

# Supporting Information

## Synergy of Activating Substrate and Introducing C-H $\cdots$ O Interaction to Achieve Rh<sub>2</sub>(II)-Catalyzed Asymmetric Cycloisomerization of 1,n-Enynes

Rui Wu<sup>1†</sup>, Kai Chen<sup>2†</sup>, Jun Ma<sup>1†</sup>, Zhi-Xiang Yu<sup>3\*</sup> & Shifa Zhu<sup>1\*</sup>

<sup>1</sup>Key Laboratory of Functional Molecular Engineering of Guangdong Province, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510641, China

<sup>2</sup>College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, China

<sup>3</sup>Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China

<sup>†</sup>These authors contributed equally

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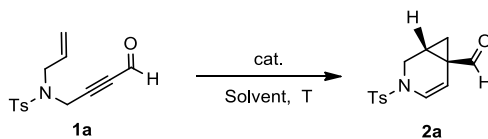
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## 1. General information

All reactions were carried out under an inert atmosphere of dry N<sub>2</sub> in Schlenk tube. Tetrahydrofuran and toluene were distilled from sodium and benzophenone prior to use. Dichloromethane and dichloroethane were distilled from CaH<sub>2</sub> prior to use. Other solvents were used as received from Adamas-beta®. <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F NMR spectra were recorded on Bruker AVANCE 400 MHz or 600 MHz, <sup>1</sup>H NMR and <sup>13</sup>C NMR chemical shifts were determined relative to internal standard TMS at δ 0.0 and <sup>19</sup>F NMR chemical shifts were determined relative to CFC<sub>l</sub><sub>3</sub> as external standard. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Optical rotations were measured on ADP440+B+S. HRMS (EI) and HRMS (ESI) were determined on Waters Micromass GCT Premier, Agilent Technologies 6224 TOF LC/MS, and APEX III 7.0 TESLA FTMS spectrometers, respectively. Infrared (IR) spectra were recorded on a Nicolet 210 spectrophotometer. All other reagents and solvents were used as received from commercial sources, unless specified otherwise, or prepared as described in the literature. Complexes Rh<sub>2</sub>(R-TPCP)<sub>4</sub>, Rh<sub>2</sub>(R-BPCP)<sub>4</sub>, and Rh<sub>2</sub>(R-3,5-di-BrTPCP)<sub>4</sub>, Rh<sub>2</sub>[R-3,5-di(*p*-<sup>t</sup>BuC<sub>6</sub>H<sub>4</sub>)TPCP]<sub>4</sub> which were prepared according to reported methods [1]. Other chiral Rh<sub>2</sub>(II) catalysts were purchased from Strem Chemicals, Inc. The spectral data of the known compounds were in consistence with data reported in the literature. The related literatures were signed following the spectral data.

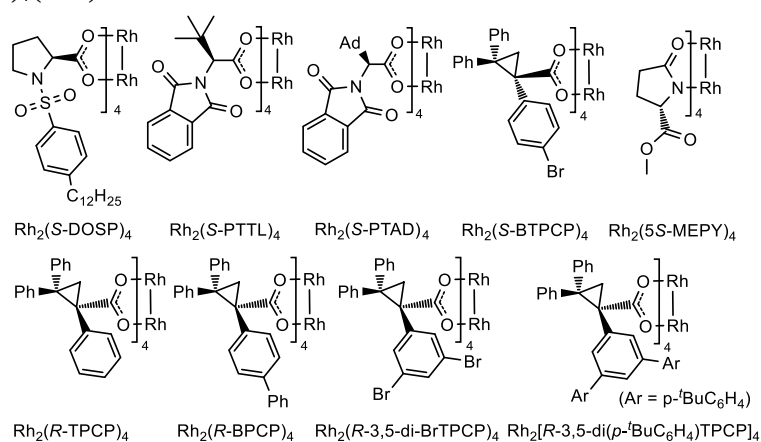
## 2. Optimization of reaction conditions

**Table S1** <sup>a</sup>



| Entry           | Cat. (x mol%)                              | Sol. | T     | Yield <sup>b</sup> | ee <sup>c</sup> |
|-----------------|--------------------------------------------|------|-------|--------------------|-----------------|
| 1               | ZnCl <sub>2</sub> (5)                      | DCE  | rt    | -                  | -               |
| 2               | Co(acac) <sub>3</sub> (5)                  | DCE  | rt    | -                  | -               |
| 3               | Fe(acac) <sub>3</sub> (5)                  | DCE  | rt    | -                  | -               |
| 4               | Ti(OiPr) <sub>4</sub> (5)                  | DCE  | rt    | -                  | -               |
| 5               | TiCl <sub>4</sub> (5)                      | DCE  | rt    | -                  | -               |
| 6               | BPh <sup>F</sup> <sub>3</sub> (5)          | DCE  | rt    | -                  | -               |
| 7               | BF <sub>3</sub> ·Et <sub>2</sub> O(5)      | DCE  | rt    | -                  | -               |
| 8               | CuCl(5)                                    | DCE  | rt    | -                  | -               |
| 9               | Cu(OAc) <sub>2</sub> (5)                   | DCE  | rt    | -                  | -               |
| 10              | Cu(OTf) <sub>2</sub> (5)                   | DCE  | rt    | -                  | -               |
| 11              | AgNO <sub>3</sub> (5)                      | DCE  | rt    | -                  | -               |
| 12              | AgF(5)                                     | DCE  | rt    | -                  | -               |
| 13              | IPrAuCl+Selectfluor(5)                     | DCE  | rt    | -                  | -               |
| 14              | Ph <sub>3</sub> PAuBF <sub>4</sub> (5)     | DCE  | rt    | trace              | -               |
| 15              | PtCl <sub>2</sub> (5)                      | DCE  | rt    | trace              | -               |
| 16              | Rh <sub>2</sub> (OPiv) <sub>4</sub> (1)    | DCE  | rt    | 89%                | -               |
| 17              | Rh <sub>2</sub> (5S-MEPY) <sub>4</sub> (1) | DCE  | rt    | trace              | -               |
| 18 <sup>d</sup> | Rh <sub>2</sub> (5S-MEPY) <sub>4</sub> (1) | DCE  | 80 °C | 36%                | 7%              |

|                 |                                                                                    |                |             |            |            |
|-----------------|------------------------------------------------------------------------------------|----------------|-------------|------------|------------|
| 19              | $\text{Rh}_2(\text{S-DOSP})_4$ (1)                                                 | DCE            | rt          | 42%        | 8%         |
| 20              | $\text{Rh}_2(\text{S-PTAD})_4$ (1)                                                 | DCE            | rt          | 34%        | 11%        |
| 21              | $\text{Rh}_2(\text{S-PTTL})_4$ (1)                                                 | DCE            | rt          | 40%        | 19%        |
| 22              | $\text{Rh}_2(\text{S-BTPCP})_4$ (1)                                                | DCE            | rt          | 94%        | 76%        |
| 23              | $\text{Rh}_2(\text{S-BTPCP})_4$ (1)                                                | Toluene        | rt          | 96%        | 89%        |
| 24              | $\text{Rh}_2(\text{R-TPCP})_4$ (1)                                                 | Toluene        | rt          | 97%        | -86%       |
| 25              | $\text{Rh}_2(\text{R-BPCP})_4$ (1)                                                 | Toluene        | rt          | 95%        | -88%       |
| 26              | $\text{Rh}_2(\text{R-3,5-di-BrTPCP})_4$ (1)                                        | Toluene        | rt          | 85%        | -46%       |
| 27              | $\text{Rh}_2[\text{R-3,5-di}(p\text{-}^t\text{BuC}_6\text{H}_4)\text{TPCP}]_4$ (1) | Toluene        | rt          | 87%        | -41%       |
| 28              | $\text{Rh}_2(\text{S-BTPCP})_4$ (1)                                                | Toluene        | 0 °C        | 91%        | 91%        |
| 29 <sup>e</sup> | <b><math>\text{Rh}_2(\text{S-BTPCP})_4</math> (0.1)</b>                            | <b>Toluene</b> | <b>0 °C</b> | <b>93%</b> | <b>91%</b> |
| 30 <sup>f</sup> | $\text{Rh}_2(\text{S-BTPCP})_4$ (0.01)                                             | Toluene        | 0 °C        | 43%        | 87%        |

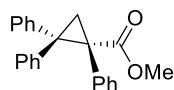


<sup>a</sup>Experiments were performed with **1a** (0.25 mmol), catalyst (x mol%) in solvent with stirring at the temperature for 12 h. (Cat. = catalyst; Sol. = solvent; rt = room temperature; ee = enantiomeric excess, Ad = 1-admantyl). <sup>b</sup>Isolated yield. <sup>c</sup>Determined by HPLC analysis with a chiral stationary phase. <sup>d</sup>120 h. <sup>e</sup>48 h. <sup>f</sup>120 h.

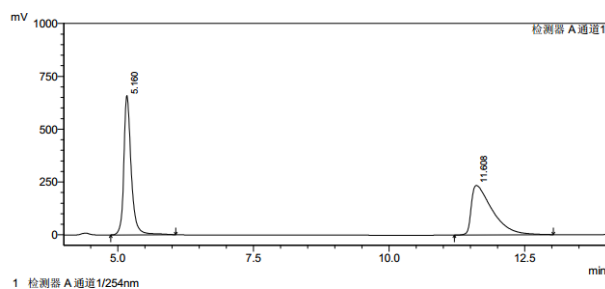
### 3. Preparation of triaryl cyclopropanecarboxylate-based dirhodium catalysts.

The catalysts of  $\text{Rh}_2(\text{R-TPCP})_4$ ,  $\text{Rh}_2(\text{R-BPCP})_4$ ,  $\text{Rh}_2(\text{R-3,5-di-BrTPCP})_4$ , and  $\text{Rh}_2[\text{R-3,5-di}(p\text{-}^t\text{BuC}_6\text{H}_4)\text{TPCP}]_4$  were prepared according to reported methods [1].

#### (R)-Methyl 1,2,2-triphenylcyclopropanecarboxylate

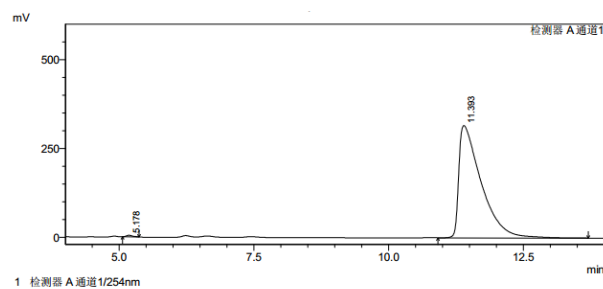
 <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.49 (d,  $J$  = 7.7 Hz, 2H), 7.31 (t,  $J$  = 7.5 Hz, 4H), 7.23 (d,  $J$  = 7.5 Hz, 1H), 7.14 – 7.03 (m, 3H), 7.00 – 6.87 (m, 5H), 3.31 (s, 3H), 2.68 (d,  $J$  = 5.4 Hz, 1H), 2.41 (d,  $J$  = 5.4 Hz, 1H). <sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 142.1, 139.7, 135.8, 132.0, 130.1, 128.8, 128.4, 127.63, 127.55, 127.0, 126.2, 52.2, 44.5, 43.3, 22.9.

Resolution of enantiomers: REGIS Whelk-O-1 column, 9 % IPA-Hexanes, 1.0mL/min, 254 nm,  $\text{RT}_1$  = 5.2 min,  $\text{RT}_2$  = 11.4 min., >99% ee.



峰表

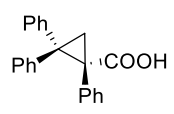
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| 1  | 5.160  | 6245815  | 659066 | 49.650  | 73.752  |
| 2  | 11.608 | 6333964  | 234556 | 50.350  | 26.248  |
| 总计 |        | 12579779 | 893622 | 100.000 | 100.000 |



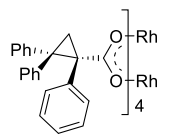
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| 2  | 11.393 | 9121524 | 316205 | 99.598  | 98.604  |
| 总计 |        | 9158312 | 320681 | 100.000 | 100.000 |

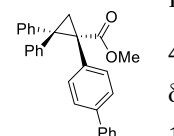
### (R)-1,2,2-Triphenylcyclopropanecarboxylic acid

  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.49 (s, 1H), 7.55 (d,  $J = 7.3$  Hz, 2H), 7.37 (dd,  $J = 14.9, 7.1$  Hz, 5H), 7.23 – 7.13 (m, 3H), 7.02 (dt,  $J = 9.9, 4.0$  Hz, 5H), 2.65 (d,  $J = 5.4$  Hz, 1H), 2.52 (d,  $J = 5.4$  Hz, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.2, 141.7, 139.5, 135.4, 132.0, 130.0, 128.8, 128.5, 127.6, 127.5, 127.1, 127.0, 126.3, 45.6, 42.8, 23.3.

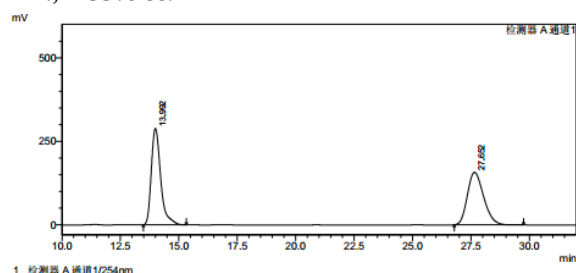
### The catalyst of $\text{Rh}_2(\text{R-TPCP})_4$

  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.27 – 7.17 (m, 6H), 7.02 (s, 3H), 6.95 (s, 2H), 6.85 – 6.77 (m, 4H), 2.37 (d,  $J = 4.7$  Hz, 1H), 1.88 (d,  $J = 5.1$  Hz, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  189.0, 142.7, 141.1, 136.4, 131.1, 130.0, 129.2, 128.0, 127.3, 127.2, 126.3, 126.1, 125.7, 46.3, 43.1, 23.3.

### (R)-Methyl 1-([1,1'-biphenyl]-4-yl)-2,2-diphenylcyclopropanecarboxylate

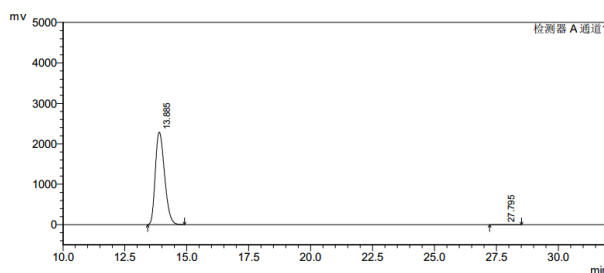
  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.51 (t,  $J = 7.0$  Hz, 4H), 7.41 – 7.19 (m, 10H), 6.98 (ddd,  $J = 23.2, 12.1, 4.2$  Hz, 5H), 3.35 (s, 3H), 2.72 (d,  $J = 5.5$  Hz, 1H), 2.44 (d,  $J = 5.5$  Hz, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 142.1, 140.8, 139.7, 139.6, 134.9, 132.3, 130.0, 128.8, 128.7, 128.4, 127.7, 127.2, 127.0, 126.23, 126.21, 52.2, 44.7, 42.9, 23.0.

Resolution of enantiomers: DAICEL Chiralcel® OA-H, 1% IPA-Hexanes, 1.0mL/min, 254 nm,  $\text{RT}_1 = 13.9$  min,  $\text{RT}_2 = 27.8$  min.; > 99% ee.



峰表

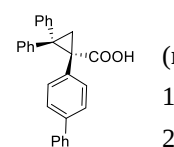
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| 1  | 13.902 | 8052422  | 288824 | 51.493  | 64.752  |
| 2  | 27.795 | 7585444  | 157112 | 48.507  | 35.248  |
| 总计 |        | 15637866 | 445736 | 100.000 | 100.000 |



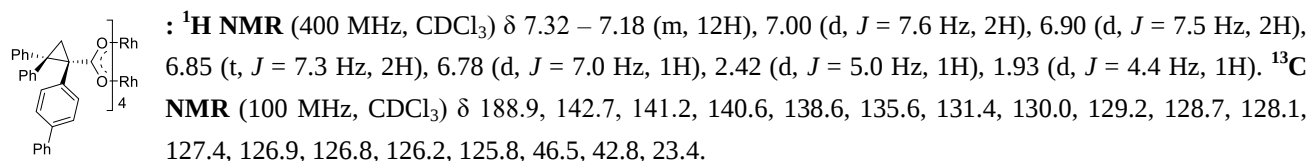
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| 1  | 13.885 | 59273183 | 2286440 | 99.900  | 99.940  |
| 2  | 27.795 | 59541    | 1363    | 0.100   | 0.060   |
| 总计 |        | 59332724 | 2287802 | 100.000 | 100.000 |

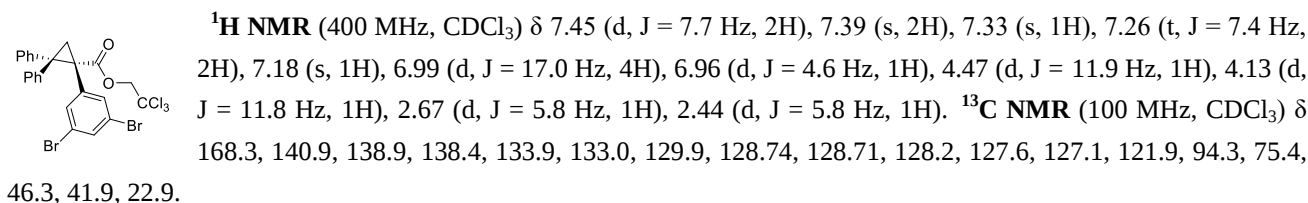
### (R)-1-([1,1'-Biphenyl]-4-yl)-2,2-diphenylcyclopropanecarboxylic acid

  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.74 (s, 1H), 7.46 (d,  $J = 7.6$  Hz, 4H), 7.36 – 7.19 (m, 10H), 6.99 – 6.85 (m, 5H), 2.58 (d,  $J = 5.3$  Hz, 1H), 2.43 (d,  $J = 5.3$  Hz, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  177.4, 141.8, 140.8, 139.8, 139.6, 134.6, 132.4, 130.0, 128.9, 128.8, 128.6, 127.8, 127.3, 127.1, 126.4, 126.3, 45.9, 42.6, 23.5.

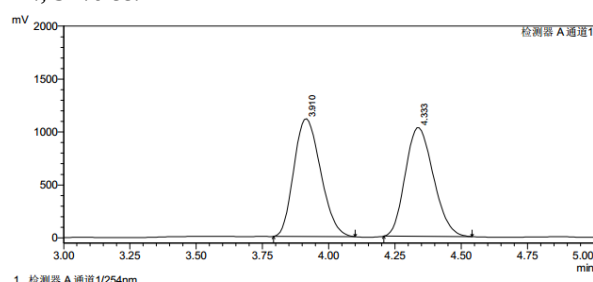
### The catalyst of Rh<sub>2</sub>(R-*p*-BPCP)<sub>4</sub>



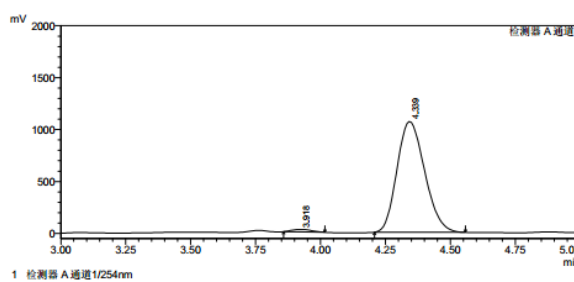
### 2,2,2-Trichloroethyl (R)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropane-1-carboxylate



Resolution of enantiomers: DAICEL Chiralcel® OA-H, 5% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 3.9 min, RT<sub>2</sub> = 4.3 min.; 97% ee.

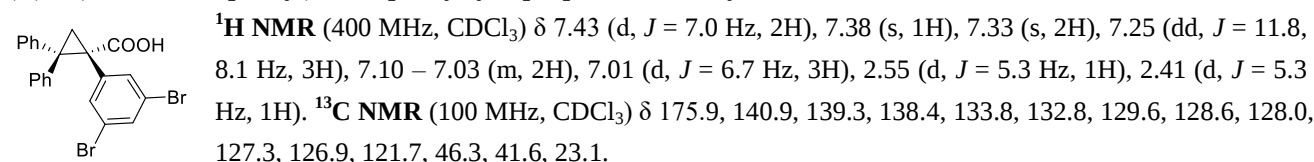


| 峰# | 保留时间  | 面积       | 高度      | 面积 %    | 高度 %    |
|----|-------|----------|---------|---------|---------|
| 1  | 3.910 | 7822816  | 1112171 | 50.673  | 52.040  |
| 2  | 4.333 | 7614885  | 1024960 | 49.327  | 47.960  |
| 总计 |       | 15437700 | 2137131 | 100.000 | 100.000 |

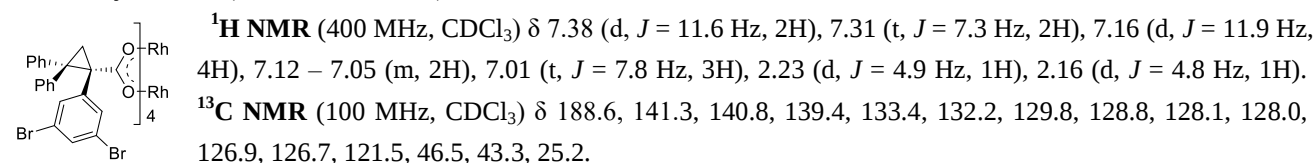


| 峰# | 保留时间  | 面积      | 高度      | 面积 %    | 高度 %    |
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| 1  | 3.918 | 124547  | 23578   | 1.545   | 2.164   |
| 2  | 4.339 | 7935842 | 1065823 | 98.455  | 97.836  |
| 总计 |       | 8060389 | 1089401 | 100.000 | 100.000 |

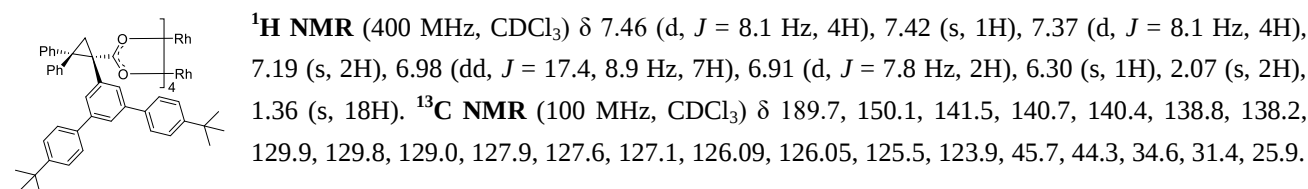
### (R)-1-(3,5-Dibromophenyl)-2,2-diphenylcyclopropane-1-carboxylic acid



### The catalyst of Rh<sub>2</sub>(R-3,5-di-BrTPCP)<sub>4</sub>

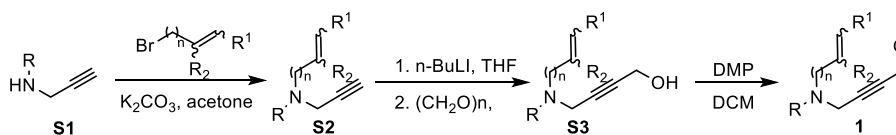


### The catalyst of Rh<sub>2</sub>[R-3,5-di(*p*-<sup>t</sup>BuC<sub>6</sub>H<sub>4</sub>)TPCP]<sub>4</sub>



## 4. Preparation of 1,*n*-enyne

### General procedure A [2]:



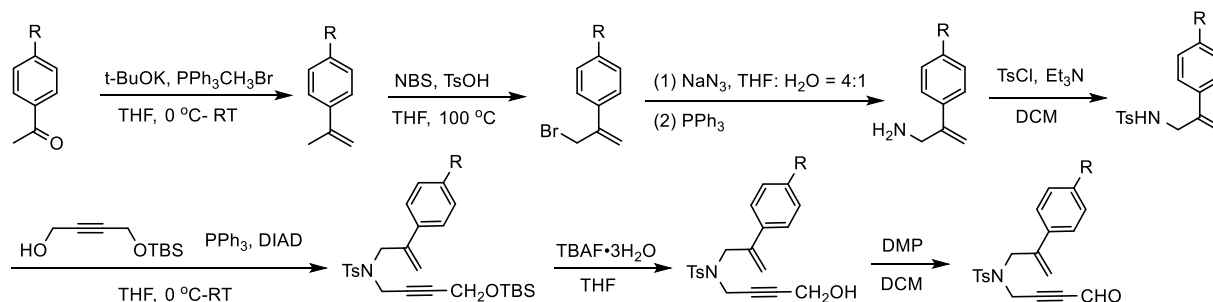
To the solution of **S1** (5.0 mmol, 1.0 equiv) in acetone (20 mL),  $K_2CO_3$  (25.0 mmol, 5.0 equiv) and 3-bromoprop-1-ene (6.0 mmol, 1.2 equiv) was added and stirred at 80 °C under  $N_2$ . After 12 h, the reaction mixture was extracted with EtOAc. Combined organic layers were washed with brine, dried over  $MgSO_4$ , and evaporated. Crude products were purified by column chromatography (PE: EA = 5: 1).

