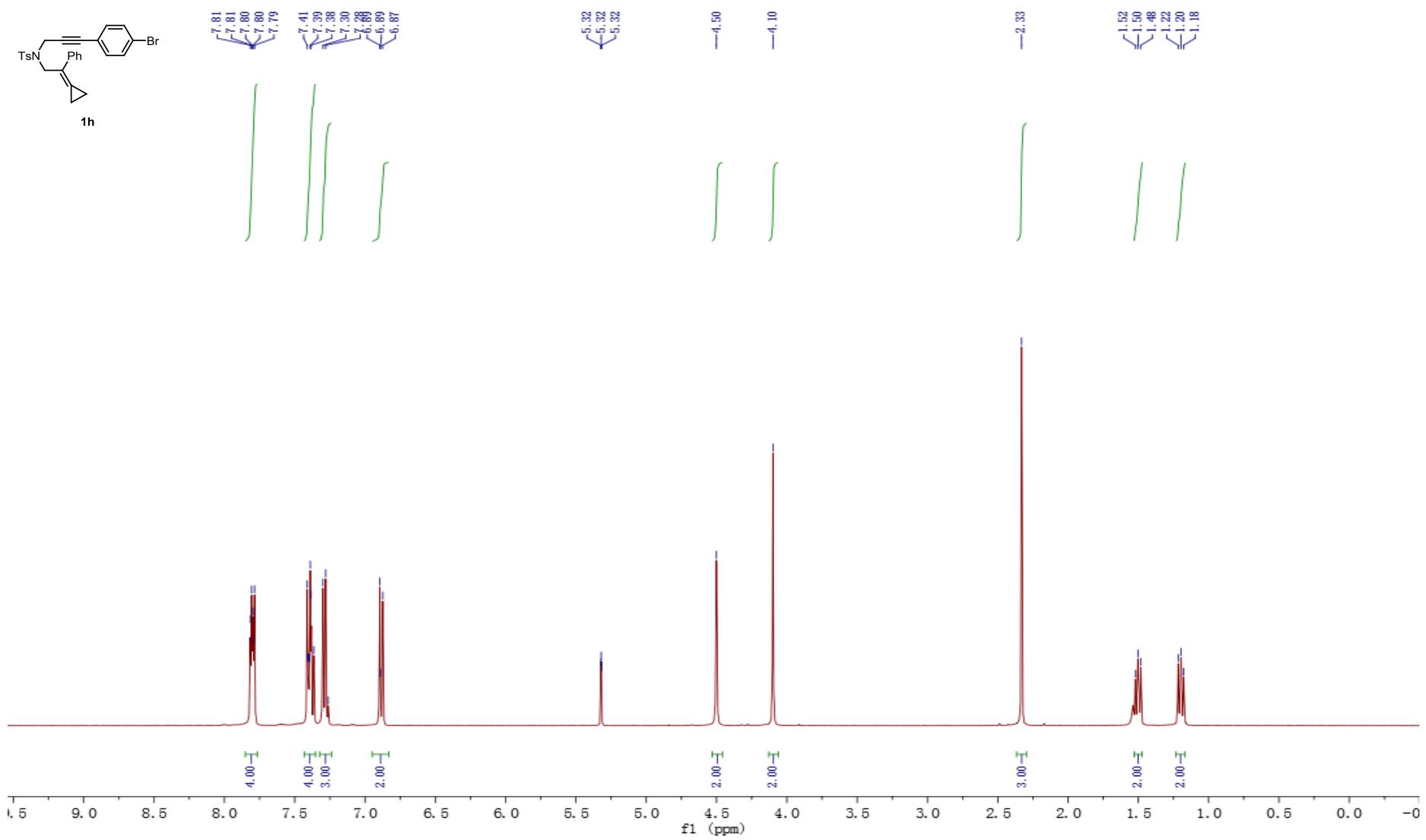


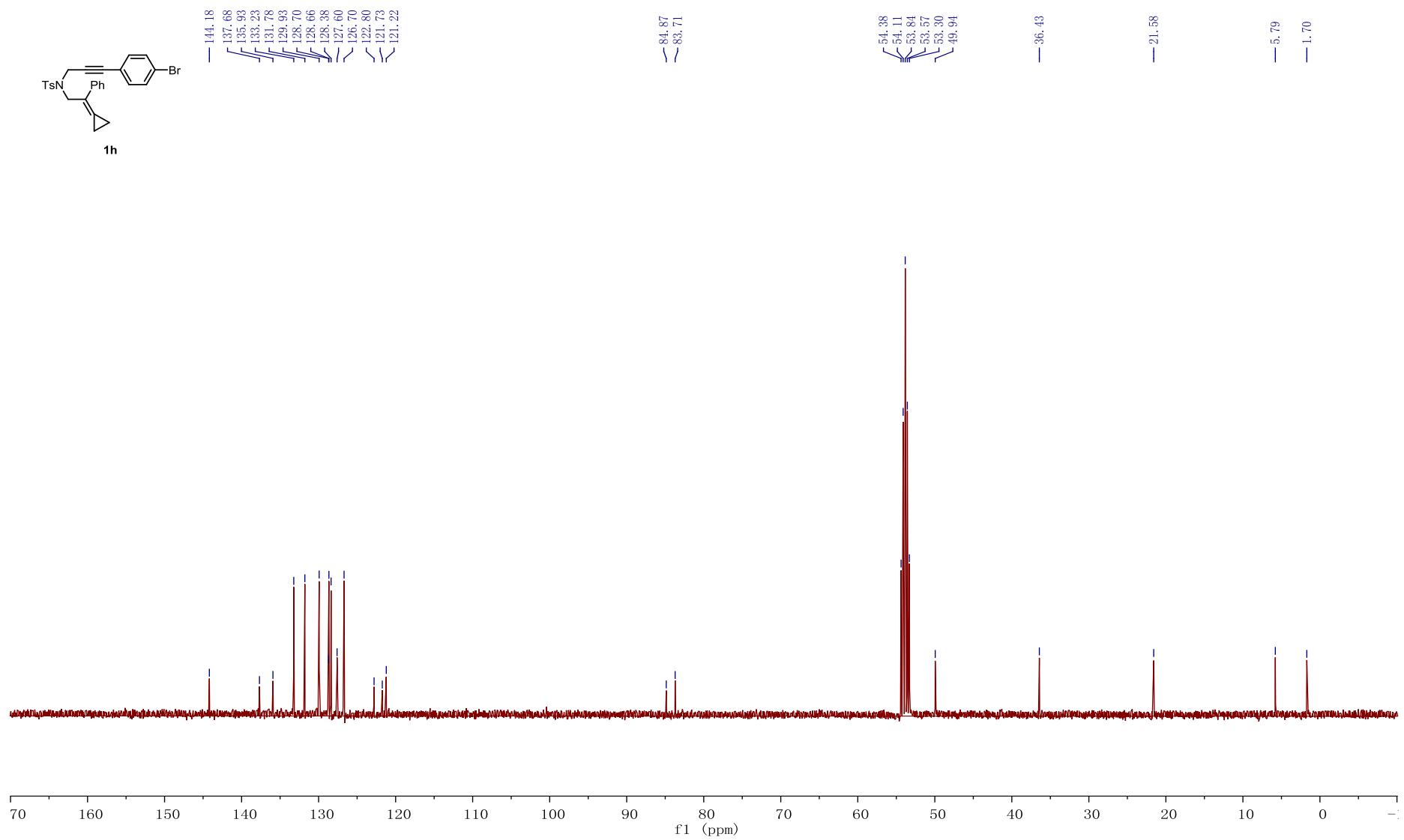


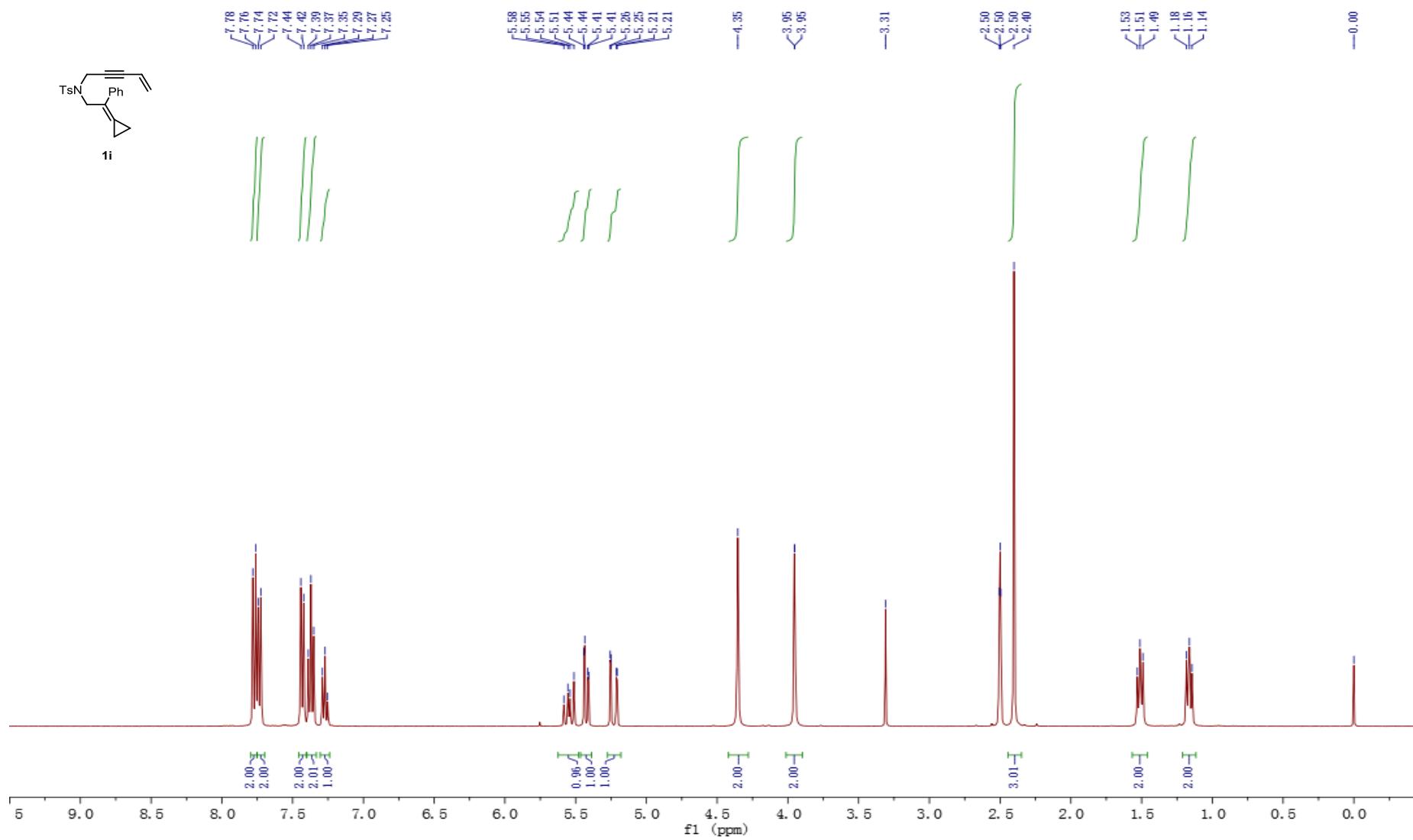


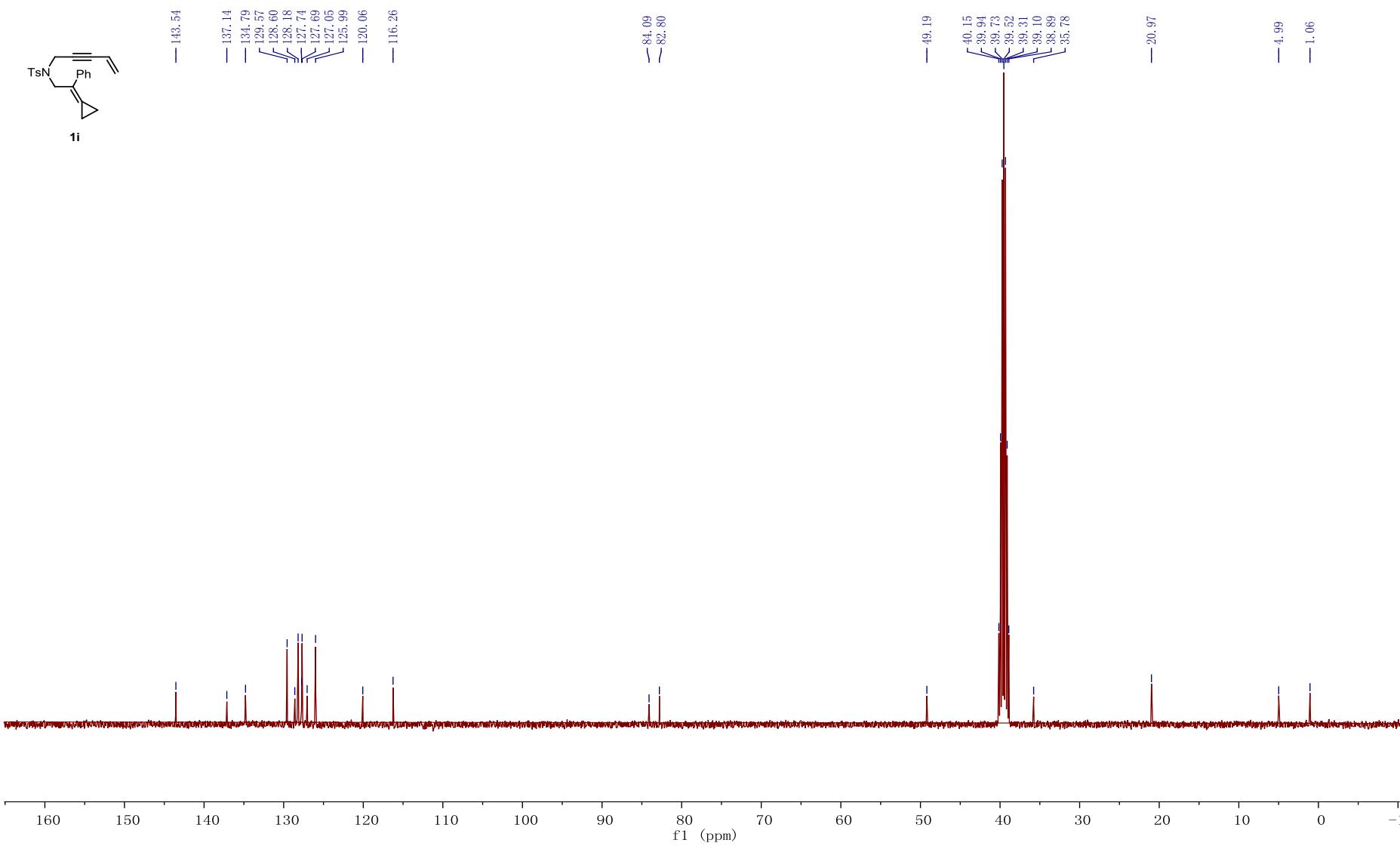


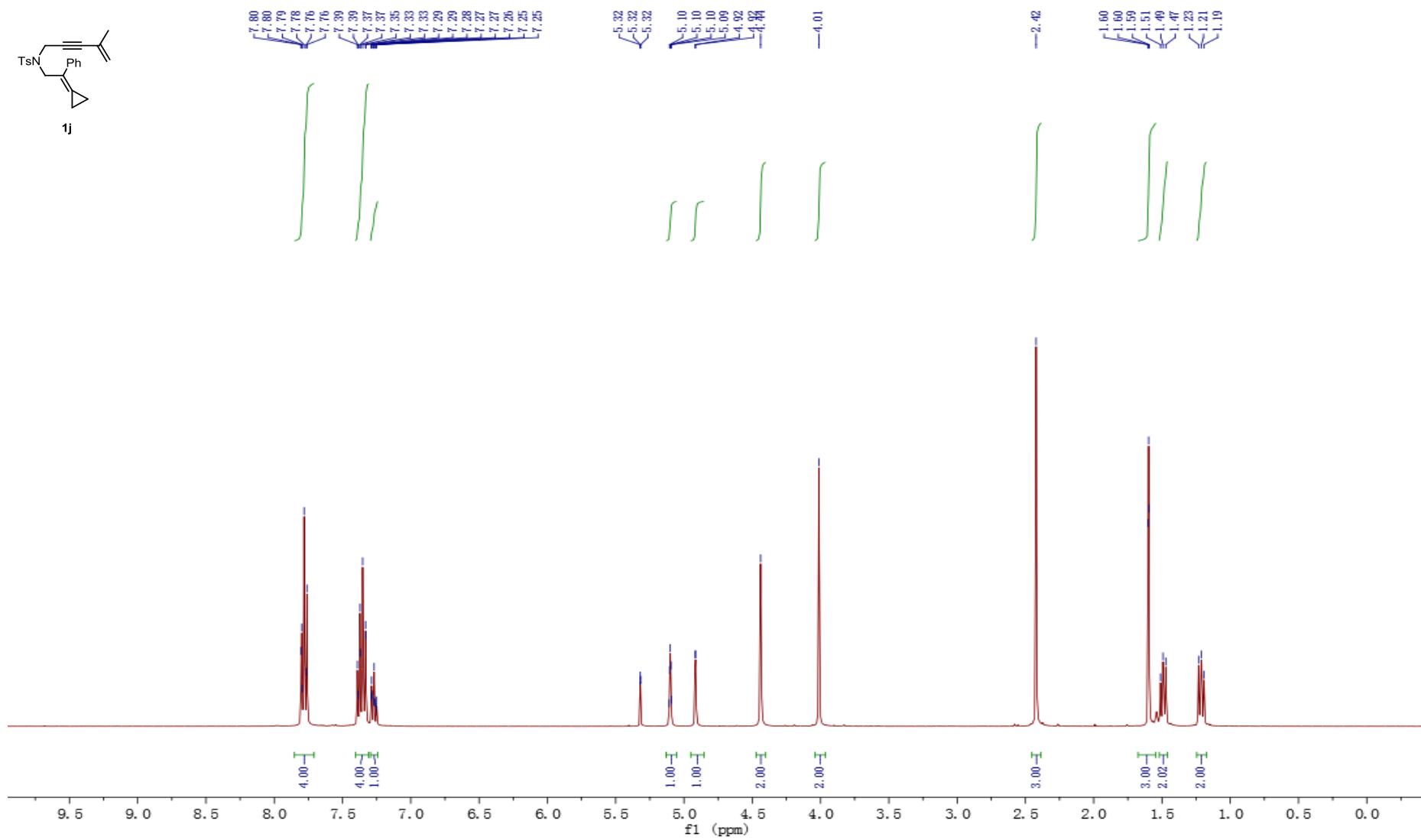
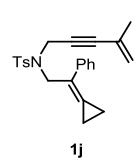