The obtained **S2** (4.0 mmol, 1.0 equiv) was dissolved in THF (15 mL), and  $n-BuLi$  (6 mmol, 1.5 equiv, 1 M in THF) was slowly added into the corresponding solution at -78 °C under  $N_2$ . After 1 h, the  $(CH_2O)_n$  (20.0 mmol, 5.0 equiv) was then added. The resulting mixture was stirred overnight under room temperature and was then quenched with saturated  $NH_4Cl$  solution. The mixture was extracted with EtOAc. Combined organic layers were washed with brine, dried over  $MgSO_4$ , and evaporated. Crude products were purified by column chromatography (PE: EA = 2: 1).

The DMP (1.2 equiv) was added into the solution of **S3** in DCM. The reaction was monitored by TLC until disappearance of the starting material. The reaction mixture was quenched with saturated  $Na_2S_2O_3$  and  $NaHCO_3$  solution. The mixture was extracted with DCM. Combined organic layers were washed with brine, dried over  $MgSO_4$ , and evaporated. Crude products were purified by column chromatography (PE: EA = 5: 1).

The substrates such as **1a**, **1b**, **1c**, **1e**, **1m**, **1p**, **1q**, **1r**, **1t** and **1f** were synthesized according to **General procedure A**.

#### General procedure B [3,4]:



In an oven dried flask, methyl triphenylphosphonium bromide (10.0 mmol, 1.0 eq) and  $t-BuOK$  ((20 mmol, 2.0 eq) were added. The flask was evacuated and backfilled with  $N_2$  (this process was repeated three times), Then THF (16 mL) was added. The suspension was cooled to 0 °C, and the resulting yellow suspension was stirred at 0 °C for 45 min. To this suspension, a solution of acetyl benzene (10.0 mmol, 1.0 eq) in THF (7 mL) was dropwise and the resulting mixture was warmed gradually to room temperature and stirred at room temperature for 16 h. Reaction mixture was quenched with diluent hydrochloric acid. The mixture which was then extracted with EA. The filtrate was concentrated under reduced pressure to yield a yellow oil. Purification by column chromatography using petroleum ether as eluent afforded product.

In an oven dried flask, the methyl styrene (8.0 mmol, 1.0 equiv.) and dry THF (6.0 mL) were added. Then,  $N$ -bromosuccinimide (16.0 mmol, 2 equiv.) and  $TsOH$  (2.4 mmol, 0.3 equiv.) were added into this system and the mixture was refluxed at 100 °C for 4 h. Next, the reaction system was cooled to room temperature and then was poured into petroleum ether (60 mL), followed by wash with  $H_2O$  (20.0 mL  $\times$  3). Organic phase was dried with  $MgSO_4$  and concentrated under reduced pressure to obtain a yellow oil. Purification by column chromatography using petroleum

ether afforded the product as a colorless oil.

The (3-bromoprop-1-en-2-yl)benzene dissolved in THF/H<sub>2</sub>O (4/1, 20 mL) was treated with NaN<sub>3</sub> (8.0 mmol, 1.2 eq) for 1 h at room temperature, and PPh<sub>3</sub> (10.1 mmol, 1.5 eq) was then added to the reaction mixture. After stirring for 12 h at ambient temperature, the mixture was concentrated under reduced pressure to remove most of the THF. The resulting suspension was diluted with conc. HCl and extracted with Et<sub>2</sub>O. The aqueous layer was then basified by adding solid KOH and extracted with Et<sub>2</sub>O. The combined organic phases were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure to give the crude allylic amine, which was pure enough to use in the next step without further purification.

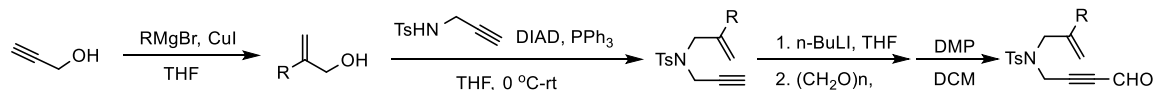
To a suspension of 4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (1.0 eq), PPh<sub>3</sub> (1.3 eq) and alcohol (1.1 eq in THF (0.25 M) was added DIAD (1.3 equiv) dropwise at 0 °C under N<sub>2</sub>, the mixture was stirred at room temperature until amide was completely consumed. The mixture was transferred to flask and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:20) to give enyne.

The obtained enyne was dissolved in THF (0.25 M), then TBAF·3H<sub>2</sub>O (1.2 eq) was added and the solution was extracted with EA/H<sub>2</sub>O, the organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and evaporated under reduced pressure. The obtained crude product was purified by flash column chromatography (EtOAc/PE = 1:2) to give the product.

The oxidation reaction was operated according to **General procedure A**.

The substrates **1g** and **1i** were synthesized according to the first two steps of **General procedure B** and **General procedure A**. The substrates **1j** and **1k** were synthesized according to **General procedure B**.

### General Procedure C [3]:



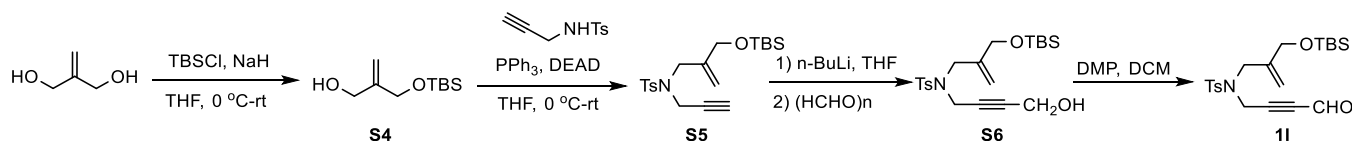
To a dried flask was added CuI (1.8 mmol, 15 mol%) and RMgBr (0.5 M, 29.3 mmol, 2.5 eq) at room temperature, the mixture was then allowed to stir for 30 min. Propargyl alcohol (11.7 mmol) in THF (10 mL) was added dropwise at room temperature. The reaction mixture was then heated to reflux for 24 h. After cooling to room temperature, saturated NH<sub>4</sub>Cl aq. was added dropwise carefully. The organic phase was separated and the aqueous phase was extracted with Et<sub>2</sub>O. The combined organic phases were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and the solvent was removed under reduced pressure. The obtained crude product was purified by flash column chromatography (hexane/ethyl acetate = 3/1) to give allylic alcohol.

To a suspension of 4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (1.1 eq), PPh<sub>3</sub> (1.3 eq) and allylic alcohol (1.0 eq in THF (0.25 M) was added DEAD (1.3 equiv) dropwise at 0 °C under N<sub>2</sub>, the mixture was stirred at room temperature until alcohol was completely consumed. The mixture was transferred to flask and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:20) to give enyne.

The subsequent procedures were operated according to **General procedure A**.

The substrates such as **1h** and the crude **1d** (using MnO<sub>2</sub> as oxidant) were synthesized according to **General procedure C**.

#### Procedure D:



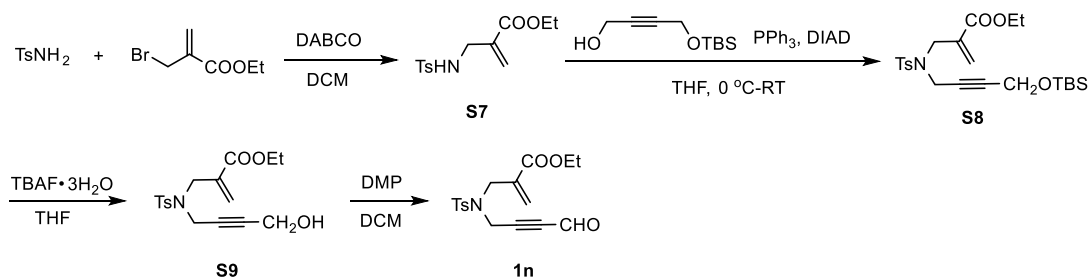
To a dried flask was added 50 mL dry THF under  $N_2$ , followed by addition of NaH (33 mmol, 1.1 equiv). To this solution at 0 °C was added 2-methyleneprop-1,3-diol (2.64 g, 1.0 equiv) dropwise. Mixture was then brought to room temperature and stirred for 45 min. TBSCl (4.98 g, 1.1 equiv) was added in one portion and the mixture was stirred overnight. The reaction was quenched with saturated aqueous  $NH_4Cl$  and extracted with EA for three times. The organic layer was washed with brine, dried over  $Na_2SO_4$ , filtered and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:4) to give the **S4** as clear oil, 6.0 g, 99% yield.

To a suspension of 4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (6.9 g, 1.1 equiv),  $PPh_3$  (10.3 g, 1.3 equiv) and **S4** (6.0 g, 1.0 equiv) in THF was added DEAD (6.79 g, 1.3 equiv) dropwise at 0 °C under  $N_2$ , the mixture was stirred at room temperature until **S4** was completely consumed. The mixture was transferred to flask and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:20) to give **S5** as white solid, 64% yield.

The obtained **S5** (1.0 equiv) was dissolved in THF, and n-BuLi (1.2 equiv, 2.5 M in THF) was slowly added into the corresponding solution at -78 °C under  $N_2$ . After 1 h, the  $(CH_2O)_n$  (3.0 equiv) was then added in one portion. The resulting mixture was stirred overnight under room temperature and was then quenched with saturated  $NH_4Cl$  solution. The mixture was extracted with EtOAc for three times. Combined organic layers were washed with brine, dried over  $MgSO_4$ , and evaporated. The Crude products were purified by column chromatography (PE: EA = 2: 1) to give 7.9 g **S6** as yellow oil, 98% yield.

The DMP (1.2 equiv) was added into the solution of **S6** in DCM under air. The reaction was monitored by TLC until disappearance of the starting material. The reaction mixture was quenched with saturated  $Na_2S_2O_3$  and  $NaHCO_3$  solution. The mixture was extracted with DCM. Combined organic layers were washed with brine, dried over  $MgSO_4$ , and evaporated. Crude products were purified by flash chromatography (PE: EA = 5:1) to give yellow liquid **11**, 87% yield.

#### Procedure E:



To a flame dried flask was added toluene 4-methylbenzenesulfonamide (6.0 eq) in DCM. DABCO was added (1.3 eq) and then ethyl 2-(bromomethyl)acrylate (1.0 eq) was added in a solution of DCM dropwise using syringe pump. The reaction was left overnight. The mixture was poured into a separatory funnel and water was added. The aqueous was extracted with DCM for three times and the collected organic phase was washed with water and brine. The organic solution was dried with  $Na_2SO_4$  and collected by vacuum into a round bottom flask. The solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (Hexanes/ EtOAc = 5:1) to afford **S7** in 74%

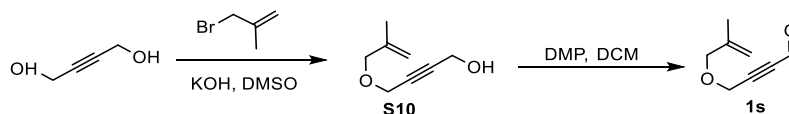
yield as the yellow oil.

To a flame dried flask was added  $\text{PPh}_3$  (1.3 eq) in dry THF, 4-((tert-butyldimethylsilyl)oxy)but-2-yn-1-ol (1.0 eq) and **S7** (1.05 eq) under nitrogen, then the reaction mixture was transferred to 0 °C, DIAD (1.3 eq) was added dropwise and the mixture was moved to room temperature, stirred for 4 hours. The mixture was evaporated under reduced pressure and purified by column chromatography (PE:EA = 10:1) to the **S8** in 94% yield as the yellow oil.

To a solution of **S8** (1.0 eq) in THF (0.25 M) was added TBAF•3H<sub>2</sub>O (1.2 eq) at room temperature and the mixture was stirred for 5 minutes. The mixture was poured into a separatory funnel and water was added. The aqueous was extracted with EA for three times and the collected organic phase was washed with brine. The organic phase was dried with Na<sub>2</sub>SO<sub>4</sub> and collected by vacuum into a round bottom flask. The crude product was purified by column chromatography (Hexanes/ EtOAc = 2:1) to afford **S9** in 59% yield as the yellow oil.

To a solution of **S9** (1.0 eq) in DCM (0.1 M) was added DMP (1.2 eq) slowly at room temperature. The reaction was monitored by TLC until **S9** was completely consumed. The mixture was poured into a saturated solution of NaHCO<sub>3</sub> and Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> and stirred until the mixture became clear. The clear mixture was extracted with DCM for three times and the collected organic phase was washed with brine. The organic phase was dried with Na<sub>2</sub>SO<sub>4</sub> and collected by vacuum into a round bottom flask. The solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (Hexanes/ EtOAc = 3:1) to afford the product in 74% yield.

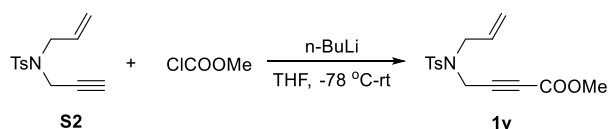
#### Procedure F:



To a suspension of KOH (2.24 g, 40 mmol) in DMSO (20 mL) were added 3-bromo-2-methylprop-1-ene (1.07g, 8 mmol) and 2-Butyne-1,4-diol (3.44g, 40 mmol). The mixture was then stirred for 2 h, poured into water, and extracted with DCM. The aqueous phase was then acidified with aqueous HCl (6 M) and further extracted with DCM. The combined organic phases were reduced in volume, washed with water, dried with MgSO<sub>4</sub>, and concentrated in vacuo. Crude products were purified by column chromatography (PE: EA = 3: 1).

The DMP (1.2 equiv) was added into the solution of **S10** in DCM. The reaction was monitored by TLC until disappearance of the starting material. The reaction mixture was quenched with saturated Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> and NaHCO<sub>3</sub> solution. The mixture was extracted with DCM. Combined organic layers were washed with brine, dried over MgSO<sub>4</sub>, and evaporated. Crude products were purified by flash chromatography with DCM.

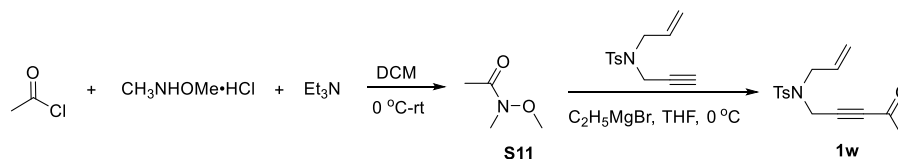
#### Procedure G:



**S2** was obtained according to the general procedure A. To obtained **S2**(1.0 eq) was dissolved in THF(0.5 M), and n-BuLi (1.2 eq, 2.5 M) was added dropwise to the corresponding solution at -78 °C. After 1 h, Methyl Carbonochloridate was added in one portion. The mixture was stirred overnight at room temperature and was then quenched with saturated NH<sub>4</sub>Cl solution. The mixture was extracted with EA for three times and the combined organic layers was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and evaporated under reduced pressure. The residue was purified by silica gel column

chromatography (EtOAc/PE = 1:3) to give **1v** as yellow oil.

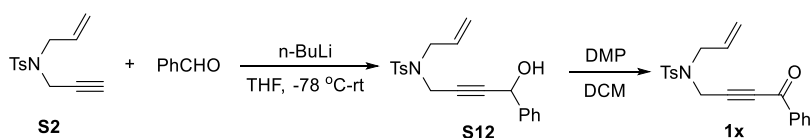
**Procedure H [5]:**



**S11** was prepared according to the procedures reported in literatures [5].  $\text{NEt}_3$  (2.0 equiv.) was added to a stirred solution of N,O-dimethylhydroxylamine hydrochloride (1.0 equiv.) in  $\text{CH}_2\text{Cl}_2$  at 0 °C. Acetyl chloride (82.8 mmol) was added dropwise at 0 °C. The resulting mixture was stirred at ambient temp. overnight. The reaction was quenched with  $\text{NaHCO}_3(\text{aq})$ . The aq. layer was separated and extracted with  $\text{CH}_2\text{Cl}_2$  for three times. The combined organic extracts were washed with aq. HCl (1 M) and brine, and dried with  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure, and the residue was used directly to next step without further purification.

The enyne (1.3 eq) was dissolved in THF, and  $\text{EtMgBr}$  (1.6 equiv, 1 M in THF) was added dropwise into the corresponding solution at 0 °C. The resulting mixture was stirred at 0 °C for 1 h to prepare the enynemagnesium bromide solution. To a solution of Weinreb amide **S11** (1.0 eq) in THF at 0 °C was slowly added the prepared enynemagnesium bromide solution. The resulting mixture was stirred at room temperature overnight. The saturated aqueous  $\text{NH}_4\text{Cl}$  solution was added to quench the reaction and the reaction mixture was extracted with EtOAc for three times. The combined organic layers were washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , filtered and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:3) to give the title ketones **1w** as yellow oil.

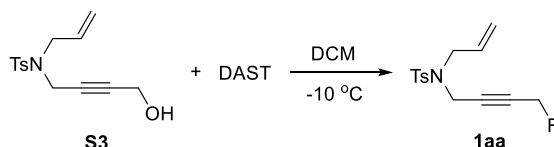
**Procedure I:**



**S2** was obtained according to the general procedure A. To obtained **S12** (1.0 eq) was dissolved in THF (0.5 M), and  $n\text{-BuLi}$  (1.2 eq, 2.5 M) was added dropwise to the corresponding solution at -78 °C. After 1 h, benzaldehyde was added in one portion. The mixture was stirred overnight under room temperature and was then quenched with saturated  $\text{NH}_4\text{Cl}$  solution. The mixture was extracted with EA for three times and the combined organic layers was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , filtered and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:3) to give **S12** as yellow oil.

The DMP (1.2 equiv) was added into the solution of **S12** in DCM. The reaction was monitored by TLC until disappearance of the starting material. The reaction mixture was quenched with saturated  $\text{Na}_2\text{S}_2\text{O}_3$  and  $\text{NaHCO}_3$ . The mixture was extracted with DCM. Combined organic layers were washed with brine, dried over  $\text{MgSO}_4$ , and evaporated. crude products were purified by column chromatography (PE: EA = 5: 1) to give **1x**.

**Procedure J:**



To a solution of alcohol (1.0 eq) in anhydrous DCM was added DAST (1.25 eq) dropwise under nitrogen at -10 °C, and the reaction mixture was stirred at this temperature and monitored by TLC until the alcohol was total consumed. Water was added and the resulting mixture was extracted with DCM for three times. The combined organic phase was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/PE = 1:5) to give **1aa** as yellow oil.

#### N-allyl-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (**1a**)

**1a** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.91 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.90 – 5.63 (m, 1H), 5.43 – 5.19 (m, 2H), 4.27 (s, 2H), 3.84 (d, *J* = 6.5 Hz, 2H), 2.43 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 175.4, 144.2, 135.4, 131.5, 129.7, 127.7, 120.6, 89.1, 84.5, 49.7, 36.0, 21.5.

#### N-allyl-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide-D<sub>2</sub> (**1a-D**)

**1a-D** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.90 (s, 1H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.72 (ddt, *J* = 16.6, 10.0, 6.5 Hz, 1H), 5.34 – 5.22 (m, 2H), 3.82 (d, *J* = 6.5 Hz, 2H), 2.42 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 175.6, 144.3, 135.3, 131.5, 129.8, 127.7, 120.6, 89.0, 84.5, 49.7, 35.6 (t, *J* = 22.0 Hz), 21.5.

#### N-(2-methylallyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (**1b**)

**1b** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.00 (s, 1H), 4.96 (s, 1H), 4.21 (s, 2H), 3.74 (s, 2H), 2.42 (s, 3H), 1.77 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 175.5, 144.2, 138.8, 135.3, 129.7, 127.7, 116.2, 89.0, 84.6, 53.2, 35.7, 21.5, 19.6.

#### N-(2-methylenebutyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (**1c**)

**1c** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.86 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.01 (s, 1H), 4.98 (s, 1H), 4.20 (s, 2H), 3.77 (s, 2H), 2.42 (s, 3H), 2.09 (q, *J* = 7.4 Hz, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 175.5, 144.3, 144.2, 135.3, 129.7, 127.8, 114.3, 89.1, 84.6, 52.0, 35.7, 25.8, 21.5, 11.9.

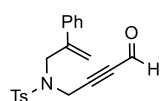
#### N-(3,3-dimethyl-2-methylenebutyl)-N-(4-hydroxybut-2-yn-1-yl)-4-methylbenzenesulfonamide (**1d**)

**1d** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.08 (d, *J* = 13.7 Hz, 2H), 4.09 (s, 2H), 3.93 (s, 2H), 3.86 (s, 2H), 2.43 (s, 4H), 1.11 (s, 9H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 150.2, 143.5, 136.2, 129.4, 128.0, 111.2, 84.0, 78.6, 50.7, 48.0, 35.7, 35.4, 29.2, 21.5.

#### N-(but-2-en-1-yl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (**1e**)

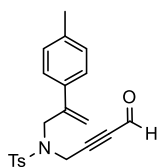
**1e** (E/Z = 6/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.90 (s, 1H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.83 – 5.68 (m, 1H), 5.45 – 5.28 (m, 1H), 4.25 (s, 2H), 3.76 (d, *J* = 6.8 Hz, 2H), 2.42 (s, 3H), 1.70 (d, *J* = 6.1 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 175.5, 144.1, 135.5, 132.5, 129.7, 127.7, 124.1, 89.5, 84.5, 49.0, 35.7, 21.5, 17.7.

#### N-(4-oxobut-2-yn-1-yl)-N-(2-phenylallyl)-4-methylbenzenesulfonamide (**1f**)



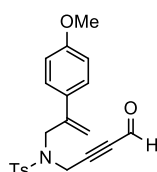
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.85 (s, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.54 – 7.47 (m, 2H), 7.33 (m, *J* = 15.2, 7.4 Hz, 5H), 5.59 (s, 1H), 5.31 (s, 1H), 4.27 (s, 2H), 4.13 (s, 2H), 2.42 (s, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.4, 144.4, 141.1, 137.2, 134.9, 129.8, 128.6, 128.4, 127.9, 126.4, 117.8, 88.9, 84.9, 50.7, 35.7, 21.5.

**N-(4-oxobut-2-yn-1-yl)-N-(2-(p-tolyl)allyl) 4-methylbenzenesulfonamide (1g)**



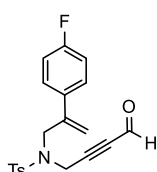
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.76 (s, 1H), 7.65 (d, *J* = 7.9 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 7.8 Hz, 2H), 5.47 (s, 1H), 5.17 (s, 1H), 4.16 (s, 2H), 4.04 (s, 2H), 2.34 (s, 3H), 2.26 (s, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.4, 144.3, 140.8, 138.3, 134.9, 134.2, 129.7, 129.3, 127.9, 126.3, 117.0, 89.0, 84.9, 50.8, 35.7, 21.6, 21.2.

**N-(2-(4-methoxyphenyl)allyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1h)**



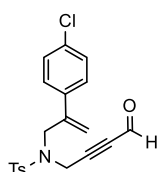
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.78 (s, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.9 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.9 Hz, 2H), 5.44 (s, 1H), 5.12 (s, 1H), 4.16 (s, 2H), 4.05 (s, 2H), 3.74 (s, 3H), 2.36 (s, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.3, 159.8, 144.4, 140.2, 134.9, 129.7, 129.4, 127.9, 127.6, 116.1, 113.9, 89.0, 84.9, 55.3, 50.9, 35.6, 21.6.

**N-(2-(4-fluorophenyl)allyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1i)**



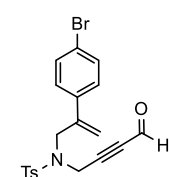
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.56 – 7.47 (m, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.05 (m, 2H), 5.56 (s, 1H), 5.30 (s, 1H), 4.25 (s, 2H), 4.14 (s, 2H), 2.45 (s, 3H). **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>) δ -113.4. **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.3, 162.8 (d, *J* = 247.9 Hz), 144.5, 140.0, 134.8, 133.1 (d, *J* = 3.4 Hz), 129.8, 128.2 (d, *J* = 8.1 Hz), 127.9, 117.8, 115.5 (d, *J* = 21.6 Hz), 88.6, 84.9, 50.8, 35.7, 21.5.

**N-(2-(4-chlorophenyl)allyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1j)**



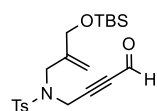
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.77 (s, 1H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.37 (d, *J* = 7.5 Hz, 2H), 7.24 (m, 4H), 5.50 (s, 1H), 5.24 (s, 1H), 4.16 (s, 2H), 4.03 (s, 2H), 2.35 (s, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.3, 144.5, 140.0, 135.5, 134.7, 134.3, 129.8, 128.7, 127.9, 127.7, 118.4, 88.6, 85.0, 50.7, 35.7, 21.6.

**N-(2-(4-bromophenyl)allyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1k)**



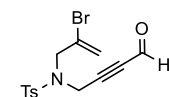
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 8.86 (s, 1H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 5.59 (s, 1H), 5.33 (s, 1H), 4.24 (s, 2H), 4.11 (s, 2H), 2.44 (s, 3H). **<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) δ 175.3, 144.5, 140.2, 136.0, 134.8, 131.7, 129.8, 128.0, 127.9, 122.6, 118.4, 88.6, 85.0, 50.7, 35.7, 21.6.

**N-(2-(((tert-butyldimethylsilyl)oxy)methyl)allyl)-N-(4-oxobut-2-yn-1-yl)benzenesulfonamide (1l)**



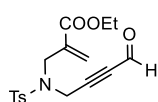
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 5.33 (s, 1H), 5.11 (s, 1H), 4.25 (s, 2H), 4.12 (s, 2H), 3.82 (s, 2H), 2.42 (s, 3H), 0.91 (s, 9H), 0.08 (s, 6H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.3, 144.3, 141.8, 135.2, 129.7, 127.8, 114.9, 89.0, 84.7, 63.5, 49.3, 35.9, 25.9, 21.5, 18.3, -5.44.

**N-(2-bromoallyl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1m)**



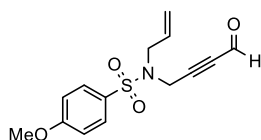
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.93 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 5.93 (s, 1H), 5.71 (s, 1H), 4.31 (s, 2H), 4.08 (s, 2H), 2.44 (s, 3H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 175.3, 144.6, 135.3, 129.8, 127.7, 126.5, 121.1, 88.4, 84.7, 54.6, 36.3, 21.6.

**Ethyl 2-(((4-methyl-N-(4-oxobut-2-yn-1-yl)phenyl)sulfonamido)methyl)acrylate (1n)**



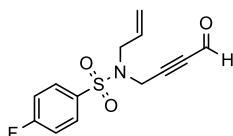
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.90 (s, 1H), 7.75 (d,  $J$  = 8.0 Hz, 2H), 7.33 (d,  $J$  = 8.1 Hz, 2H), 6.41 (s, 1H), 5.93 (s, 1H), 4.30 (s, 2H), 4.27 – 4.18 (m, 2H), 4.09 (s, 2H), 2.43 (s, 3H), 1.33 – 1.29 (m, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  175.4, 165.6, 144.4, 135.4, 134.9, 129.8, 128.1, 127.7, 89.1, 84.5, 61.2, 47.5, 37.3, 21.5, 14.1.

**N-allyl-N-(4-oxobut-2-yn-1-yl)-4-methoxybenzenesulfonamide (1o)**



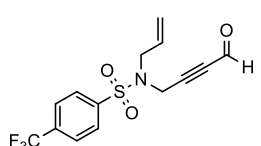
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.96 (s, 1H), 7.79 (d,  $J$  = 8.9 Hz, 2H), 7.01 (d,  $J$  = 8.9 Hz, 2H), 5.75 (m, 1H), 5.37 – 5.20 (m, 2H), 4.28 (s, 2H), 3.89 (s, 3H), 3.84 (d,  $J$  = 6.5 Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  175.5, 163.5, 131.5, 129.9, 129.8, 120.6, 114.3, 89.2, 84.6, 55.7, 49.7, 36.0.

**N-allyl-N-(4-oxobut-2-yn-1-yl)-4-fluorobenzenesulfonamide (1p)**



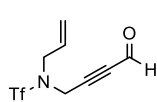
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.96 (s, 1H), 7.87 (m, 2H), 7.22 (m, 2H), 5.83 – 5.63 (m, 1H), 5.40 – 5.22 (m, 2H), 4.29 (s, 2H), 3.84 (d,  $J$  = 6.5 Hz, 2H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -104.1.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  175.3, 165.5 (d,  $J$  = 255.9 Hz), 134.5 (d,  $J$  = 3.5 Hz), 131.2, 130.4 (d,  $J$  = 9.4 Hz), 120.9, 116.4 (d,  $J$  = 22.7 Hz), 88.5, 84.6, 49.7, 36.0.

**N-allyl-N-(4-oxobut-2-yn-1-yl)-4-(trifluoromethyl)benzenesulfonamide (1q)**



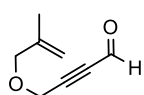
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.91 (s, 1H), 8.00 (d,  $J$  = 8.4 Hz, 2H), 7.81 (d,  $J$  = 8.4 Hz, 2H), 5.83 – 5.64 (m, 1H), 5.34 – 5.30 (m, 2H), 4.32 (s, 2H), 3.87 (d,  $J$  = 6.5 Hz, 2H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.2.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  175.1, 142.1, 134.9 (q,  $J$  = 33.0 Hz), 130.9, 128.2, 126.3 (q,  $J$  = 3.7 Hz), 123.1 (d,  $J$  = 272.9 Hz), 121.1, 87.8, 84.6, 49.8, 36.0.

**N-allyl-N-(4-oxobut-2-yn-1-yl)-1,1,1-trifluoromethanesulfonamide (1r)**



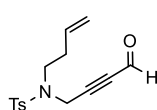
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.23 (s, 1H), 5.94 – 5.67 (m, 1H), 5.43 (m, 2H), 4.38 (s, 2H), 4.12 (s, 2H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -76.0.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  175.6, 130.0, 122.2, 119.7 (q,  $J$  = 322.3 Hz), 87.1, 84.4, 50.7, 36.8.

**4-((2-methylallyl)oxy)but-2-ynal (1s)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.25 (s, 1H), 5.01 (s, 1H), 4.98 (s, 1H), 4.34 (s, 2H), 4.00 (s, 2H), 1.77 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.2, 140.8, 113.7, 92.4, 85.4, 74.3, 56.7, 19.4.

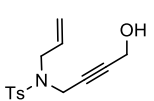
**N-(but-3-en-1-yl)-N-(4-oxobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1t)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.91 (s, 1H), 7.72 (d,  $J$  = 8.2 Hz, 2H), 7.31 (d,  $J$  = 8.2 Hz, 2H), 5.76 (m, 1H), 5.31 – 4.94 (m, 2H), 4.31 (s, 2H), 3.27 (t,  $J$  = 7.3 Hz, 2H), 2.41 (s, 3H), 2.34 (q,  $J$  = 7.0 Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  175.5, 144.1, 135.3, 134.1, 129.7, 127.6, 117.6, 89.2, 84.4, 46.3, 36.7, 32.2, 21.5.

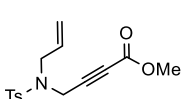
**1u** was prepared according to the general **procedure A**.

**N-allyl-N-(4-hydroxybut-2-yn-1-yl)-4-methylbenzenesulfonamide (1u)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J$  = 8.2 Hz, 2H), 7.27 (d,  $J$  = 8.2 Hz, 2H), 5.66 (ddt,  $J$  = 16.6, 9.5, 6.4 Hz, 1H), 5.31 – 5.11 (m, 2H), 3.94 (s, 2H), 3.76 (d,  $J$  = 6.5 Hz, 2H), 2.53 (s, 1H), 2.38 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.8, 135.8, 131.9, 129.5, 127.8, 119.9, 84.1, 78.0, 50.4, 49.2, 36.1, 21.5.

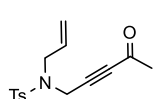
**Methyl-4-((N-allyl-4-methylphenyl)sulfonamido)but-2-ynoate (1v)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J$  = 7.9 Hz, 2H), 7.32 (d,  $J$  = 7.9 Hz, 2H), 5.81 – 5.65 (m, 1H),

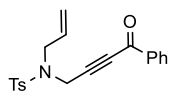
5.37 – 5.18 (m, 2H), 4.20 (s, 2H), 3.81 (d,  $J = 6.4$  Hz, 2H), 3.69 (s, 3H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  152.9, 144.0, 135.3, 131.5, 129.7, 127.6, 120.5, 80.4, 77.0, 52.7, 49.6, 35.8, 21.5

**N-allyl-N-(4-oxopent-2-yn-1-yl)-4-methylbenzenesulfonamide (1w)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.0$  Hz, 2H), 7.34 (d,  $J = 8.0$  Hz, 2H), 5.84 – 5.67 (m, 1H), 5.40 – 5.23 (m, 2H), 4.25 (s, 2H), 3.85 (d,  $J = 6.5$  Hz, 2H), 2.44 (s, 3H), 2.12 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  183.2, 144.1, 135.6, 131.5, 129.7, 127.7, 120.5, 84.7, 84.2, 49.6, 35.9, 32.3, 21.5.

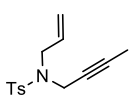
**N-allyl-N-(4-oxo-4-phenylbut-2-yn-1-yl)-4-methylbenzenesulfonamide (1x)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (d,  $J = 8.2$  Hz, 2H), 7.76 (d,  $J = 8.3$  Hz, 2H), 7.61 (t,  $J = 7.4$  Hz, 1H), 7.43 (t,  $J = 7.8$  Hz, 2H), 7.21 (d,  $J = 8.0$  Hz, 2H), 6.04 – 5.55 (m, 1H), 5.44 – 5.04 (m, 2H), 4.38 (s, 2H), 3.92 (d,  $J = 6.5$  Hz, 2H), 2.21 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.8, 144.2, 136.0, 135.4, 134.3, 131.6, 129.8, 129.4, 128.6, 127.7, 120.6, 86.9, 83.4, 49.8, 36.2, 21.4.

**1y** was prepared according to the procedures reported in literature [6].

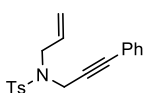
**N-allyl-N-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (1y)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 7.8$  Hz, 2H), 7.26 (d,  $J = 7.8$  Hz, 2H), 5.72 – 5.65 (m, 1H), 5.25 – 5.15 (m, 2H), 3.97 (s, 2H), 3.75 (d,  $J = 6.1$  Hz, 2H), 2.37 (s, 3H), 1.49 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.3, 136.1, 132.2, 129.3, 127.8, 119.5, 81.6, 71.5, 49.0, 36.3, 21.4, 3.2.

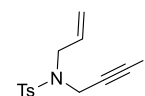
**1z** was prepared according to the procedures reported in literature [7].

**N-allyl-N-(3-phenylprop-2-yn-1-yl)-4-methylbenzenesulfonamide (1z)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.1$  Hz, 2H), 7.30 – 7.22 (m, 5H), 7.06 (d,  $J = 7.3$  Hz, 2H), 5.85 – 5.75 (m, 1H), 5.41 – 5.21 (m, 2H), 4.30 (s, 2H), 3.89 (d,  $J = 6.4$  Hz, 2H), 2.33 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 136.0, 132.1, 131.5, 129.5, 128.4, 128.1, 127.8, 122.2, 120.0, 85.7, 81.7, 49.3, 36.7, 21.4.

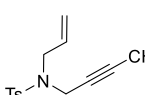
**N-allyl-N-(4-fluorobut-2-yn-1-yl)-4-methylbenzenesulfonamide (1aa)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.3$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 5.74 (dd,  $J = 17.0$ , 10.1 Hz, 1H), 5.36 – 5.20 (m, 2H), 4.74 (t,  $J = 1.7$  Hz, 1H), 4.62 (t,  $J = 1.7$  Hz, 1H), 4.16 (d,  $J = 7.0$  Hz, 2H), 3.82 (d,  $J = 6.5$  Hz, 2H), 2.44 (s, 3H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -215.7.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.8, 135.8, 131.8, 129.5, 127.8, 120.1, 82.8 (d,  $J = 11.9$  Hz), 79.4 (d,  $J = 22.3$  Hz), 70.1 (d,  $J = 166.1$  Hz), 49.3, 36.0 (d,  $J = 3.0$  Hz), 21.5.

**1ab** was prepared according to the procedures reported in literature [7].

**N-allyl-N-(4-methoxybut-2-yn-1-yl)-4-methylbenzenesulfonamide (1ab)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 8.3$  Hz, 2H), 7.30 (d,  $J = 8.6$  Hz, 2H), 5.74 (ddt,  $J = 16.5$ , 10.0, 6.4 Hz, 1H), 5.26 (ddd,  $J = 13.6$ , 11.1, 1.2 Hz, 2H), 4.13 (s, 2H), 3.82 (d,  $J = 6.0$  Hz, 4H), 3.19 (s, 3H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 136.0, 132.0, 129.5, 127.8, 119.9, 81.4, 79.1, 59.5, 57.4, 49.1, 36.1, 21.5.

## 5. General procedure for Rh-catalyzed reactions

**General procedure for asymmetric cycloisomerization of 1,n-enynals.** To a toluene solution of **1** (0.25 mmol, 1 mL) in Schlenk tube with a magnetic bar was added  $\text{Rh}_2(\text{S-BTPCP})_4$  (0.00025 mmol, 0.1 mol%, 0.44 mg, the catalyst was dissolved in toluene) at 0 °C under  $\text{N}_2$ . The sealed tube was then stirred at 0 °C under nitrogen atmosphere for 48 h. The

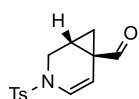
mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: ethyl acetate/petroleum ether) to afford the desired product **2**.

**Procedure for gram-scale reaction:** To a toluene solution of **1a** (4.5 mmol, 18 mL) in Schlenk tube with a magnetic bar was added Rh<sub>2</sub>(S-BTPCP)<sub>4</sub> (0.0045 mmol, 0.1 mol%, 7.9 mg) at 0 °C under N<sub>2</sub>. The sealed tube was then stirred at 0 °C under nitrogen atmosphere for 48 h. The mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: ethyl acetate/petroleum ether) to afford the desired product **2a**.

**Procedures for the oxidation of alcohol and asymmetric cycloisomerization of 1d:** To a solution of alcohol (5.2 mmol, 1.0 eq) in DCM (25 ml) was added MnO<sub>2</sub> (40 eq). The reaction was monitored by TLC until the alcohol was completely consumed. The mixture was filtered by short silica gel and was then concentrated to give the product accompanied by unknown inseparable byproduct. The purity which was determined by <sup>1</sup>H NMR using 1-methyl-4-nitrobenzene as internal standard was 83% in wt%.

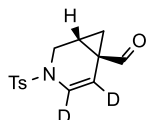
To a toluene solution of **1d** (100 mg, 83% wt%, 1mL) in Schlenk tube with a magnetic bar was added Rh<sub>2</sub>(S-BTPCP)<sub>4</sub> (1 mol%, the catalyst was dissolved in toluene) at room temperature under N<sub>2</sub>. The sealed tube was then stirred for 60 h under nitrogen atmosphere. The mixture was then concentrated and the residue was purified by chromatography on silica gel to afford the desired product.

### 3-Tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (**2a**)



Colorless oil, 63.0 mg, 93%, 91% ee, (gram scale (4.5mmol): 1.1g 86%, 90% ee) purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 6.51 (d, *J* = 8.2 Hz, 1H), 5.84 (d, *J* = 8.2 Hz, 1H), 4.11 (d, *J* = 11.9 Hz, 1H), 2.98 (m, 1H), 2.45 (s, 3H), 2.28 (m, 1H), 1.60 (m, 1H), 1.27 (m, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.8, 144.2, 134.5, 129.9, 127.0, 122.7, 106.4, 40.2, 29.39, 29.37, 22.2, 21.6. IR (KBr) ν<sub>max</sub> 2924, 2859, 2724, 2369, 1711, 1645, 1596, 1492, 1458, 1407, 1349, 1268, 1216, 1166, 1117, 1088, 1059, 1023, 994, 958, 931, 866, 815, 765, 708, 682, 643, 602, 544, 497, 468. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>14</sub>H<sub>16</sub>NO<sub>3</sub>S<sup>+</sup>: 278.0845, found 278.0846.

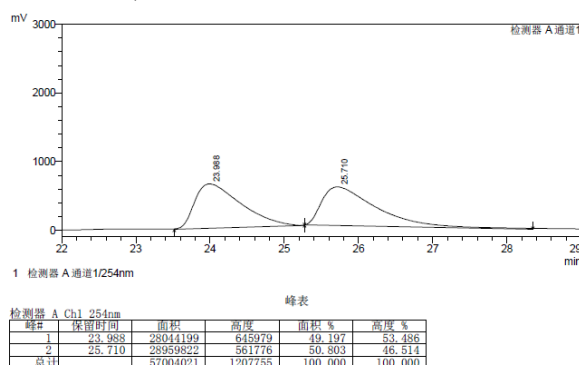
### 3-Tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde-d<sub>2</sub> (**2a-D**)

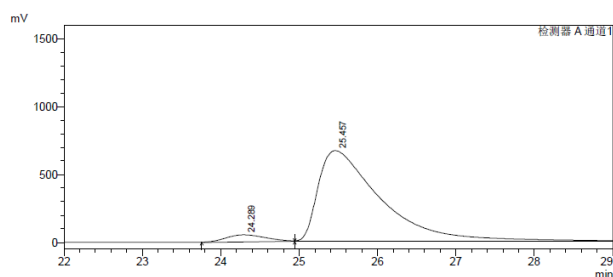


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 4.11 (dd, *J* = 11.9, 1.4 Hz, 1H), 2.98 (dd, *J* = 11.9, 2.3 Hz, 1H), 2.46 (s, 3H), 2.28 (td, *J* = 7.0, 3.4 Hz, 1H), 1.61 (dd, *J* = 9.1, 4.8 Hz, 1H), 1.26 (dd, *J* = 6.7, 4.9 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.8, 144.2, 134.5, 130.0, 127.0, 123.3 – 120.9 (m), 107.5 – 104.5 (m), 40.2, 29.31, 29.28, 22.2, 21.6. HRMS (ESI)

[M+H]<sup>+</sup> calculated for C<sub>14</sub>H<sub>14</sub>D<sub>2</sub>NO<sub>3</sub>S<sup>+</sup>: 280.0971, found 280.0965.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 24.0 min, RT<sub>2</sub> = 25.7 min. [α]<sub>D</sub><sup>25</sup> = +36.2 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



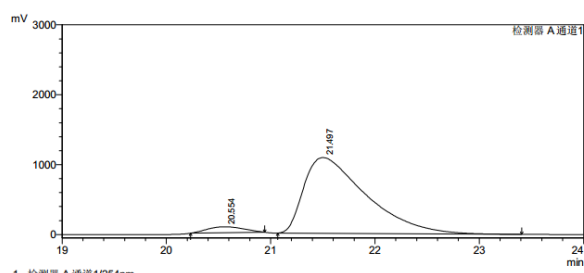


1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 24.289 | 1876004  | 52457  | 4.720   | 7.275   |
| 2  | 25.457 | 37868761 | 668597 | 95.280  | 92.725  |
| 总计 |        | 39744766 | 721055 | 100.000 | 100.000 |

2a



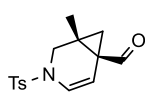
1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积       | 高度      | 面积 %    | 高度 %    |
|----|--------|----------|---------|---------|---------|
| 1  | 20.554 | 2077230  | 85567   | 4.410   | 7.317   |
| 2  | 21.497 | 45027130 | 1083937 | 95.590  | 92.683  |
| 总计 |        | 47104360 | 1169504 | 100.000 | 100.000 |

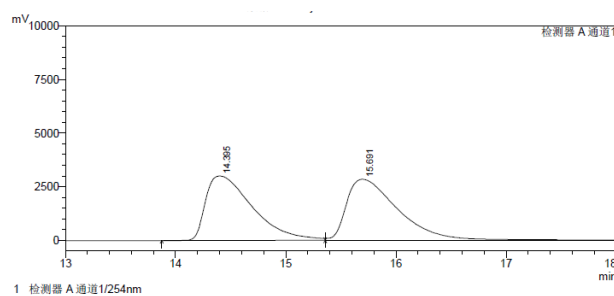
2a-D

### 1-Methyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2b)



Colorless oil, 65.5 mg, 90%, 94% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.23 (s, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.46 (d, *J* = 8.0 Hz, 1H), 5.80 (d, *J* = 8.0 Hz, 1H), 3.90 (d, *J* = 11.9 Hz, 1H), 2.70 (d, *J* = 11.9 Hz, 1H), 2.43 (s, 3H), 1.68 (d, *J* = 4.8 Hz, 1H), 1.47 (d, *J* = 4.8 Hz, 1H), 1.37 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 198.5, 144.2, 134.6, 130.0, 127.0, 122.4, 107.8, 46.5, 39.9, 34.7, 28.5, 21.6, 16.8. IR (KBr) ν<sub>max</sub> 2960, 2924, 2853, 2362, 2333, 1640, 1596, 1527, 1352, 1340, 1257, 1215, 1165, 1090, 1007, 965, 813, 764, 590, 544, 478, 433. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>15</sub>H<sub>18</sub>NO<sub>3</sub>S<sup>+</sup>: 292.1002, found 292.1001.

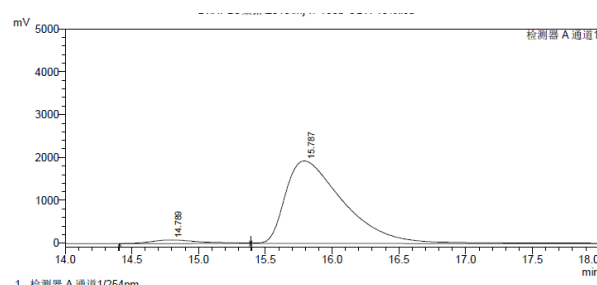
Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 14.8 min, RT<sub>2</sub> = 15.8 min. [α]<sub>D</sub><sup>25</sup> = +21.7 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积        | 高度      | 面积 %    | 高度 %    |
|----|--------|-----------|---------|---------|---------|
| 1  | 14.395 | 90579747  | 3000127 | 49.789  | 51.334  |
| 2  | 15.691 | 91345873  | 2844146 | 50.211  | 48.666  |
| 总计 |        | 181925620 | 5844273 | 100.000 | 100.000 |

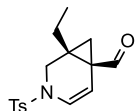


1 检测器 A 通道1/254nm

峰表

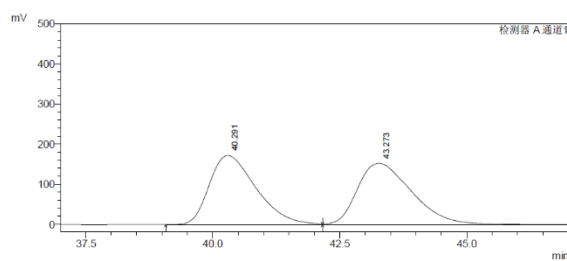
| 峰# | 保留时间   | 面积       | 高度      | 面积 %    | 高度 %    |
|----|--------|----------|---------|---------|---------|
| 1  | 14.789 | 1978628  | 85419   | 3.256   | 4.254   |
| 2  | 15.787 | 58790050 | 1922661 | 96.744  | 95.746  |
| 总计 |        | 60768678 | 2008080 | 100.000 | 100.000 |

### 1-Ethyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2c)



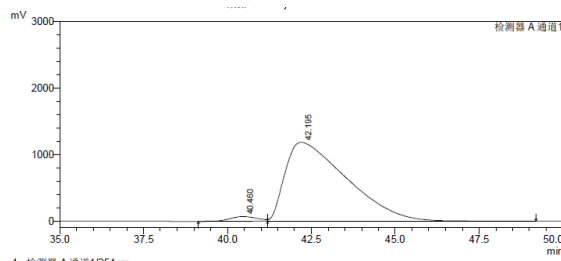
Colorless oil, 69.7 mg, 92%, 93% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.24 (s, 1H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 6.45 (d, *J* = 8.0 Hz, 1H), 5.83 (d, *J* = 8.0 Hz, 1H), 3.94 (d, *J* = 11.8 Hz, 1H), 2.80 (d, *J* = 11.8 Hz, 1H), 2.43 (s, 3H), 1.81 (dq, *J* = 14.9, 7.5 Hz, 1H), 1.67 (m, 2H), 1.41 (d, *J* = 4.8 Hz, 1H), 0.96 (t, *J* = 7.5 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 198.3, 144.2, 134.7, 130.0, 127.0, 122.4, 108.3, 45.6, 44.1, 34.7, 28.1, 24.2, 21.6, 11.3. IR (KBr) ν<sub>max</sub> 2959, 2923, 2851, 2363, 2332, 1639, 1626, 1352, 1259, 1216, 1166, 1092, 1016, 764, 665, 598, 539, 516, 479, 433. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>16</sub>H<sub>20</sub>NO<sub>3</sub>S<sup>+</sup>: 306.1158, found 306.1158.

Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 40.5 min, RT<sub>2</sub> = 42.2 min. [α]<sub>D</sub><sup>25</sup> = +58.7 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



1 检测器 A 通道 1/254nm

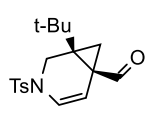
| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 40.291 | 11063755 | 172378 | 49.179  | 52.985  |
| 2  | 43.273 | 11433152 | 152955 | 50.821  | 47.015  |
| 总计 |        | 22496907 | 325333 | 100.000 | 100.000 |



1 检测器 A 通道 1/254nm

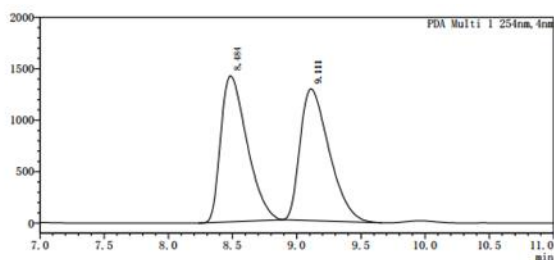
| 峰# | 保留时间   | 面积        | 高度      | 面积 %    | 高度 %    |
|----|--------|-----------|---------|---------|---------|
| 1  | 40.460 | 5521837   | 70805   | 3.552   | 5.639   |
| 2  | 42.195 | 149946470 | 1184844 | 96.448  | 94.361  |
| 总计 |        | 155468307 | 1255650 | 100.000 | 100.000 |

### 1-(tert-butyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2d)



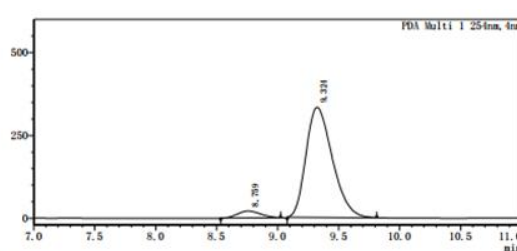
Yellow oil, 66.6 mg, 80%, 90% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.24 (s, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 6.52 (d, *J* = 8.1 Hz, 1H), 5.84 (d, *J* = 8.1 Hz, 1H), 4.29 – 4.12 (m, 3H), 3.24 (d, *J* = 12.4 Hz, 1H), 2.44 (s, 3H), 2.35 (d, *J* = 5.1 Hz, 1H), 1.71 (d, *J* = 5.2 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 196.5, 168.2, 144.5, 134.5, 130.1, 127.1, 124.3, 106.8, 62.3, 43.5, 41.8, 36.1, 24.7, 21.6, 14.1. IR (KBr) ν<sub>max</sub> 2958, 1855, 1728, 1694, 1659, 1582, 1442, 1406, 1384, 1350, 1263, 1163, 1096, 1025, 689, 576, 545, 465, 423. HRMS (ESI) [M+Na]<sup>+</sup> calculated for C<sub>18</sub>H<sub>23</sub>NO<sub>3</sub>S Na<sup>+</sup>: 356.1291, found 356.1286.

Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 20% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 8.5 min, RT<sub>2</sub> = 9.1 min. [α]<sub>D</sub><sup>25</sup> = -18.4 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



<峰表>

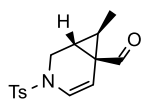
| 峰号 | 保留时间  | 面积       | 高度      | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|-------|----------|---------|------|----|-----------|---------|
| 1  | 8.484 | 20217468 | 1419624 | mg/L | M  | RT: 8.484 | 50.014  |
| 2  | 9.111 | 20206149 | 1281356 | mg/L | M  | RT: 9.111 | 49.986  |
| 总计 |       | 40423617 | 2700980 |      |    |           | 100.000 |



<峰表>

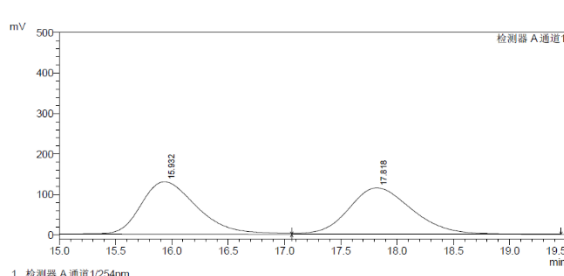
| 峰号 | 保留时间  | 面积      | 高度     | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|-------|---------|--------|------|----|-----------|---------|
| 1  | 8.759 | 275222  | 20968  | mg/L | M  | RT: 8.759 | 5.222   |
| 2  | 9.324 | 4995254 | 331969 | mg/L | M  | RT: 9.324 | 94.778  |
| 总计 |       | 5270476 | 352937 |      |    |           | 100.000 |

### 7-Methyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2e)

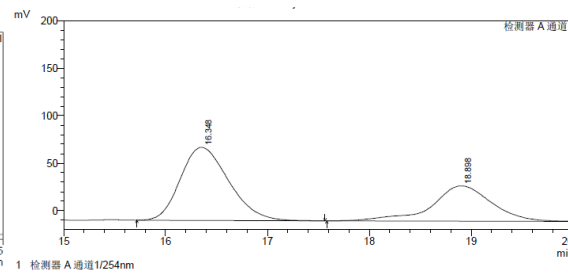


Yellow oil, 51.2 mg, 70% ((*R, R, R*)-**2n**/*(R, S, R)*-**2n** = 6/1), 25% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. The configuration was determined following the literature. <sup>13</sup>-<sup>14</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.29 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 6.45 (d, *J* = 8.3 Hz, 1H), 5.83 (d, *J* = 8.3 Hz, 1H), , 4.10 (d, *J* = 11.8 Hz, 1H), 2.83 (dd, *J* = 11.8, 2.3 Hz, 1H), 2.43 (s, 3H), 2.30 (d, *J* = 6.8 Hz, 1H), 1.58 – 1.53 (m, 1H), 1.21 (d, *J* = 6.4 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 198.5, 144.1, 134.4, 129.9, 127.0, 122.0, 108.0, 39.9, 36.9, 34.7, 33.7, 21.6, 12.7. IR (KBr) ν<sub>max</sub> 2924, 2858, 2724, 1714, 1646, 1596, 1493, 1458, 1407, 1352, 1273, 1216, 1165, 1117, 1089, 976, 931, 866, 815, 765, 708, 682, 646, 602, 540, 497, 468. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>15</sub>H<sub>18</sub>NO<sub>3</sub>S<sup>+</sup>: 292.1002, found 292.1002.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 16.3 min, RT<sub>2</sub> = 18.9 min.

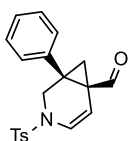


| 峰表 |        |         |        |         |         |
|----|--------|---------|--------|---------|---------|
| 峰# | 保留时间   | 面积      | 高度     | 面积 %    | 高度 %    |
| 1  | 16.892 | 4487012 | 129393 | 49.931  | 53.030  |
| 2  | 17.818 | 4499423 | 114606 | 50.069  | 46.970  |
| 总计 |        | 8986435 | 244000 | 100.000 | 100.000 |



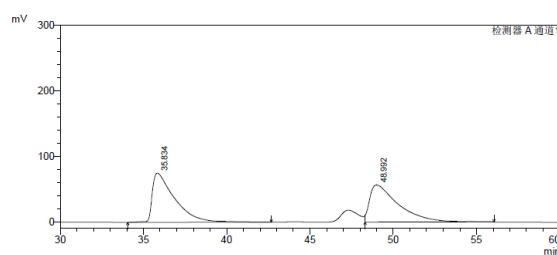
| 峰表 |        |         |        |         |         |
|----|--------|---------|--------|---------|---------|
| 峰# | 保留时间   | 面积      | 高度     | 面积 %    | 高度 %    |
| 1  | 16.348 | 2537754 | 76867  | 62.571  | 67.423  |
| 2  | 18.898 | 1518028 | 37140  | 37.429  | 32.577  |
| 总计 |        | 4055782 | 114007 | 100.000 | 100.000 |

### 1-Phenyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2f)

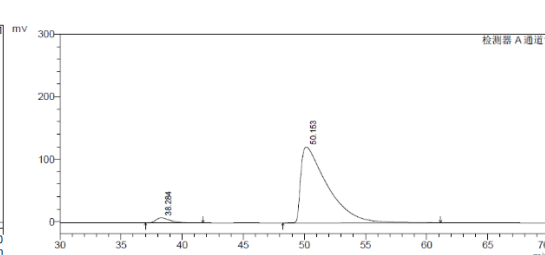


Colorless oil, 76.5 mg, 87%, 93% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (s, 1H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.34 (t, *J* = 10.4 Hz, 7H), 6.56 (d, *J* = 8.1 Hz, 1H), 6.02 (d, *J* = 8.1 Hz, 1H), 4.10 (d, *J* = 12.0 Hz, 1H), 2.98 (d, *J* = 11.9 Hz, 1H), 2.46 (s, 3H), 2.17 (d, *J* = 5.1 Hz, 1H), 1.97 (d, *J* = 5.1 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.4, 144.3, 135.7, 134.6, 130.0, 129.4, 129.2, 128.5, 127.1, 123.1, 107.4, 47.8, 46.8, 34.9, 24.6, 21.6. IR (KBr) ν<sub>max</sub> 2922, 2852, 2428, 1853, 1807, 1712, 1601, 1584, 1570, 1553, 1521, 1502, 1488, 1454, 1442, 1402, 1387, 1273, 1166, 1114, 1047, 974, 902, 850, 767, 680, 591, 472. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>20</sub>H<sub>20</sub>NO<sub>3</sub>S<sup>+</sup>: 354.1158, found 354.1158.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 5% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 38.3 min, RT<sub>2</sub> = 50.2 min. [α]<sub>D</sub><sup>25</sup> = +46.3 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)

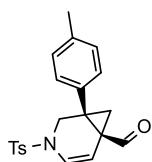


| 峰表 |        |          |        |         |         |
|----|--------|----------|--------|---------|---------|
| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
| 1  | 38.834 | 6979130  | 75013  | 50.663  | 56.910  |
| 2  | 48.892 | 6796583  | 56798  | 49.337  | 43.090  |
| 总计 |        | 13775714 | 131811 | 100.000 | 100.000 |



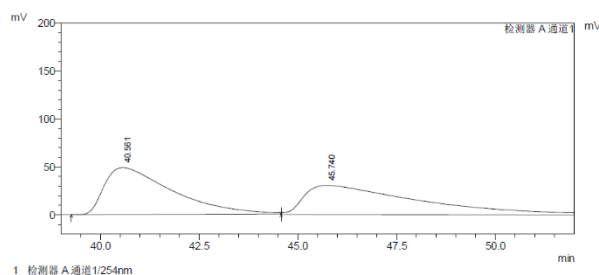
| 峰表 |        |          |        |         |         |
|----|--------|----------|--------|---------|---------|
| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
| 1  | 38.284 | 652282   | 7987   | 3.414   | 8.158   |
| 2  | 50.183 | 18455742 | 121702 | 96.586  | 93.842  |
| 总计 |        | 19108024 | 129689 | 100.000 | 100.000 |

### 1-(p-Tolyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2g)

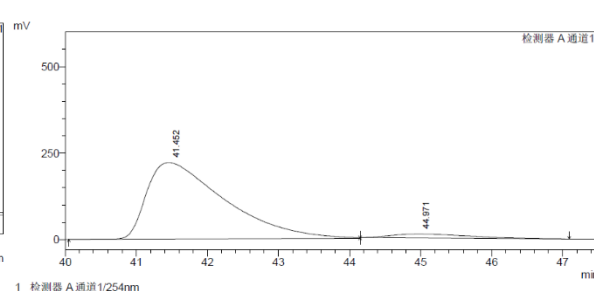


Colorless oil, 83.1 mg, 90%, 91% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 7.7 Hz, 2H), 7.15 - 7.12 (m, 4H), 6.53 (d, *J* = 8.1 Hz, 1H), 5.98 (d, *J* = 8.1 Hz, 1H), 4.05 (d, *J* = 11.9 Hz, 1H), 2.93 (d, *J* = 11.9 Hz, 1H), 2.43 (s, 3H), 2.32 (s, 3H), 2.12 (d, *J* = 4.9 Hz, 1H), 1.92 (d, *J* = 5.0 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.6, 144.2, 138.4, 134.6, 132.6, 130.0, 129.8, 129.2, 127.1, 123.0, 107.5, 47.8, 46.5, 34.9, 24.6, 21.6, 21.1. IR (KBr) ν<sub>max</sub> 3026, 2957, 2922, 2848, 2366, 2336, 1708, 1646, 1518, 1490, 1390, 1273, 1166, 1045, 1017, 973, 934, 905, 849, 765, 712, 685, 658, 585, 545, 497, 470, 450. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>21</sub>H<sub>22</sub>NO<sub>3</sub>S<sup>+</sup>: 368.1315, found 368.1314.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 1% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 41.5 min, RT<sub>2</sub> = 45.0 min. [α]<sub>D</sub><sup>25</sup> = +55.6 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)

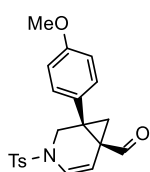


| 峰表 |        |          |       |         |
|----|--------|----------|-------|---------|
| 峰# | 保留时间   | 面积       | 高度    | 面积 %    |
| 1  | 40.561 | 5521864  | 44658 | 49.436  |
| 2  | 45.740 | 5647891  | 27873 | 50.564  |
| 总计 |        | 11169755 | 72531 | 100.000 |



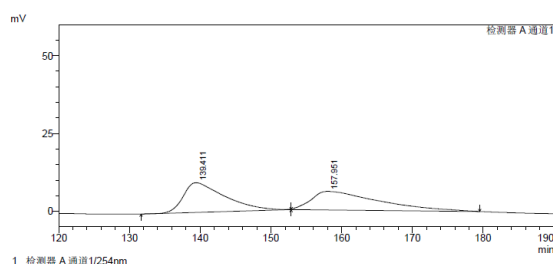
| 峰表 |        |          |        |         |
|----|--------|----------|--------|---------|
| 峰# | 保留时间   | 面积       | 高度     | 面积 %    |
| 1  | 41.452 | 16805144 | 220698 | 95.273  |
| 2  | 44.971 | 833796   | 11175  | 4.727   |
| 总计 |        | 17638940 | 231873 | 100.000 |

### 1-(4-Methoxyphenyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde(2h)

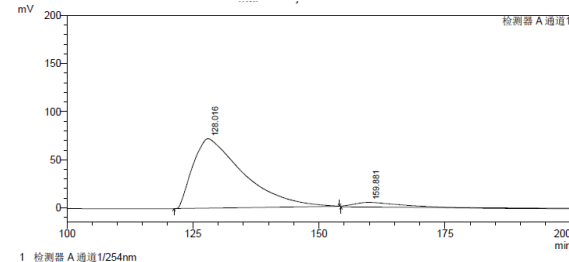


Colorless oil, 79.5 mg, 83%, 91% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (s, 1H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 8.6 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 6.52 (d, *J* = 8.1 Hz, 1H), 5.97 (d, *J* = 8.1 Hz, 1H), 4.04 (d, *J* = 11.8 Hz, 1H), 3.79 (s, 3H), 2.91 (d, *J* = 11.8 Hz, 1H), 2.44 (s, 3H), 2.11 (d, *J* = 5.1 Hz, 1H), 1.92 (d, *J* = 5.1 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.7, 159.5, 144.2, 134.7, 130.5, 130.0, 127.6, 127.1, 123.0, 114.5, 107.5, 55.3, 47.8, 46.2, 35.0, 24.8, 21.6. IR (KBr) ν<sub>max</sub> 2926, 2836, 2331, 1702, 1645, 1588, 1497, 1357, 1301, 1293, 1182, 1163, 1078, 1021, 995, 933, 848, 784, 755, 692, 614, 553, 501, 470. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>21</sub>H<sub>22</sub>NO<sub>4</sub>S<sup>+</sup>: 384.1264, found 384.1264.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 1% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 128.0 min, RT<sub>2</sub> = 159.9 min. [α]<sub>D</sub><sup>25</sup> = -18.1 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)

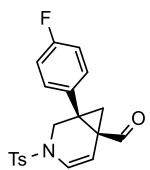


| 峰表 |         |         |       |         |
|----|---------|---------|-------|---------|
| 峰# | 保留时间    | 面积      | 高度    | 面积 %    |
| 1  | 138.411 | 3951624 | 9591  | 49.922  |
| 2  | 157.951 | 3963958 | 5973  | 50.078  |
| 总计 |         | 7915582 | 15564 | 100.000 |



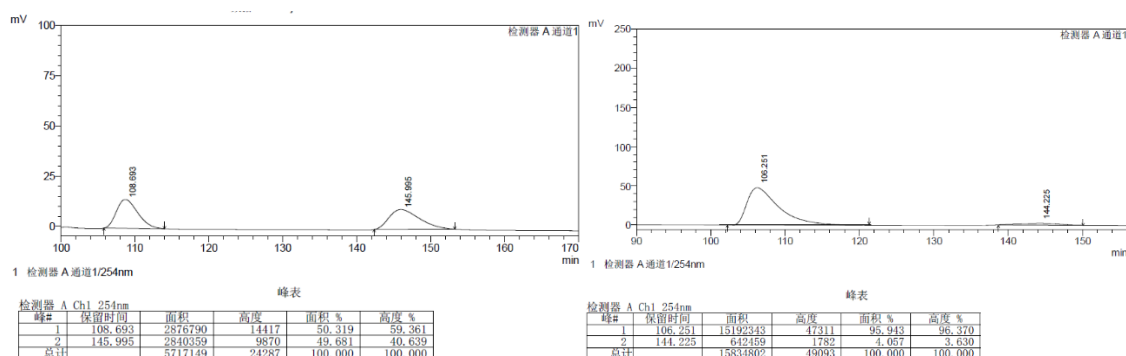
| 峰表 |         |          |       |         |
|----|---------|----------|-------|---------|
| 峰# | 保留时间    | 面积       | 高度    | 面积 %    |
| 1  | 128.016 | 50346535 | 72198 | 95.521  |
| 2  | 159.881 | 2360894  | 4910  | 4.479   |
| 总计 |         | 52707429 | 77108 | 100.000 |

### 1-(4-Fluorophenyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2i)

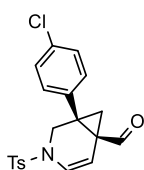


Colorless oil, 78.1 mg, 84%, 92% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.43 (s, 1H), 7.65 (d, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.29 – 7.22 (m, 2H), 7.02 (t, *J* = 8.3 Hz, 2H), 6.54 (d, *J* = 8.1 Hz, 1H), 5.98 (d, *J* = 8.1 Hz, 1H), 4.05 (d, *J* = 12.0 Hz, 1H), 2.91 (d, *J* = 12.0 Hz, 1H), 2.44 (s, 3H), 2.11 (d, *J* = 5.1 Hz, 1H), 1.94 (d, *J* = 5.1 Hz, 1H). <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -112.5. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.1, 162.4 (d, *J* = 248.6 Hz), 144.3, 134.6, 131.5 (d, *J* = 3.5 Hz), 131.1 (d, *J* = 8.3 Hz), 130.1, 127.0, 123.2, 116.2 (d, *J* = 21.7 Hz), 107.3, 47.7, 46.1, 34.9, 24.7, 21.6. IR (KBr) ν<sub>max</sub> 2961, 2924, 2853, 2740, 2431, 2369, 2189, 1710, 1660, 1515, 1488, 1443, 1404, 1390, 1353, 1228, 1166, 1026, 976, 927, 837, 794, 712, 686, 660, 624, 584, 543, 408, 498, 468, 430. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>20</sub>H<sub>19</sub>FO<sub>3</sub>S<sup>+</sup>: 372.1064, found 372.1063.

Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 106.3 min, RT<sub>2</sub> = 144.2 min. [α]<sub>D</sub><sup>25</sup> = +66.1 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)

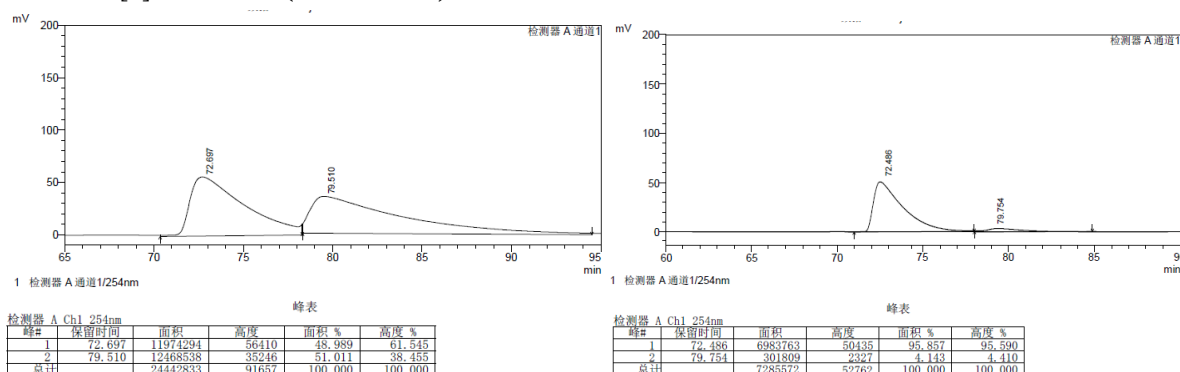


### 1-(4-Chlorophenyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2j)

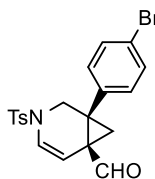


Colorless oil, 82.4 mg, 86%, 92% ee, purified by chromatograph ( $\text{SiO}_2$ ), PE/EA = 5/1.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.43 (s, 1H), 7.64 (d,  $J$  = 8.0 Hz, 2H), 7.42 – 7.29 (m, 4H), 7.21 (d,  $J$  = 8.2 Hz, 2H), 6.54 (d,  $J$  = 8.1 Hz, 1H), 5.97 (d,  $J$  = 8.1 Hz, 1H), 4.05 (d,  $J$  = 11.9 Hz, 1H), 2.91 (d,  $J$  = 11.9 Hz, 1H), 2.44 (s, 3H), 2.11 (d,  $J$  = 5.3 Hz, 1H), 1.94 (d,  $J$  = 5.3 Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  197.0, 144.4, 134.52, 134.46, 134.2, 130.7, 130.1, 129.5, 127.0, 123.3, 107.2, 47.6, 46.1, 34.9, 24.5, 21.6. IR (KBr)  $\nu_{\text{max}}$  2966, 2920, 2848, 2361, 2331, 1707, 1691, 1642, 1592, 1491, 1393, 1273, 1165, 1089, 1045, 1009, 972, 929, 821, 769, 742, 683, 653, 627, 569, 497, 473, 450. HRMS (ESI)  $[\text{M}+\text{H}]^+$  calculated for  $\text{C}_{20}\text{H}_{19}\text{ClNO}_3\text{S}^+$ : 388.0769, found 388.0767.

Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm,  $\text{RT}_1$  = 72.5 min,  $\text{RT}_2$  = 79.7 min.  $[\alpha]_{\text{D}}^{25}$  = +79.0 (c 0.5,  $\text{CH}_2\text{Cl}_2$ )

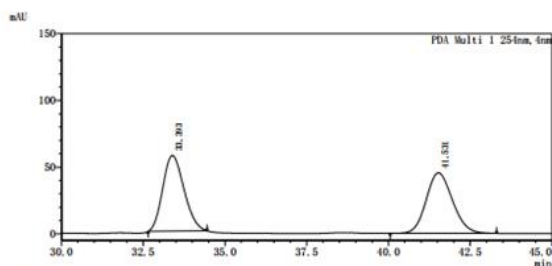


### 1-(4-bromophenyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2k)



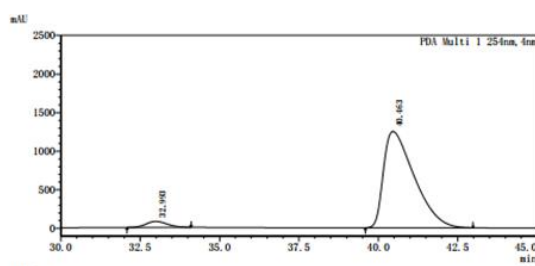
Yellow oil, 94.8 mg, 88%, 92% ee, purified by chromatograph ( $\text{SiO}_2$ ), PE/EA = 5/1.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.43 (s, 1H), 7.64 (d,  $J$  = 8.2 Hz, 2H), 7.46 (d,  $J$  = 8.3 Hz, 2H), 7.33 (d,  $J$  = 8.1 Hz, 2H), 7.15 (d,  $J$  = 8.3 Hz, 2H), 6.54 (d,  $J$  = 8.1 Hz, 1H), 5.97 (d,  $J$  = 8.1 Hz, 1H), 4.05 (d,  $J$  = 12.0 Hz, 1H), 2.90 (d,  $J$  = 12.0 Hz, 1H), 2.44 (s, 3H), 2.11 (d,  $J$  = 5.1 Hz, 1H), 1.94 (d,  $J$  = 5.2 Hz, 1H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  197.0, 144.4, 134.7, 134.5, 132.4, 131.1, 130.1, 127.1, 123.3, 122.6, 107.2, 47.6, 46.2, 34.9, 24.5, 21.6. IR (KBr)  $\nu_{\text{max}}$  2922, 1710, 1580, 1492, 1351, 1273, 1167, 1009, 934, 820, 685, 543, 463, 421. HRMS (ESI)  $[\text{M}+\text{H}]^+$  calculated for  $\text{C}_{20}\text{H}_{19}\text{BrNO}_3\text{S}^+$ : 432.0265, found 432.0264.