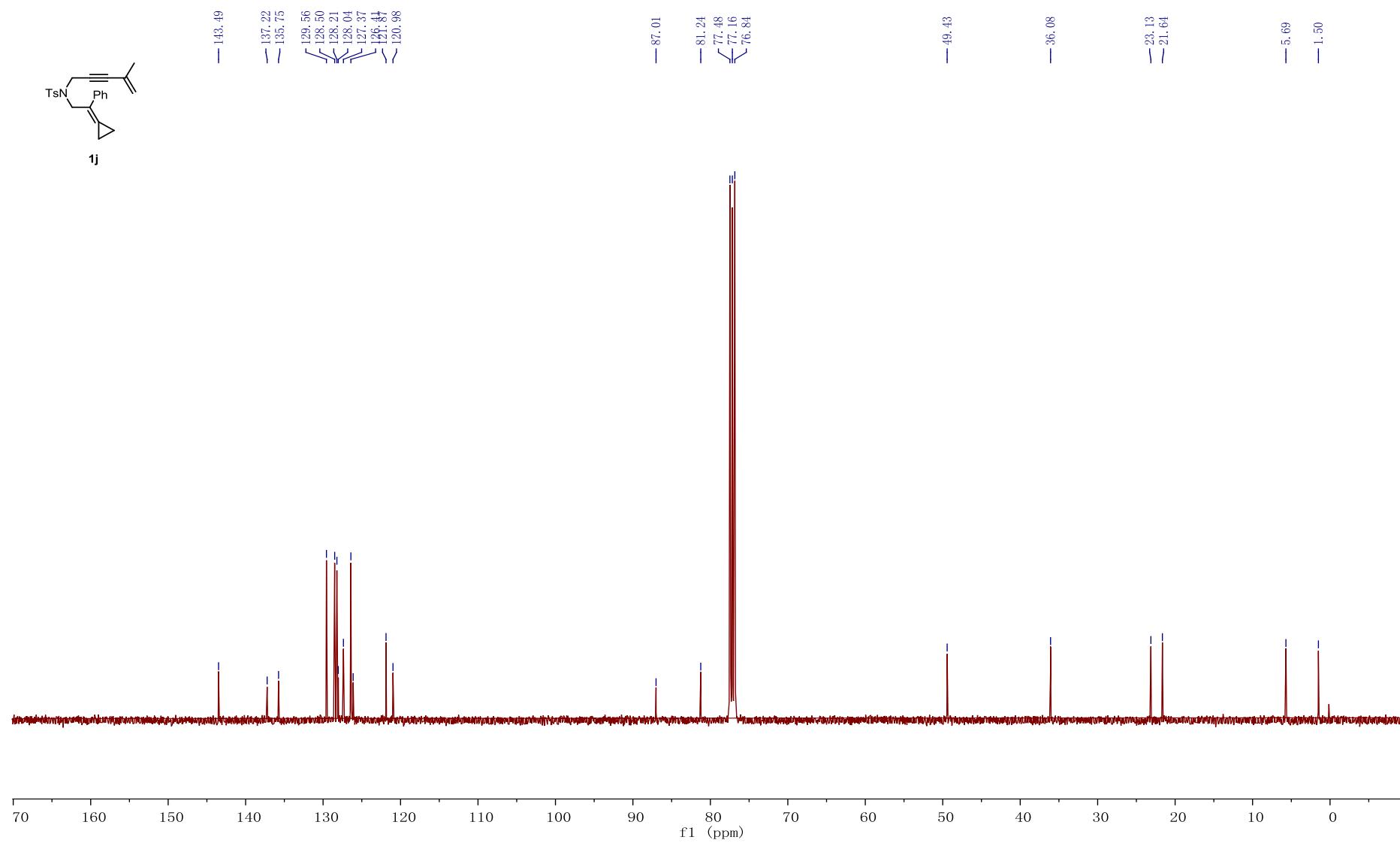


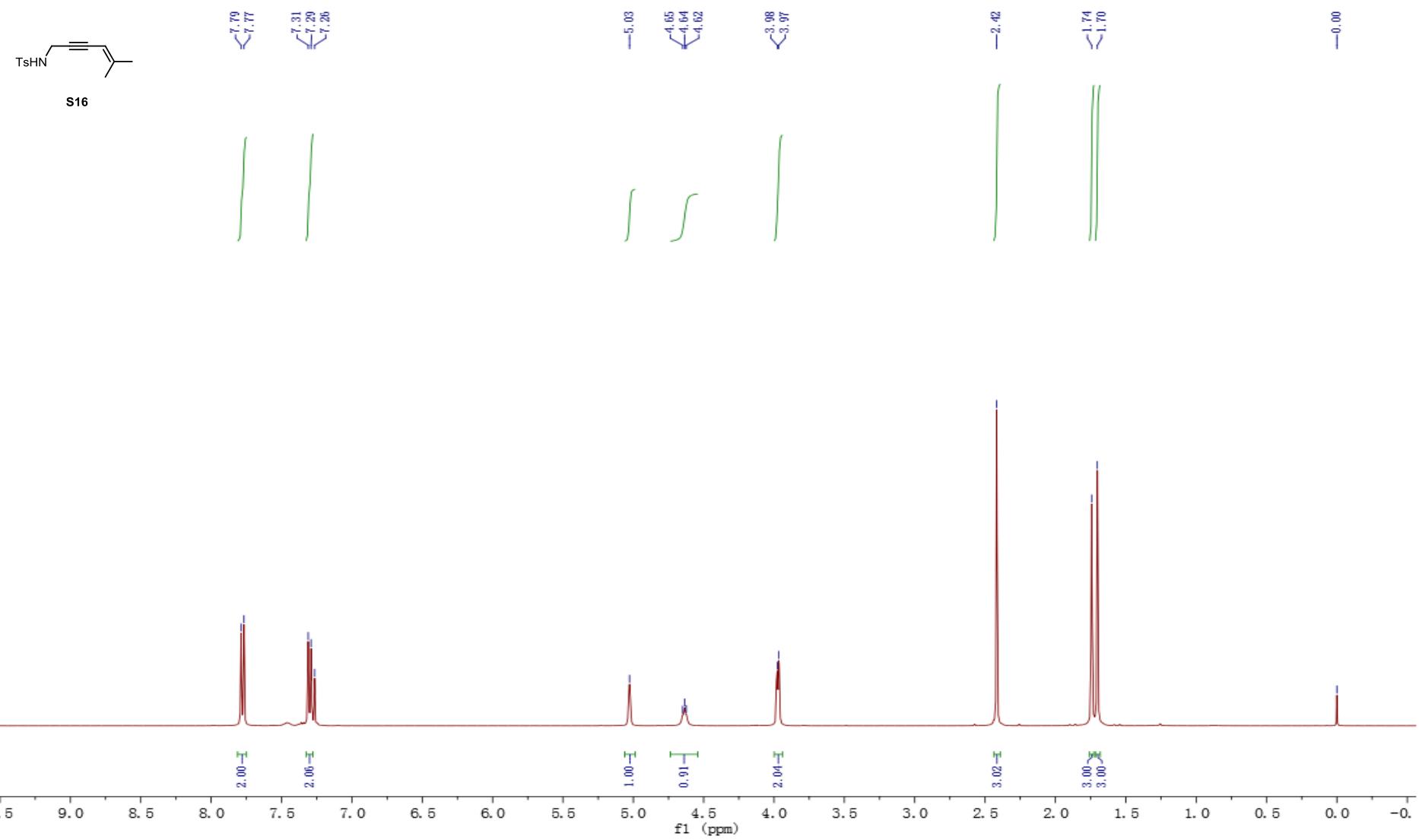


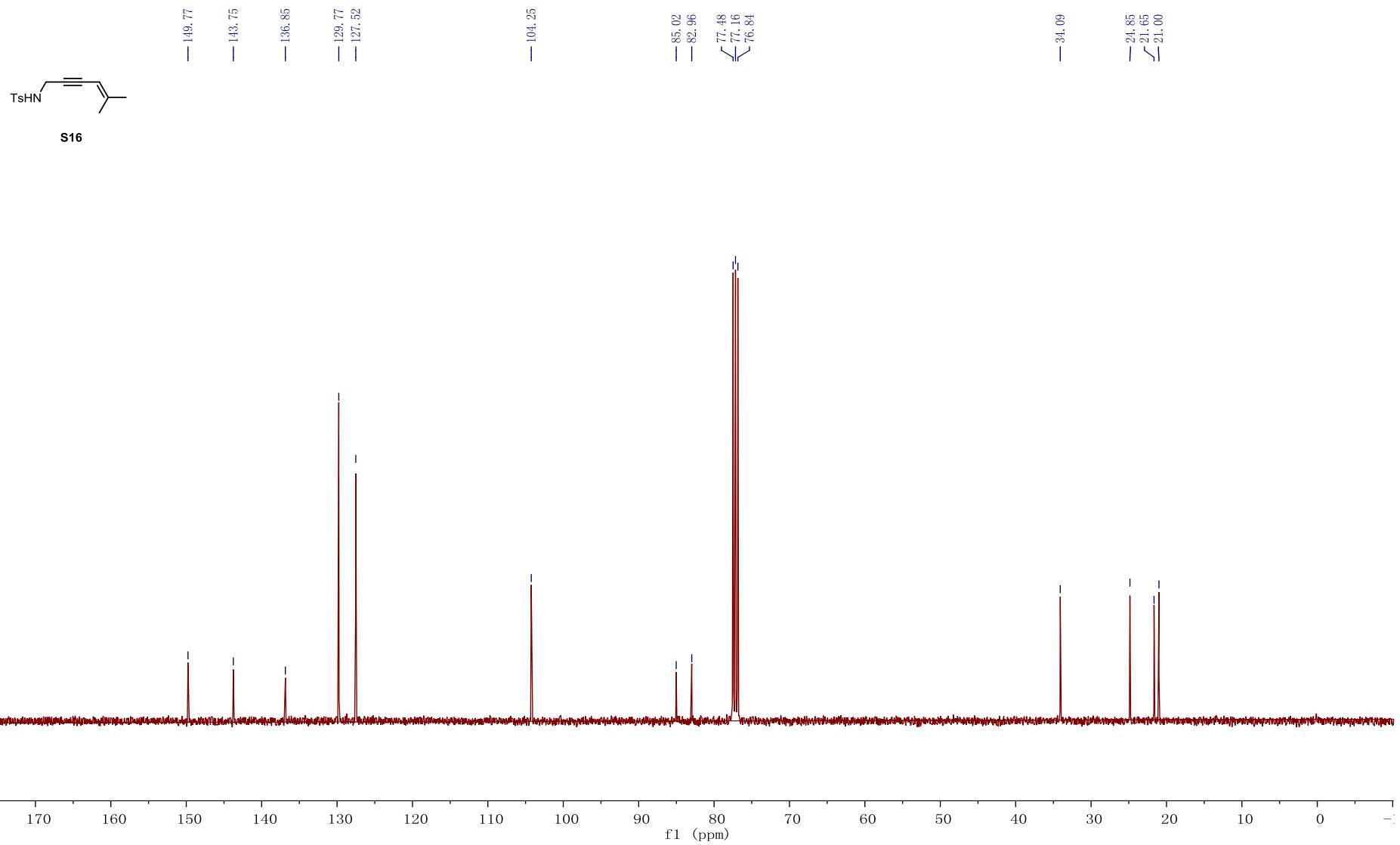


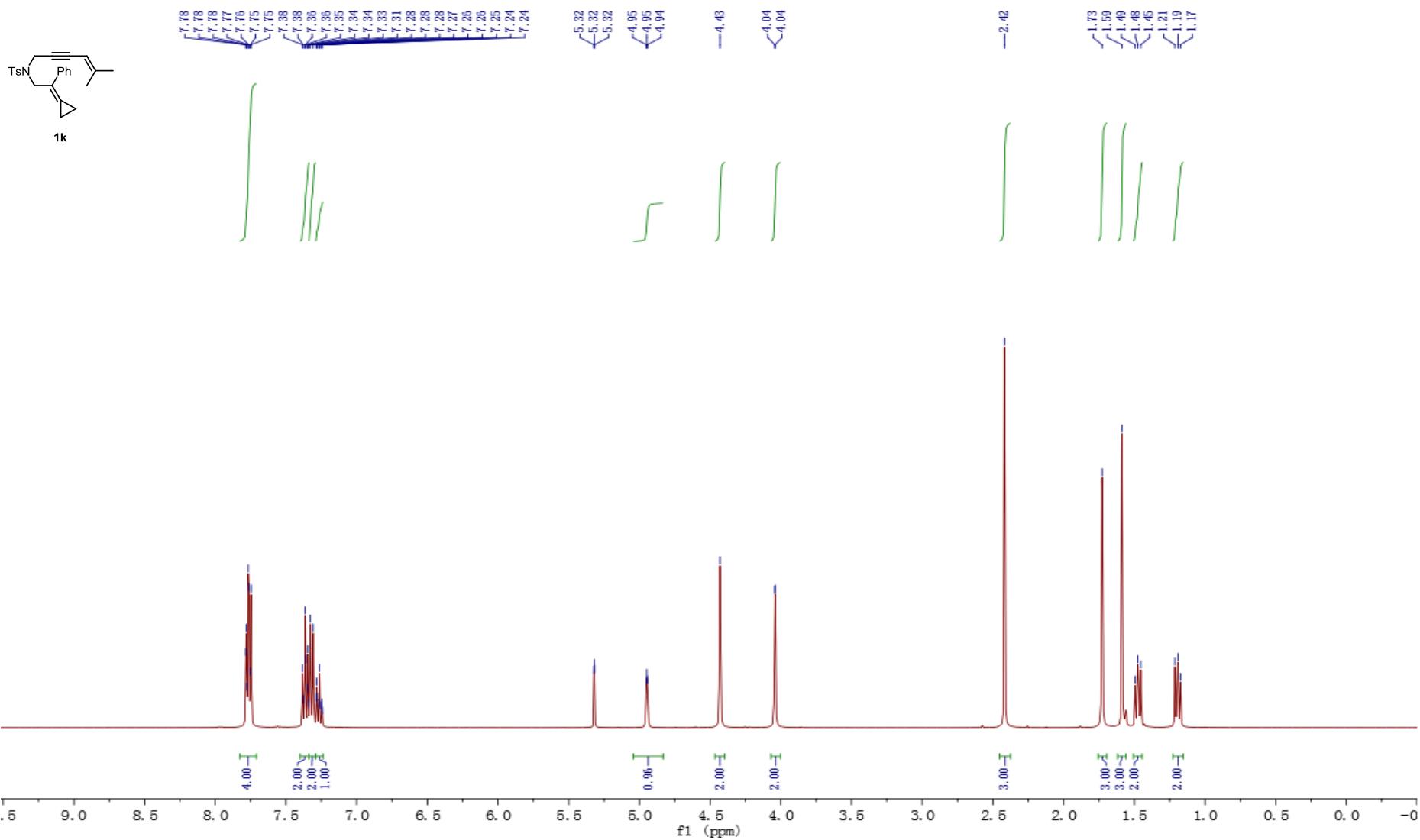


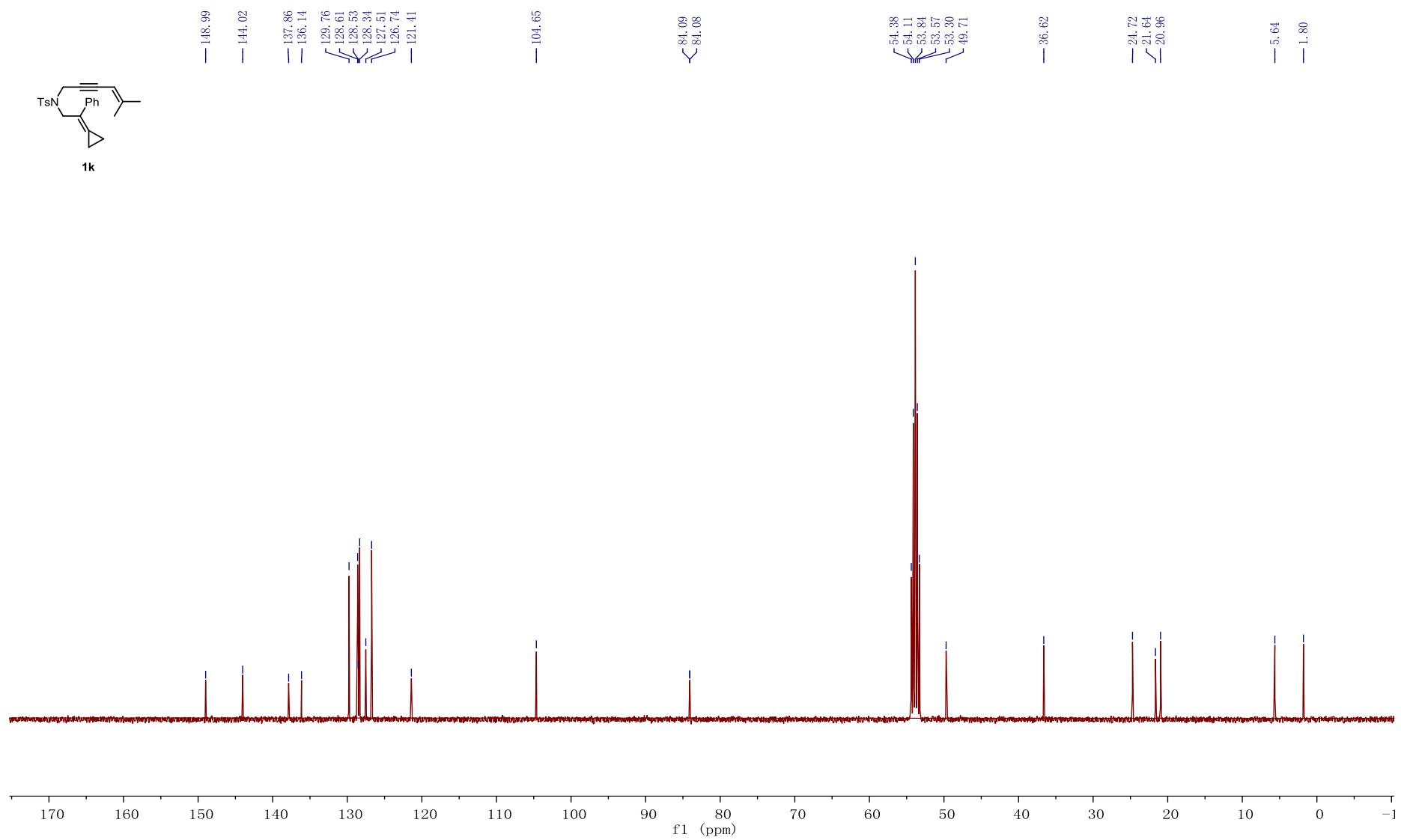


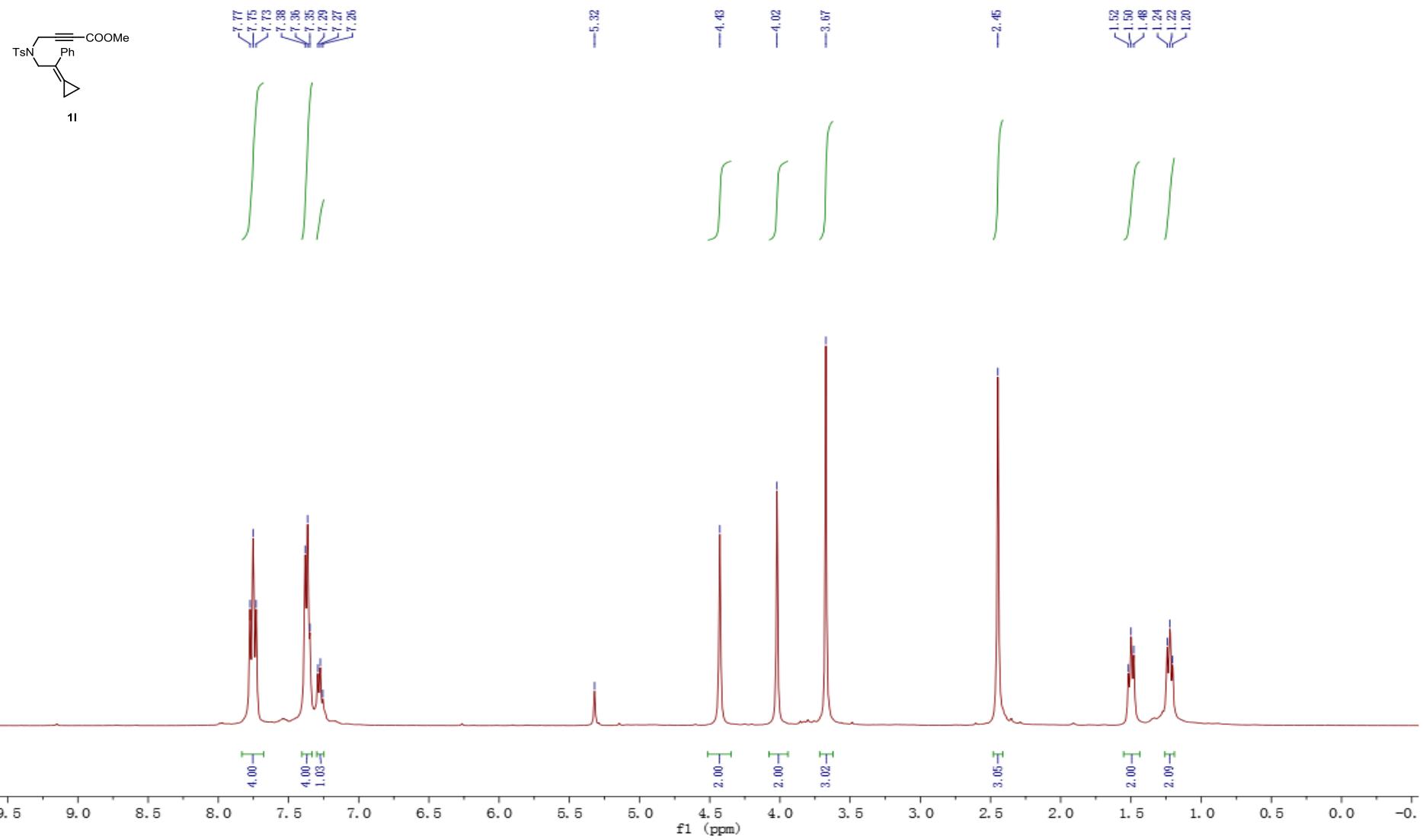


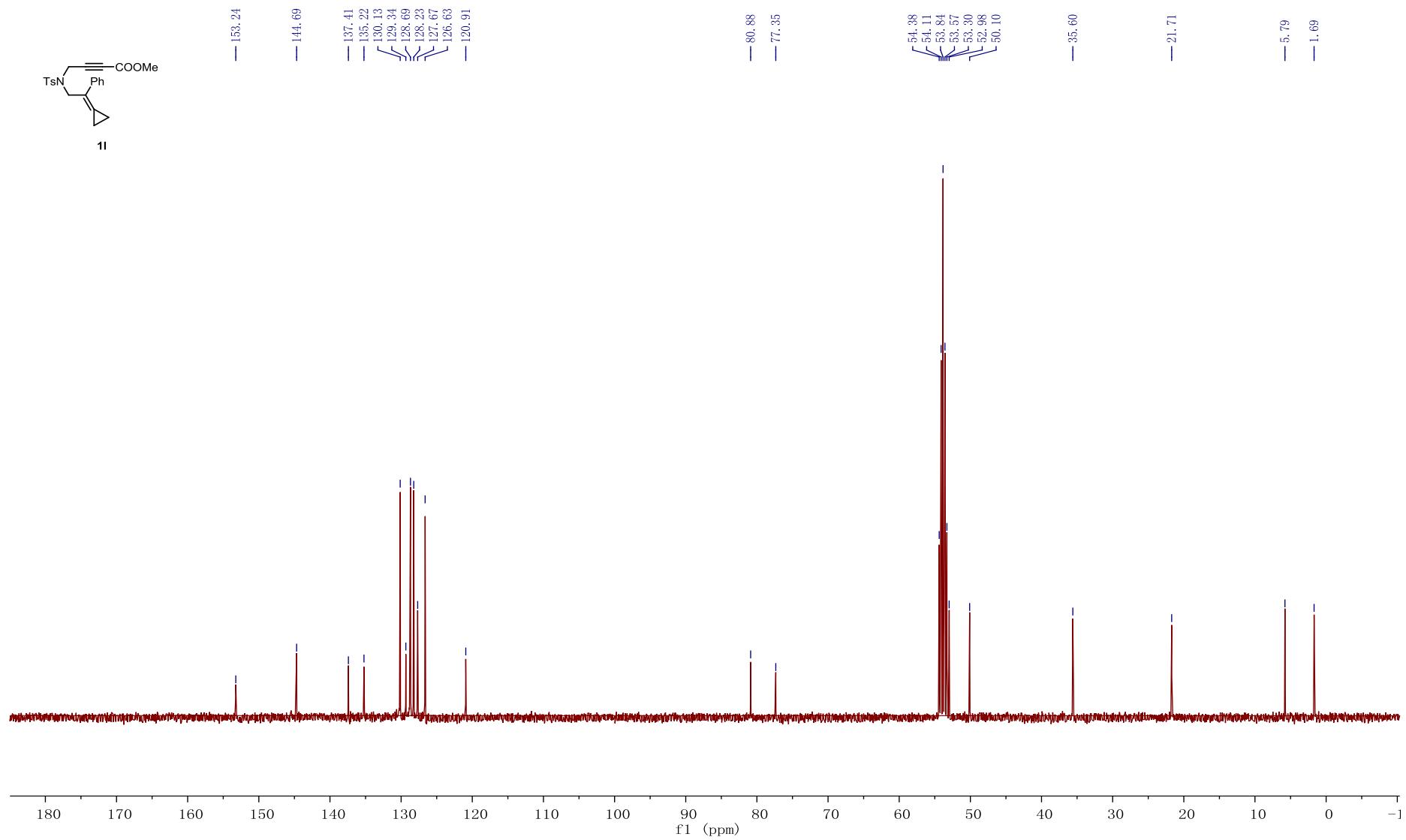


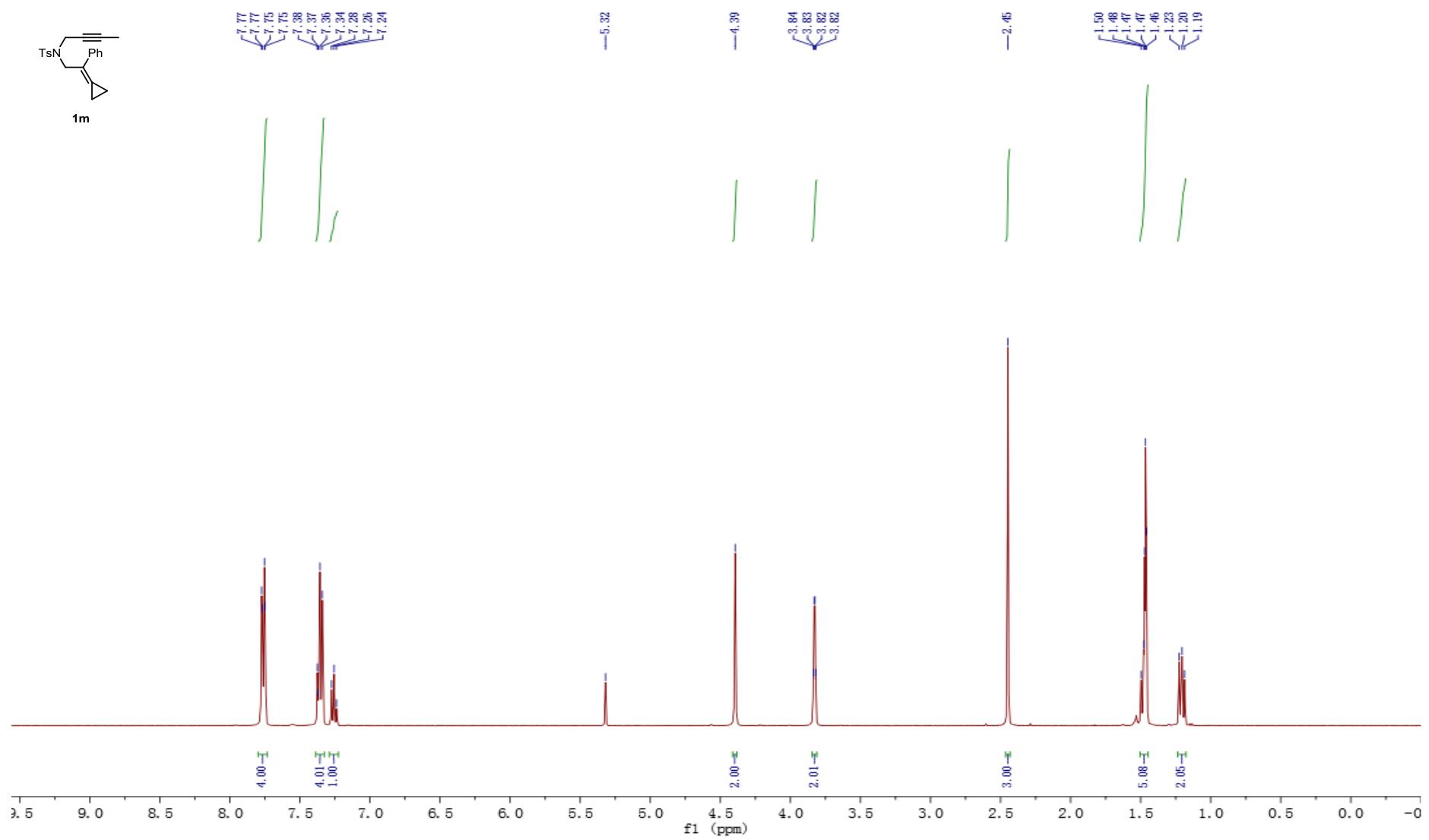


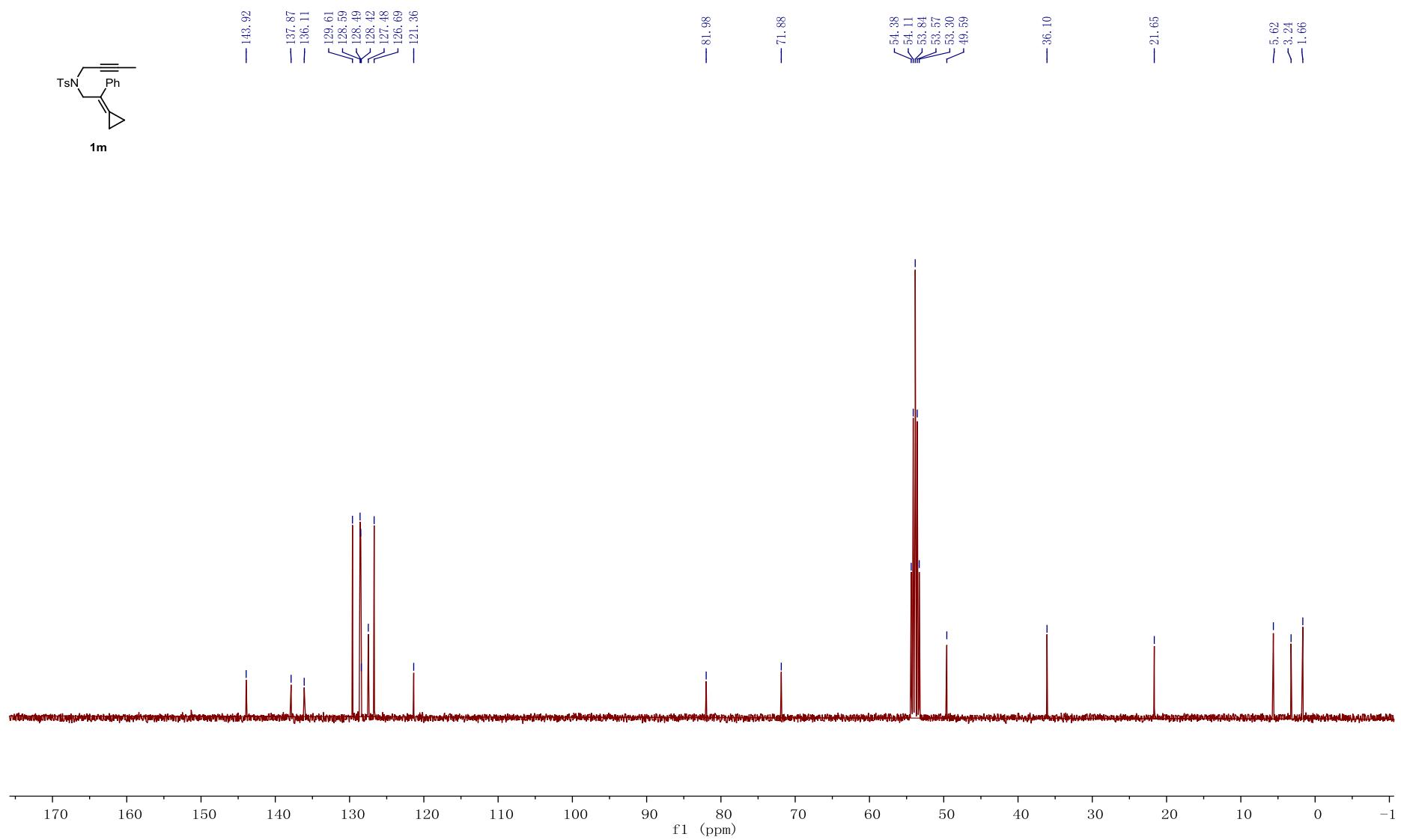


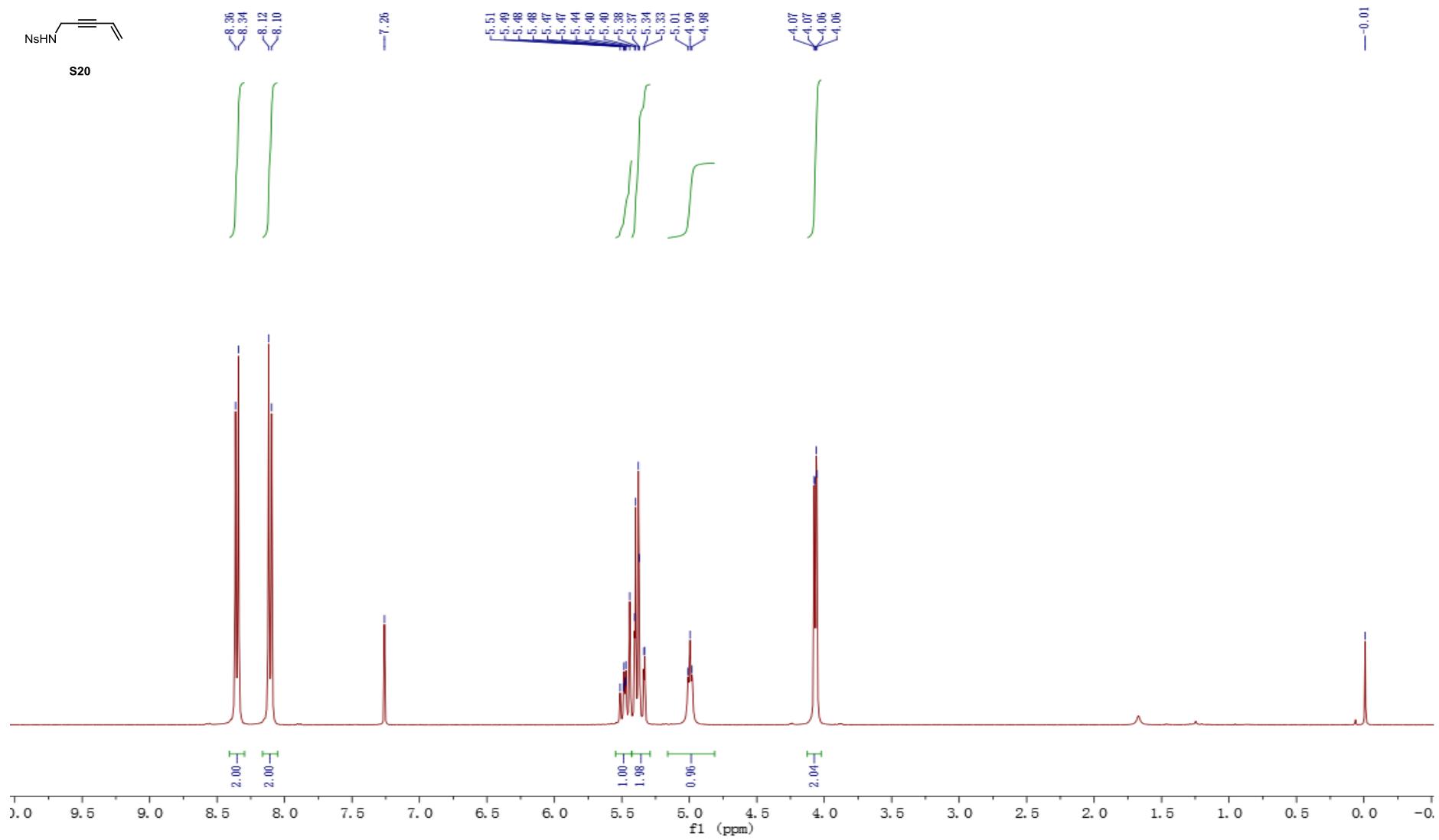


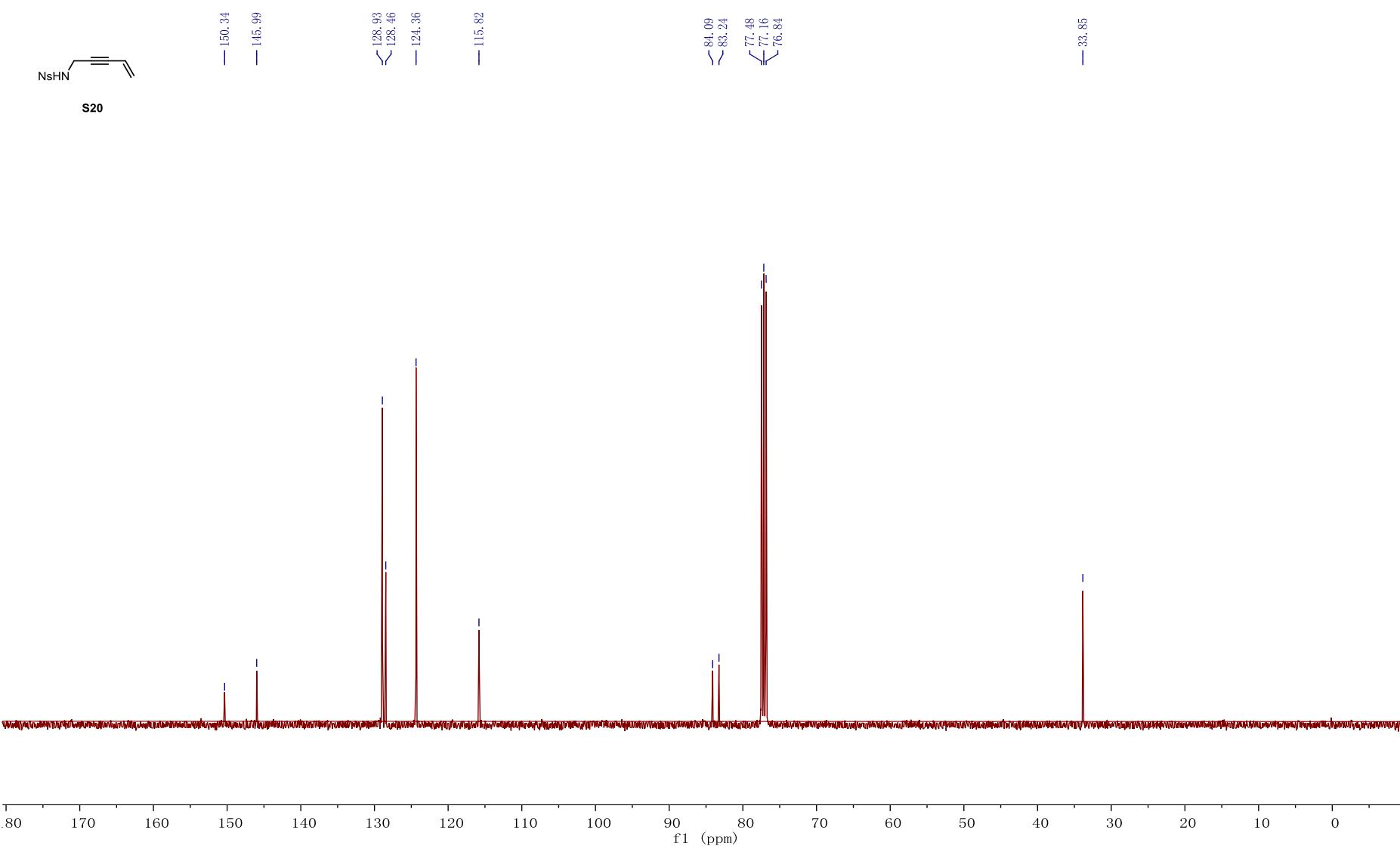


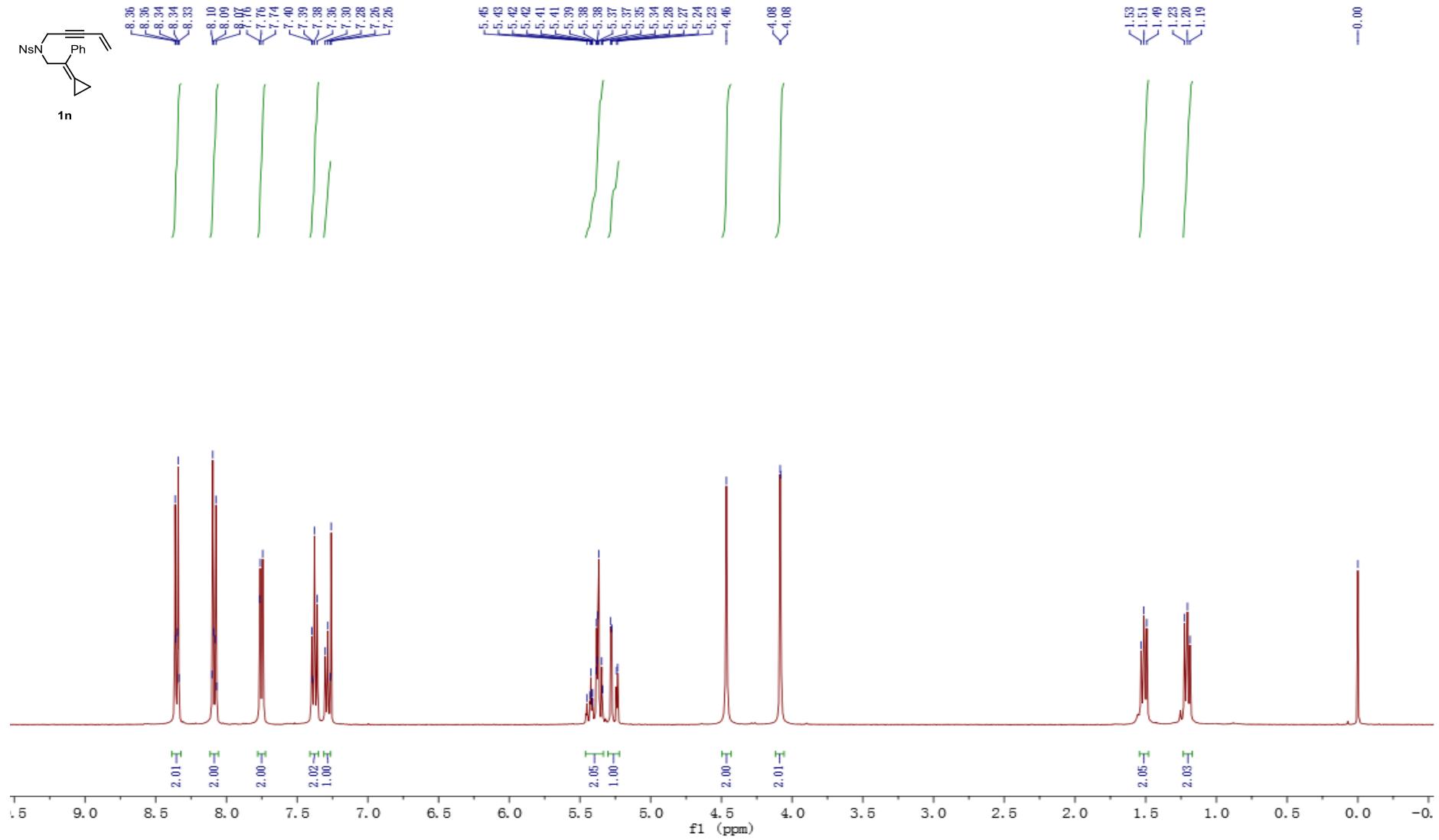


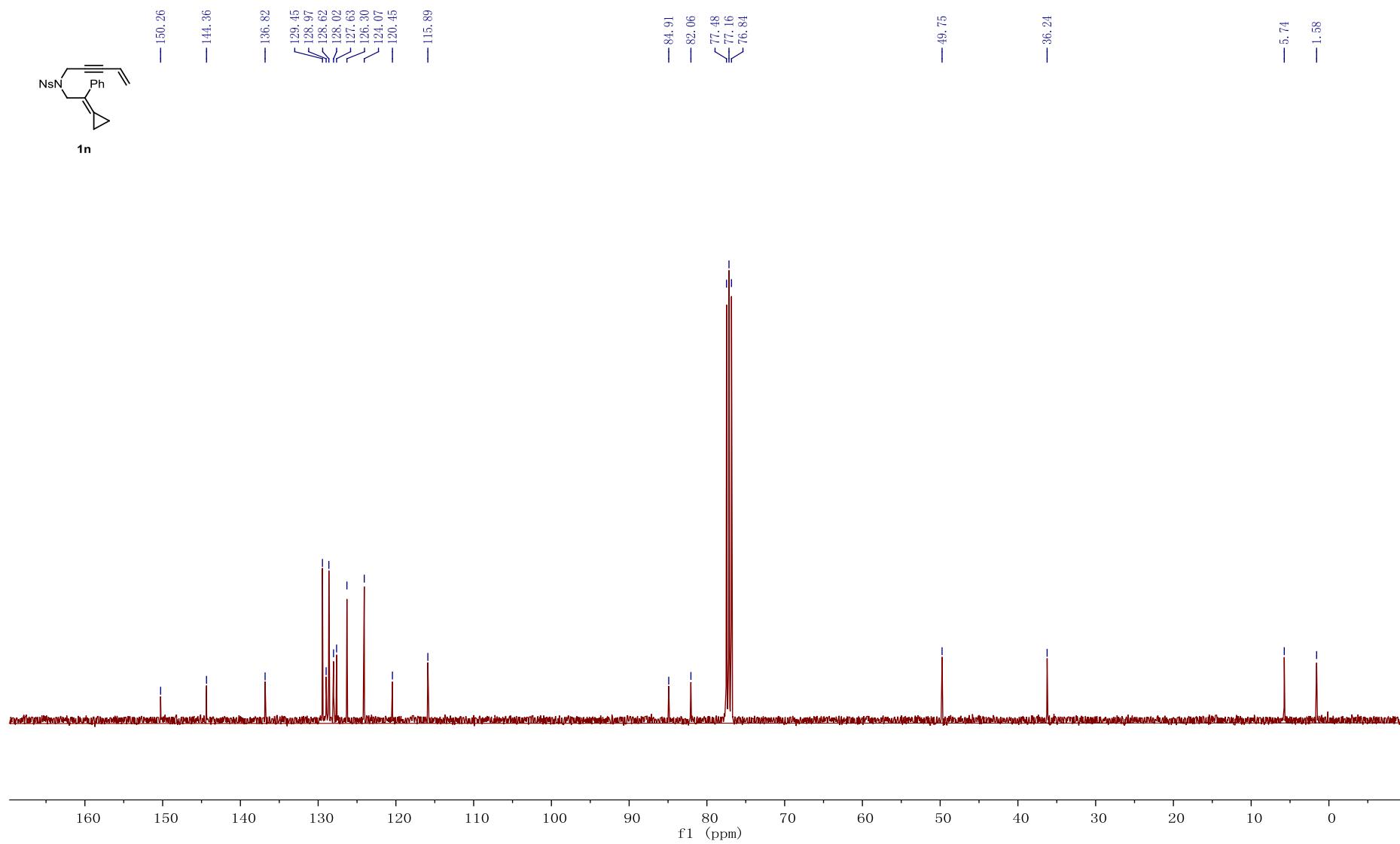


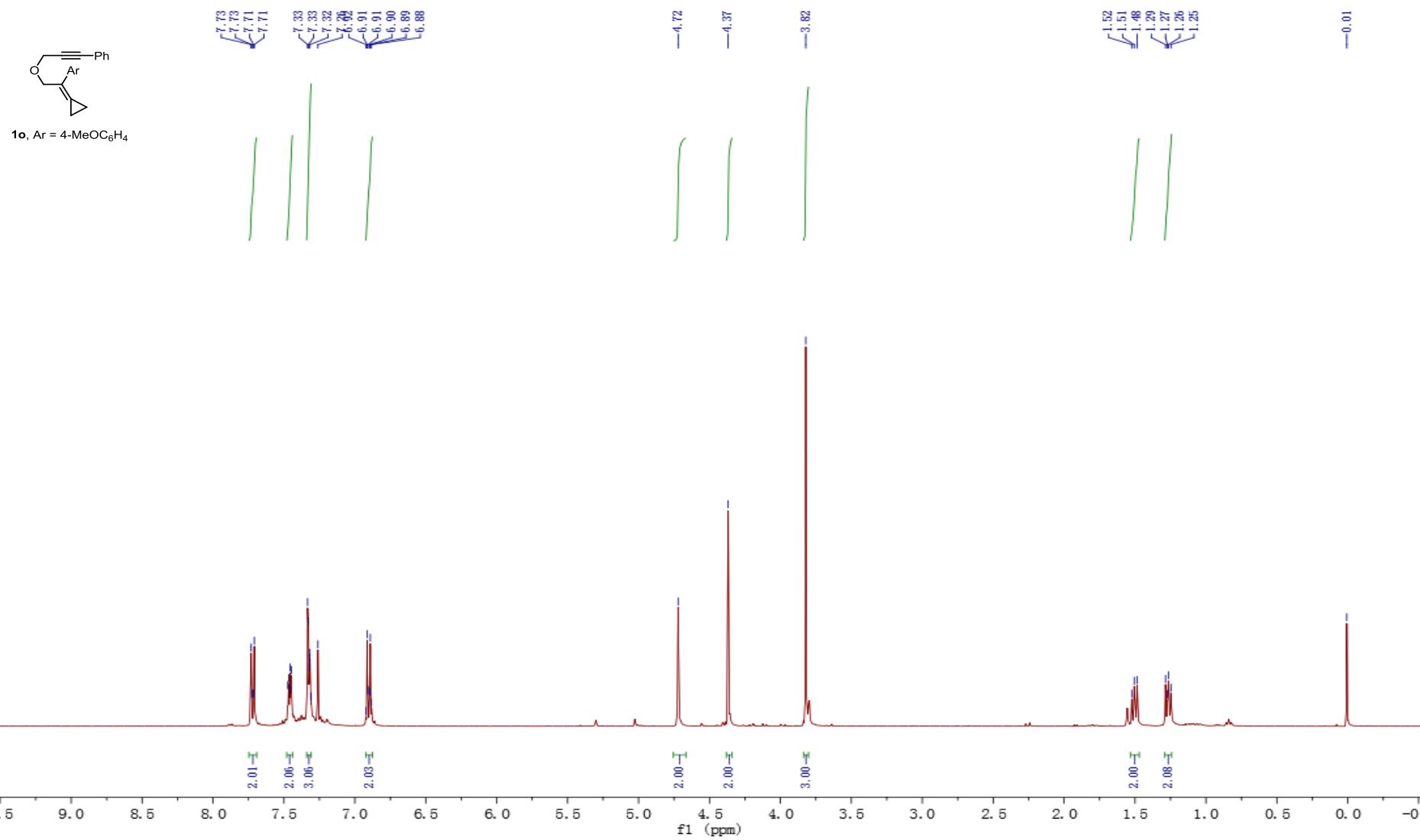


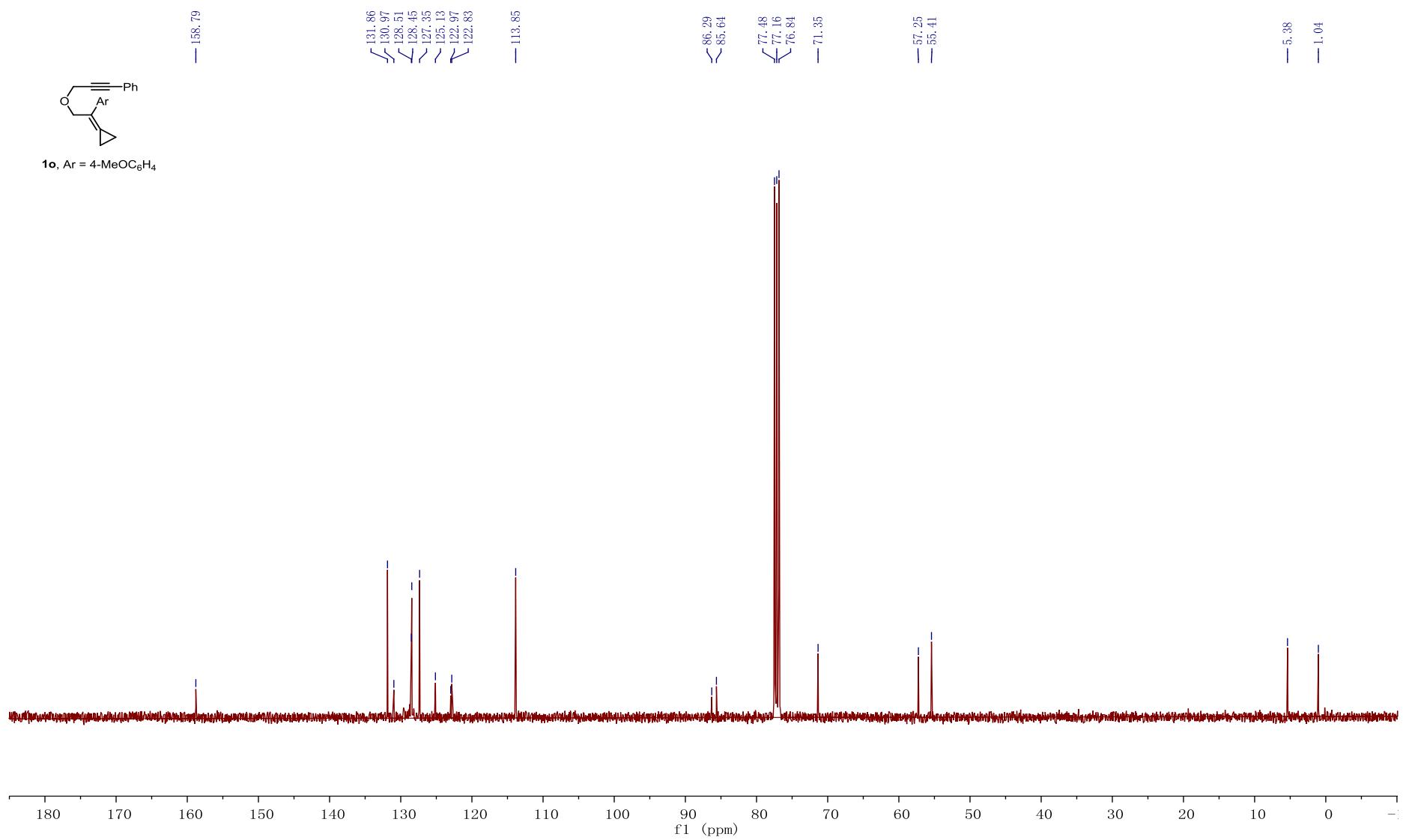


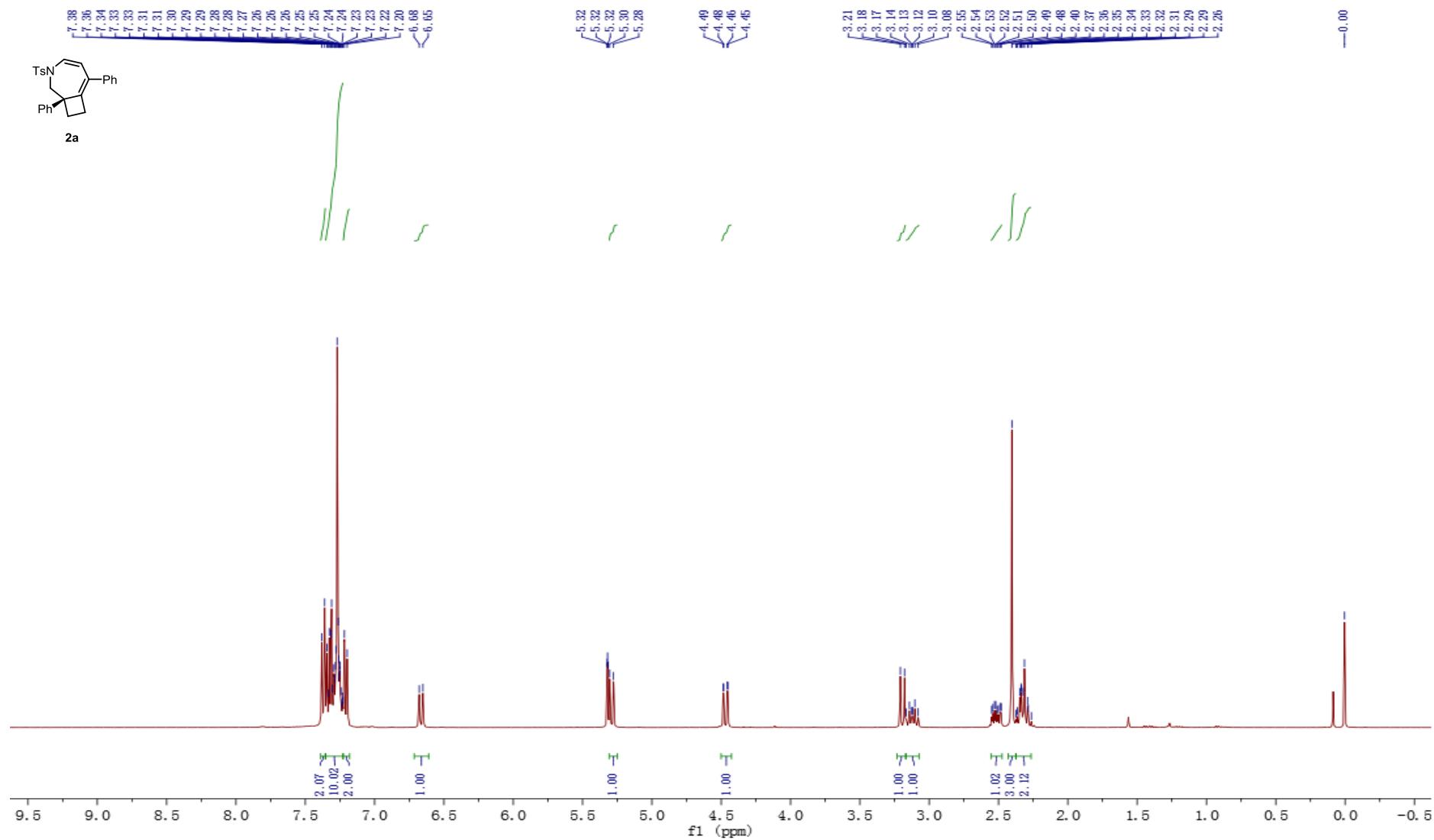


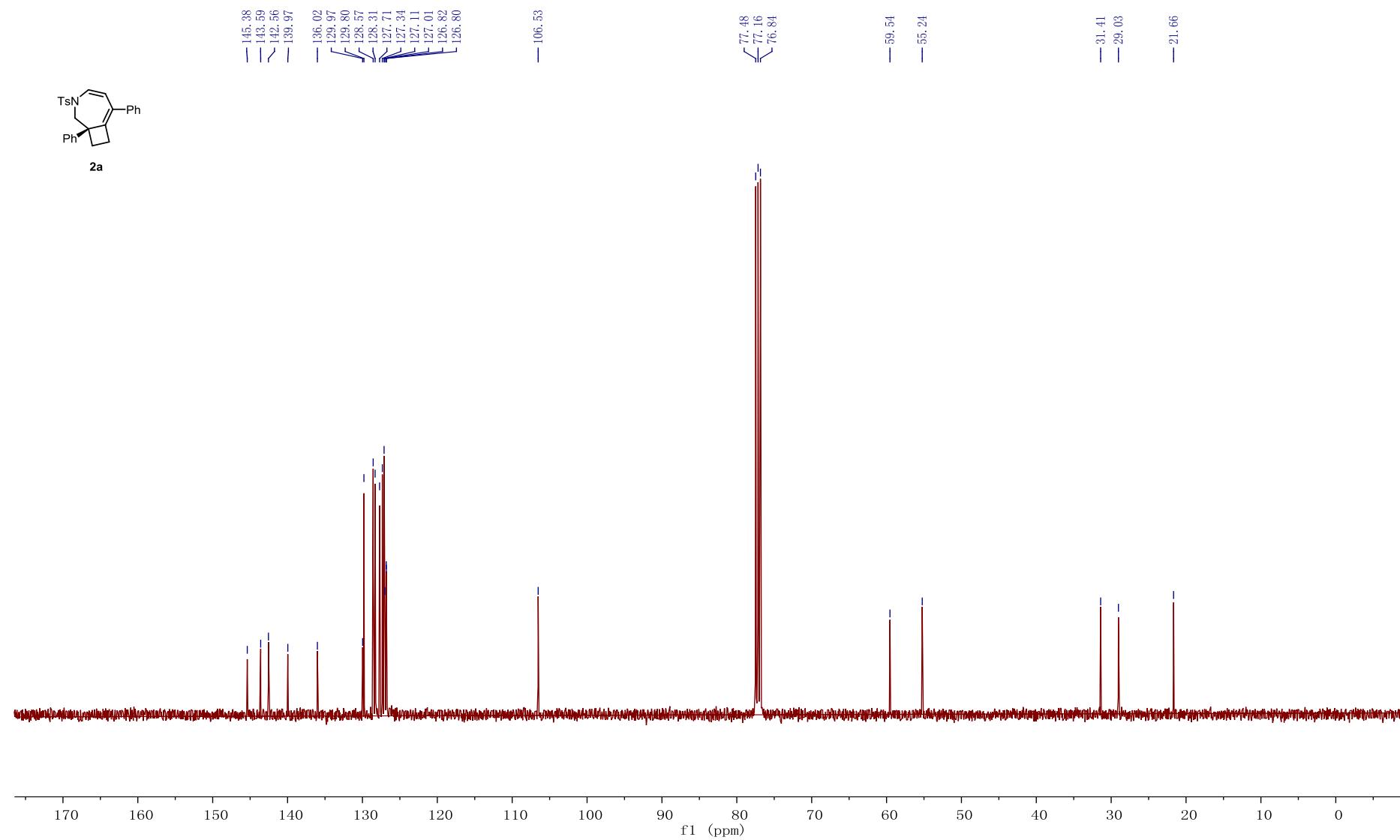


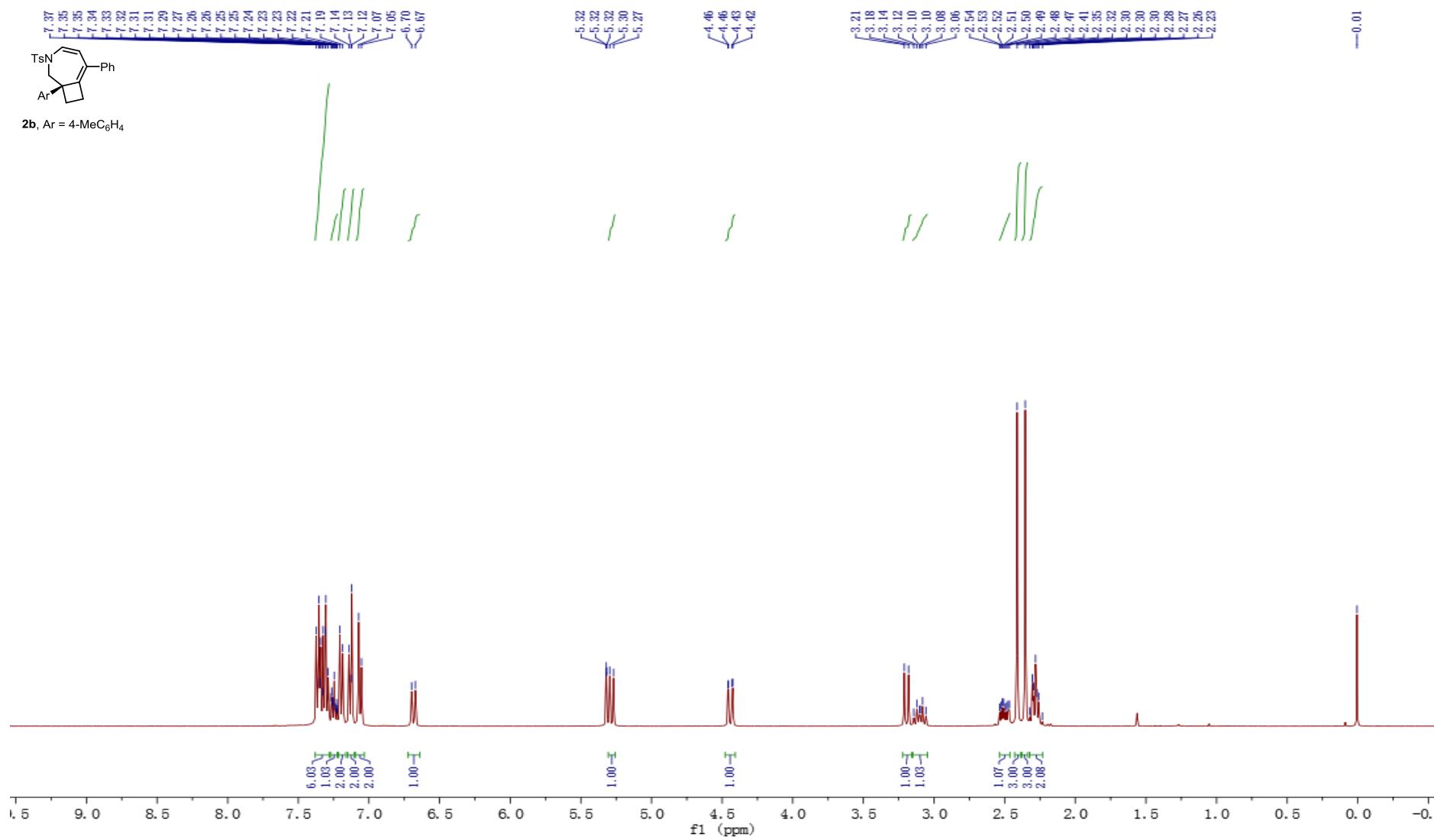


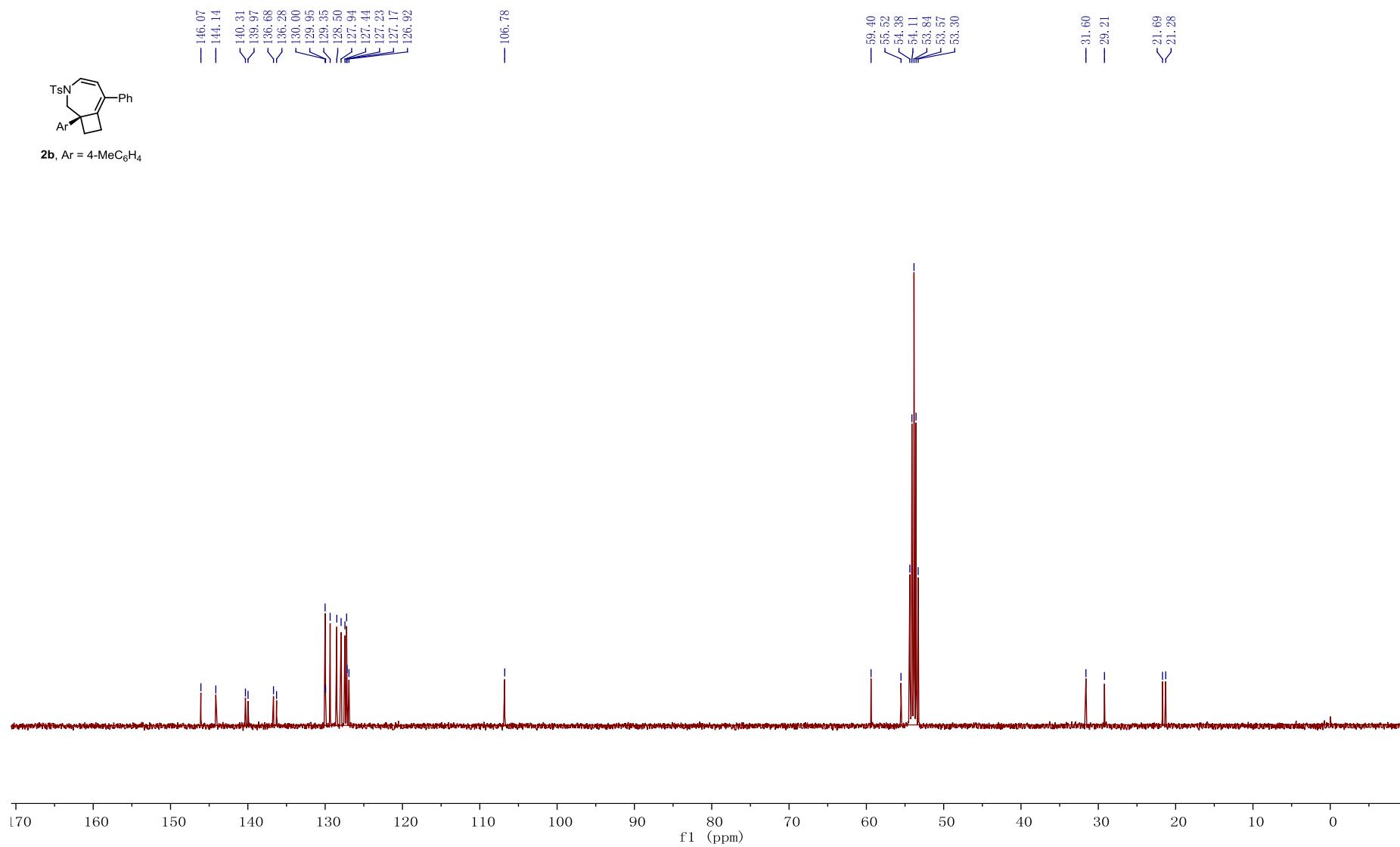


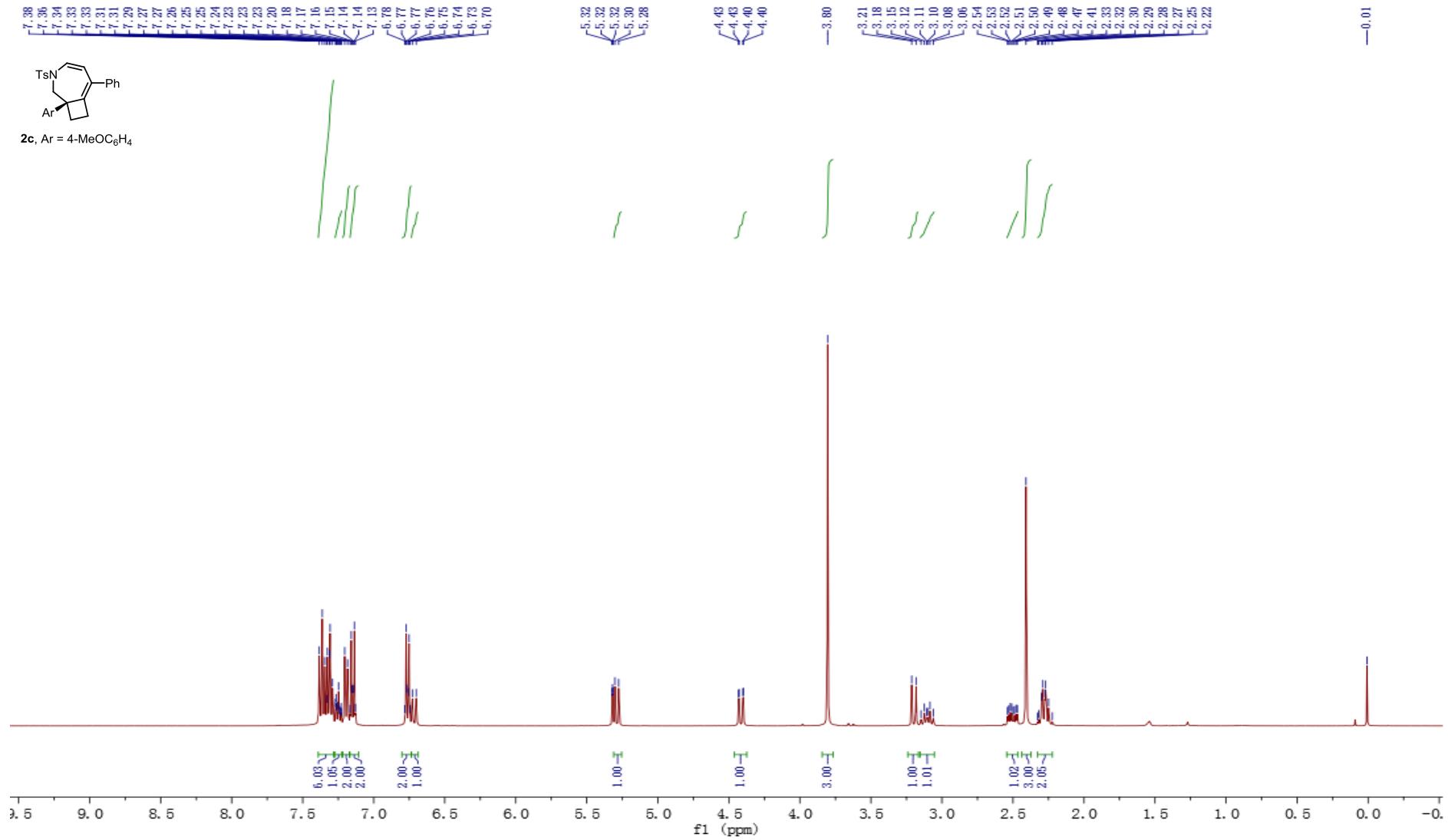


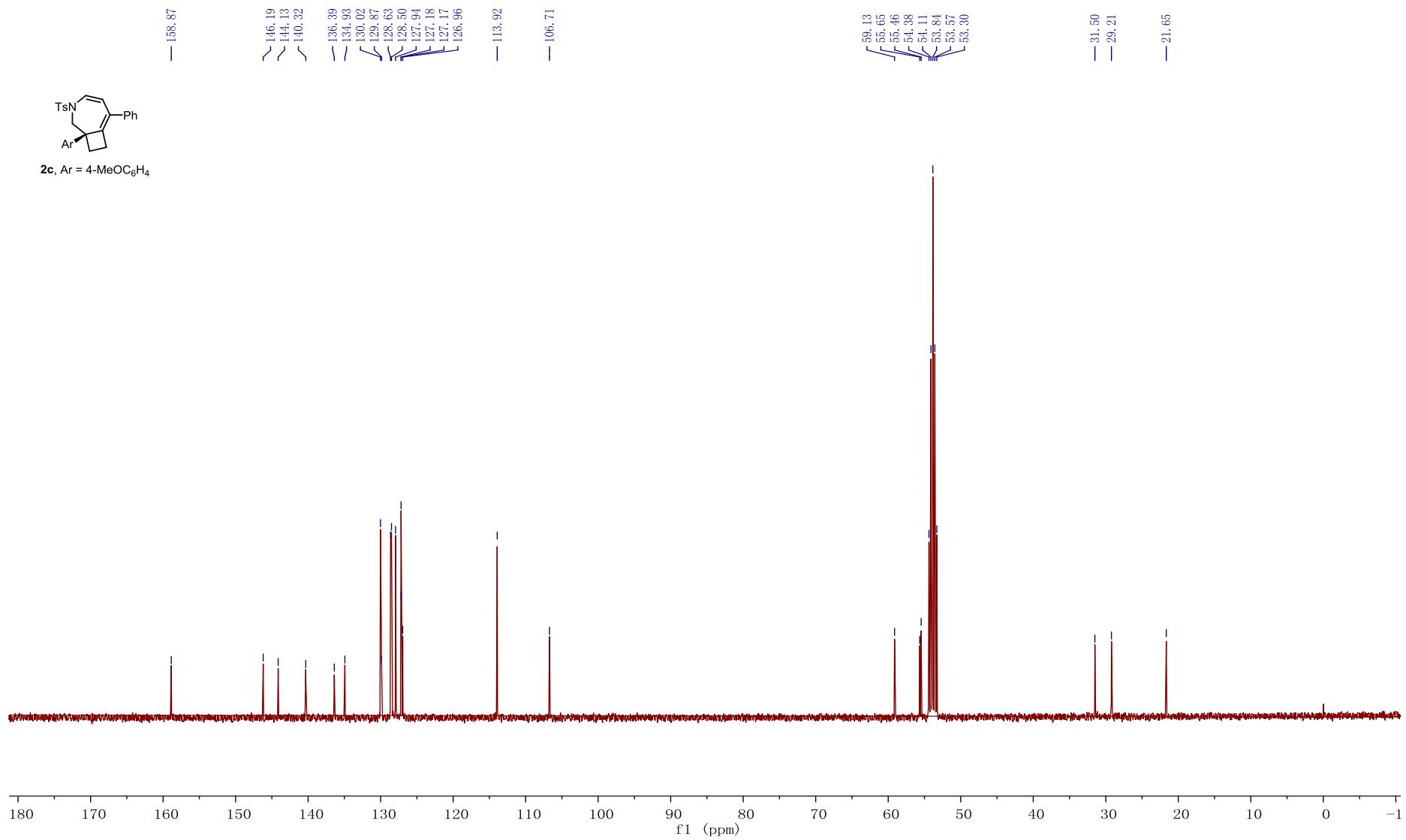


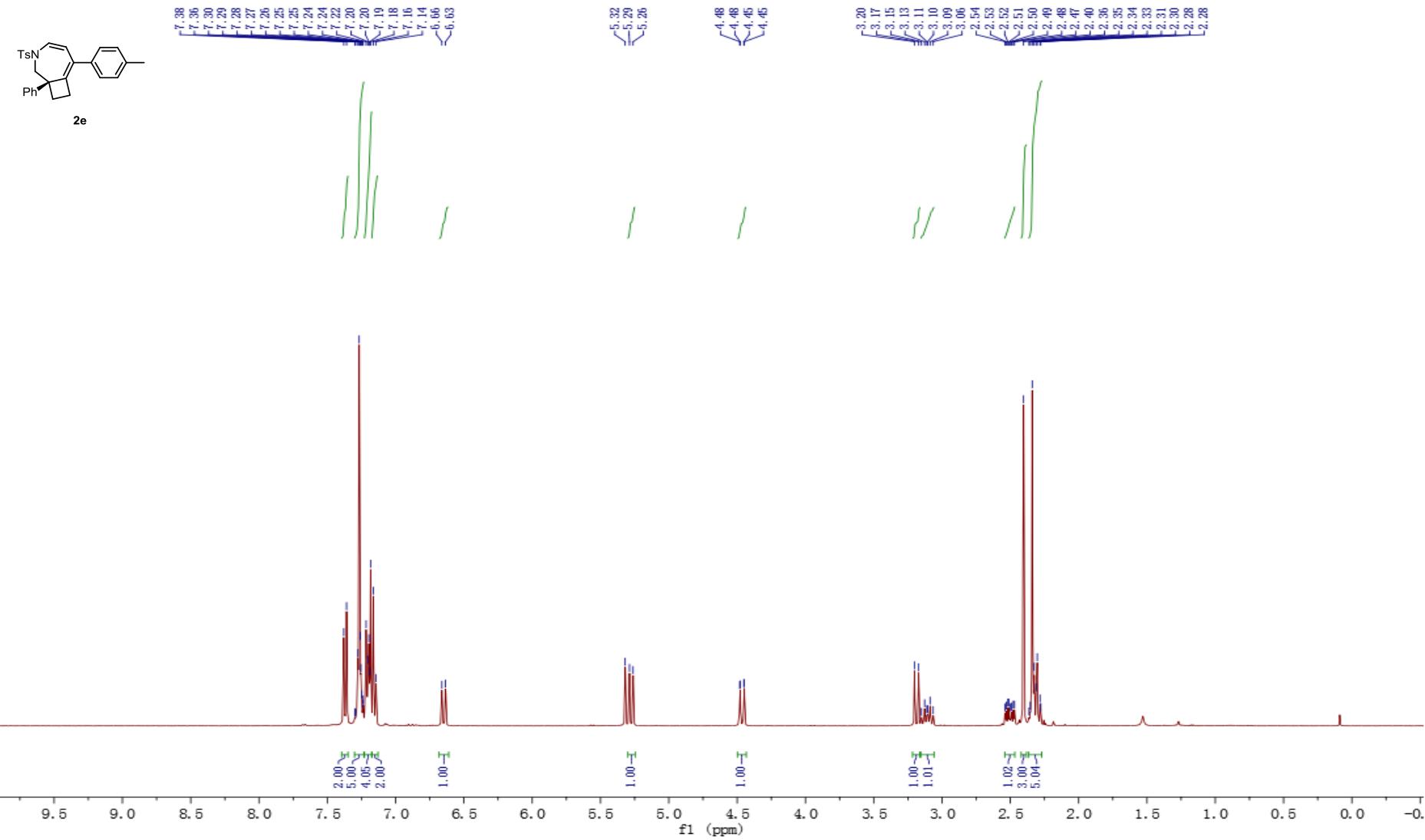


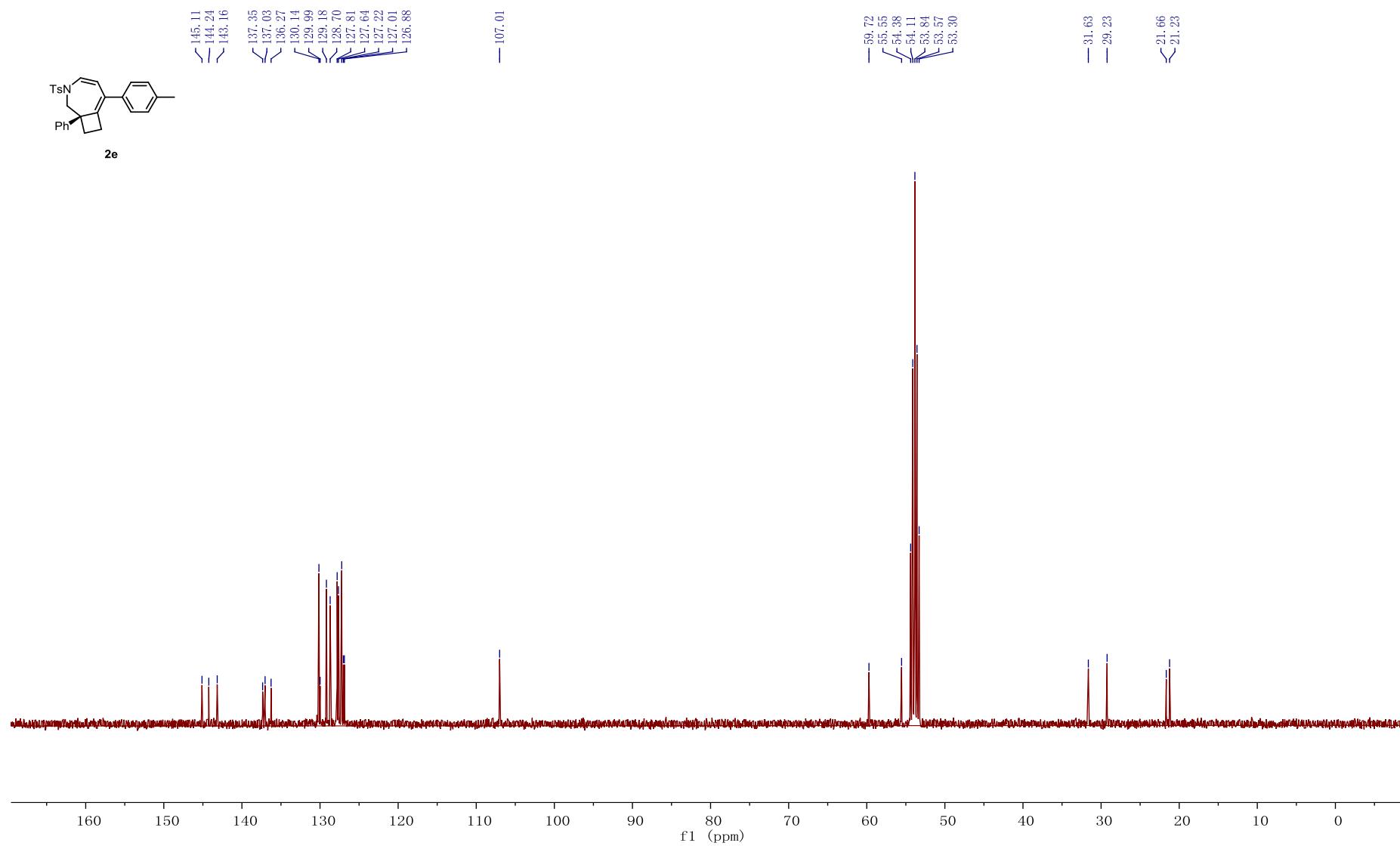


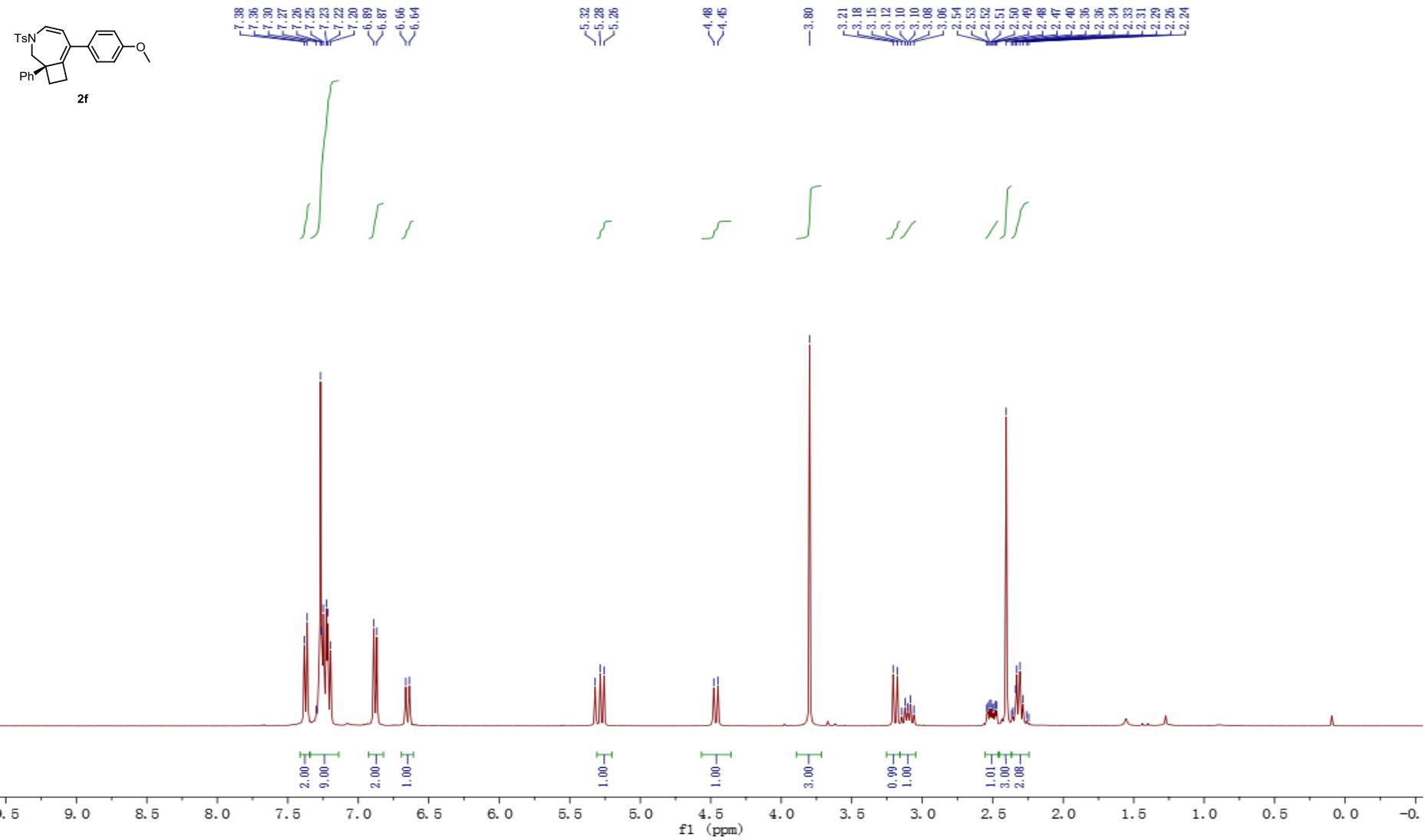