Resolution of enantiomers: FLM Chiral INC column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $\text{RT}_1$  = 33.4 min,  $\text{RT}_2$  = 41.5 min.  $[\alpha]_{\text{D}}^{25}$  = -23.2 (c 0.5,  $\text{CH}_2\text{Cl}_2$ )



<峰表>

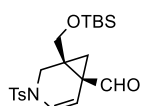
| 峰号 | 保留时间   | 面积      | 高度     | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|------|----|-----------|---------|
| 1  | 33.293 | 2572327 | 56987  | mg/L | M  | RT:33.293 | 50.282  |
| 2  | 41.531 | 2545672 | 45360  | mg/L | M  | RT:41.531 | 49.718  |
| 总计 |        | 5117999 | 102047 |      |    |           | 100.000 |



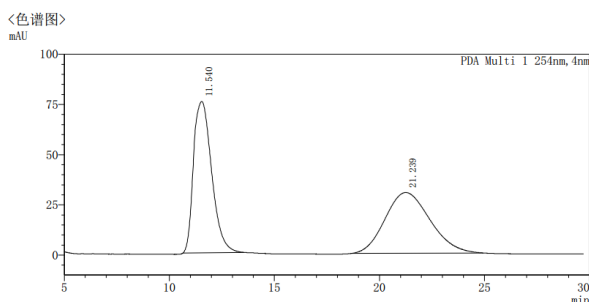
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| 峰号 | 保留时间   | 面积       | 高度      | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|--------|----------|---------|------|----|-----------|---------|
| 1  | 32.993 | 3580095  | 76948   | mg/L | M  | RT:32.993 | 4.084   |
| 2  | 40.463 | 84085119 | 1248849 | mg/L | M  | RT:40.463 | 95.916  |
| 总计 |        | 87665215 | 1325798 |      |    |           | 100.000 |

### 1-(((tert-butyldimethylsilyl)oxy)methyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (21)

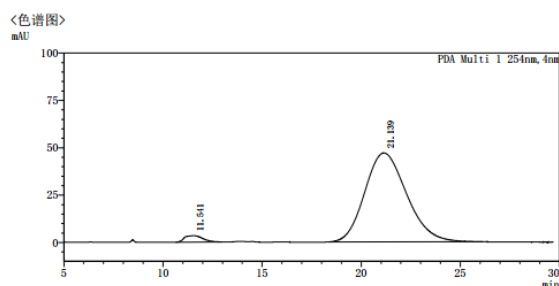


White solid, MP: 84-87 °C, 93.7 mg, 89%, 94% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 9.29 (s, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.50 (d, *J* = 8.1 Hz, 1H), 5.82 (d, *J* = 8.1 Hz, 1H), 3.98 (d, *J* = 11.8 Hz, 1H), 3.90 (d, *J* = 11.3 Hz, 1H), 3.68 (d, *J* = 11.3 Hz, 1H), 3.00 (d, *J* = 11.8 Hz, 1H), 2.45 (s, 3H), 1.79 (d, *J* = 4.7 Hz, 1H), 1.38 (d, *J* = 4.8 Hz, 1H), 0.83 (s, 9H), 0.01 (d, *J* = 3.2 Hz, 6H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 197.7, 144.2, 134.5, 129.9, 127.1, 122.6, 107.9, 62.6, 45.3, 43.2, 33.6, 25.9, 25.7, 21.5, 18.1, -5.55, -5.60. **IR** (KBr) ν<sub>max</sub> 3594, 2940, 2859, 1706, 1647, 1464, 1404, 1353, 1255, 1169, 1092, 1006, 906, 842, 779, 680, 591, 546. **HRMS** (ESI) [M+Na]<sup>+</sup> calculated for C<sub>21</sub>H<sub>31</sub>NO<sub>4</sub>SSiNa<sup>+</sup> 444.1635, found 444.1638. Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 11.5 min, RT<sub>2</sub> = 21.1 min. [α]<sub>D</sub><sup>25</sup> = -13.2 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



<峰表>

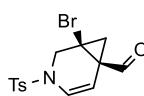
| 峰号 | 保留时间   | 面积      | 高度     | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|------|----|-----------|---------|
| 1  | 11.540 | 4542260 | 75412  | mg/L | M  | RT:11.540 | 50.282  |
| 2  | 21.239 | 4491377 | 30223  | mg/L | M  | RT:21.239 | 49.718  |
| 总计 |        | 9033637 | 105636 |      |    |           | 100.000 |



<峰表>

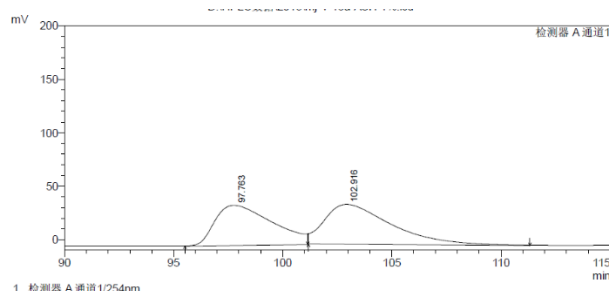
| 峰号 | 保留时间   | 面积      | 高度    | 浓度单位 | 标记 | 化合物名 | 面积%     |
|----|--------|---------|-------|------|----|------|---------|
| 1  | 11.541 | 218450  | 3401  |      | M  |      | 3.074   |
| 2  | 21.139 | 6887965 | 46958 |      | M  |      | 96.926  |
| 总计 |        | 7106415 | 50359 |      |    |      | 100.000 |

### 1-Bromo-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2m)



Yellow oil, 77.1 mg, 87%, 93% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 9.09 (s, 1H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.36 (d, *J* = 8.3 Hz, 2H), 6.52 (d, *J* = 7.9 Hz, 1H), 5.82 (d, *J* = 7.9 Hz, 1H), 4.36 (d, *J* = 12.2 Hz, 1H), 3.13 (d, *J* = 12.2 Hz, 1H), 2.45 (s, 3H), 2.13 (dd, *J* = 6.8, 1.1 Hz, 1H), 1.66 (d, *J* = 6.8 Hz, 1H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 196.7, 144.7, 134.5, 130.2, 127.0, 123.8, 105.9, 47.6, 41.2, 32.7, 29.7, 28.7. **IR** (KBr) ν<sub>max</sub> 2959, 2925, 2850, 2728, 2363, 2332, 1734, 1703, 1681, 1628, 1594, 1447, 1349, 1162, 1216, 1118, 970, 813, 757, 703, 663, 590, 548, 478. **HRMS** (ESI) [M+H]<sup>+</sup> calculated for C<sub>14</sub>H<sub>15</sub>BrNO<sub>3</sub>S<sup>+</sup>: 355.9951, found 355.9951.

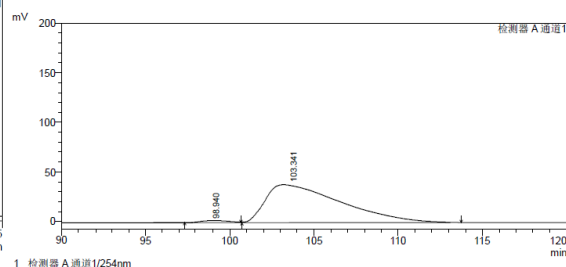
Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 1% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 98.9 min, RT<sub>2</sub> = 103.3 min. [α]<sub>D</sub><sup>25</sup> = +21.6 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



1 检测器 A 通道 1/254nm

峰表

| 峰# | 保留时间    | 面积       | 高度    | 面积 %    | 高度 %    |
|----|---------|----------|-------|---------|---------|
| 1  | 97.763  | 7314371  | 37515 | 49.027  | 50.110  |
| 2  | 102.916 | 7604697  | 37351 | 50.973  | 49.890  |
| 总计 |         | 14919068 | 74866 | 100.000 | 100.000 |

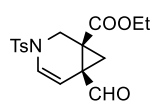


1 检测器 A 通道 1/254nm

峰表

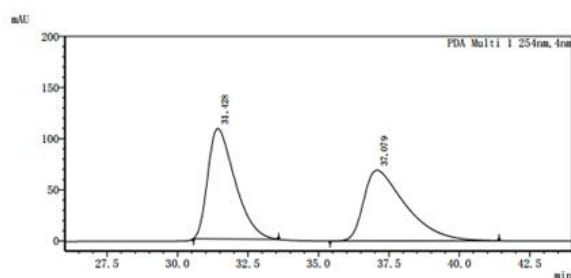
| 峰# | 保留时间    | 面积      | 高度    | 面积 %    | 高度 %    |
|----|---------|---------|-------|---------|---------|
| 1  | 98.940  | 299147  | 1592  | 3.627   | 3.857   |
| 2  | 103.341 | 7948284 | 39683 | 96.373  | 96.143  |
| 总计 |         | 8247431 | 41275 | 100.000 | 100.000 |

### Ethyl (1S,6S)-6-formyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-1-carboxylate (2n)



Colorless oil, 67.2 mg, 77%, 94% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 3/1. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.24 (s, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 6.52 (d, *J* = 8.1 Hz, 1H), 5.84 (d, *J* = 8.1 Hz, 1H), 4.29 – 4.12 (m, 3H), 3.24 (d, *J* = 12.4 Hz, 1H), 2.44 (s, 3H), 2.35 (d, *J* = 5.1 Hz, 1H), 1.71 (d, *J* = 5.2 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 196.5, 168.2, 144.5, 134.5, 130.1, 127.1, 124.3, 106.8, 62.3, 43.5, 41.8, 36.1, 24.7, 21.6, 14.1. IR (KBr) ν<sub>max</sub> 2921, 1443, 1256, 1166, 1101, 753. HRMS (ESI) [M+Na]<sup>+</sup> calculated for C<sub>17</sub>H<sub>19</sub>NO<sub>5</sub>Na<sup>+</sup>: 372.0876, found 372.0867.

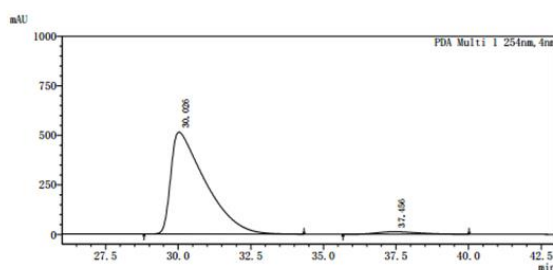
Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 20% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 31.4 min, RT<sub>2</sub> = 37.1 min. [α]<sub>D</sub><sup>25</sup> = +144.7 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



<峰表>

PDA Ch1 254nm

| 峰号 | 保留时间   | 面积       | 高度     | 浓度单位 | 标记 | 化合物名       | 面积%     |
|----|--------|----------|--------|------|----|------------|---------|
| 1  | 31.428 | 7261761  | 107988 | mg/L | M  | RT: 31.428 | 50.274  |
| 2  | 37.079 | 7182567  | 69168  | mg/L | M  | RT: 37.079 | 49.726  |
| 总计 |        | 14444328 | 177155 |      |    |            | 100.000 |

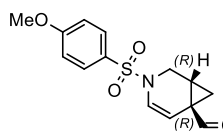


<峰表>

PDA Ch1 254nm

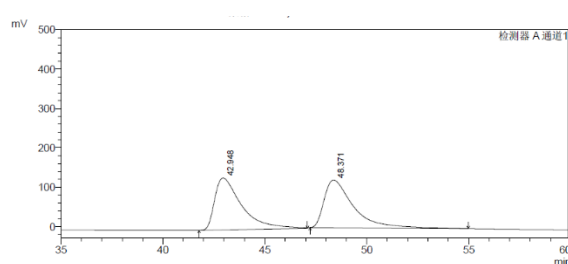
| 峰号 | 保留时间   | 面积       | 高度     | 浓度单位 | 标记 | 化合物名       | 面积%     |
|----|--------|----------|--------|------|----|------------|---------|
| 1  | 30.026 | 42549733 | 514260 | mg/L | M  | RT: 30.026 | 97.088  |
| 2  | 37.456 | 1276146  | 12849  | mg/L | M  | RT: 37.456 | 2.912   |
| 总计 |        | 43825878 | 527109 |      |    |            | 100.000 |

### (1R,6R)-3-((4-Methoxyphenyl)sulfonyl)-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde(2o)



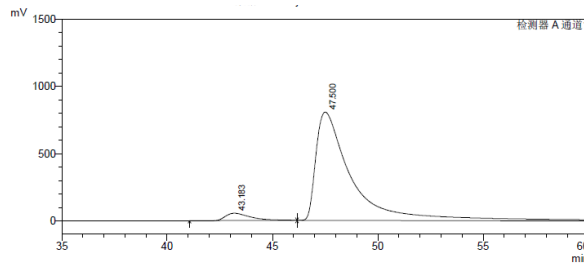
Yellow solid, MP: 187-189 °C, 64.1 mg, 87%, 92% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.01 (d, *J* = 8.3 Hz, 2H), 6.51 (d, *J* = 8.2 Hz, 1H), 5.83 (d, *J* = 8.2 Hz, 1H), 4.09 (d, *J* = 11.9 Hz, 1H), 3.89 (s, 3H), 2.97 (d, *J* = 11.9 Hz, 1H), 2.28 (t, *J* = 7.7 Hz, 1H), 1.61 (dd, *J* = 9.0, 4.7 Hz, 1H), 1.33 – 1.25 (m, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.8, 163.3, 129.2, 129.1, 122.8, 114.5, 106.1, 55.7, 40.2, 29.39, 29.36, 22.2. IR (KBr) ν<sub>max</sub> 2958, 2923, 2849, 2720, 2362, 2332, 1738, 1707, 1594, 1462, 1411, 1349, 1307, 1261, 1161, 1051, 1021, 958, 567, 801, 740, 687, 604, 513, 468, 441, 427. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>14</sub>H<sub>16</sub>NO<sub>4</sub>S<sup>+</sup>: 294.0795, found 294.0794.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 43.2 min, RT<sub>2</sub> = 47.5 min. [α]<sub>D</sub><sup>25</sup> = +78.9 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 42.948 | 12207640 | 131821 | 49.718  | 51.977  |
| 2  | 48.371 | 12346083 | 121791 | 50.282  | 48.023  |
| 总计 |        | 24553723 | 253612 | 100.000 | 100.000 |



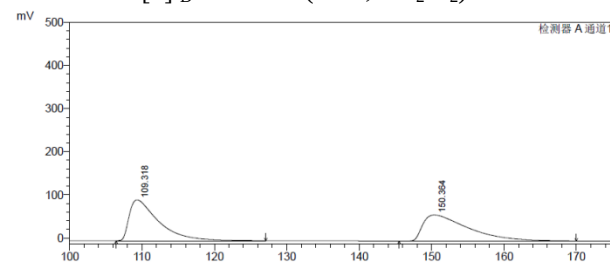
峰表

| 峰# | 保留时间   | 面积        | 高度     | 面积 %    | 高度 %    |
|----|--------|-----------|--------|---------|---------|
| 1  | 43.183 | 4305954   | 64423  | 4.243   | 6.328   |
| 2  | 47.500 | 97185878  | 805559 | 95.757  | 93.672  |
| 总计 |        | 101491833 | 859982 | 100.000 | 100.000 |

### 3-((4-Fluorophenyl)sulfonyl)-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde(2p)

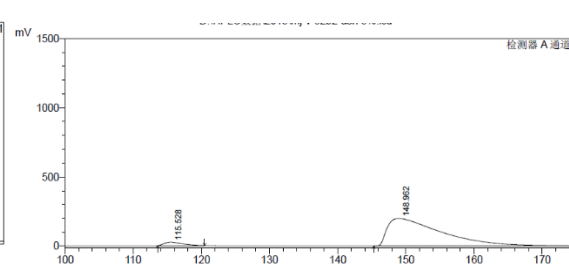
Colorless oil, 63.0 mg, 89%, 92% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.86 (s, 1H), 7.80 (dd, *J* = 8.9, 5.0 Hz, 2H), 7.31 – 7.09 (m, 2H), 6.47 (d, *J* = 8.2 Hz, 1H), 5.86 (d, *J* = 8.1 Hz, 1H), 4.09 (d, *J* = 12.0 Hz, 1H), 2.98 (dd, *J* = 11.9, 2.5 Hz, 1H), 2.29 (ddt, *J* = 9.0, 6.8, 2.1 Hz, 1H), 1.61 (dd, *J* = 9.0, 4.8 Hz, 1H), 1.22 (dd, *J* = 6.9, 4.8 Hz, 1H). <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -103.9. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.6, 165.4 (d, *J* = 256.2 Hz), 133.6 (d, *J* = 3.3 Hz), 129.7 (d, *J* = 9.4 Hz), 122.3, 116.7 (d, *J* = 22.7 Hz), 107.1, 40.3, 29.3, 29.3, 22.2. IR (KBr) ν<sub>max</sub> 2925, 2834, 2740, 1743, 1712, 1647, 1515, 1479, 1442, 1404, 1352, 1258, 1174, 1065, 1003, 935, 873, 748, 712, 669, 594, 537, 468, 430. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>13</sub>H<sub>13</sub>FO<sub>3</sub>S<sup>+</sup>: 282.0595, found 282.0595.

Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 5% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 115.5 min, RT<sub>2</sub> = 149.0 min. [α]<sub>D</sub><sup>25</sup> = +41.9 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



峰表

| 峰# | 保留时间    | 面积       | 高度     | 面积 %    | 高度 %    |
|----|---------|----------|--------|---------|---------|
| 1  | 109.318 | 26806032 | 94680  | 50.400  | 61.001  |
| 2  | 150.364 | 26380676 | 60531  | 49.600  | 38.999  |
| 总计 |         | 53186707 | 155211 | 100.000 | 100.000 |



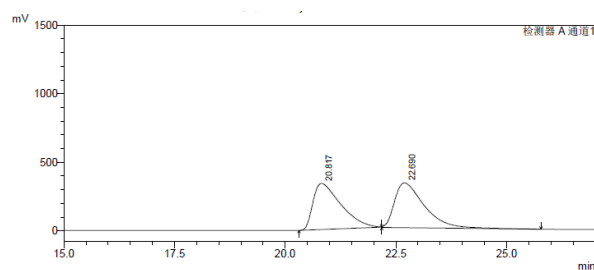
峰表

| 峰# | 保留时间    | 面积        | 高度     | 面积 %    | 高度 %    |
|----|---------|-----------|--------|---------|---------|
| 1  | 115.528 | 4843766   | 24502  | 4.190   | 10.968  |
| 2  | 148.962 | 110771184 | 198892 | 95.810  | 89.032  |
| 总计 |         | 115614950 | 223394 | 100.000 | 100.000 |

### 3-((4-(Trifluoromethyl)phenyl)sulfonyl)-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2q)

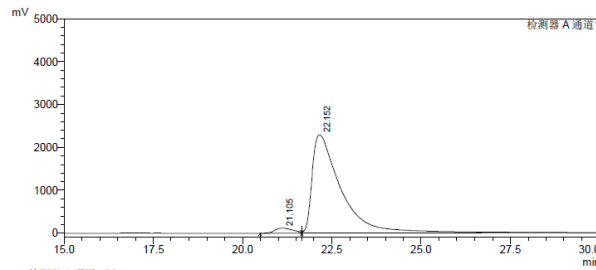
Yellow oil, 69.3 mg, 84%, 94% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.86 (s, 1H), 7.92 (d, *J* = 8.2 Hz, 2H), 7.82 (d, *J* = 8.3 Hz, 2H), 6.48 (d, *J* = 8.2 Hz, 1H), 5.91 (d, *J* = 8.2 Hz, 1H), 4.12 (d, *J* = 12.0 Hz, 1H), 3.01 (d, *J* = 14.2 Hz, 1H), 2.30 (t, *J* = 8.0 Hz, 1H), 1.62 (dd, *J* = 9.0, 4.9 Hz, 1H), 1.19 (dd, *J* = 6.7, 5.0 Hz, 1H). <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.2. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.4, 141.0, 134.9 (d, *J* = 33.3 Hz), 127.5, 126.6 (q, *J* = 3.7 Hz), 123.1 (d, *J* = 273.0 Hz), 122.0, 107.8, 40.4, 29.3, 29.2, 22.3. IR (KBr) ν<sub>max</sub> 2927, 2831, 2724, 2362, 2333, 1715, 1644, 1527, 1463, 1403, 1323, 1256, 1173, 1114, 1061, 1019, 993, 932, 869, 842, 743, 713, 669, 610, 591, 537, 464, 429. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>14</sub>H<sub>13</sub>F<sub>3</sub>NO<sub>3</sub>S<sup>+</sup>: 332.0563, found 332.0562.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 21.1 min, RT<sub>2</sub> = 22.2 min. [α]<sub>D</sub><sup>25</sup> = +95.6 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 20.817 | 14665452 | 336059 | 49.095  | 50.759  |
| 2  | 22.690 | 15205974 | 326014 | 50.905  | 49.241  |
| 总计 |        | 29871426 | 662073 | 100.000 | 100.000 |

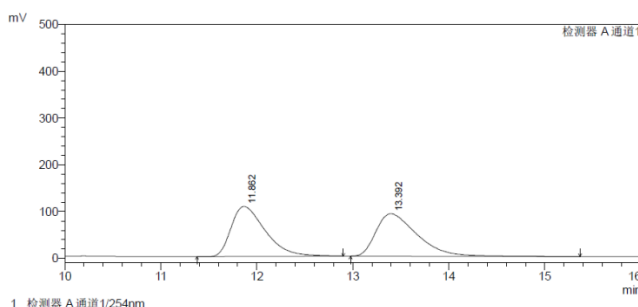


峰表

| 峰# | 保留时间   | 面积        | 高度      | 面积 %    | 高度 %    |
|----|--------|-----------|---------|---------|---------|
| 1  | 21.105 | 4156737   | 113109  | 3.060   | 4.931   |
| 2  | 22.152 | 131669597 | 2296307 | 96.940  | 95.069  |
| 总计 |        | 135826334 | 2415416 | 100.000 | 100.000 |

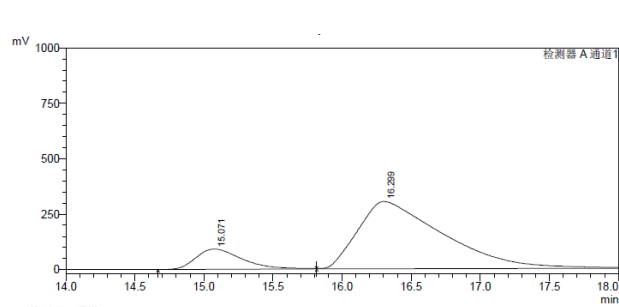
### 3-((Trifluoromethyl)sulfonyl)-3-azabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2r)

Yellow oil, 58.7 mg, 92%, 72% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) 8.98 (s, 1H), 6.35 (d, *J* = 8.1 Hz, 1H), 6.16 (d, *J* = 8.1 Hz, 1H), 4.23 (d, *J* = 12.5 Hz, 1H), 3.45 (d, *J* = 12.5 Hz, 1H), 2.47 (ddt, *J* = 9.0, 6.9, 2.1 Hz, 1H), 1.85 (dd, *J* = 9.0, 5.3, 1H), 1.59 (t, *J* = 6.1 Hz, 1H). <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -75.0. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 196.8, 120.9, 119.7 (d, *J* = 323.6 Hz), 111.0, 41.7, 29.4, 29.0, 21.9. IR (KBr) ν<sub>max</sub> 2927, 2831, 2724, 1715, 1645, 1461, 1407, 1353, 1240, 1170, 1115, 780, 743, 715, 687, 661, 585, 441. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>8</sub>H<sub>9</sub>F<sub>3</sub>NO<sub>3</sub>S<sup>+</sup>: 256.0250, found 256.0250. Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 15.1 min, RT<sub>2</sub> = 16.3 min. [α]<sub>D</sub><sup>25</sup> = +13.5 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



峰表

| 峰# | 保留时间   | 面积      | 高度     | 面积 %    | 高度 %    |
|----|--------|---------|--------|---------|---------|
| 1  | 11.862 | 2666298 | 107313 | 49.388  | 54.104  |
| 2  | 13.392 | 2732391 | 91031  | 50.612  | 45.896  |
| 总计 |        | 5398690 | 198345 | 100.000 | 100.000 |



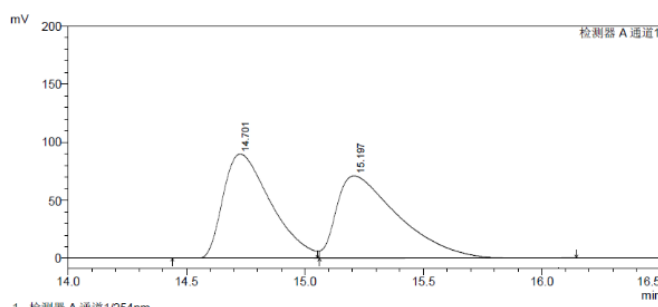
峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 15.071 | 2144432  | 91839  | 14.020  | 23.191  |
| 2  | 16.299 | 13151099 | 304180 | 85.980  | 76.809  |
| 总计 |        | 15295532 | 396018 | 100.000 | 100.000 |

### 1-Methyl-3-oxabicyclo[4.1.0]hept-4-ene-6-carbaldehyde (2s)

Colorless oil, 33.9 mg, 99%, 20% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 10/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.34 (s, 1H), 6.37 (d, *J* = 5.8 Hz, 1H), 5.78 (d, *J* = 5.8 Hz, 1H), 4.02 (d, *J* = 10.9 Hz, 1H), 3.52 (d, *J* = 10.9 Hz, 1H), 1.83 (s, 2H), 1.36 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 199.0, 142.5, 102.7, 66.6, 38.4, 29.7, 28.2, 14.9. IR (KBr) ν<sub>max</sub> 2925, 2831, 2723, 1716, 1649, 1466, 1447, 1408, 1392, 1339, 1215, 1091, 1062, 1033, 968, 933, 891, 811, 764, 671, 544, 506, 490, 442. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>8</sub>H<sub>11</sub>O<sub>2</sub><sup>+</sup>: 139.0754, found 139.0754.