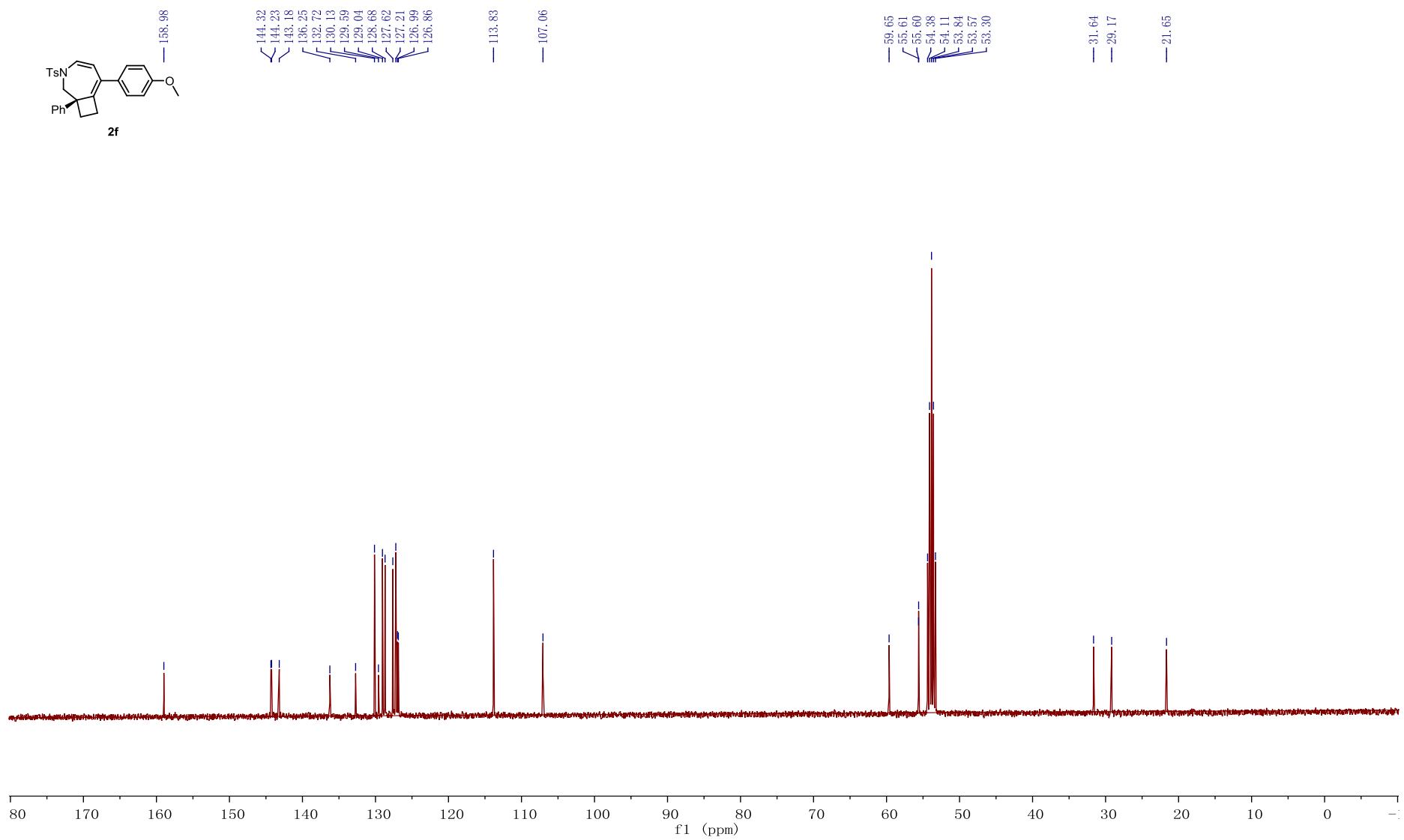


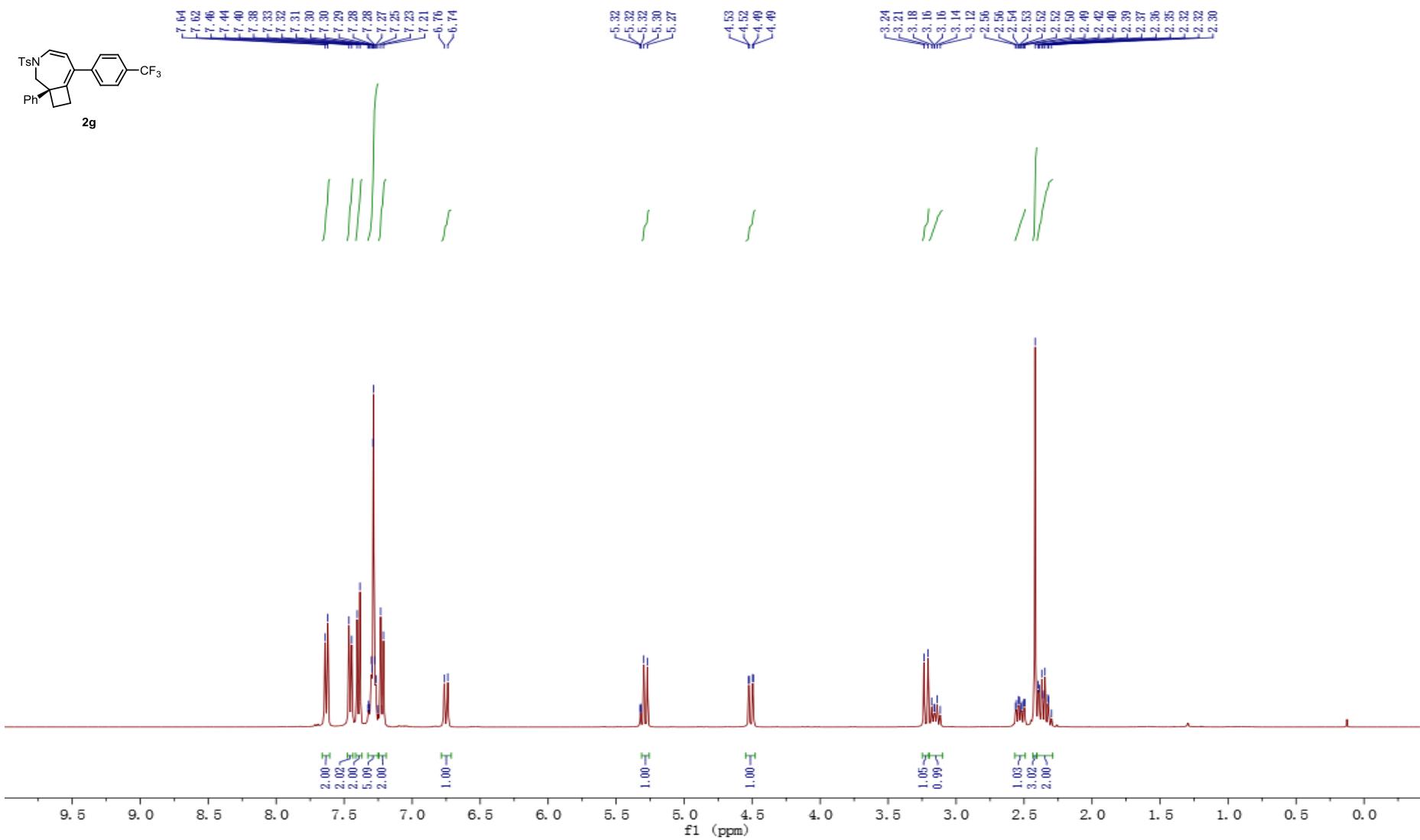


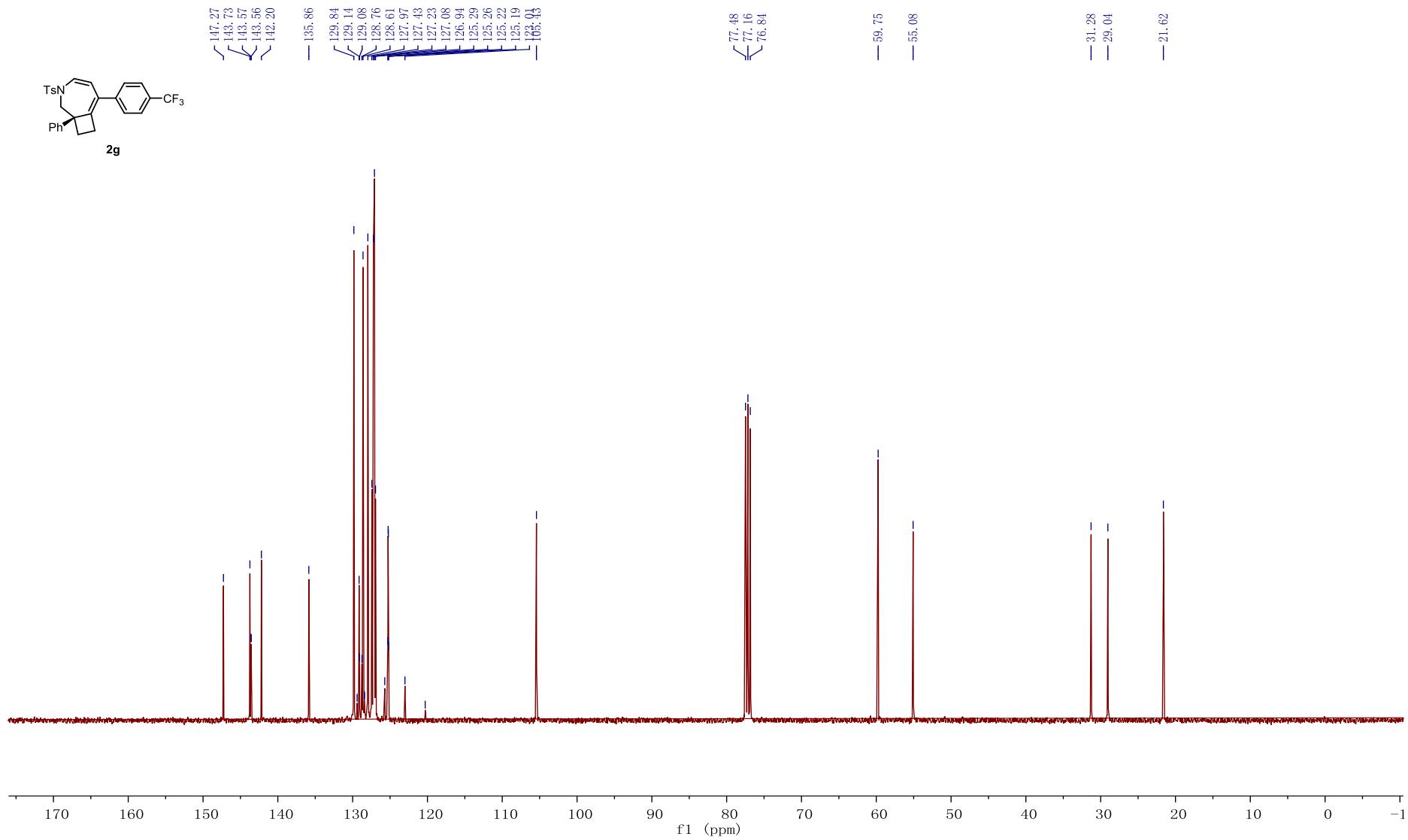


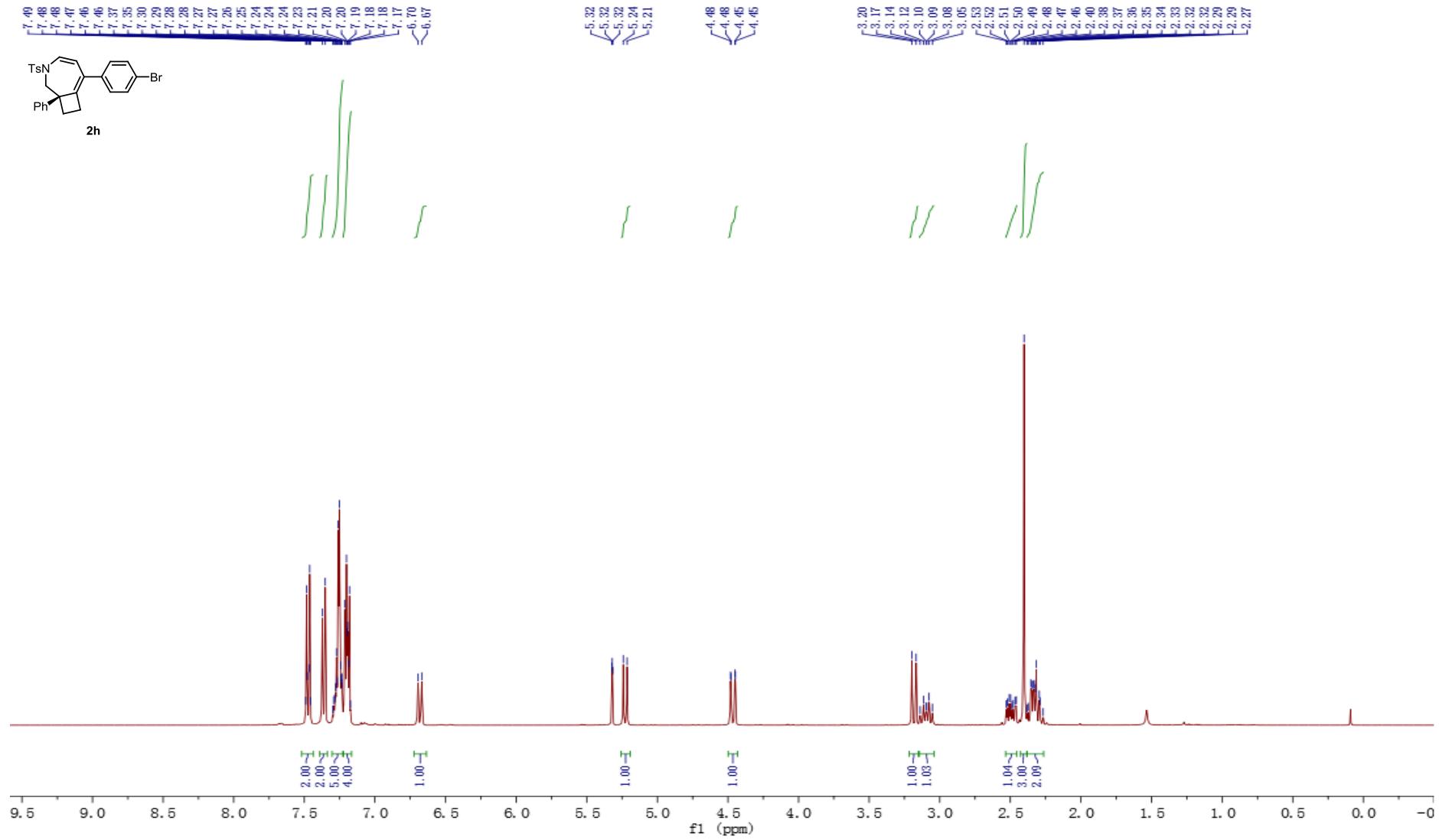


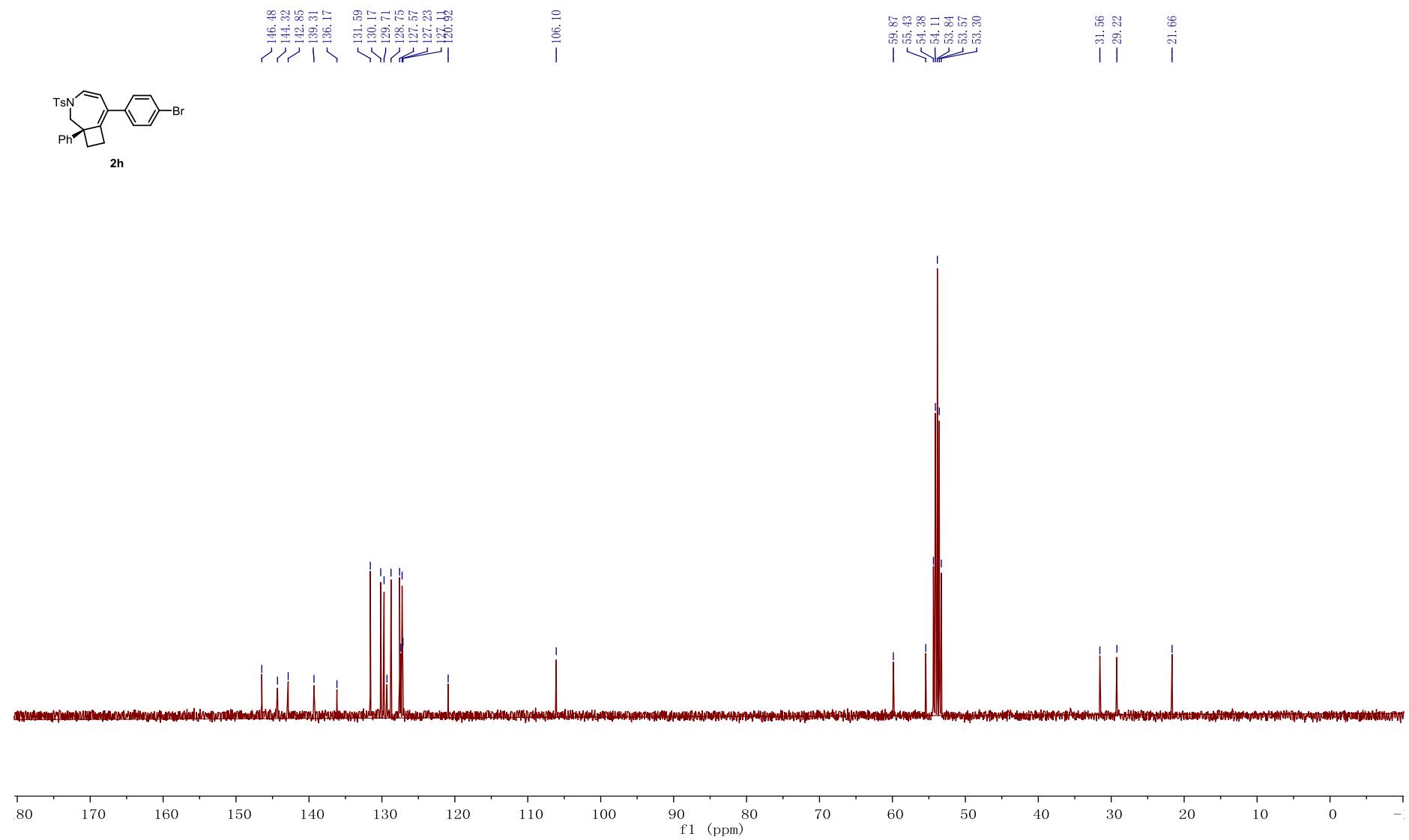


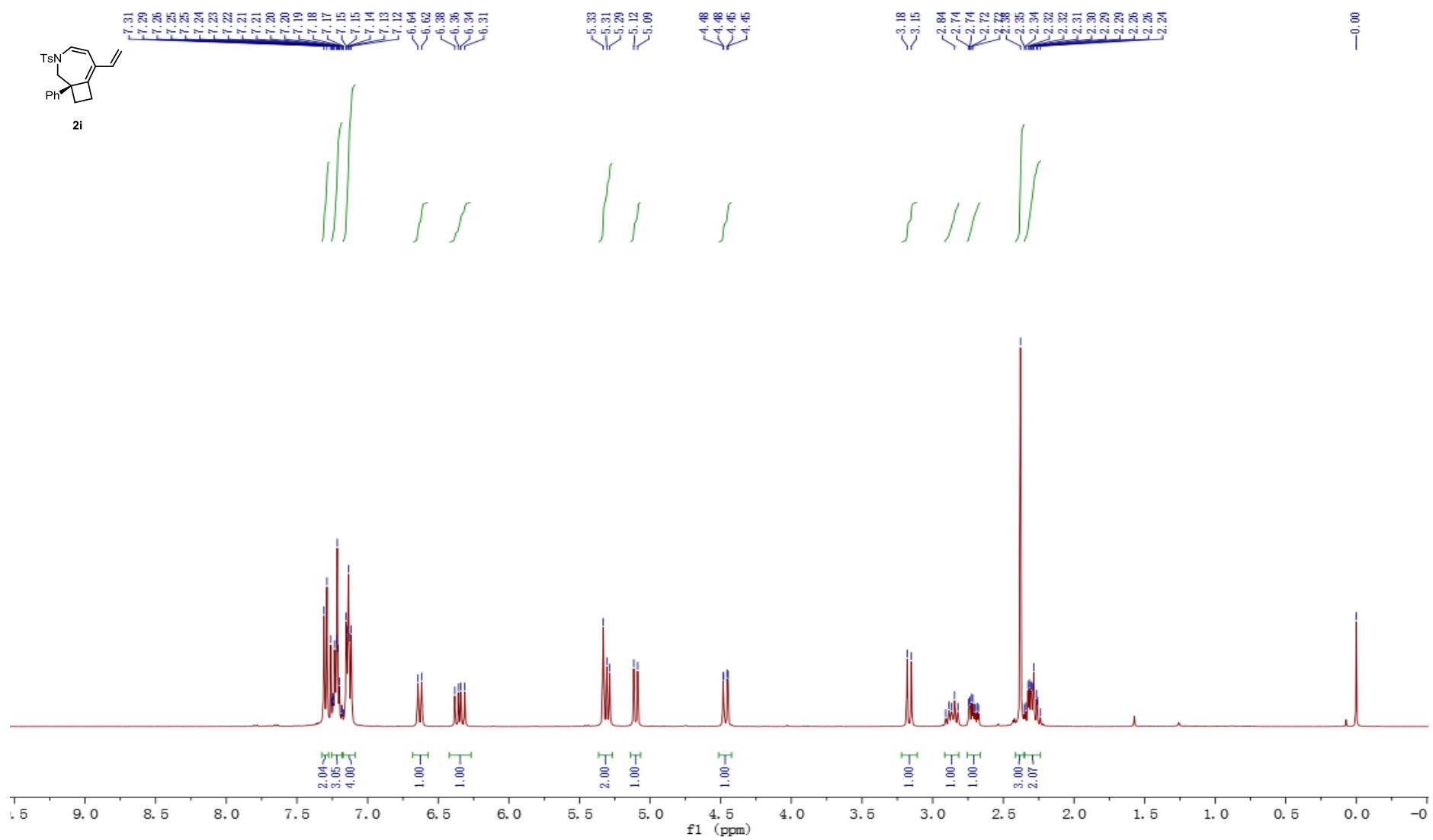


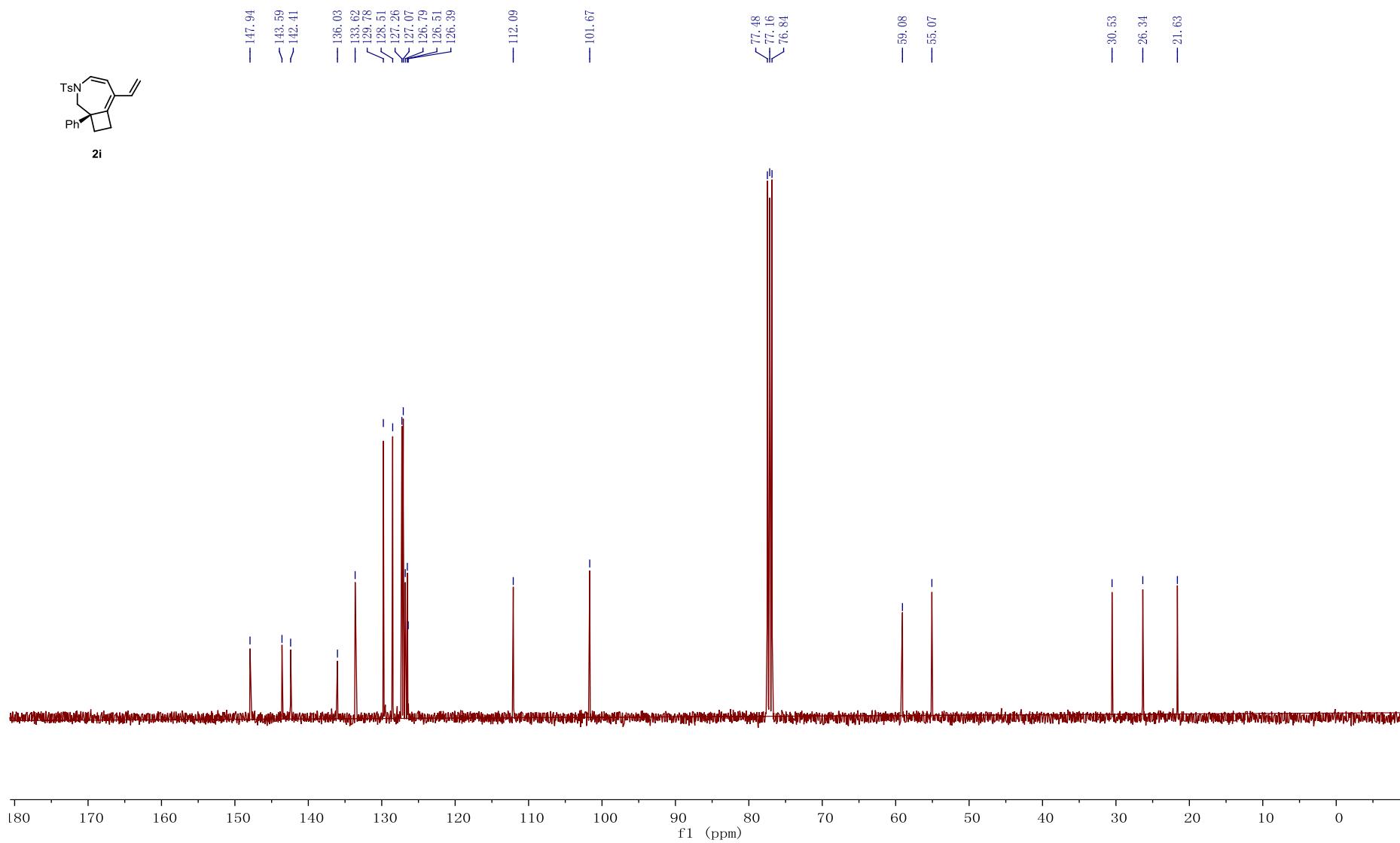


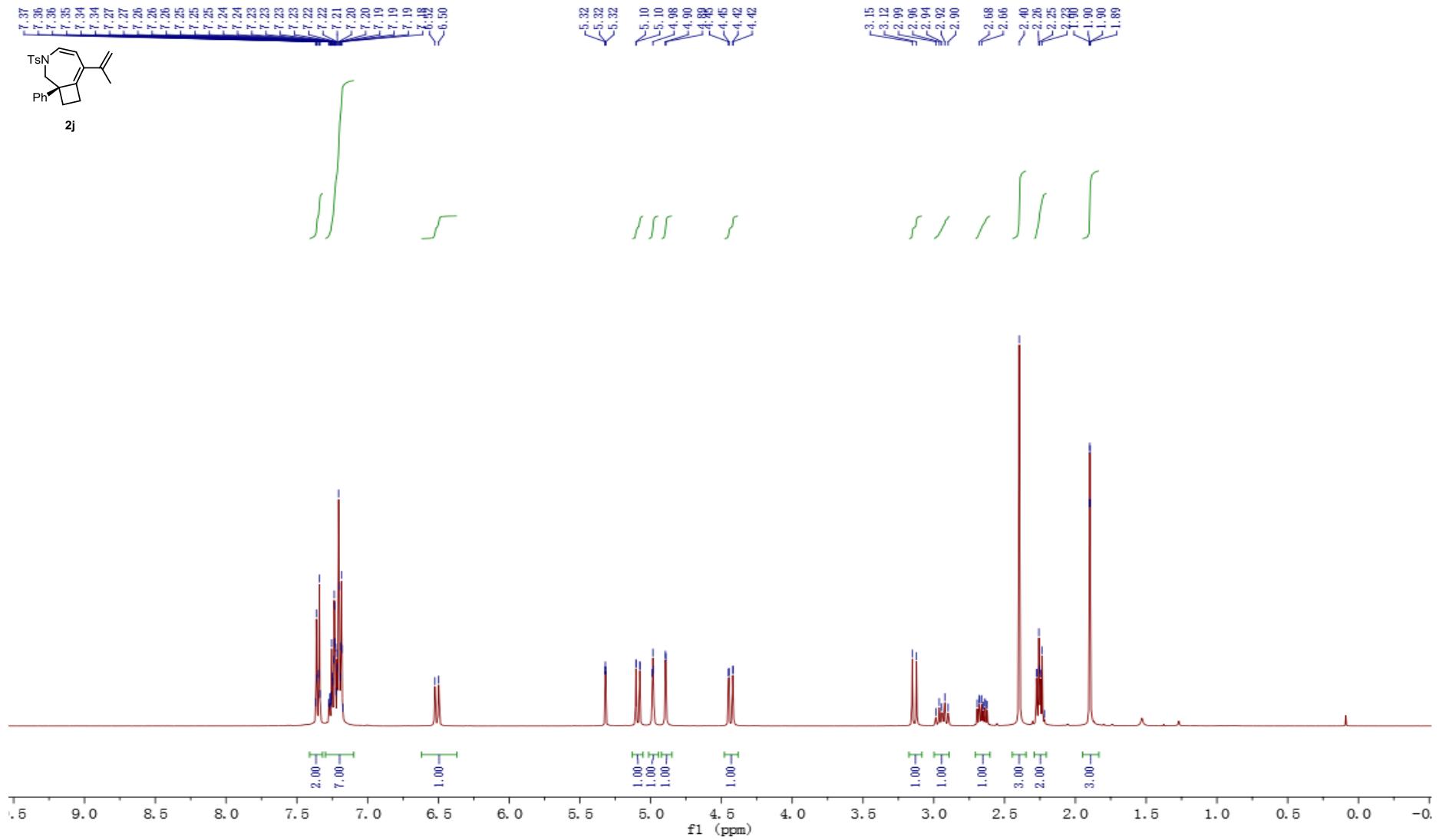


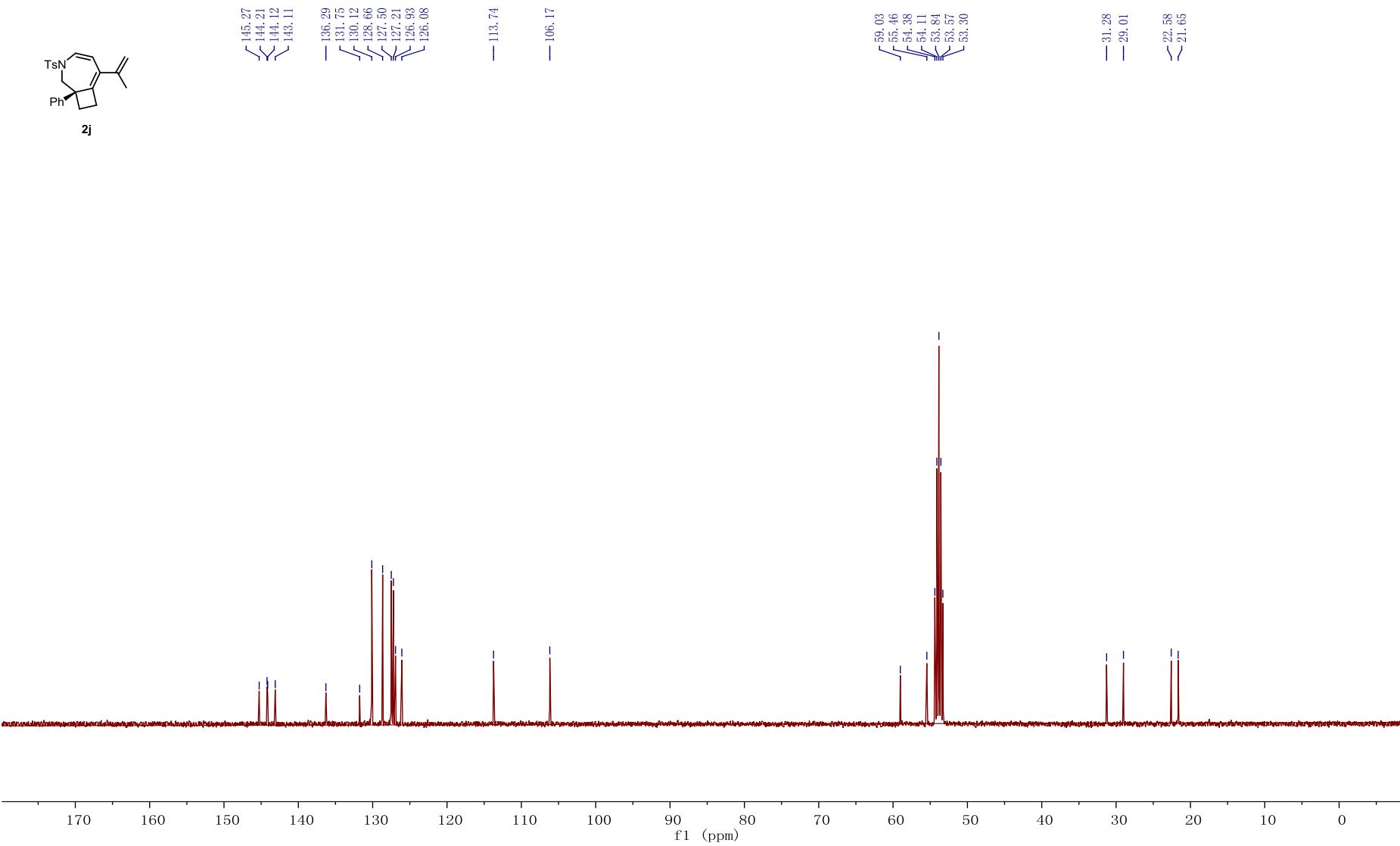


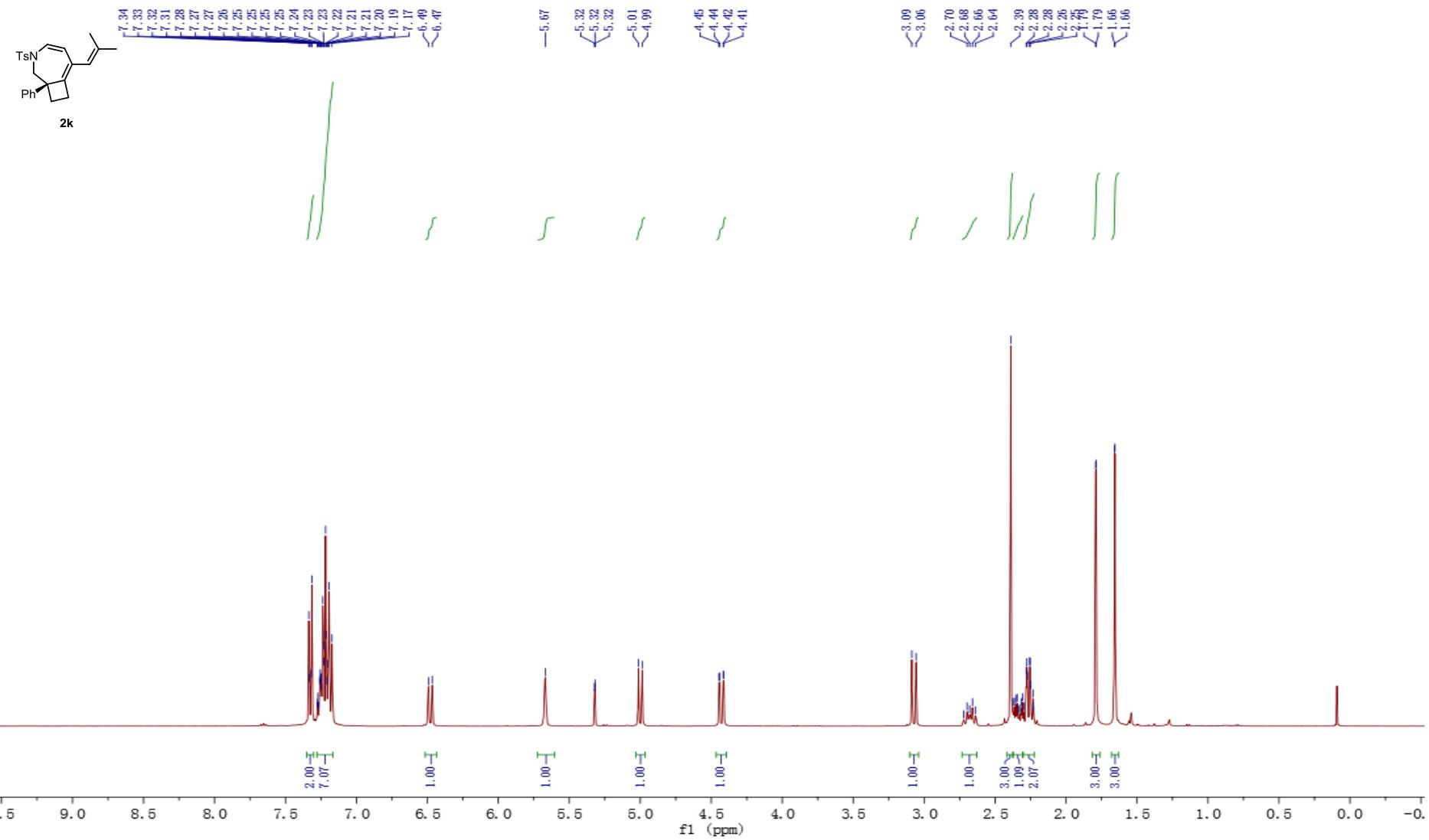


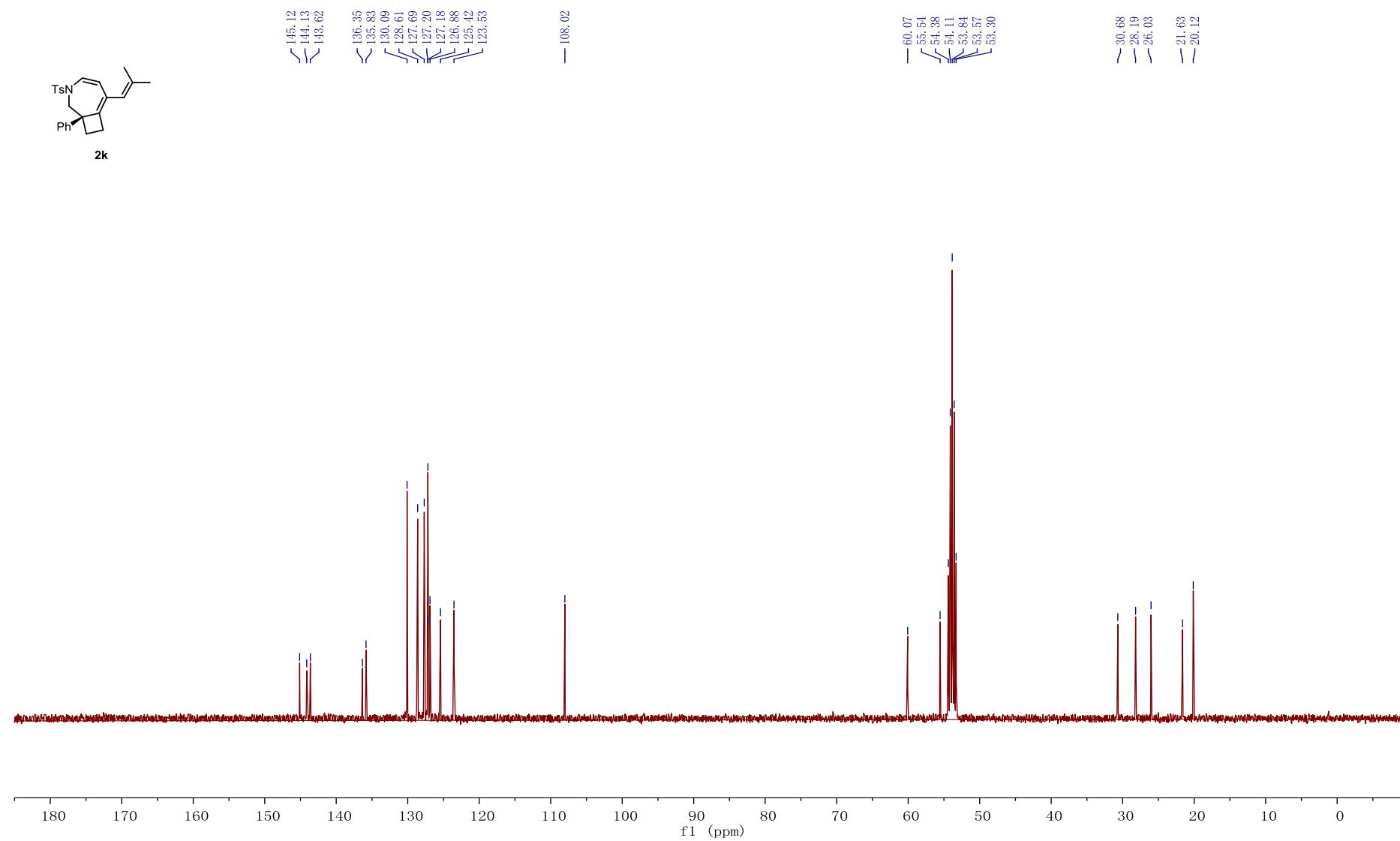


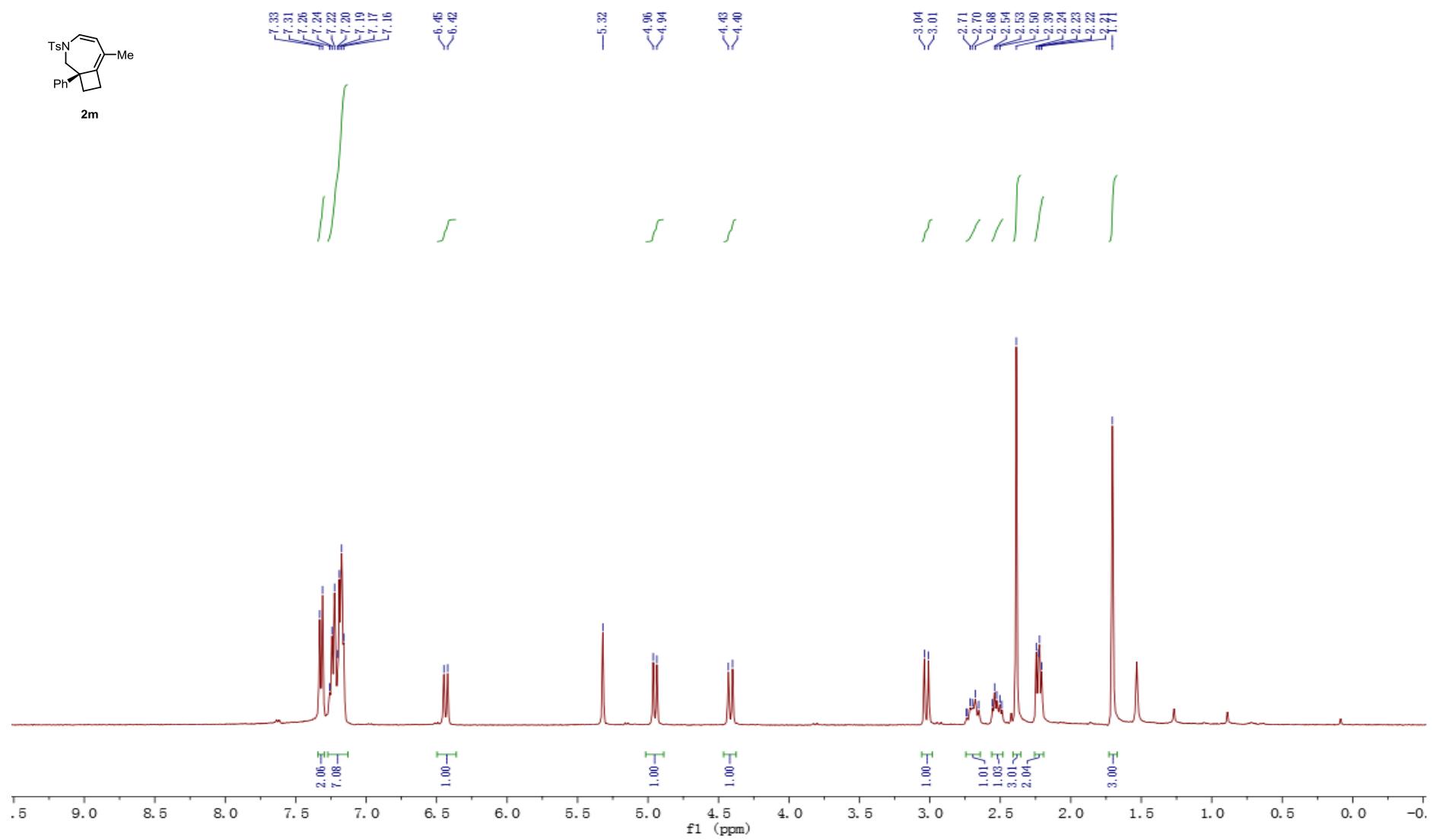


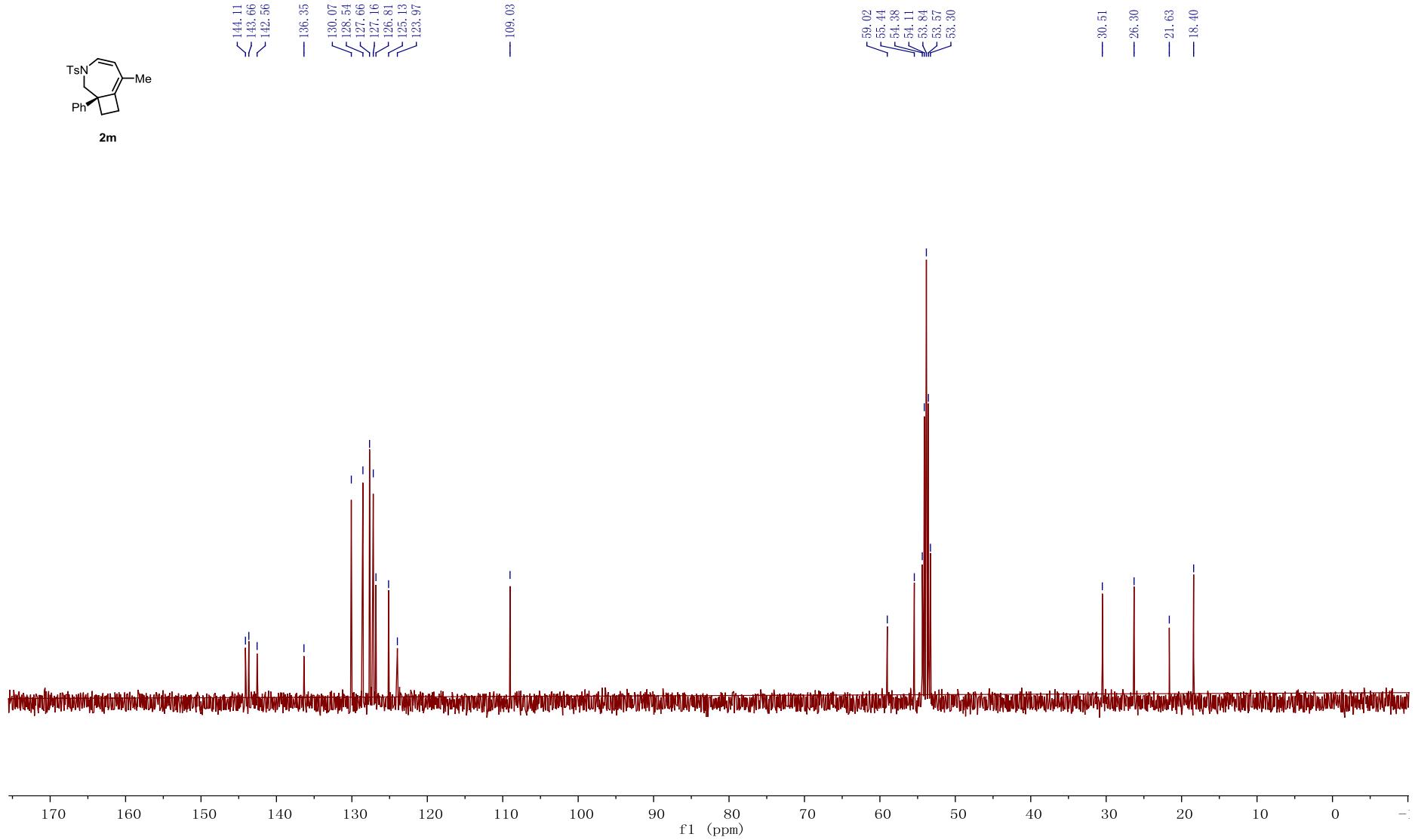


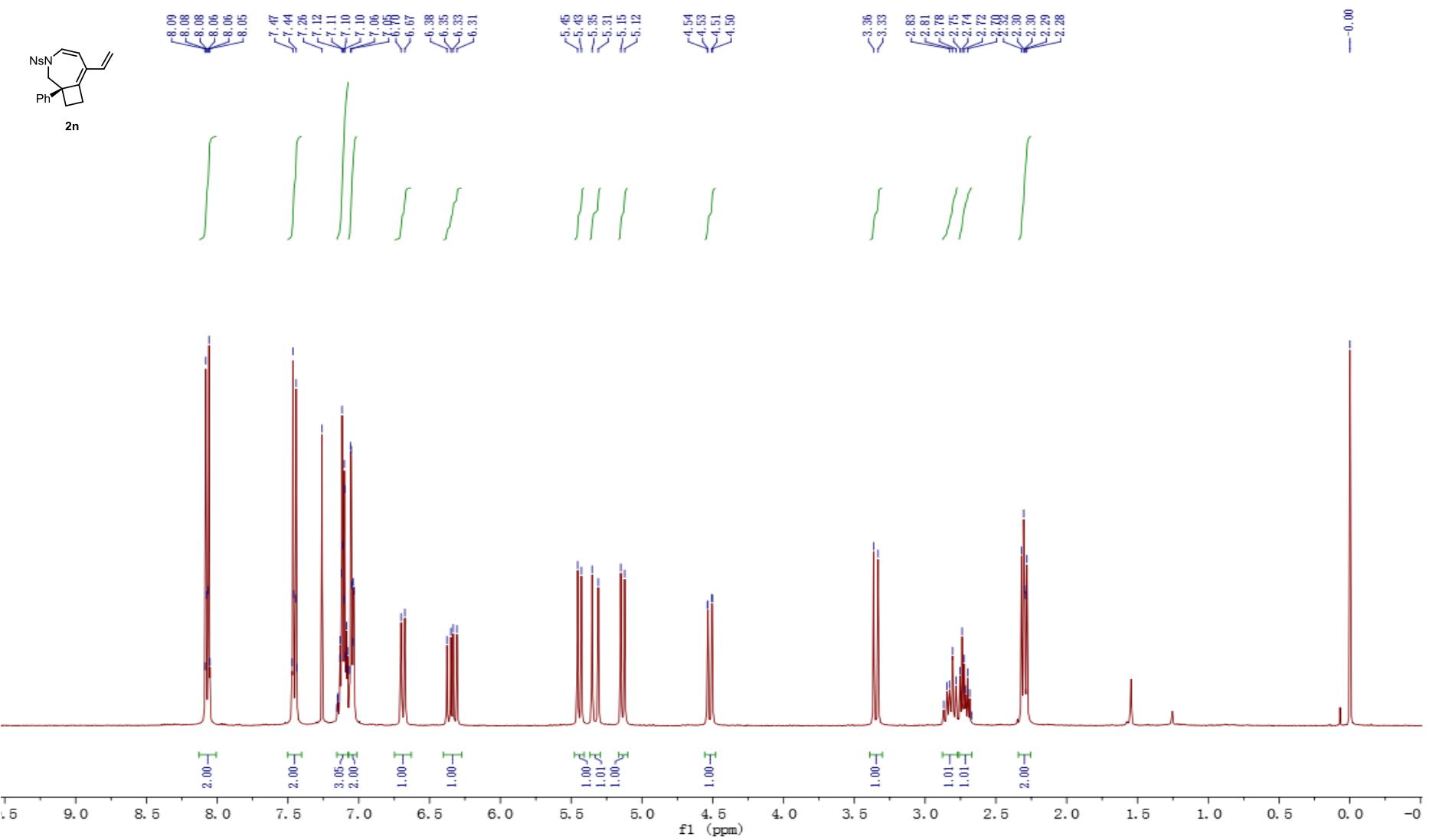


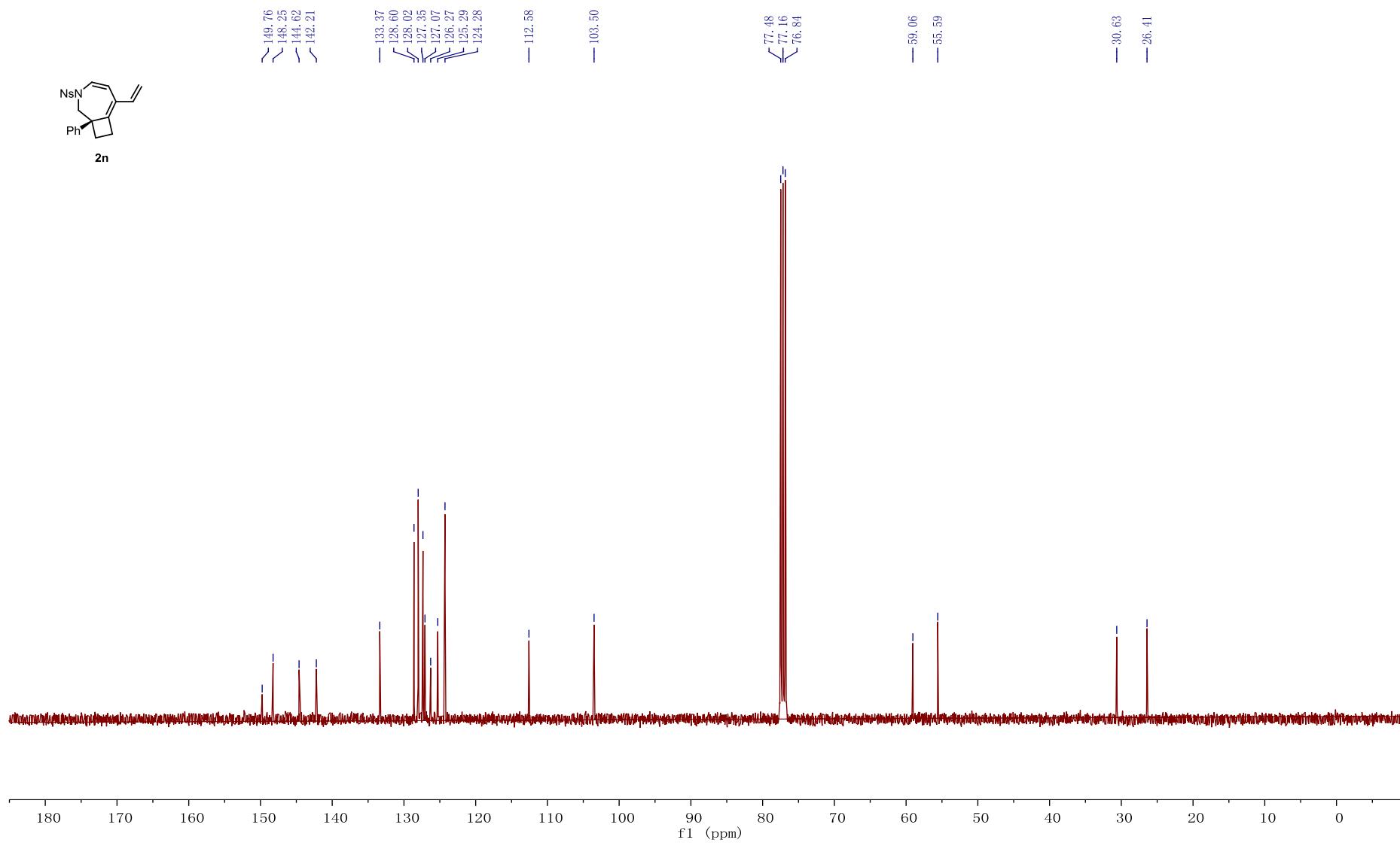


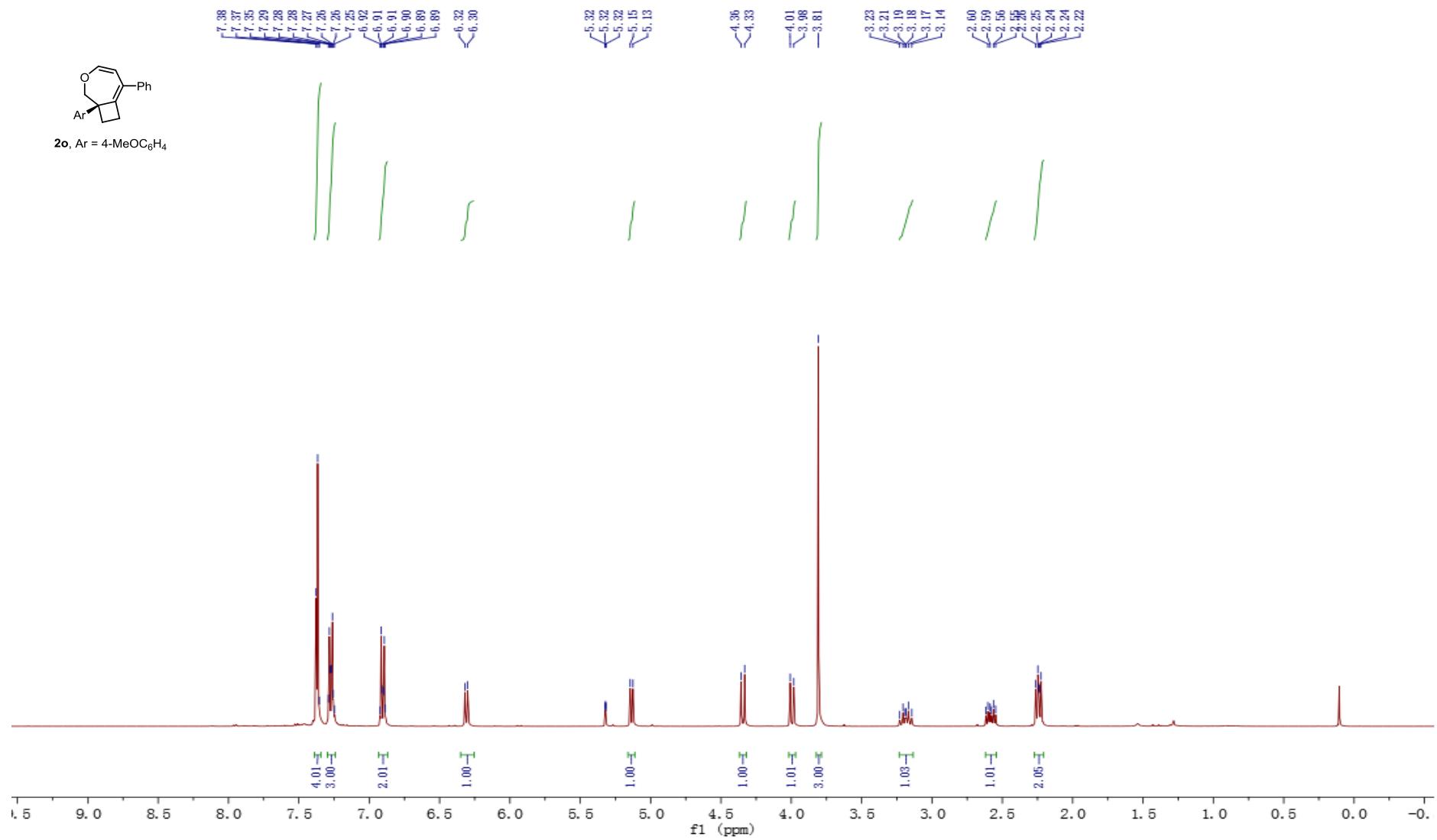


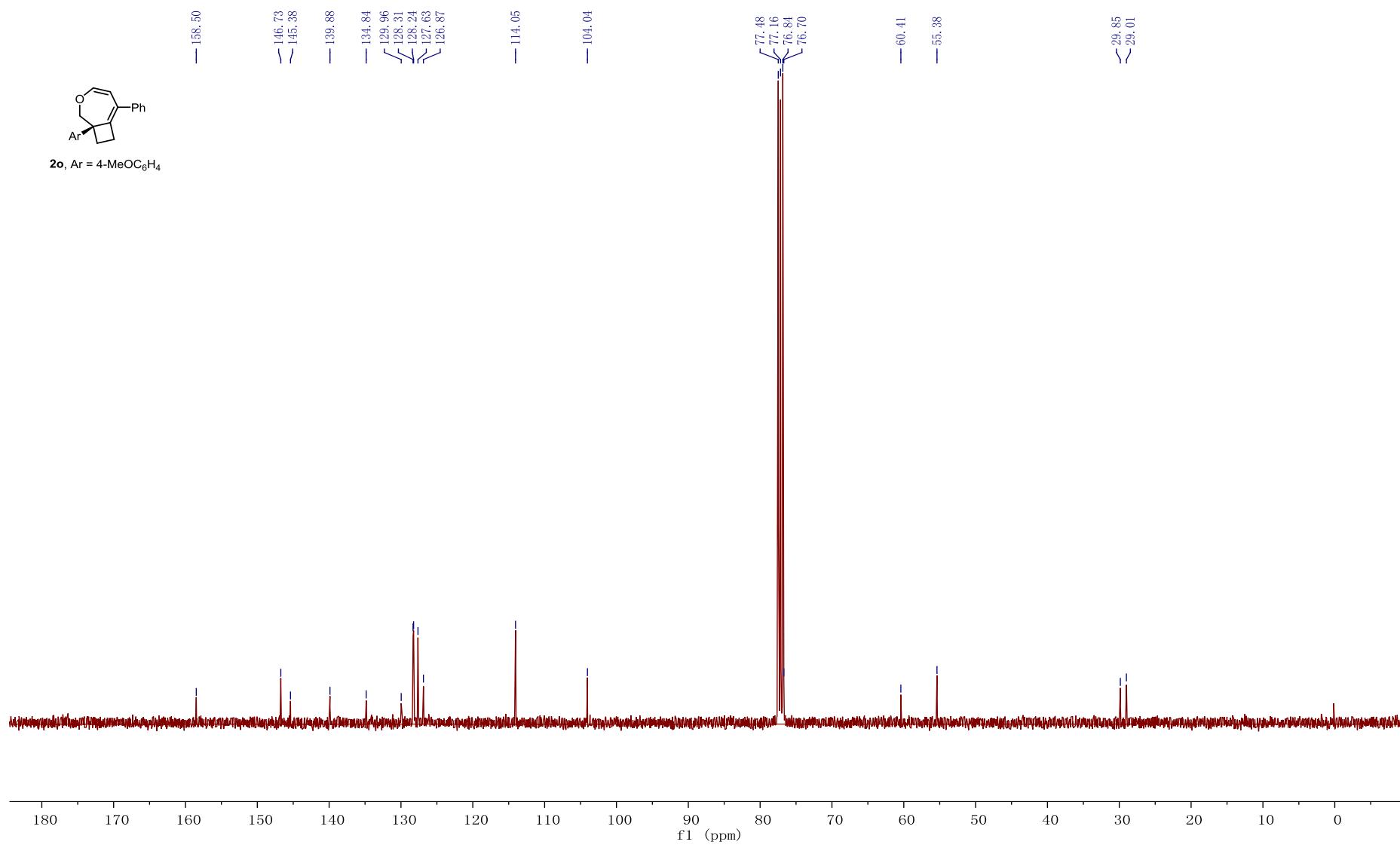


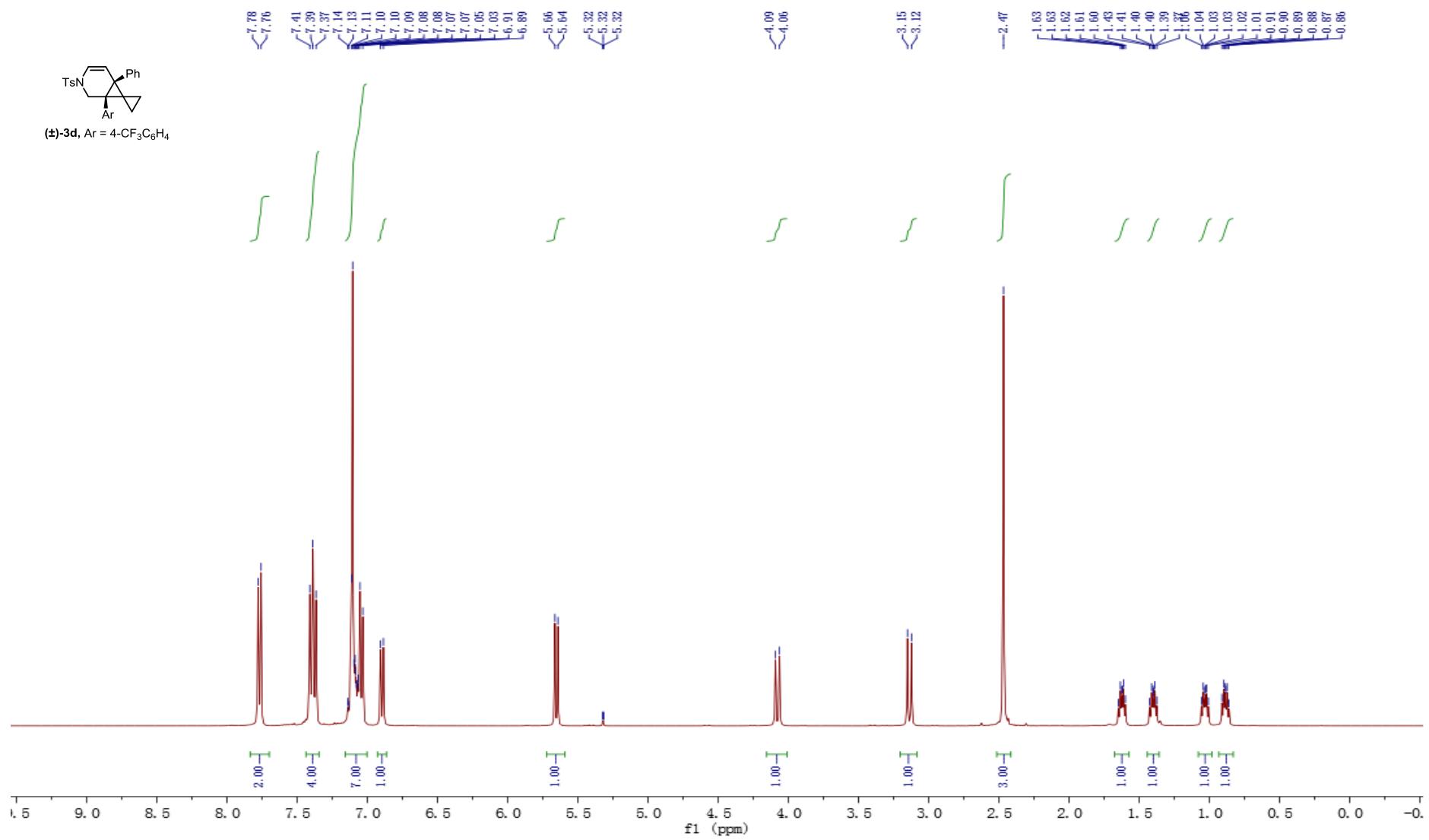


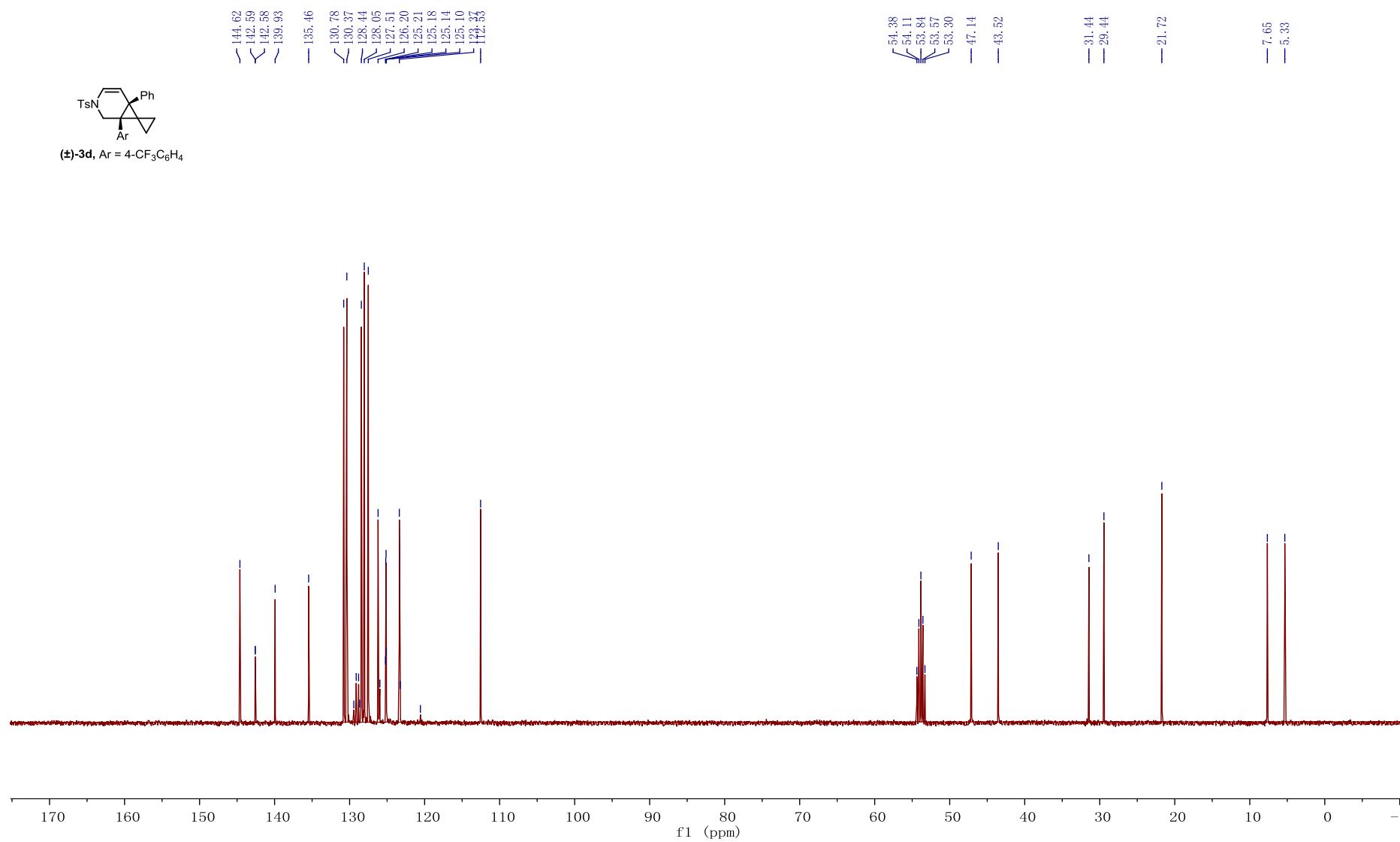


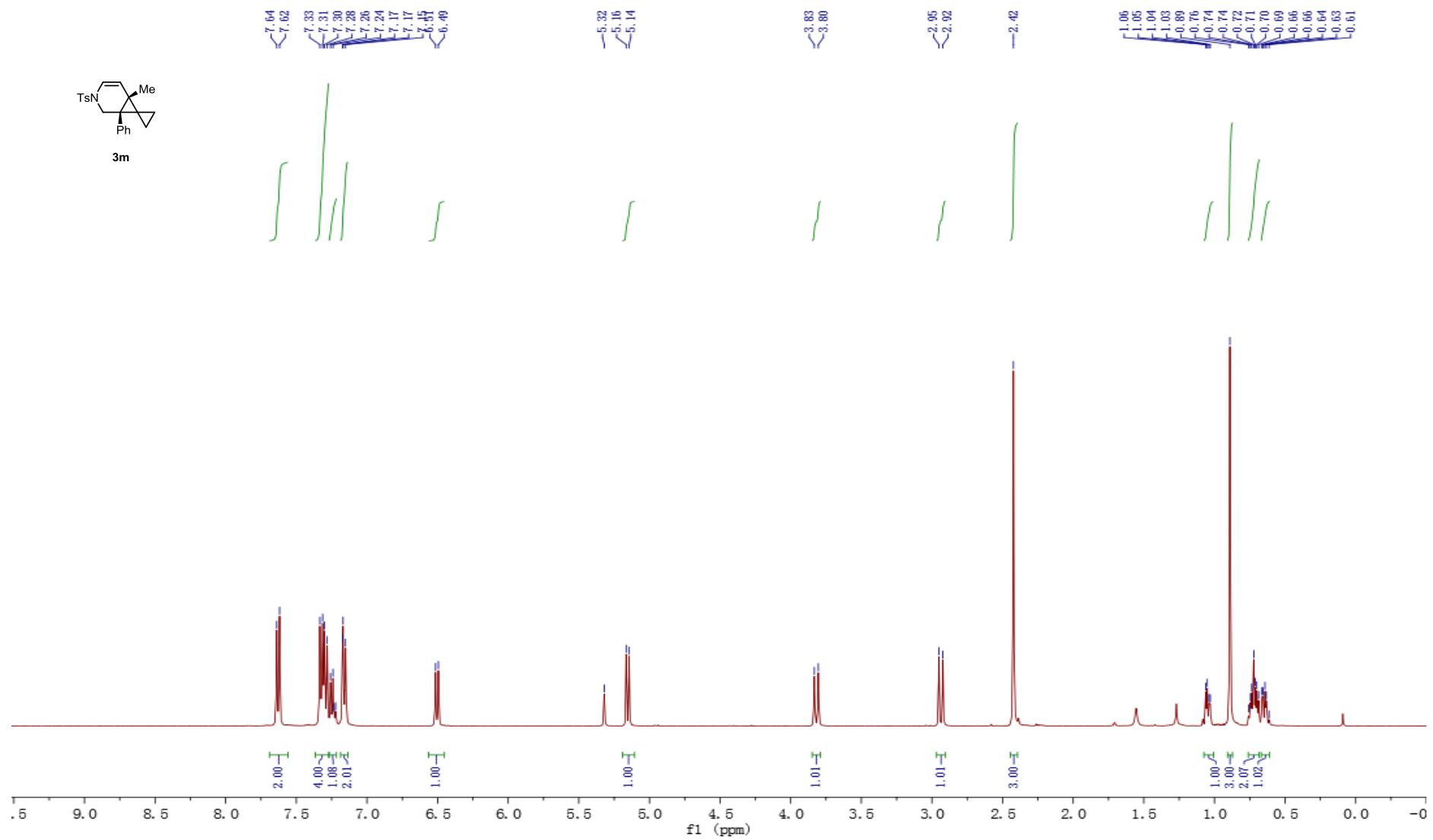


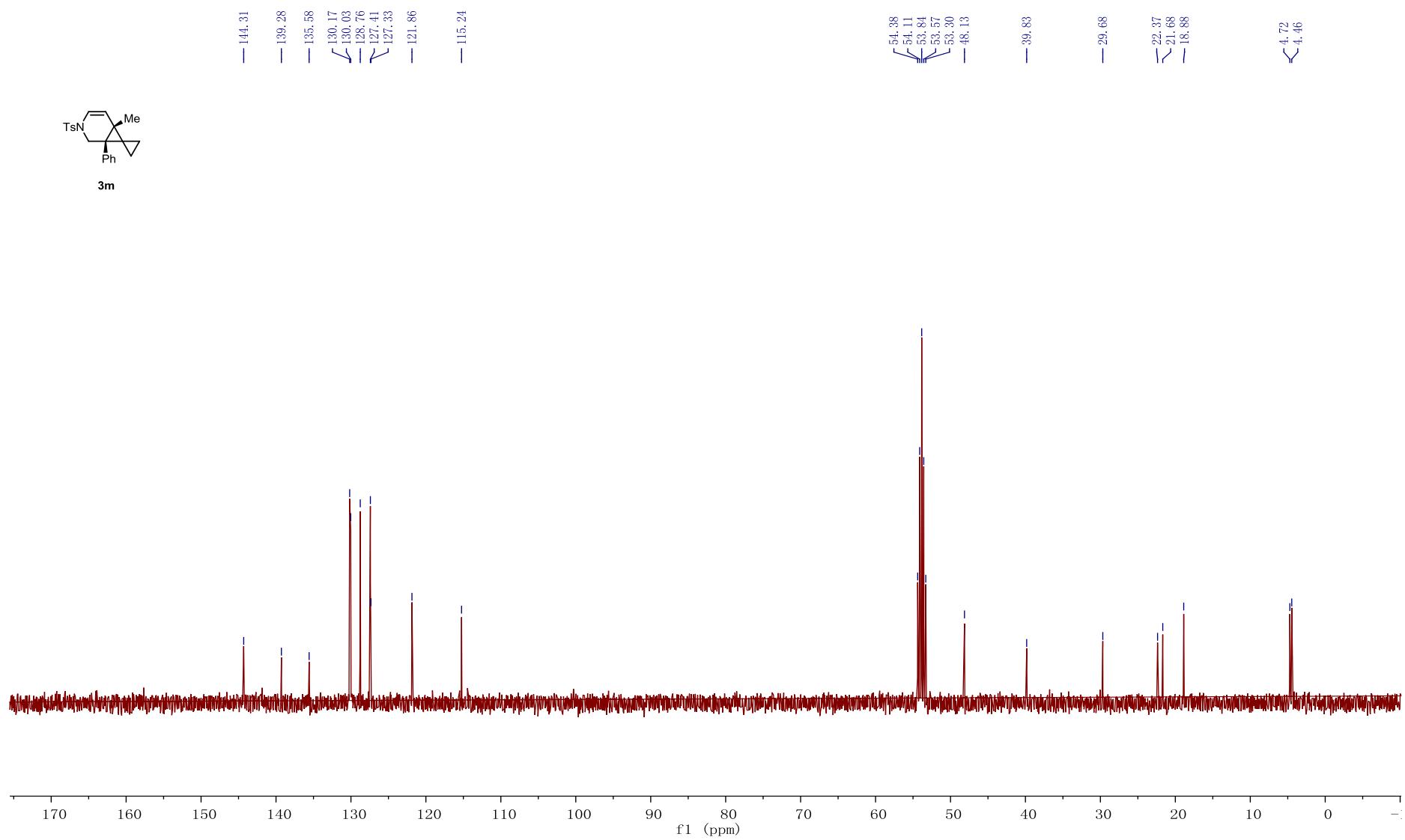




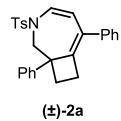




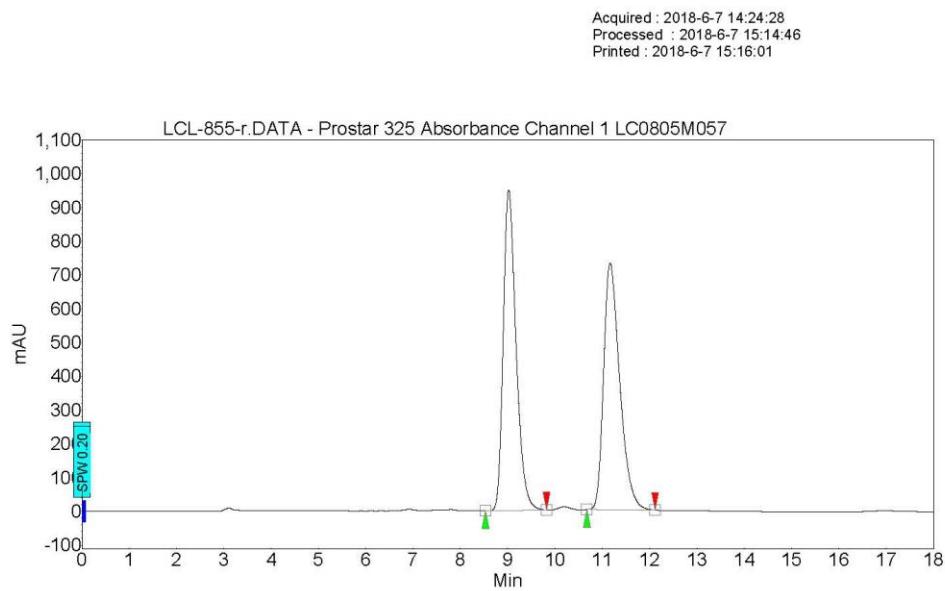




## VII. High Performance Liquid Chromatography (HPLC) Data

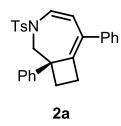


Chromatogram : LCL-855-r\_channel1

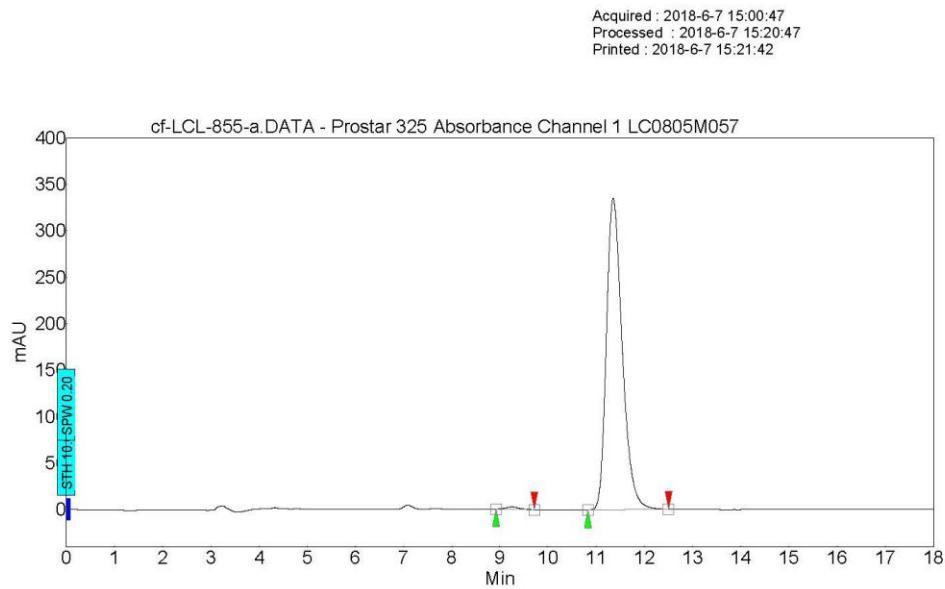


Peak results :

Index	Name	Time [Min]	Amount [% Areal]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	9.02	50.71	948.7	296.8	50.706
2	-	11.17	49.29	730.4	288.6	49.294
Total			100.00	1679.1	585.4	100.000

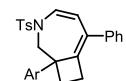


### Chromatogram : cf-LCL-855-a\_channel1



### Peak results :

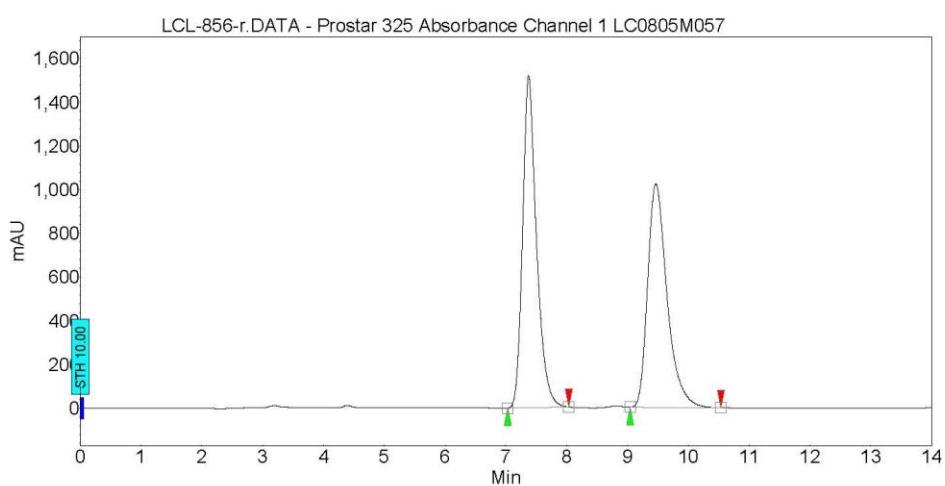
Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
2	-	9.26	0.68	2.7	0.9	0.683
1	-	11.35	99.32	335.0	127.6	99.317
Total			100.00	337.7	128.5	100.000



(±)-2b, Ar = 4-MeC<sub>6</sub>H<sub>4</sub>

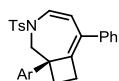
### Chromatogram : LCL-856-r\_channel1

Acquired : 2018-6-14 15:54:04  
Processed : 2018-6-14 17:36:13  
Printed : 2018-6-14 17:39:31



### Peak results :

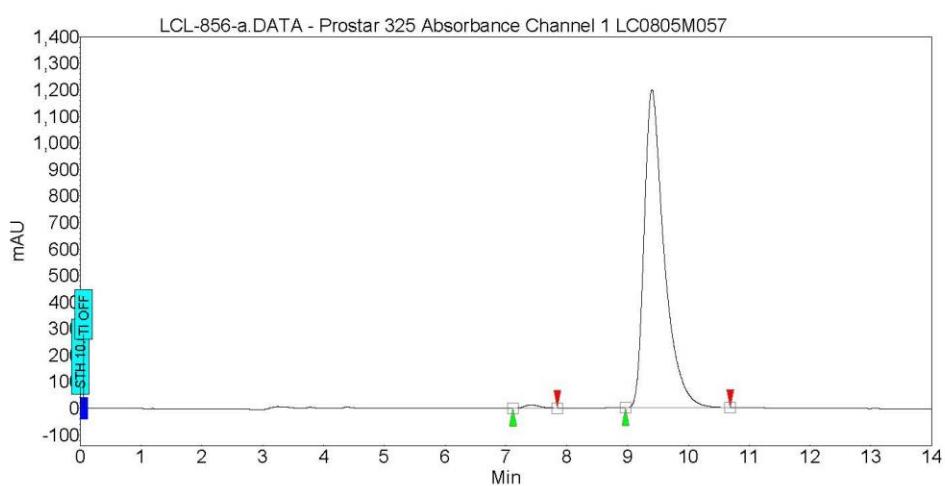
Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	7.37	51.50	1520.7	401.2	51.497