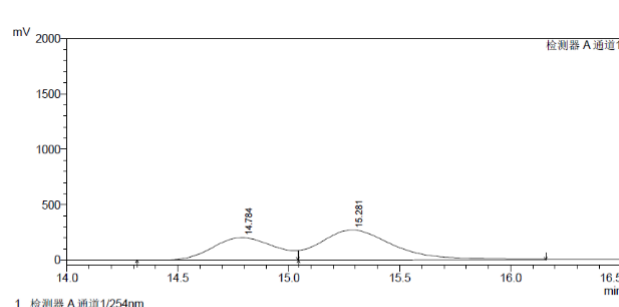
Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 1% IPA-Hexanes, 0.5 mL/min, 254 nm, RT<sub>1</sub> = 14.8 min, RT<sub>2</sub> = 15.3 min. [α]<sub>D</sub><sup>25</sup> = +3.1 (c 0.2, CH<sub>2</sub>Cl<sub>2</sub>)



1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积      | 高度     | 面积 %    | 高度 %    |
|----|--------|---------|--------|---------|---------|
| 1  | 14.701 | 3095254 | 95746  | 49.783  | 60.897  |
| 2  | 15.197 | 3122196 | 61480  | 50.217  | 39.103  |
| 总计 |        | 6217450 | 157226 | 100.000 | 100.000 |

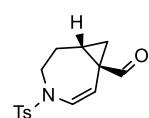


1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积      | 高度     | 面积 %    | 高度 %    |
|----|--------|---------|--------|---------|---------|
| 1  | 14.784 | 4001057 | 199417 | 40.221  | 42.979  |
| 2  | 15.281 | 5946824 | 264565 | 59.779  | 57.021  |
| 总计 |        | 9947881 | 463982 | 100.000 | 100.000 |

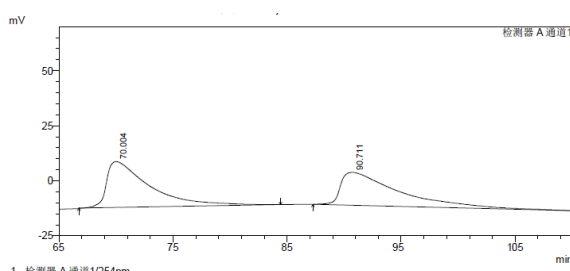
#### 4-Tosyl-4-azabicyclo[5.1.0]oct-2-ene-1-carbaldehyde (2t)



Yellow oil, 54.7 mg, 75%, 4% ee, purified by chromatograph (SiO<sub>2</sub>), PE/EA = 5/1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.87 (s, 1H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.3 Hz, 2H), 6.60 (d, *J* = 10.1 Hz, 1H), 5.23 (d, *J* = 10.1 Hz, 1H), 3.70 (dd, *J* = 13.5, 8.6 Hz, 1H), 3.30 (dd, *J* = 13.4, 9.1 Hz, 1H), 2.53-2.38 (m, 4H), 1.98 - 1.86 (m, 1H), 1.67 - 1.60 (m, 1H), 1.53 (dd, *J* = 9.1, 4.3 Hz, 1H), 0.96 (dd, *J* = 6.9, 4.4 Hz, 1H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 199.8, 144.0, 135.7, 129.9, 126.9, 126.0, 104.4, 46.1, 34.6, 27.8, 27.7, 24.9, 21.6. IR (KBr) ν<sub>max</sub> 2925, 2859, 2724, 1711, 1648, 1597, 1492, 1448, 1406, 1384, 1340, 1272, 1219, 1164, 1110, 1077, 1019, 995, 969, 931, 867, 832, 824, 804, 682, 629, 601, 544, 497, 486, 464. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>15</sub>H<sub>18</sub>NO<sub>3</sub>S<sup>+</sup>: 292.1002, found 292.1002.

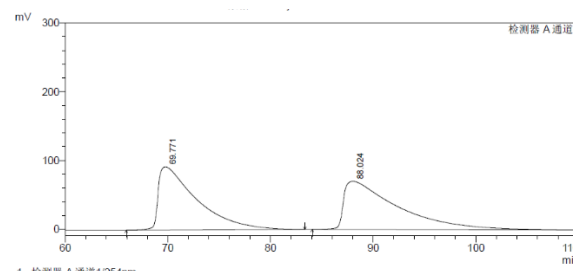
Resolution of enantiomers: REGIS Whelk-O-1 column, 10% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 69.8 min, RT<sub>2</sub> = 88.0 min.



1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积       | 高度    | 面积 %    | 高度 %    |
|----|--------|----------|-------|---------|---------|
| 1  | 70.004 | 5459384  | 20828 | 50.695  | 58.223  |
| 2  | 90.711 | 5309589  | 14944 | 49.305  | 41.777  |
| 总计 |        | 10768973 | 35772 | 100.000 | 100.000 |



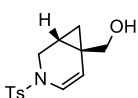
1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 69.771 | 23975671 | 91783  | 48.018  | 56.669  |
| 2  | 88.024 | 25954706 | 70179  | 51.982  | 43.331  |
| 总计 |        | 49930377 | 161963 | 100.000 | 100.000 |

## 6. The derivatization of azabicyclo[4.1.0]hept-4-ene

### 3-Tosyl-3-azabicyclo[4.1.0]hept-4-en-6-yl)methanol (2u) [8]

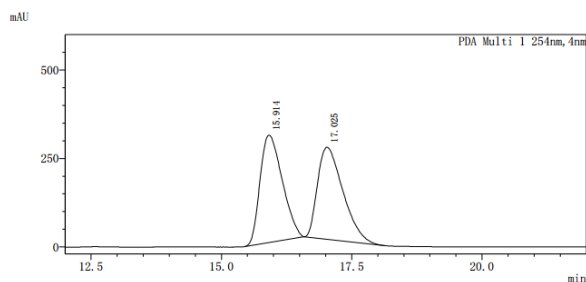


The substrates **2a** (139mg, 90% ee, 0.5 mmol) and NaBH<sub>4</sub> (2.0 equiv, 1.0 mmol) were taken in 2mL MeOH at room temperature. The reaction was monitored by TLC until disappearance of the starting material. Then the reaction mixture was purified by silica gel column chromatography to obtain the product **5** (Colorless oil, 114.5mg, 82%, 90% ee, PE/EA = 2/1)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.39 – 7.28 (m, 2H), 6.43 (dd, *J* = 8.2, 0.9 Hz, 1H), 5.41 (dd, *J* = 8.2, 0.9 Hz, 1H), 3.98 – 3.85 (m, 1H), 3.53 (d, *J* = 11.1 Hz, 1H), 3.35 (d, *J* = 11.2 Hz, 1H), 3.03 (dd, *J* = 11.6, 2.8 Hz, 1H), 2.42 (s, 3H), 1.69 (s, 1H), 1.54 – 1.42 (m, 1H), 0.76 (ddd, *J* = 8.7, 4.7, 0.9 Hz, 1H), 0.55 (t, *J* = 5.2 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 143.8, 134.8, 129.8, 127.0, 122.1, 112.2, 68.2, 40.9, 23.3, 21.5, 19.9, 17.7. IR (KBr) ν<sub>max</sub> 3341, 3095, 3027, 2924, 1656, 1597, 1493, 1406, 1350, 1215, 1165, 1117, 1053, 1042, 984, 958, 945, 899, 867, 766, 707, 683,

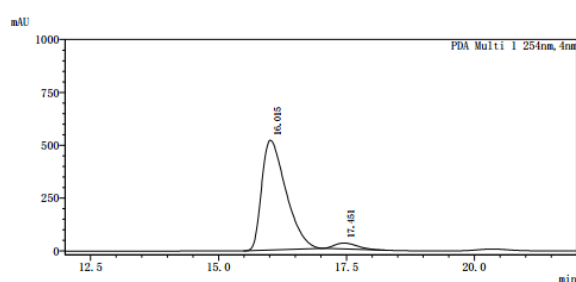
644, 602, 555, 545, 491, 466. **HRMS** (ESI)  $[M+H]^+$  calculated for  $C_{14}H_{18}NO_3S^+$ : 280.1002, found 280.1004.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $RT_1 = 16.0$  min,  $RT_2 = 17.5$  min.  $[\alpha]_D^{20} = +52.2$  (c 0.5,  $CH_2Cl_2$ )



<峰表>

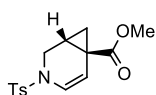
| 峰号 | 保留时间   | 面积       | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|--------|----------|------|----|-----------|---------|
| 1  | 15.914 | 9001643  | mg/L | M  | RT:15.914 | 50.403  |
| 2  | 17.025 | 8857724  | mg/L | M  | RT:17.025 | 49.597  |
| 总计 |        | 17859368 |      |    |           | 100.000 |



<峰表>

| 峰号 | 保留时间   | 面积       | 高度     | 浓度单位 | 标记 | 化合物名      | 面积%     |
|----|--------|----------|--------|------|----|-----------|---------|
| 1  | 16.015 | 17155259 | 519706 | mg/L | M  | RT:16.015 | 95.292  |
| 2  | 17.451 | 847646   | 27523  | mg/L | M  | RT:17.451 | 4.708   |
| 总计 |        | 18002905 | 547229 |      |    |           | 100.000 |

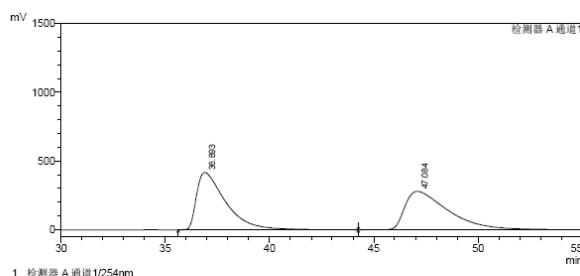
### Methyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene-6-carboxylate (**2v**) [9]



The substrates **2a** (139 mg, 90% ee, 0.5 mmol), NaOClO (3.0 equiv, 1.5 mmol),  $NaH_2PO_4$  (4.0 equiv, 2.0 mmol) were taken in the mixed solvent 2-Methyl-2-butene/tBuOH/ $H_2O$  (3/3/1, 7 mL) at room temperature. The reaction was monitored by TLC until disappearance of the starting material. Then the reaction mixture was purified by flash column chromatography with DCM. The obtained product was dissolved in DMF (4 mL), then MeI (2.0 equiv, 1.0 mmol) and  $K_2CO_3$  (2.0 equiv, 1 mmol) were added. After the reaction was completely proceed, the reaction mixture was extracted with water and DCM. Combined organic layers were washed with brine, dried over  $MgSO_4$ , and evaporated. **6** was obtained by column chromatography (Colorless oil, 110.4mg, 72%, 89% ee, PE/EA = 2/1).

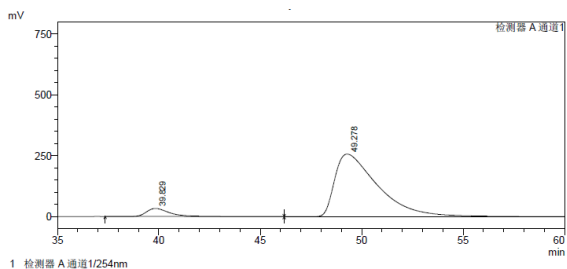
**$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.65 (d,  $J = 8.3$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 6.39 (d,  $J = 8.5$  Hz, 1H), 5.79 (d,  $J = 8.5$  Hz, 1H), 4.00 (d,  $J = 11.7$  Hz, 1H), 3.67 (s, 3H), 2.95 (d,  $J = 14.2$  Hz, 1H), 2.42 (s, 3H), 2.26 (t,  $J = 7.9$  Hz, 1H), 1.56 (dd,  $J = 9.0, 4.1$  Hz, 1H), 0.99 (dd,  $J = 6.8, 4.2$  Hz, 1H).  **$^{13}C$  NMR** (100 MHz,  $CDCl_3$ )  $\delta$  172.6, 144.0, 134.6, 129.9, 127.1, 121.4, 108.6, 52.2, 40.0, 29.9, 23.8, 21.5, 20.6. **IR** (KBr)  $\nu_{max}$  2924, 1750, 1646, 1603, 1624, 1460, 1403, 1247, 1171, 1065, 1034, 1008, 683, 544, 478, 468, 450. **HRMS** (ESI)  $[M+H]^+$  calculated for  $C_{15}H_{18}NO_4S^+$ : 308.0951, found 308.0951.

Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm,  $RT_1 = 39.8$  min,  $RT_2 = 49.3$  min.  $[\alpha]_D^{20} = +36.1$  (c 0.5,  $CH_2Cl_2$ )



峰表

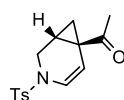
| 峰号 | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 36.893 | 40833731 | 417318 | 49.884  | 59.886  |
| 2  | 47.084 | 41026651 | 279540 | 50.116  | 40.114  |
| 总计 |        | 81861382 | 696858 | 100.000 | 100.000 |



峰表

| 峰号 | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 39.829 | 2340942  | 32709  | 5.836   | 11.304  |
| 2  | 49.278 | 37768638 | 256643 | 94.164  | 88.696  |
| 总计 |        | 40109580 | 289353 | 100.000 | 100.000 |

### 3-Tosyl-3-azabicyclo[4.1.0]hept-4-en-6-yl)ethan-1-one (**2w**)

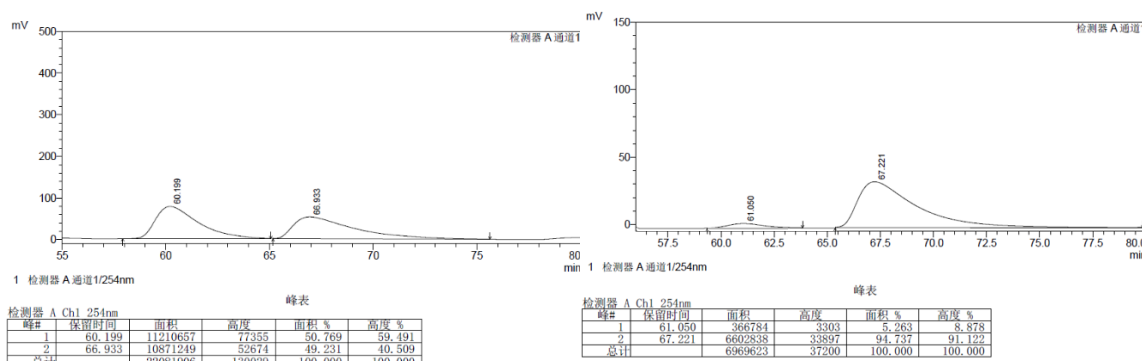


The substrates **2a** (139 mg, 90% ee, 0.5 mmol) was dissolved in THF (2 mL) at 0 °C, MeMgBr (1.5 equiv, 0.75 mmol, 1.0 mol/L) was added into the solution. After 2 h, the solvent was removed. The mixture was

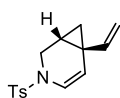
redissolved in DCM, and DMP (1.2 equiv, 0.6 mmol) was then added. The reaction mixture was stirred at room temperature for 2h. Then, the mixture was purified by silica gel column chromatography to obtain the product **11** (Colorless oil, 110.6 mg, 76%, 90 % ee, PE/EA = 5/1)

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.47 (d, *J* = 8.3 Hz, 1H), 5.79 (d, *J* = 8.3 Hz, 1H), 4.01 (d, *J* = 11.9 Hz, 1H), 2.99 (dd, *J* = 11.9, 2.6 Hz, 1H), 2.44 (s, 3H), 2.32 – 2.21 (m, 1H), 2.17 (s, 3H), 1.62 (dd, *J* = 9.0, 4.1 Hz, 1H), 1.01 (dd, *J* = 6.9, 4.1 Hz, 1H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 205.5, 144.1, 134.5, 129.9, 127.0, 121.9, 108.6, 40.2, 31.1, 28.7, 26.7, 25.7, 21.6. **IR** (KBr) ν<sub>max</sub> 3046, 3002, 2935, 2925, 2861, 1715, 1667, 1641, 1594, 1453, 1405, 1347, 1164, 1117, 931, 763, 708, 683, 544, 470. **HRMS** (ESI) [*M*+*H*]<sup>+</sup> calculated for C<sub>15</sub>H<sub>18</sub>NO<sub>3</sub>S<sup>+</sup>: 292.1002, found 292.1004.

Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 1% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 61.0 min, RT<sub>2</sub> = 67.2 min. [*α*]<sub>D</sub><sup>20</sup> = -52.0 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



### 3-Tosyl-6-vinyl-3-azabicyclo[4.1.0]hept-4-ene (**3**) [10]

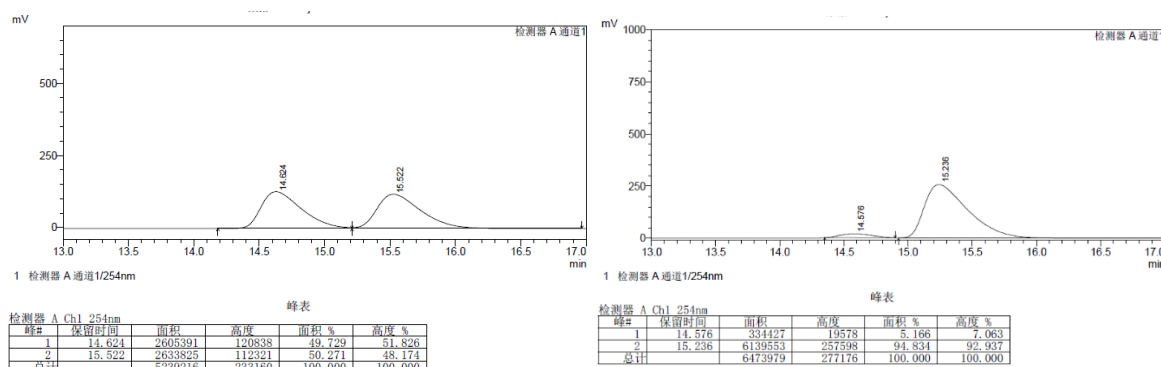


The MePh<sub>3</sub>PBr (2.0 equiv, 1.0 mmol) was dissolved in THF (2mL) at -78 °C, then n-BuLi (1.5 equiv, 0.75 mmol, 2.5 mol/L) was added dropwise. After 2 h, the substrates **2a** (139mg, 90% ee, 0.5 mmol) in

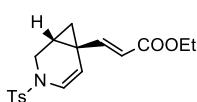
THF (2mL) was added into the mixture. The reaction was monitored by TLC until disappearance of the starting material. Then the reaction mixture was purified by silica gel column chromatography to obtain the product **7** (Colorless oil, 116.5mg, 85%, 90% ee, PE/EA = 5/1)

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 6.42 (d, *J* = 8.3 Hz, 1H), 5.52 – 5.37 (m, 2H), 5.06 – 4.90 (m, 2H), 3.92 (d, *J* = 11.6 Hz, 1H), 3.04 (dd, *J* = 11.6, 2.7 Hz, 1H), 2.42 (s, 3H), 1.57 (t, *J* = 7.4 Hz, 1H), 0.97 (dd, *J* = 8.6, 4.5 Hz, 1H), 0.82 (dd, *J* = 6.0, 4.7 Hz, 1H). **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>) δ 143.8, 141.6, 134.8, 129.8, 127.1, 121.3, 111.4, 111.3, 40.5, 27.6, 22.7, 21.5, 19.5. **IR** (KBr) ν<sub>max</sub> 3061, 2924, 1945, 1826, 1652, 1641, 1496, 1451, 1436, 1421, 1291, 1260, 1116, 1043, 1026, 992, 946, 912, 815, 762, 707, 644, 601, 535, 466, 432. **HRMS** (ESI) [*M*+*H*]<sup>+</sup> calculated for C<sub>15</sub>H<sub>18</sub>NO<sub>2</sub>S<sup>+</sup>: 276.1053, found 276.1054.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 1% IPA-Hexanes, 1.0mL/min, 254 nm, RT<sub>1</sub> = 14.6 min, RT<sub>2</sub> = 15.2 min. [*α*]<sub>D</sub><sup>20</sup> = +30.3 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



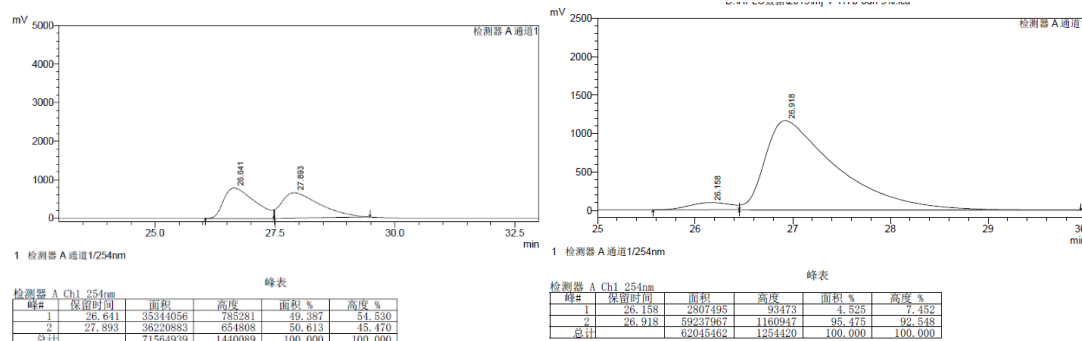
### Ethyl (E)-3-((1R,6R)-3-tosyl-3-azabicyclo[4.1.0]hept-4-en-6-yl)acrylate (4) [11]



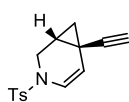
The substrates **2a** (139mg, 90% ee, 0.5 mmol) and  $\text{Ph}_3\text{PCHCOOEt}$  (1.2 equiv, 0.6 mmol) were dissolved in DCM at room temperature. The reaction was monitored by TLC until disappearance of the starting material. Then the reaction mixture was purified by silica gel column chromatography to obtain the product **8** (Colorless oil, 114.0mg, 83%, 91 % ee, PE/EA = 5/1)

**$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J$  = 8.3 Hz, 2H), 7.32 (d,  $J$  = 8.0 Hz, 2H), 6.52 – 6.40 (m, 2H), 5.80 (d,  $J$  = 15.7 Hz, 1H), 5.43 (d,  $J$  = 8.4 Hz, 1H), 4.16 (q,  $J$  = 7.1 Hz, 2H), 3.98 (d,  $J$  = 11.7 Hz, 1H), 3.04 (dd,  $J$  = 11.8, 2.8 Hz, 1H), 2.43 (s, 3H), 1.80 (ddd,  $J$  = 8.9, 6.3, 2.9 Hz, 1H), 1.26 (t,  $J$  = 7.1 Hz, 3H), 1.21 (dd,  $J$  = 8.8, 4.7 Hz, 1H), 1.07 (dd,  $J$  = 6.5, 4.8 Hz, 1H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.5, 152.2, 144.0, 134.6, 129.9, 127.1, 122.2, 117.9, 109.3, 60.3, 40.4, 29.4, 24.6, 21.6, 19.8, 14.3. **IR** (KBr)  $\nu_{\text{max}}$  3030, 2957, 2925, 2894, 2364, 2333, 2244, 1725, 1646, 1595, 1493, 1458, 1270, 1183, 1058, 1024, 983, 936, 867, 815, 767, 707, 683, 545, 568, 477, 435. **HRMS** (ESI)  $[\text{M}+\text{H}]^+$  calculated for  $\text{C}_{18}\text{H}_{22}\text{NO}_4\text{S}^+$ : 348.1264, found 348.1266.

Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm,  $\text{RT}_1$  = 26.2 min,  $\text{RT}_2$  = 26.9 min.  $[\alpha]_{\text{D}}^{20}$  = +55.5 (c 0.5,  $\text{CH}_2\text{Cl}_2$ )



### 6-Ethynyl-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene (5) [12]

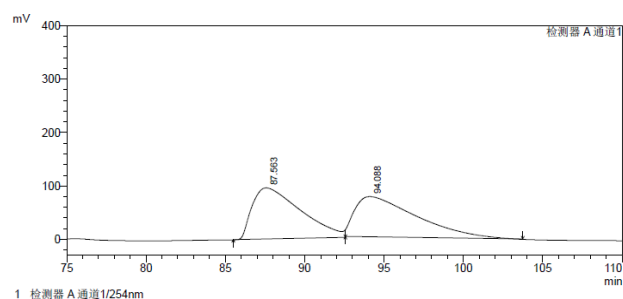


The substrates **2a** (139 mg, 90% ee, 0.5 mmol) and  $\text{Ph}_3\text{P}$  (2.0 equiv, 1.0 mmol) were dissolved in DCM (2 mL) at room temperature, and the  $\text{CBr}_4$  (1.5 equiv, 0.75mmol) solution in DCM (2mL) was added dropwise. After **2a** was completely consumed, the solvent was removed. Then obtained mixture was redissolved in THF (2 mL) and  $\text{nBuLi}$  (3.0 equiv, 1.5mmol) was added dropwise at  $-78^\circ\text{C}$ . After 2 h, saturated  $\text{NH}_4\text{Cl}$  solution was added into the reaction. The mixture was extracted with  $\text{EtOAc}$ . Combined organic layers were washed with brine, dried over  $\text{MgSO}_4$ , chromatography to obtain the product **9** (Colorless oil, 112.1 mg, 82%, 90 % ee, PE/EA = 5/1)

**$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J$  = 8.3 Hz, 2H), 7.33 (d,  $J$  = 8.0 Hz, 2H), 6.34 (d,  $J$  = 8.2 Hz, 1H), 5.37 (d,  $J$  = 8.2 Hz, 1H), 3.93 (d,  $J$  = 11.7 Hz, 1H), 3.04 (dd,  $J$  = 11.8, 2.5 Hz, 1H), 2.43 (s, 3H), 2.02 – 1.92 (m, 1H), 1.88 (s, 1H), 1.25 (dd,  $J$  = 8.8, 4.6 Hz, 1H), 0.91 (dd,  $J$  = 6.5, 4.6 Hz, 1H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.0, 134.5, 129.9, 127.0,

121.0, 111.8, 87.0, 64.5, 39.9, 29.3, 23.5, 21.5, 8.6. **IR** (KBr)  $\nu_{\text{max}}$  3291, 2958, 2113, 1644, 1608, 1528, 1407, 1357, 1285, 1186, 1117, 1091, 997, 969, 765, 665, 590, 548, 498, 468. **HRMS** (ESI)  $[M+H]^+$  calculated for  $C_{15}H_{16}NO_2S^+$ : 274.0896, found 274.0897.