2	-	9.47	48.50	1023.1	377.8	48.503
Total			100.00	2543.8	779.0	100.000



**2b**, Ar = 4-MeC<sub>6</sub>H<sub>4</sub>

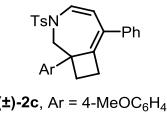
### Chromatogram : LCL-856-a\_channel1

Acquired : 2018-6-14 16:12:05  
Processed : 2018-6-14 17:40:56  
Printed : 2018-6-14 17:45:08

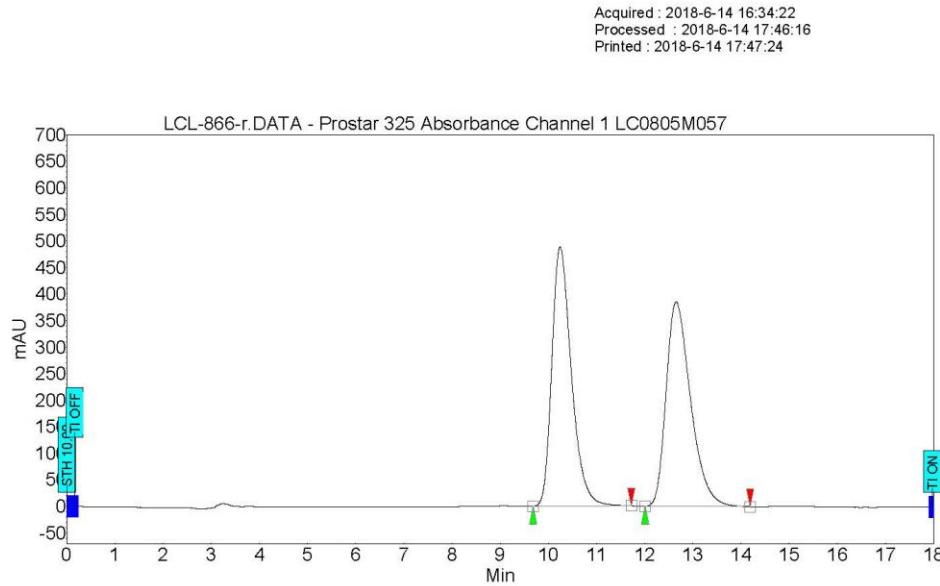


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	7.42	0.78	12.5	3.6	0.784
2	-	9.40	99.22	1198.4	456.4	99.216
Total			100.00	1210.9	460.0	100.000

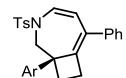


### Chromatogram : LCL-866-r\_channel1



### Peak results :

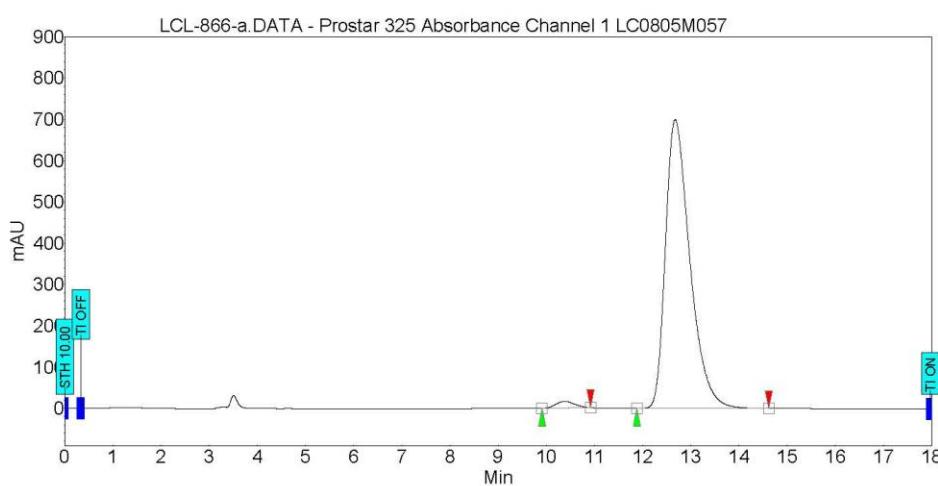
Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	10.25	50.26	488.8	229.5	50.255
2	-	12.65	49.74	385.3	227.2	49.745
Total			100.00	874.1	456.7	100.000



**2c**, Ar = 4-MeOC<sub>6</sub>H<sub>4</sub>

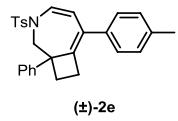
### Chromatogram : LCL-866-a\_channel1

Acquired : 2018-6-14 16:55:49  
Processed : 2018-6-14 17:50:30  
Printed : 2018-6-14 17:52:09