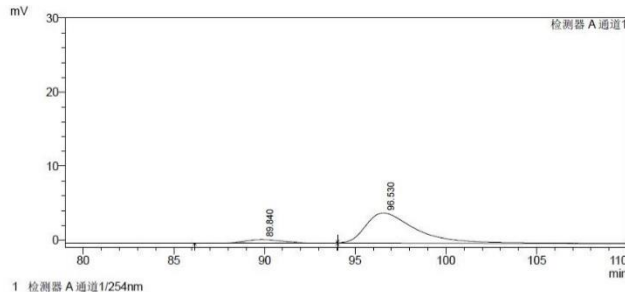
Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 1% IPA-Hexanes, 1.0 mL/min, 254 nm,  $RT_1 = 89.8$  min,  $RT_2 = 96.5$  min.  $[\alpha]_D^{20} = +4.0$  (c 0.5,  $CH_2Cl_2$ )



1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积 %    | 高度 %    |
|----|--------|----------|--------|---------|---------|
| 1  | 87.563 | 20383160 | 95650  | 49.859  | 55.951  |
| 2  | 94.088 | 20498344 | 75304  | 50.141  | 44.049  |
| 总计 |        | 40881504 | 170953 | 100.000 | 100.000 |

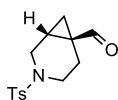


1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积     | 高度   | 面积 %    | 高度 %    |
|----|--------|--------|------|---------|---------|
| 1  | 89.840 | 44821  | 410  | 5.355   | 9.192   |
| 2  | 96.530 | 792139 | 4048 | 94.645  | 90.808  |
| 总计 |        | 836960 | 4457 | 100.000 | 100.000 |

### 3-Tosyl-3-azabicyclo[4.1.0]heptane-6-carbaldehyde (6) [13]



The substrates **2a** (139 mg, 90% ee, 0.5 mmol) was dissolved in DCM (2 mL) at room temperature,  $Et_3SiH$  (2.0 equiv, 1.0 mmol) and TFA (2.0 equiv, 1.0 mmol) were subsequently added into the solution. The reaction was stirred at room temperature overnight. The mixture was purified by silica gel column

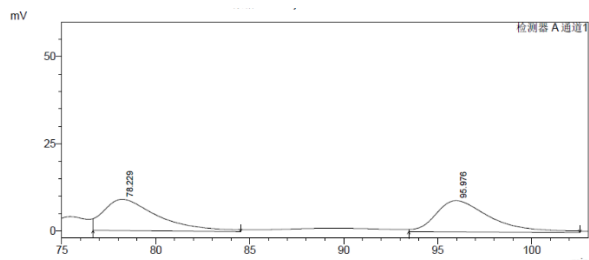
chromatography to obtain the product **10** (Colorless oil, 99.7 mg, 71%, 90 % ee, PE/EA = 5/1)

**$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  8.62 (s, 1H), 7.64 (d,  $J = 8.2$  Hz, 2H), 7.34 (d,  $J = 8.1$  Hz, 2H), 3.93 (d,  $J = 11.8$  Hz, 1H), 3.56 (dd,  $J = 11.1, 7.4$  Hz, 1H), 2.81 (dd,  $J = 11.8, 4.1$  Hz, 1H), 2.78 – 2.70 (m, 1H), 2.45 (s, 3H), 2.18 (td,  $J = 11.9, 5.0$  Hz, 1H), 1.80 (ddd,  $J = 14.3, 11.8, 6.6$  Hz, 1H), 1.72 – 1.64 (m, 1H), 1.45 (dd,  $J = 9.3, 5.0$  Hz, 1H), 1.33 – 1.25 (m, 1H).

**$^{13}C$  NMR** (100 MHz,  $CDCl_3$ )  $\delta$  199.7, 143.8, 133.4, 129.8, 127.5, 43.9, 43.1, 29.4, 21.5, 21.2, 20.1, 17.8. **IR** (KBr)  $\nu_{\text{max}}$  2925, 2850, 2728, 1734, 1704, 1645, 1637, 1495, 1349, 1284, 1258, 1163, 1118, 1091, 1055, 934, 903, 812, 545, 469.

**HRMS** (ESI)  $[M+H]^+$  calculated for  $C_{14}H_{18}NO_3S^+$ : 280.1002, found 280.1004.

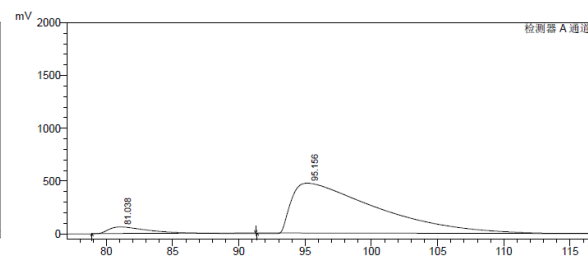
Resolution of enantiomers: DAICEL Chiralcel® AS-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $RT_1 = 81.0$  min,  $RT_2 = 95.2$  min.  $[\alpha]_D^{20} = +5.5$  (c 0.5,  $CH_2Cl_2$ )



1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积      | 高度    | 面积 %    | 高度 %    |
|----|--------|---------|-------|---------|---------|
| 1  | 78.229 | 1807246 | 8969  | 49.929  | 50.138  |
| 2  | 95.976 | 1812393 | 8920  | 50.071  | 49.862  |
| 总计 |        | 3619639 | 17888 | 100.000 | 100.000 |

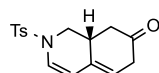


1 检测器 A 通道1/254nm

峰表

| 峰# | 保留时间   | 面积        | 高度     | 面积 %    | 高度 %    |
|----|--------|-----------|--------|---------|---------|
| 1  | 81.038 | 11243678  | 61556  | 5.036   | 11.542  |
| 2  | 95.156 | 212043018 | 471147 | 94.964  | 88.458  |
| 总计 |        | 223286697 | 533303 | 100.000 | 100.000 |

### 2-Tosyl-1,2,8,8a-tetrahydroisoquinolin-7(6H)-one (7)

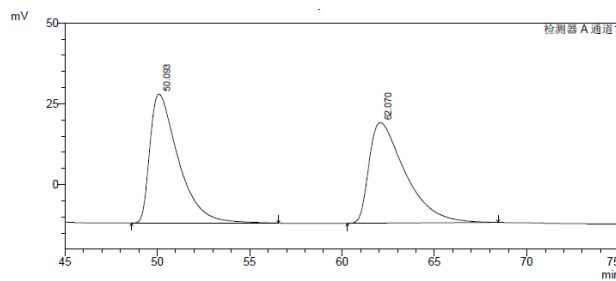


The reaction was operated following the literature [14] with **5** (54 mg, 90% ee). The product **9** (37.8 mg, 63%, 90 % ee, PE/EA = 3/1) was obtained.

**$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.67 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 6.73 (d,  $J = 8.0$  Hz, 1H), 5.60 – 5.44 (m, 2H), 3.93 (d,  $J = 6.9$  Hz, 1H), 3.14 – 2.83 (m, 2H), 2.75 – 2.64 (m, 2H), 2.48 (dd,  $J = 14.3, 4.0$  Hz, 1H), 2.43 (s, 3H),

2.18 – 2.08 (m, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 207.2, 144.3, 134.7, 131.4, 130.0, 127.0, 125.5, 118.5, 109.5, 48.6, 42.2, 40.1, 33.6, 21.6.

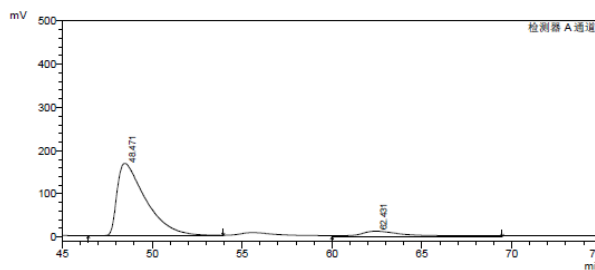
Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 5% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 48.5 min, RT<sub>2</sub> = 62.4 min. [α]<sub>D</sub><sup>20</sup> = -21.0 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



1 检测器 A 通道 1/254nm

峰表

| 峰# | 保留时间   | 面积      | 高度    | 面积%     | 高度%     |
|----|--------|---------|-------|---------|---------|
| 1  | 50.093 | 4290964 | 39938 | 50.288  | 56.236  |
| 2  | 62.070 | 4241778 | 31081 | 49.712  | 43.764  |
| 总计 |        | 8532742 | 71019 | 100.000 | 100.000 |

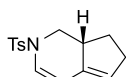


1 检测器 A 通道 1/254nm

峰表

| 峰# | 保留时间   | 面积       | 高度     | 面积%     | 高度%     |
|----|--------|----------|--------|---------|---------|
| 1  | 48.471 | 18638344 | 167502 | 94.885  | 94.359  |
| 2  | 62.431 | 1004734  | 10014  | 5.115   | 5.641   |
| 总计 |        | 19643078 | 177515 | 100.000 | 100.000 |

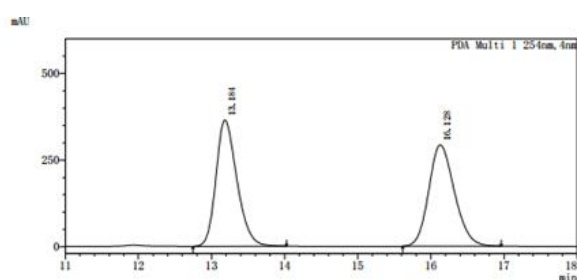
## 2-tosyl-2,6,7,7a-tetrahydro-1H-cyclopenta[c]pyridine (8)



The reaction was operated following the literature [14] with **5** (54 mg, 90% ee). The product **10** (20 mg, 37%, 90 % ee, PE/EA = 3/1) was obtained.

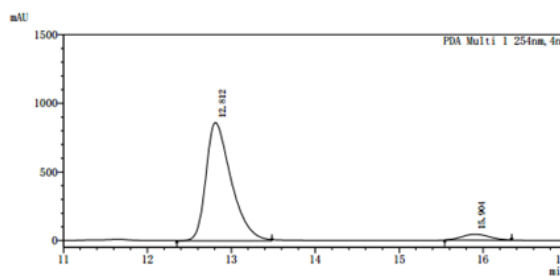
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.67 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 2H), 6.71 (d, *J* = 7.8 Hz, 1H), 5.63 (d, *J* = 7.9 Hz, 1H), 5.43 (s, 1H), 4.14 (dd, *J* = 10.9, 4.4 Hz, 1H), 2.67 (s, 1H), 2.57 (t, *J* = 11.6 Hz, 1H), 2.42 (s, 3H), 2.34 (d, *J* = 8.5 Hz, 2H), 2.10 (dd, *J* = 12.2, 6.4 Hz, 1H), 1.26 (t, *J* = 10.5 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 143.8, 136.4, 135.3, 129.8, 127.0, 126.1, 122.9, 105.3, 50.2, 41.4, 31.9, 29.1, 21.5. IR (KBr) ν<sub>max</sub> 3665, 2961, 1724, 1593, 1454, 1344, 1164, 1095, 970, 813, 688, 547. HRMS (ESI) [M+H]<sup>+</sup> calculated for C<sub>15</sub>H<sub>18</sub>NO<sub>2</sub>S<sup>+</sup>: 276.1053, found 276.1052

.Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm, RT<sub>1</sub> = 18.2 min, RT<sub>2</sub> = 16.1 min. [α]<sub>D</sub><sup>20</sup> = +72.3 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>)



<峰表>

| 峰# | 保留时间   | 面积       | 高度     | 面积%     | 高度%     |
|----|--------|----------|--------|---------|---------|
| 1  | 13.184 | 7272758  | 364512 | 50.410  | 55.496  |
| 2  | 16.128 | 7154320  | 292313 | 49.590  | 44.504  |
| 总计 |        | 14427078 | 656825 | 100.000 | 100.000 |



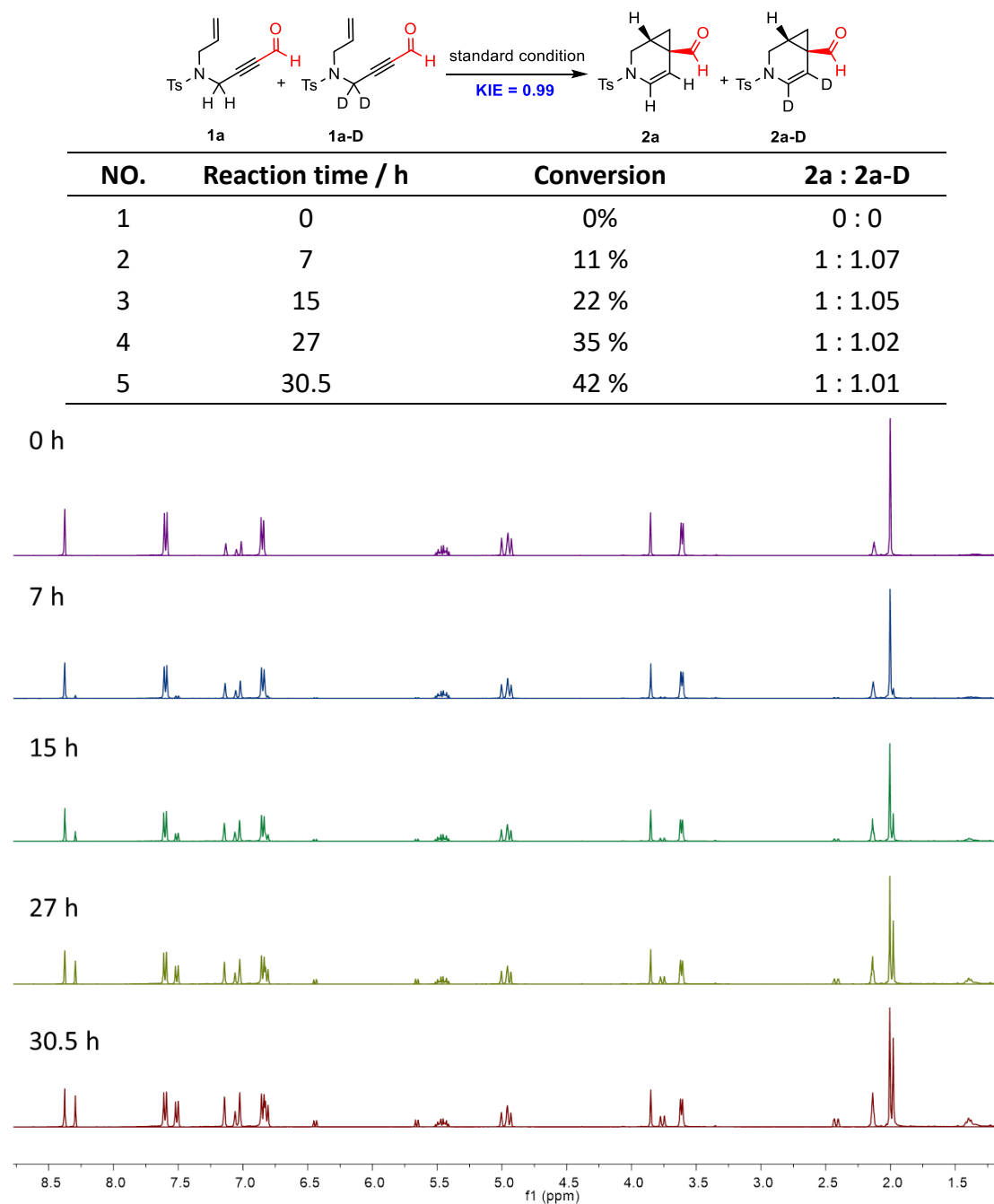
<峰表>

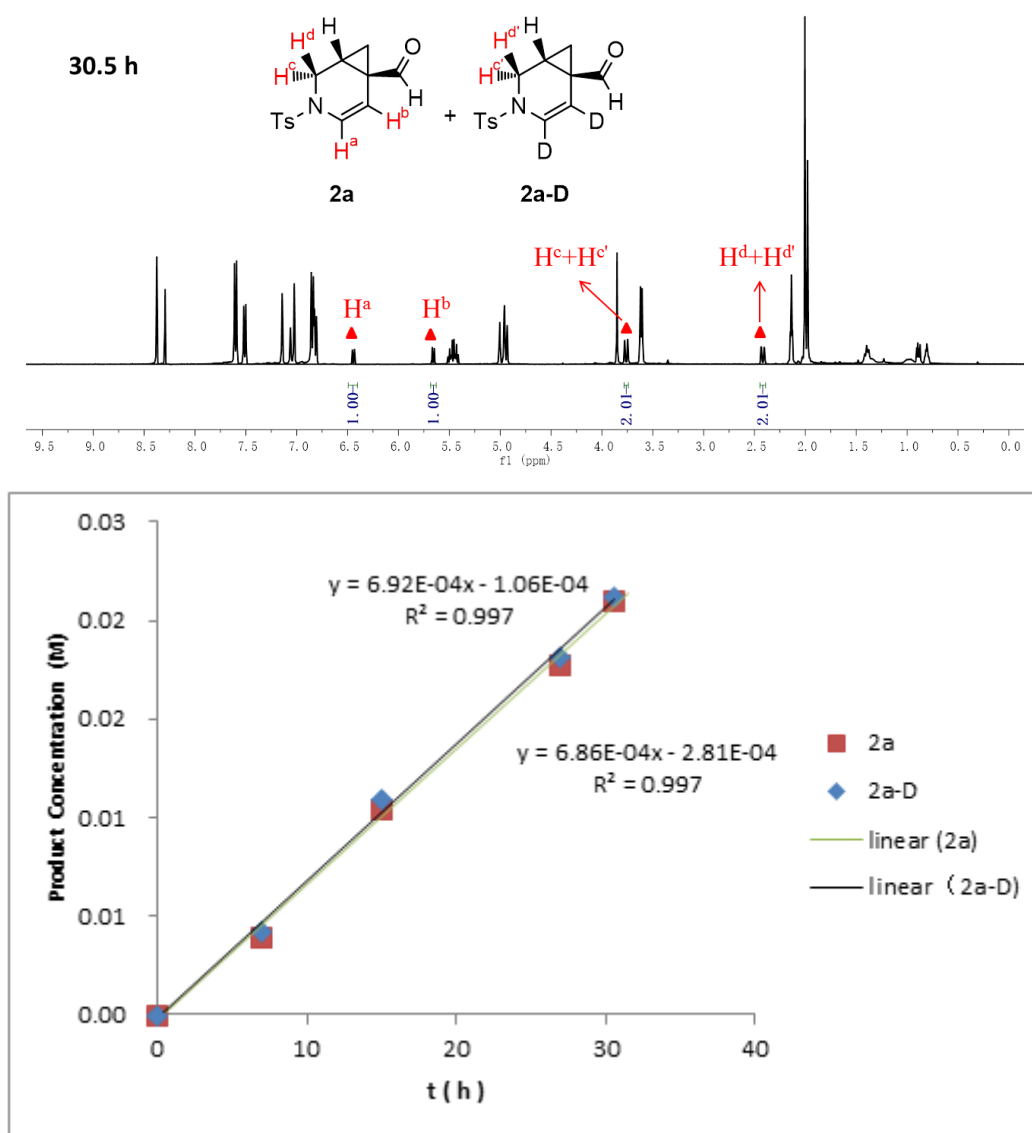
| 峰# | 保留时间   | 面积       | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|----------|--------|----|-----------|---------|
| 1  | 12.812 | 18008925 | 862161 | W  | RT:12.812 | 94.835  |
| 2  | 15.904 | 976870   | 42878  | W  | RT:15.904 | 5.145   |
| 总计 |        | 18985795 | 905039 |    |           | 100.000 |

## 7. Measure of KIE

The KIE of the reactions were measured as follows: To a toluene solution (4.0 mL) of  $\text{Rh}_2(\text{S-BTPCP})_4$  (0.1 mol%) was added equal mole of **1a** (0.2 mmol, 56 mg) and **1a-D** (0.2 mmol, 56 mg) at rt. The reaction was monitored by  $^1\text{H}$  NMR (with  $\text{D}_8$ -toluene as solvent) at different reaction time (7 h, 15 h, 27 h, 30.5 h). The ratios of **2a** and **2a-D** at different time were showed in the following table.

**Table S2.**



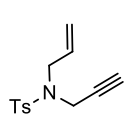


$$KIE = K_H/K_D = 6.86/6.92 = 0.99$$

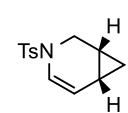
## 8. Rh-catalyzed initial investigations and control reactions

**General procedure for  $Rh_2(S-BTPCP)_4$ -catalyzed initial investigations:** To a toluene solution of **1** (0.25 mmol, 1 mL) in Schlenk tube with a magnetic bar was added  $Rh_2(S-BTPCP)_4$  (0.0025 mmol, 1 mol%, 4.4 mg) at room temperature under  $N_2$ . The sealed tube was then stirred at 80 °C under nitrogen atmosphere for 12 h. The mixture was then concentrated and the residue was purified by chromatography on silica gel to afford the desired product **2**.

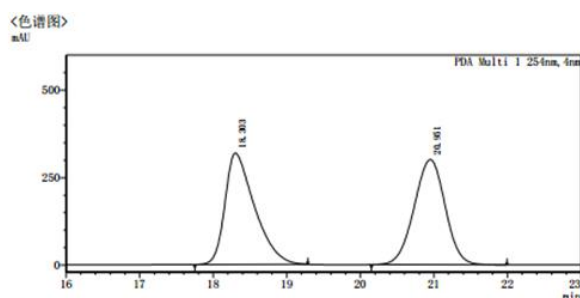
### N-allyl-N-(prop-2-yn-1-yl)-4-methylbenzenesulfonamide (**1a**)

  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.73 (d,  $J = 7.8$  Hz, 2H), 7.29 (d,  $J = 7.8$  Hz, 2H), 5.76 – 5.67 (m, 1H), 5.35 – 5.20 (m, 2H), 4.08 (s, 2H), 3.82 (d,  $J = 6.4$  Hz, 2H), 2.42 (s, 3H), 2.03 (s, 1H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  143.6, 135.9, 131.8, 129.5, 127.7, 120.0, 76.4, 73.9, 49.0, 35.8, 21.5.

### 3-tosyl-3-azabicyclo[4.1.0]hept-4-ene (**2a**)

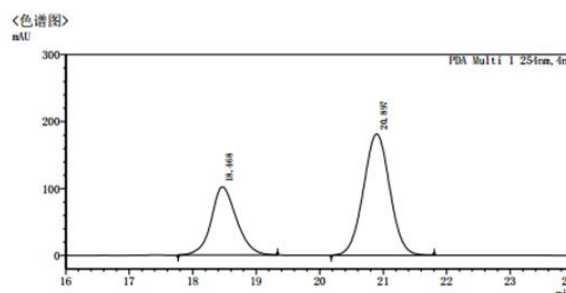
 colorless oil, 10 mg, 16% yield, 30% ee,  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.67 (d,  $J = 8.2$  Hz, 2H), 7.33 (d,  $J = 8.1$  Hz, 2H), 6.35 (d,  $J = 8.1$  Hz, 1H), 5.42 (dd,  $J = 8.0, 5.5$  Hz, 1H), 3.90 (d,  $J = 11.5$  Hz, 1H), 3.07 (dd,  $J = 11.6, 2.8$  Hz, 1H), 2.45 (s, 3H), 1.58 – 1.49 (m, 1H), 1.19 – 1.10 (m, 1H), 0.81 (td,  $J = 8.2, 4.6$  Hz, 1H), 0.37 (dd,  $J = 9.8, 4.7$  Hz, 1H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  143.6, 134.9, 129.7, 127.0, 121.1, 112.1, 77.4, 77.1, 76.7,

40.9, 21.5, 18.5, 13.4, 7.1. **IR** (KBr)  $\nu_{\text{max}}$  3661, 3067, 1734, 1591, 1346, 1163, 1110, 1019, 954, 809, 755, 682, 547. **HRMS** (ESI)  $[M+H]^+$  calculated for  $C_{13}H_{16}NO_2S^+$ : 250.0892, found 250.0892. Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $RT_1 = 18.5$  min,  $RT_2 = 20.9$  min.  $[\alpha]_D^{20} = +5.0$  (c 0.5,  $CH_2Cl_2$ )



<峰表>

| 峰号 | 保留时间   | 面积       | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|----------|--------|----|-----------|---------|
| 1  | 18.303 | 8899919  | 318495 | M  | RT:18.303 | 50.211  |
| 2  | 20.951 | 8825277  | 300317 | M  | RT:20.951 | 49.789  |
| 总计 |        | 17725196 | 618812 |    |           | 100.000 |



<峰表>

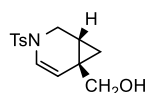
| 峰号 | 保留时间   | 面积      | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|----|-----------|---------|
| 1  | 18.468 | 2826473 | 101980 | M  | RT:18.468 | 35.116  |
| 2  | 20.897 | 5222540 | 181022 | M  | RT:20.897 | 64.884  |
| 总计 |        | 8049013 | 283001 |    |           | 100.000 |

**General procedure for  $Rh_2(OPiv)_4$ -catalyzed control reactions:** To a toluene solution of **1** (0.25 mmol, 1 mL) in Schlenk tube with a magnetic bar was added  $Rh_2(OPiv)_4$  (0.0125 mmol, 5 mol%, 7.6 mg) at room temperature under  $N_2$ . The sealed tube was then stirred at 80 °C under nitrogen atmosphere for 24 h. The mixture was then concentrated and the residue was purified by chromatography on silica gel to afford the desired product **2**.