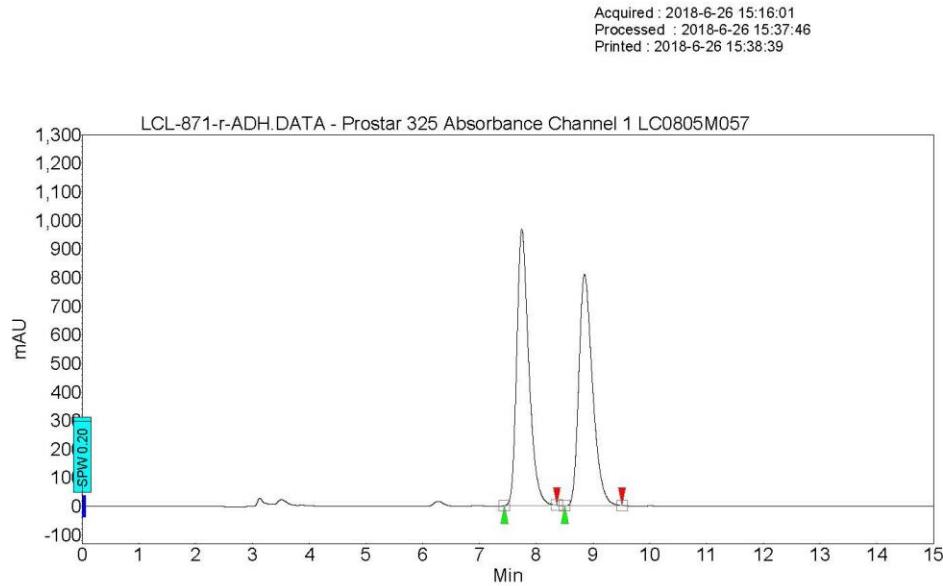


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	10.37	1.72	16.0	7.2	1.724
2	-	12.67	98.28	699.3	411.4	98.276
Total			100.00	715.3	418.6	100.000

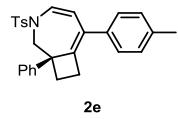


### Chromatogram : LCL-871-r-ADH\_channel1

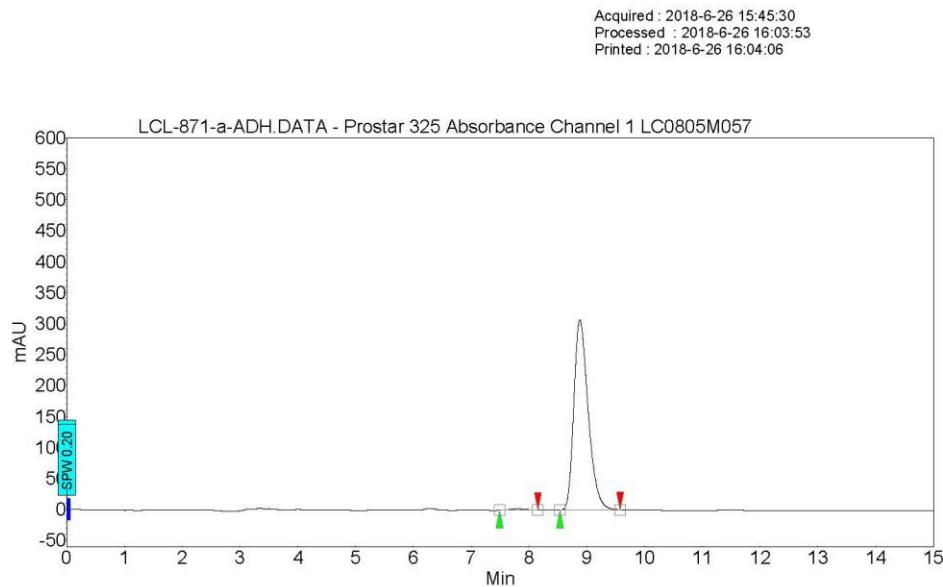


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	7.75	51.06	967.5	236.4	51.063
2	-	8.85	48.94	809.7	226.6	48.937
Total			100.00	1777.1	463.0	100.000

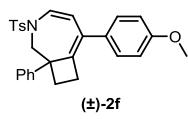


### Chromatogram : LCL-871-a-ADH\_channel1



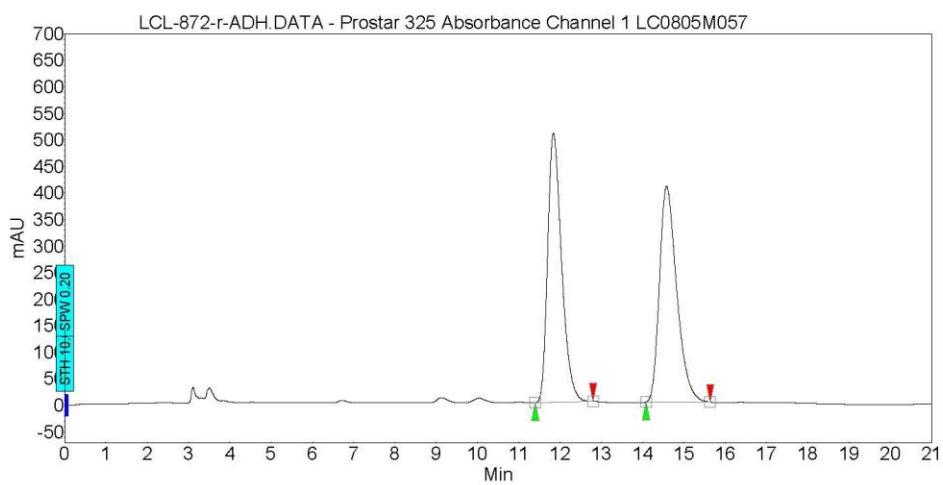
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	7.79	0.75	2.2	0.7	0.753
2	-	8.88	99.25	307.2	88.4	99.247
Total			100.00	309.3	89.0	100.000



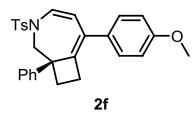
### Chromatogram : LCL-872-r-ADH\_channel1

Acquired : 2018-6-26 14:07:30  
 Processed : 2018-6-26 14:58:45  
 Printed : 2018-6-26 15:00:00

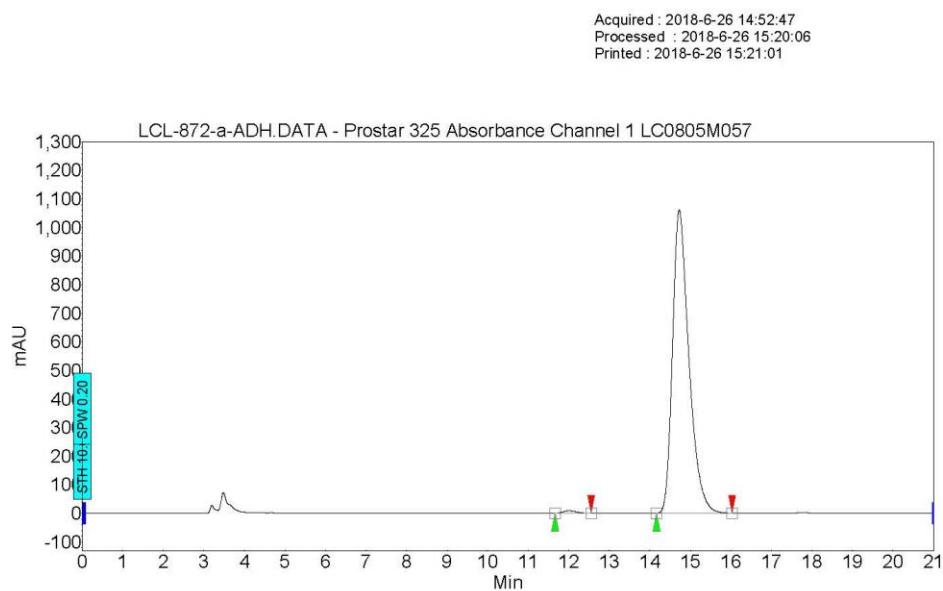


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	11.84	50.12	506.7	197.8	50.120
2	-	14.58	49.88	406.3	196.8	49.880
Total			100.00	913.0	394.6	100.000

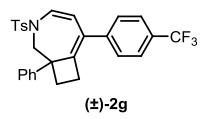


### Chromatogram : LCL-872-a-ADH\_channel1



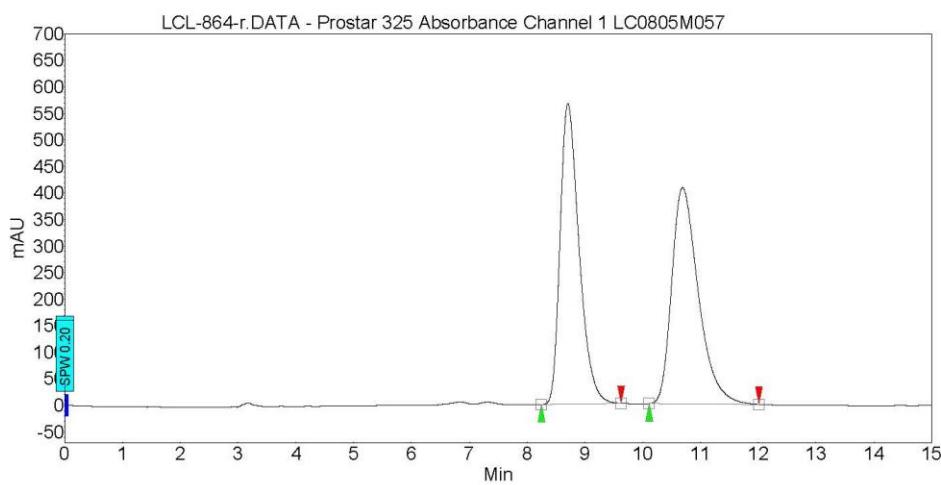
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	12.01	0.67	9.0	3.4	0.673
2	-	14.73	99.33	1061.0	496.7	99.327
Total			100.00	1070.0	500.1	100.000



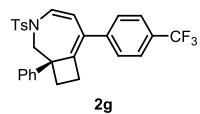
### Chromatogram : LCL-864-r\_channel1

Acquired : 2018-6-14 15:15:23  
 Processed : 2018-6-14 16:18:20  
 Printed : 2018-6-14 16:22:06

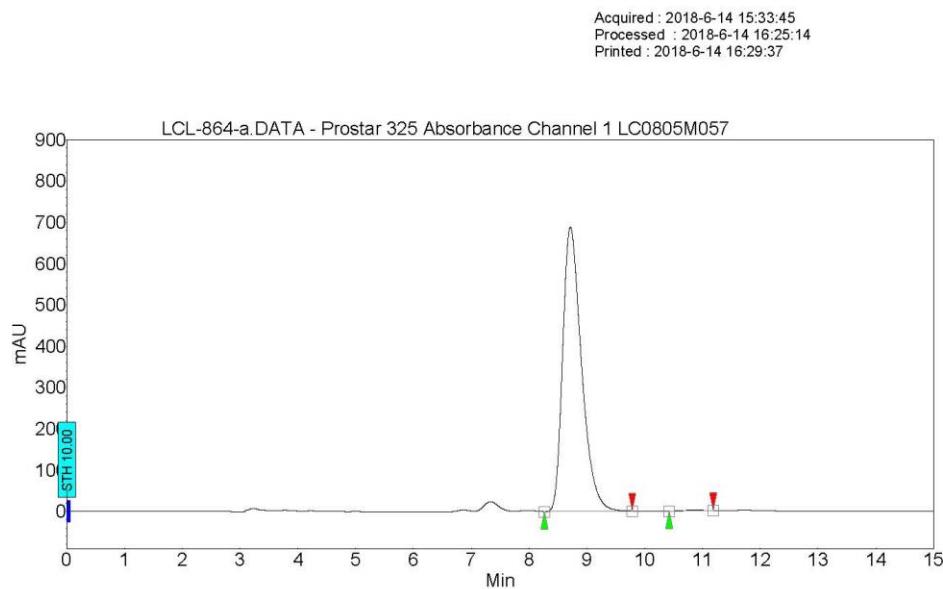


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	8.71	49.71	566.0	215.1	49.706
2	-	10.69	50.29	407.4	217.6	50.294
Total			100.00	973.5	432.8	100.000

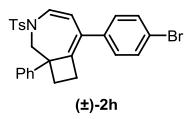


### Chromatogram : LCL-864-a\_channel1



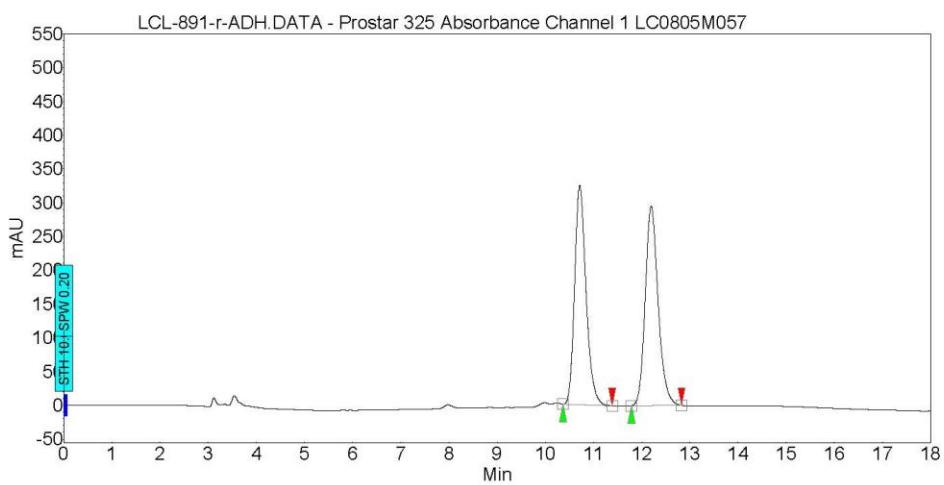
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	8.71	99.70	689.2	259.7	99.696
2	-	10.83	0.30	2.0	0.8	0.304
Total			100.00	691.2	260.5	100.000



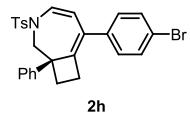
### Chromatogram : LCL-891-r-ADH\_channel1

Acquired : 2018-7-20 13:59:36  
 Processed : 2018-7-20 14:24:06  
 Printed : 2018-7-20 14:25:12

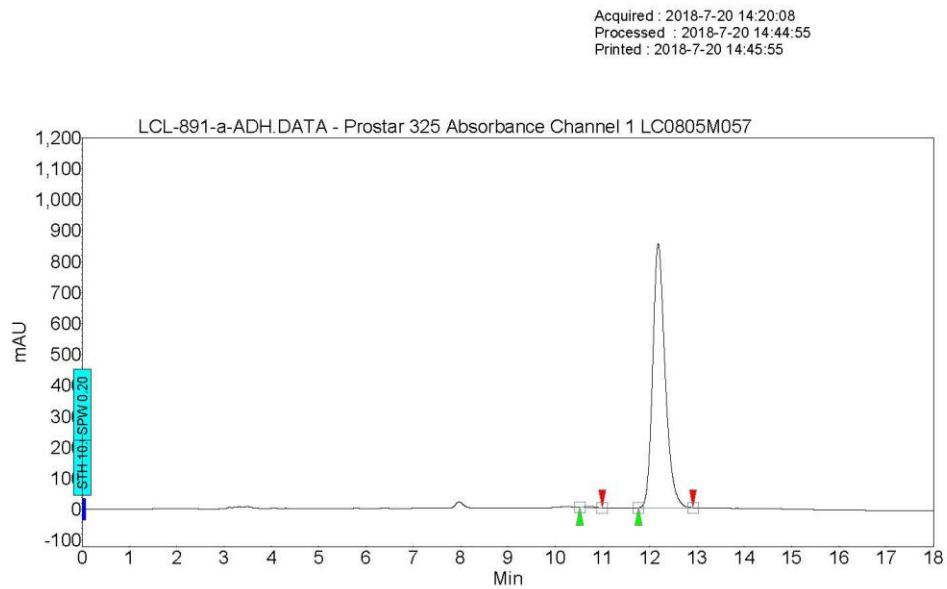


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	10.71	49.27	324.5	89.1	49.269
2	-	12.20	50.73	294.9	91.7	50.731
Total			100.00	619.4	180.7	100.000

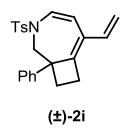


### Chromatogram : LCL-891-a-ADH\_channel1



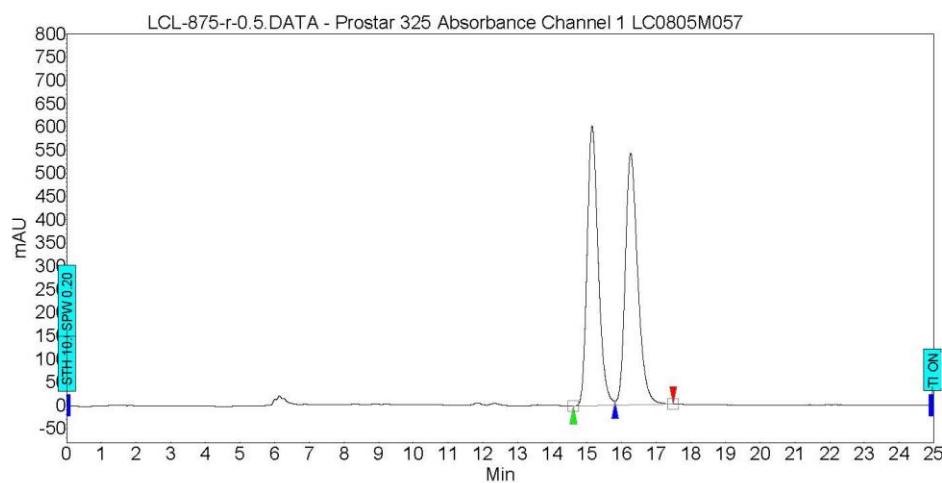
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
2	-	10.72	0.41	4.6	1.1	0.405
1	-	12.18	99.59	852.9	259.4	99.595
Total			100.00	857.5	260.5	100.000



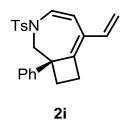
### Chromatogram : LCL-875-r-0.5\_channel1

Acquired : 2018-6-26 12:36:22  
 Processed : 2018-6-26 14:11:11  
 Printed : 2018-6-26 14:11:40

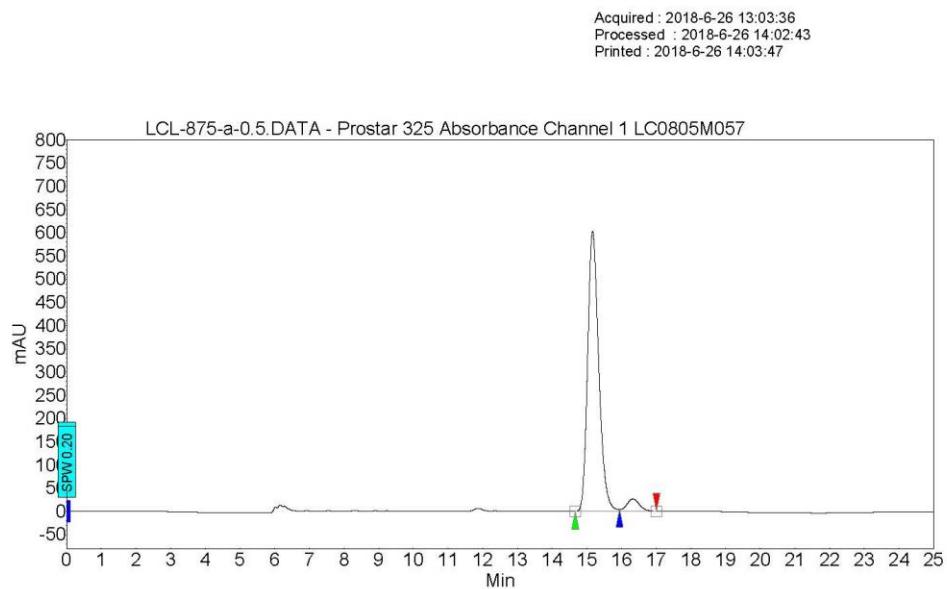


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	15.15	49.69	602.3	222.6	49.685
2	-	16.27	50.31	541.5	225.5	50.315
Total			100.00	1143.8	448.1	100.000

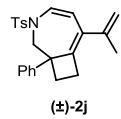


### Chromatogram : LCL-875-a-0.5\_channel1



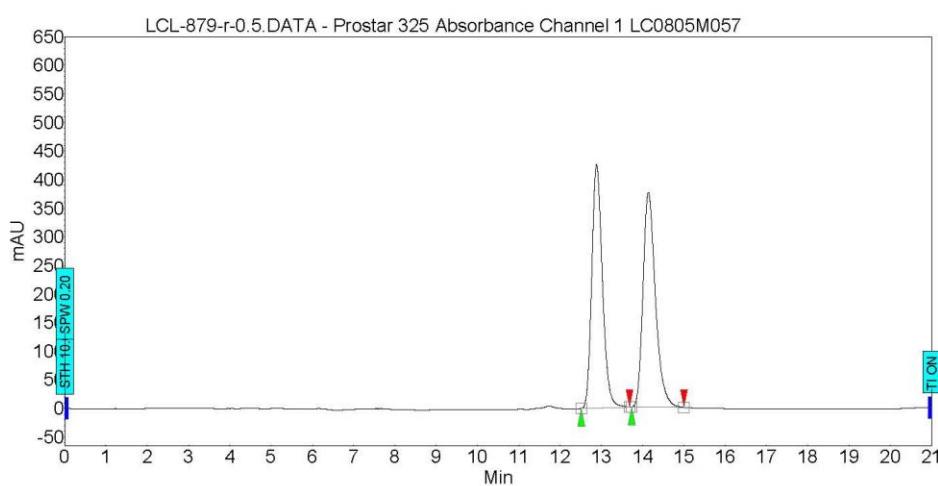
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	15.17	95.12	602.9	223.0	95.117
2	-	16.32	4.88	26.8	11.4	4.883
Total			100.00	629.7	234.5	100.000



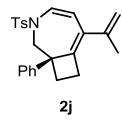
### Chromatogram : LCL-879-r-0.5\_channel1

Acquired : 2018-7-4 15:16:48  
 Processed : 2018-7-4 15:46:08  
 Printed : 2018-7-4 15:48:31

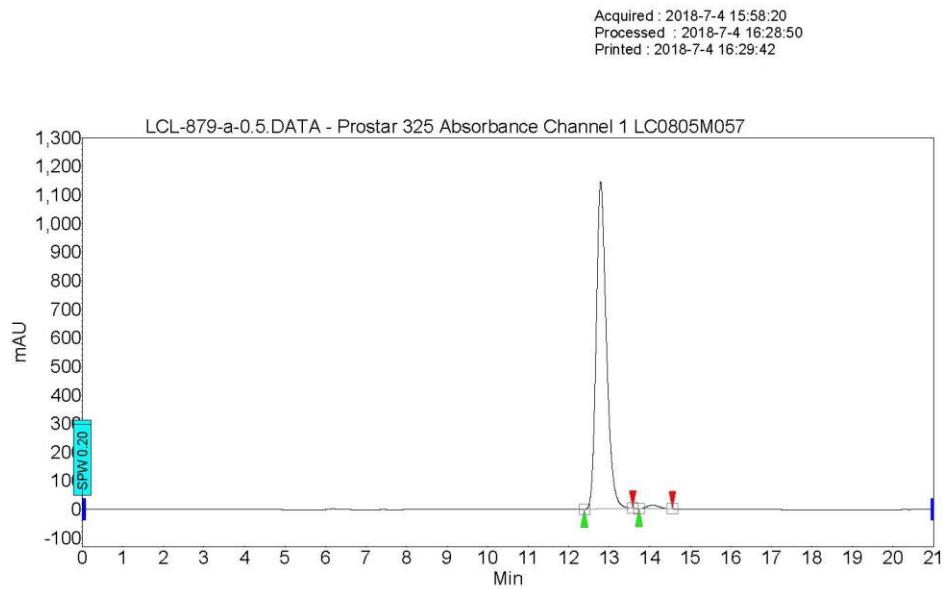


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	12.89	49.15	425.9	126.6	49.147
2	-	14.14	50.85	376.0	131.0	50.853
Total			100.00	801.9	257.7	100.000

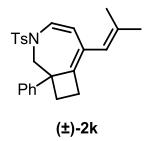


### Chromatogram : LCL-879-a-0.5\_channel1

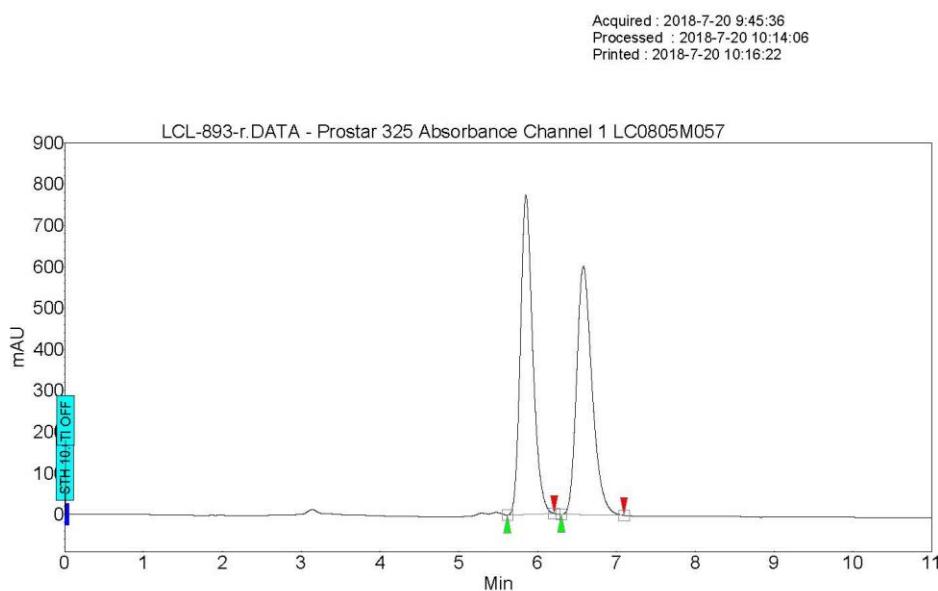


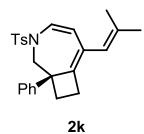
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	12.79	98.72	1145.0	332.7	98.722
2	-	14.07	1.28	12.8	4.3	1.278
Total			100.00	1157.9	337.0	100.000



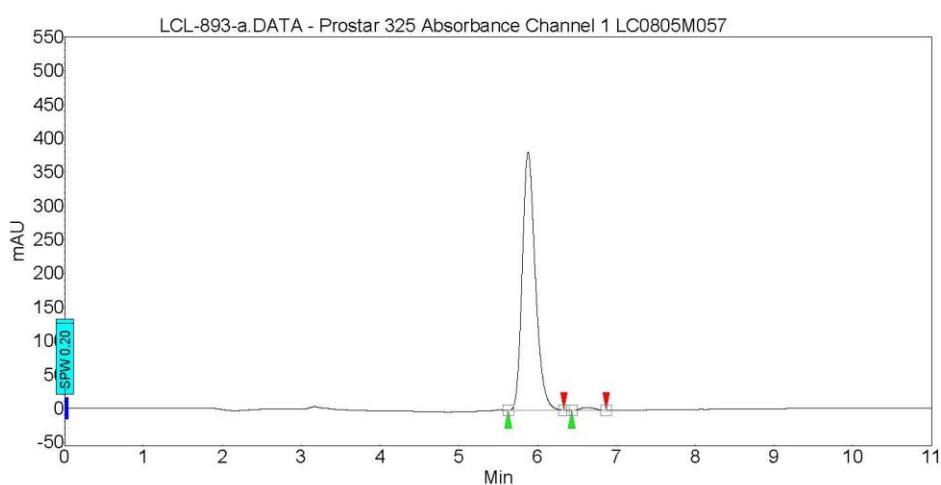
### Chromatogram : LCL-893-r\_channel1





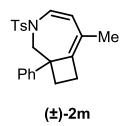
### Chromatogram : LCL-893-a\_channel1

Acquired : 2018-7-20 10:11:40  
 Processed : 2018-7-20 10:29:54  
 Printed : 2018-7-20 10:30:58



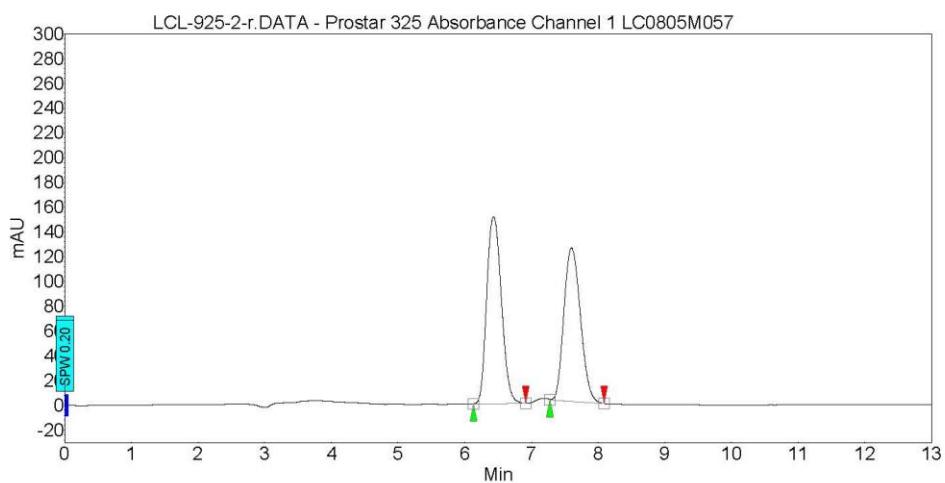
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]		Area [%] [%]
					[mAU.Min]	[%]	
1	-	5.88	98.72	382.2	73.4	98.721	
2	-	6.63	1.28	4.6	1.0	1.279	
Total			100.00	386.7	74.3	100.000	



### Chromatogram : LCL-925-2-r\_channel1

Acquired : 2018-9-6 10:20:40  
 Processed : 2018-9-6 10:40:27  
 Printed : 2018-9-6 10:41:33

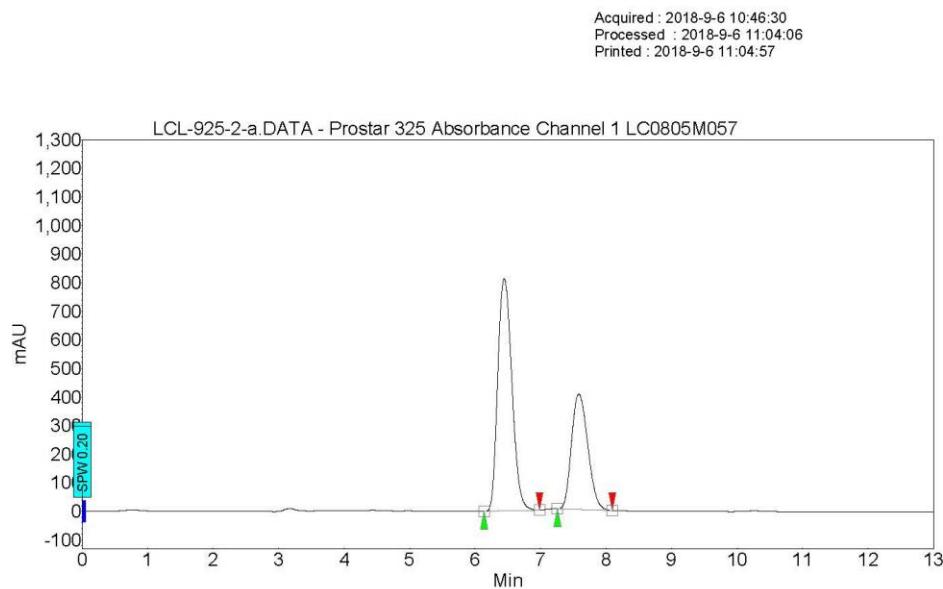


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	6.43	51.92	150.9	38.4	51.917
2	-	7.60	48.08	123.8	35.6	48.083
Total			100.00	274.7	74.0	100.000

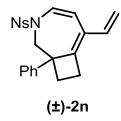


### Chromatogram : LCL-925-2-a\_channel1



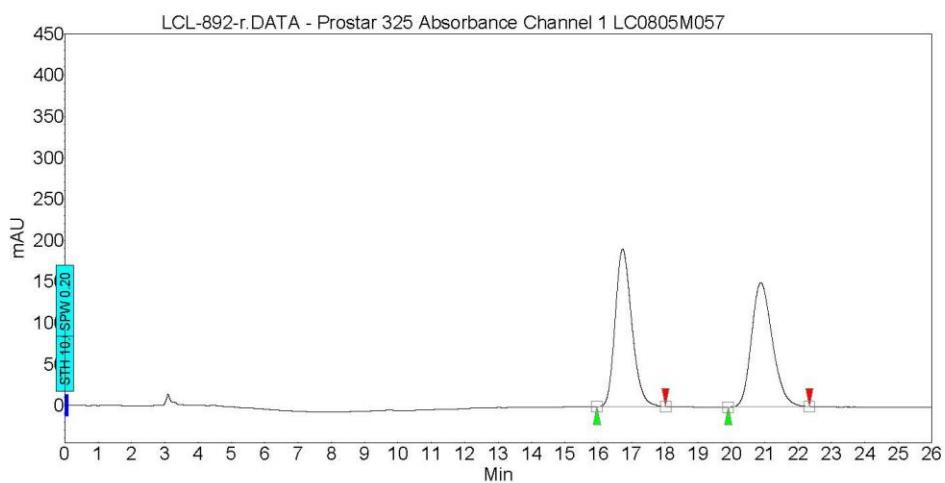
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	6.45	63.54	811.6	203.0	63.538
2	-	7.59	36.46	403.8	116.5	36.462
Total			100.00	1215.4	319.5	100.000



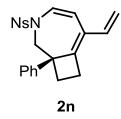
### Chromatogram : LCL-892-r\_channel1

Acquired : 2018-7-20 14:50:29  
 Processed : 2018-7-20 15:21:25  
 Printed : 2018-7-20 15:22:15

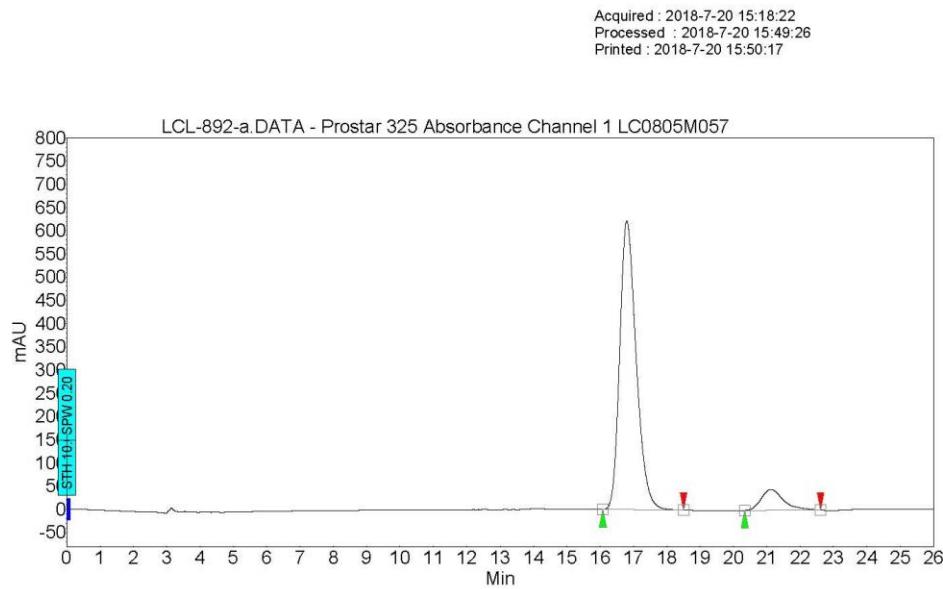


### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	16.73	50.27	190.9	110.5	50.272
2	-	20.87	49.73	150.3	109.3	49.728
Total			100.00	341.1	219.8	100.000

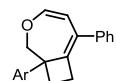


### Chromatogram : LCL-892-a\_channel1



### Peak results :

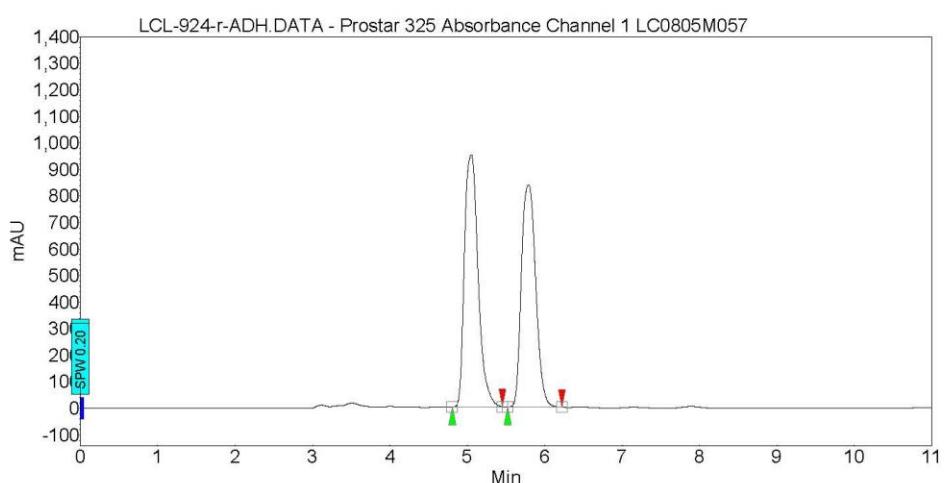
Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	16.80	91.01	621.7	355.0	91.010
2	-	21.11	8.99	44.8	35.1	8.990
Total			100.00	666.5	390.1	100.000



(±)-2o, Ar = 4-MeOC<sub>6</sub>H<sub>4</sub>

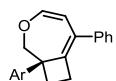
### Chromatogram : LCL-924-r-ADH\_channel1

Acquired : 2018-9-6 12:07:09  
 Processed : 2018-9-6 12:24:39  
 Printed : 2018-9-6 12:31:17



### Peak results :

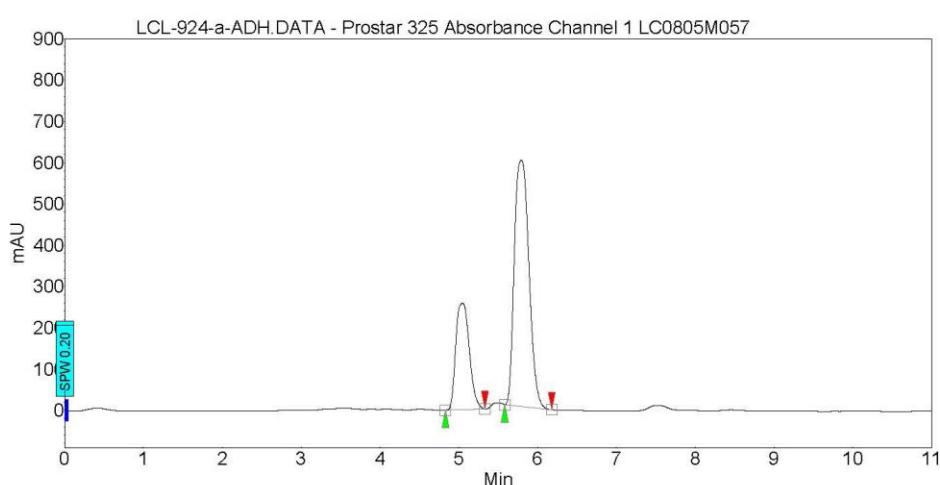
Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	5.05	51.99	950.3	193.9	51.990
2	-	5.79	48.01	837.0	179.1	48.010
Total			100.00	1787.3	373.0	100.000



**2o**, Ar = 4-MeOC<sub>6</sub>H<sub>4</sub>

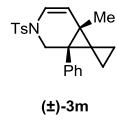
### Chromatogram : LCL-924-a-ADH\_channel1

Acquired : 2018-9-6 12:28:55  
 Processed : 2018-9-6 12:45:50  
 Printed : 2018-9-6 12:46:36



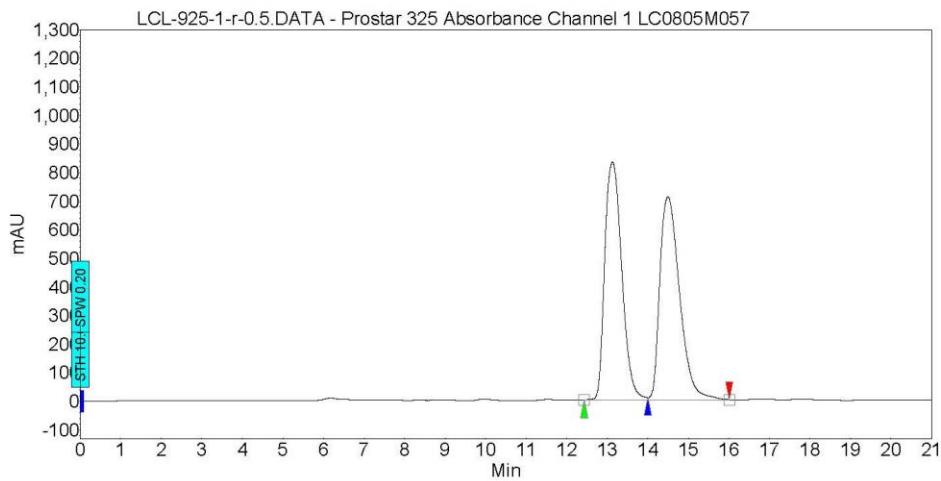
### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	5.05	28.60	257.8	51.3	28.601
2	-	5.79	71.40	596.4	128.0	71.399
Total			100.00	854.2	179.3	100.000



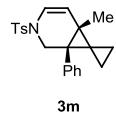
### Chromatogram : LCL-925-1-r-0.5\_channel1

Acquired : 2018-9-6 11:08:15  
 Processed : 2018-9-6 12:03:44  
 Printed : 2018-9-6 12:04:26

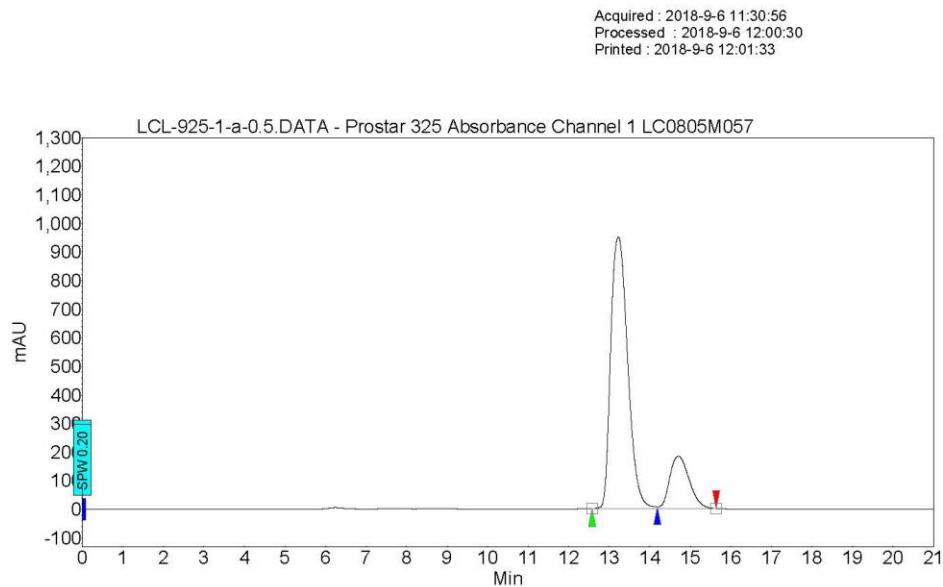


#### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	13.13	50.28	831.3	404.6	50.281
2	-	14.49	49.72	710.2	400.1	49.719
Total			100.00	1541.5	804.7	100.000



### Chromatogram : LCL-925-1-a-0.5\_channel1



### Peak results :

Index	Name	Time [Min]	Amount [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	-	13.23	81.86	950.5	460.3	81.864
2	-	14.71	18.14	183.0	102.0	18.136
Total			100.00	1133.5	562.3	100.000