#### General procedure for $Rh_2(S-BTPCP)_4$ -catalyzed control reactions:

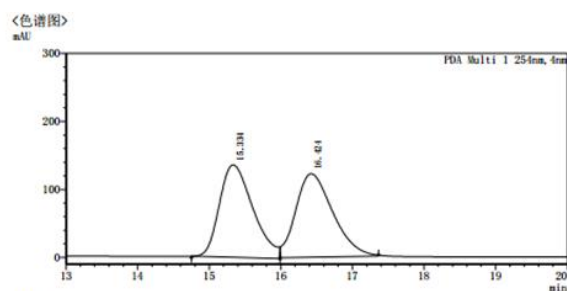
To a toluene solution of **1** (0.25 mmol, 1 mL) in Schlenk tube with a magnetic bar was added  $Rh_2(S-BTPCP)_4$  (0.0025 mmol, 1 mol%, 4.4 mg) at room temperature under  $N_2$ . The sealed tube was then stirred at 80 °C under nitrogen atmosphere for 60 h. The mixture was then concentrated and the residue was purified by chromatography on silica gel to afford the desired product **2**.

#### 3-tosyl-3-azabicyclo[4.1.0]hept-4-en-6-yl)methanol (**2u**)



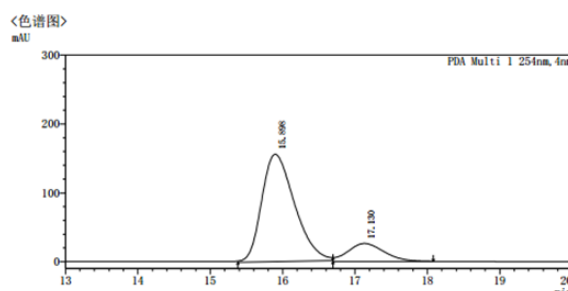
Colorless oil, 41.9 mg, 60% yield, 69% ee,  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.64 (d,  $J = 8.3$  Hz, 2H), 7.39 – 7.28 (m, 2H), 6.43 (dd,  $J = 8.2, 0.9$  Hz, 1H), 5.41 (dd,  $J = 8.2, 0.9$  Hz, 1H), 3.98 – 3.85 (m, 1H), 3.53 (d,  $J = 11.1$  Hz, 1H), 3.35 (d,  $J = 11.2$  Hz, 1H), 3.03 (dd,  $J = 11.6, 2.8$  Hz, 1H), 2.42 (s, 3H), 1.69 (s, 1H), 1.54 – 1.42 (m, 1H), 0.76 (ddd,  $J = 8.7, 4.7, 0.9$  Hz, 1H), 0.55 (t,  $J = 5.2$  Hz, 1H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  143.8, 134.8, 129.8, 127.0, 122.1, 112.2, 68.2, 40.9, 23.3, 21.5, 19.9, 17.7. **IR** (KBr)  $\nu_{\text{max}}$  3341, 3095, 3027, 2924, 1656, 1597, 1493, 1406, 1350, 1215, 1165, 1117, 1053, 1042, 984, 958, 945, 899, 867, 766, 707, 683, 644, 602, 555, 545, 491, 466.

**HRMS** (ESI)  $[M+H]^+$  calculated for  $C_{14}H_{18}NO_3S^+$ : 280.1002, found 280.1004. Resolution of enantiomers: DAICEL Chiralcel® OD-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $RT_1 = 16.9$  min,  $RT_2 = 17.1$  min.  $[\alpha]_D^{20} = +28.7$  (c 0.5,  $CH_2Cl_2$ )



<峰表>

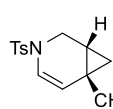
| 峰号 | 保留时间   | 面积      | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|----|-----------|---------|
| 1  | 15.334 | 4411709 | 135787 | M  | RT:15.334 | 49.971  |
| 2  | 16.424 | 4416806 | 122797 | M  | RT:16.424 | 50.029  |
| 总计 |        | 8828515 | 258584 |    |           | 100.000 |



<峰表>

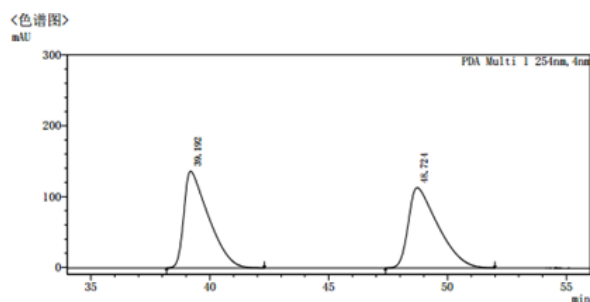
| 峰号 | 保留时间   | 面积      | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|----|-----------|---------|
| 1  | 15.898 | 4931544 | 155901 | M  | RT:15.898 | 84.441  |
| 2  | 17.130 | 908648  | 26109  | M  | RT:17.130 | 15.559  |
| 总计 |        | 5840192 | 182010 |    |           | 100.000 |

## 6-(fluoromethyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene (2aa)



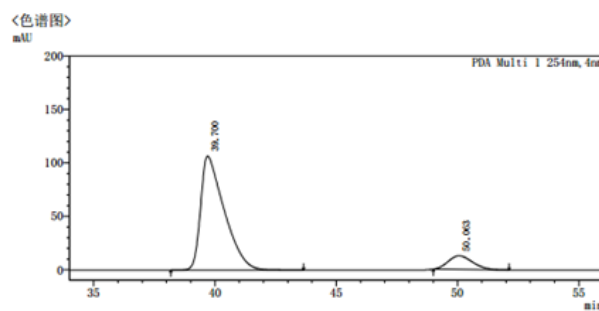
Colorless oil, 53.4 mg, 76% yield, 78% ee,  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J = 8.2$  Hz, 2H), 7.32 (d,  $J = 8.1$  Hz, 2H), 6.44 (d,  $J = 8.2$  Hz, 1H), 5.41 (d,  $J = 8.2$  Hz, 1H), 4.26 (dd,  $J = 81.5, 9.7$  Hz, 1H), 4.13 (dd,  $J = 81.1, 9.7$  Hz, 1H), 3.94 (d,  $J = 11.6$  Hz, 1H), 3.01 (dd,  $J = 11.6, 2.4$  Hz, 1H), 2.42 (s, 3H), 1.67 – 1.54 (m, 1H), 0.86 (dd,  $J = 8.7, 5.0$  Hz, 1H), 0.69 (dd,  $J = 10.1, 5.0$  Hz, 1H).  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -214.4.  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.9, 134.9, 129.9, 127.0, 122.4, 110.6,  $\delta$  88.4 (d,  $J = 170.4$  Hz), 40.5, 23.9 (d,  $J = 6.1$  Hz), 21.5, 18.3 (d,  $J = 23.9$  Hz), 17.7 (d,  $J = 6.6$  Hz). **IR** (KBr)  $\nu_{\text{max}}$  3666, 2958, 1644, 1597, 1461, 1405, 1348, 1270, 1165, 1116, 1088, 989, 949, 889, 812, 709, 677, 640, 607, 548. **HRMS** (ESI)  $[\text{M}+\text{H}]^+$  calculated for  $\text{C}_{14}\text{H}_{17}\text{FNO}_2\text{S}^+$ : 282.0959, found 282.0956.

Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $\text{RT}_1 = 39.2$  min,  $\text{RT}_2 = 48.7$  min.  $[\alpha]_{\text{D}}^{20} = +28.7$  (c 0.5,  $\text{CH}_2\text{Cl}_2$ )



<峰表>

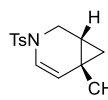
| 峰号 | 保留时间   | 面积       | 高度     | 化合物名      | 面积%     |
|----|--------|----------|--------|-----------|---------|
| 1  | 39.192 | 9872545  | 136618 | RT:39.192 | 50.014  |
| 2  | 48.724 | 9866844  | 113521 | RT:48.724 | 49.986  |
| 总计 |        | 19739389 | 250139 |           | 100.000 |



<峰表>

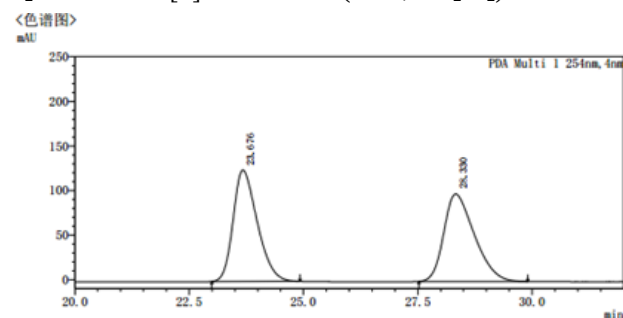
| 峰号 | 保留时间   | 化合物名      | 面积%     |
|----|--------|-----------|---------|
| 1  | 39.700 | RT:39.700 | 88.986  |
| 2  | 50.063 | RT:50.063 | 11.014  |
| 总计 |        |           | 100.000 |

## 6-(methoxymethyl)-3-tosyl-3-azabicyclo[4.1.0]hept-4-ene (2ab)



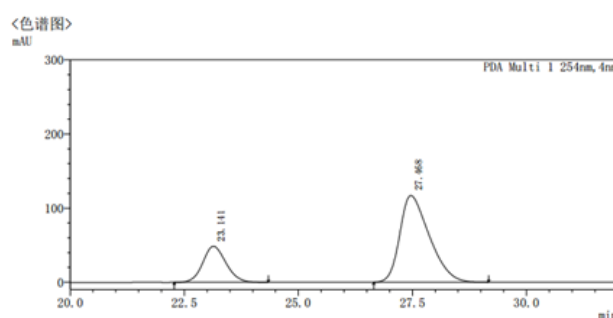
Colorless oil, 12.5 mg, 17% yield, 51% ee,  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 8.1$  Hz, 2H), 7.32 (d,  $J = 8.0$  Hz, 2H), 6.41 (d,  $J = 8.1$  Hz, 1H), 5.42 (d,  $J = 8.2$  Hz, 1H), 3.95 (d,  $J = 11.5$  Hz, 1H), 3.36 (d,  $J = 10.0$  Hz, 1H), 3.31 (s, 3H), 3.10 (d,  $J = 10.0$  Hz, 1H), 3.04 (d,  $J = 11.5$  Hz, 1H), 2.44 (s, 3H), 1.51 (t,  $J = 6.9$  Hz, 1H), 0.77 (dd,  $J = 8.5, 4.7$  Hz, 1H), 0.60 (t,  $J = 5.2$  Hz, 1H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.7, 134.9, 129.8, 127.1, 121.6, 112.8, 77.9, 58.7, 40.7, 24.1, 21.5, 17.7, 17.6. **IR** (KBr)  $\nu_{\text{max}}$  3649, 2930, 2243, 1719, 1598, 1445, 1348, 1259, 1162, 1093, 900, 814, 756, 665, 588, 546. **HRMS** (ESI)  $[\text{M}+\text{H}]^+$  calculated for  $\text{C}_{15}\text{H}_{20}\text{NO}_3\text{S}^+$ : 294.1158, found 294.1157.

Resolution of enantiomers: DAICEL Chiralcel® OJ-H column, 10% IPA-Hexanes, 1.0 mL/min, 254 nm,  $\text{RT}_1 = 23.7$  min,  $\text{RT}_2 = 28.3$  min.  $[\alpha]_{\text{D}}^{20} = +28.7$  (c 0.5,  $\text{CH}_2\text{Cl}_2$ )



<峰表>

| 峰号 | 保留时间   | 面积      | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|----|-----------|---------|
| 1  | 23.676 | 4582969 | 124795 | M  | RT:23.676 | 50.149  |
| 2  | 28.330 | 4555730 | 97899  | M  | RT:28.330 | 49.851  |
| 总计 |        | 9138699 | 222693 |    |           | 100.000 |

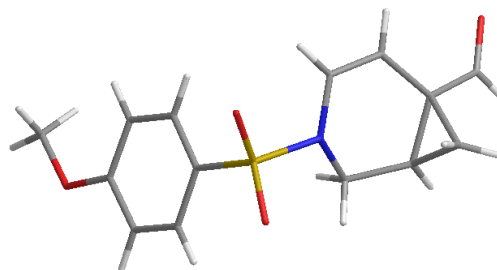
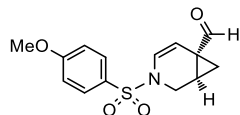


<峰表>

| 峰号 | 保留时间   | 面积      | 高度     | 标记 | 化合物名      | 面积%     |
|----|--------|---------|--------|----|-----------|---------|
| 1  | 23.141 | 1725063 | 48647  | M  | RT:23.141 | 24.687  |
| 2  | 27.468 | 5262659 | 116860 | M  | RT:27.468 | 75.313  |
| 总计 |        | 6987723 | 165507 |    |           | 100.000 |

## 9. The X-ray diffraction analysis

Crystal data and structure refinement for **2o**



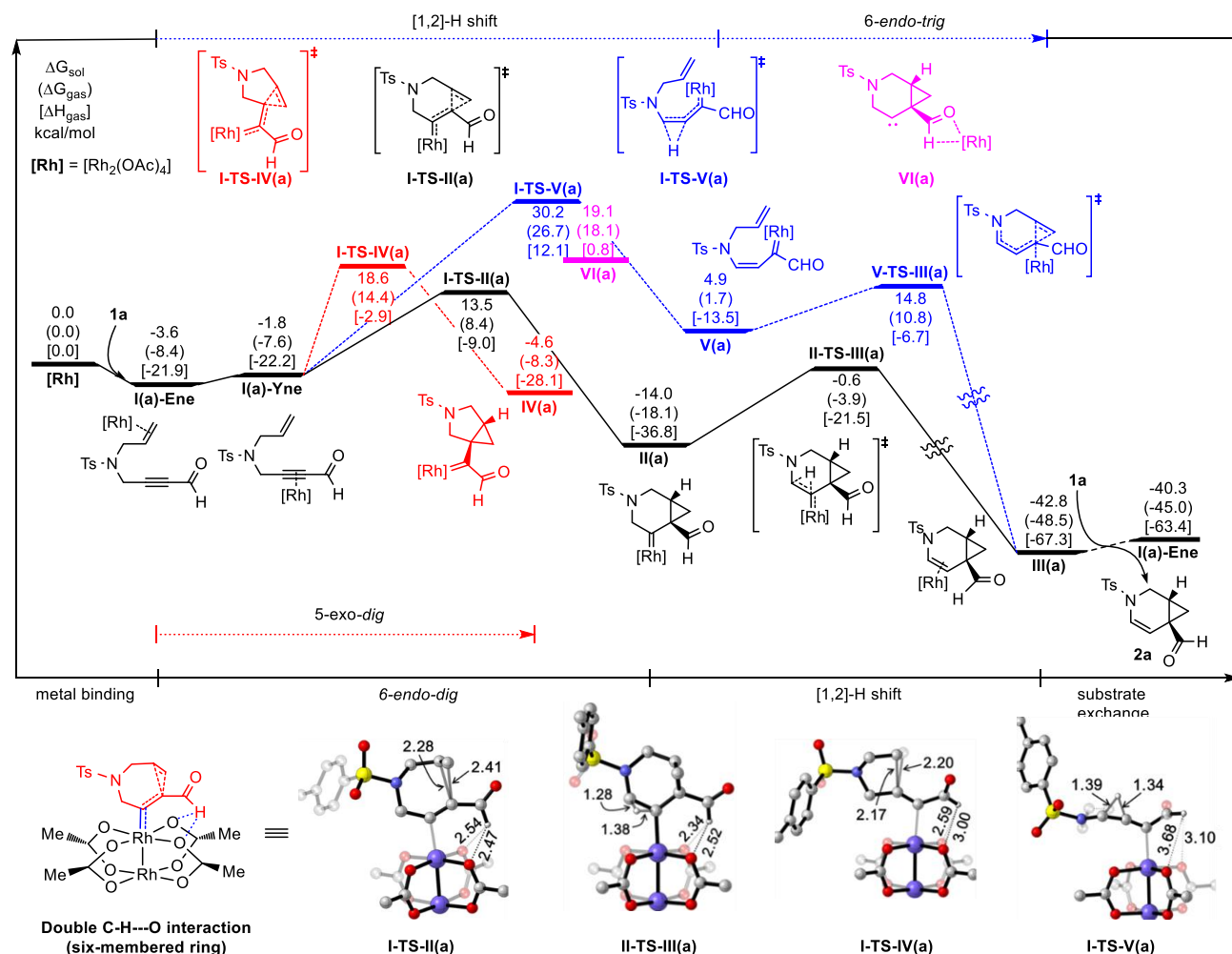
|                                                     |                                                                                                                             |
|-----------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| Identification code                                 | cd16569                                                                                                                     |
| Empirical formula                                   | C <sub>14</sub> H <sub>15</sub> NO <sub>4</sub> S                                                                           |
| Formula weight                                      | 293.33                                                                                                                      |
| Temperature                                         | 293(2) K                                                                                                                    |
| Wavelength                                          | 0.71073 Å                                                                                                                   |
| Crystal system                                      | Orthorhombic                                                                                                                |
| Space group                                         | <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>                                                                       |
| Unit cell dimensions                                | <i>a</i> = 8.1048(14) Å $\alpha$ = 90 °<br><i>b</i> = 8.8621(16) Å $\beta$ = 90 °<br><i>c</i> = 18.947(3) Å $\gamma$ = 90 ° |
| Volume                                              | 1360.9(4) Å <sup>3</sup>                                                                                                    |
| <i>Z</i>                                            | 4                                                                                                                           |
| Density (calculated)                                | 1.432 Mg/m <sup>3</sup>                                                                                                     |
| Absorption coefficient                              | 0.250 mm <sup>-1</sup>                                                                                                      |
| <i>F</i> (000)                                      | 616                                                                                                                         |
| Crystal size                                        | 0.200 x 0.170 x 0.140 mm <sup>3</sup>                                                                                       |
| Theta range for data collection                     | 2.150 to 25.987 °                                                                                                           |
| Index ranges                                        | -9 ≤ <i>h</i> ≤ 9, -8 ≤ <i>k</i> ≤ 10, -23 ≤ <i>l</i> ≤ 22                                                                  |
| Reflections collected                               | 8153                                                                                                                        |
| Independent reflections                             | 2664 [ <i>R</i> (int) = 0.0280]                                                                                             |
| Completeness to theta = 25.242 °                    | 99.9 %                                                                                                                      |
| Absorption correction                               | Semi-empirical from equivalents                                                                                             |
| Max. and min. transmission                          | 0.7456 and 0.6972                                                                                                           |
| Refinement method                                   | Full-matrix least-squares on <i>F</i> <sup>2</sup>                                                                          |
| Data / restraints / parameters                      | 2664 / 0 / 182                                                                                                              |
| Goodness-of-fit on <i>F</i> <sup>2</sup>            | 1.058                                                                                                                       |
| Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )] | <i>R</i> <sub>1</sub> = 0.0362, <i>wR</i> <sub>2</sub> = 0.0940                                                             |
| <i>R</i> indices (all data)                         | <i>R</i> <sub>1</sub> = 0.0399, <i>wR</i> <sub>2</sub> = 0.0971                                                             |
| Absolute structure parameter                        | 0.06(4)                                                                                                                     |
| Extinction coefficient                              | <i>n/a</i>                                                                                                                  |
| Largest diff. peak and hole                         | 0.344 and -0.171 e.Å <sup>-3</sup>                                                                                          |

## 10. Computational details

All of the calculations were performed with Gaussian 09 program [15]. The hybrid B3LYP [16] functional in conjunction with the LANL2DZ [17] basis set for rhodium (augmented with a 4f-function,  $\zeta_f(\text{Rh}) = 1.350$ ) [18] and bromide (augmented with a 3d-function,  $\zeta_d(\text{Br}) = 0.428$ ) [19], and the 6-31G(d) basis set for the other atoms [20], was applied for the optimization of all stationary points in gas phase. Frequency calculations were performed at the same level to confirm whether each stationary point was either a minimum or a transition structure. Single point calculations were carried out with Truhlar's M06 functional [21] with SDD basis set [22] for rhodium and bromine, and 6-311++G(d,p) for the other atoms in gas phase or in toluene with SMD [23] solvent model.  $\text{Rh}_2(\text{OAc})_4$  was used as the catalyst model during the investigation of reaction mechanism, to simplify the problem and reduce the computation cost. As the cyclopropanation step was the rate-determining step, the transition step **I-TS-II** with the real chiral catalyst  $\text{Rh}_2(\text{S-BTPCP})_4$  was calculated to understand the enantioselectivity. The initial conformation of  $\text{Rh}_2(\text{S-BTPCP})_4$  was generated from the mirror inversion of the crystal structure  $\text{Rh}_2(\text{R-BTPCP})_4$  (CCDC number: 830584) [24]. For all the structures, the Gibbs free energy and enthalpy were reported by adding the thermal corrections from frequency calculation to the electronic energy in gas phase or with solvent corrections from single point calculation. Conformational samplings were performed, and the most stable one was reported. Computed structures were illustrated using CYLView [25] or VMD [26]. QTAIM analysis was performed by Multiwfn [27]. The binding energy between Rh(II) catalyst and R-H species (acetaldehyde or methane) was obtained through subtracting the energies of the isolated Rh(II) catalyst and R-H species from the energy of the complex, and corrected for BSSE using counterpoise approach [28].

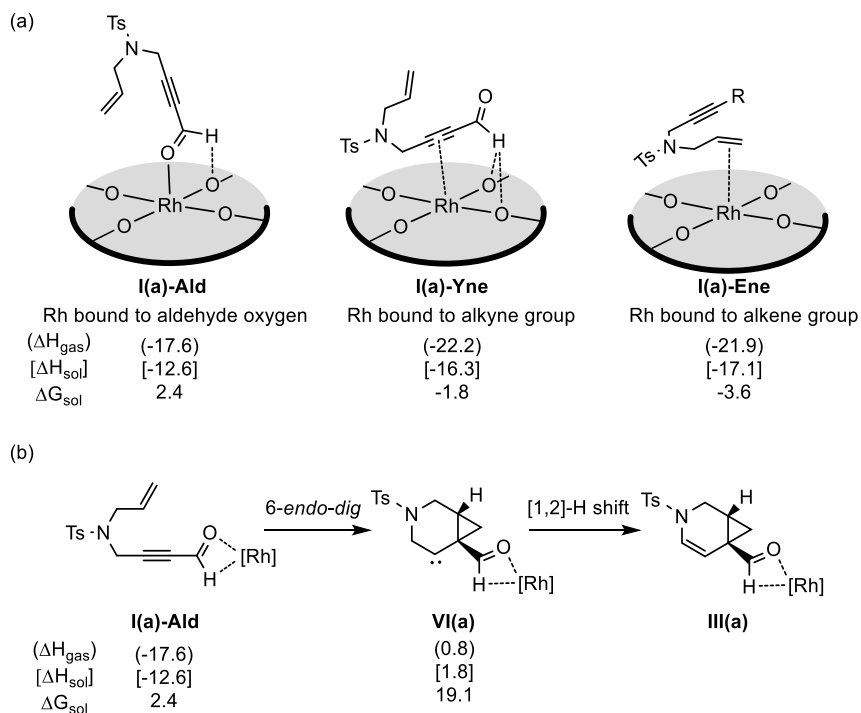
## 10.1 DFT studies of the cycloisomerization of 1, 6-enynal **1a**.

### (1) Potential energy surfaces



**Figure S1. Possible reaction pathways of the cycloisomerization of 1,6-enynal, **1a****

The dirhodium(II) catalyst could bind to the alkene group as **I(a)-Ene**, or alkyne group as **I(a)-Yne**, or aldehyde oxygen atom as **I(a)-Ald**. Among these complex structures, **I(a)-Ene** is the most stable one. The reaction starting from the complex **I(a)-Ald** will form a free carbene intermediate **VI(a)**. Considering this unstable intermediate, this reaction pathway should be impossible. Therefore, reaction starts from **I(a)-Ene**, then **I(a)-Yne**, followed by cyclopropanation or proton shift. The cyclopropanation can take place via 6-endo-dig mode or 5-exo-dig mode, and the former is more favorable than the latter by at least 5.0 kcal/mol in free energy. The subsequent [1,2]-H shift is feasible with activation free energy about 13.4 kcal/mol ( $\Delta\Delta G_{\text{toluene}}$ ) via **II-TS-III(a)**. Considering the heteroatom is crucial, the lone pair at the heteroatom may promote a [1,2]-H shift from the propargylic position to give alkenyl metal carbene intermediate **V(a)**. The free energy barrier for [1,2]-H shift via **I-TS-V(a)** is as high as 33.8 kcal/mol, much higher than that of the cyclopropanation step. Therefore, the potential reaction pathway should be the 6-endo-dig cyclopropanation/[1,2]-H shift pathway, and the first step is rate determining.



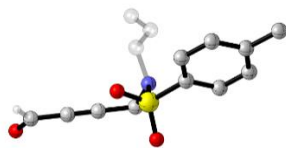
**Scheme S1. Aldehyde-activation mode**

We have also considered the possible intermediates between **I(a)** and **II(a)**, or **I(a)** and **IV(a)** from stepwise cyclopropanations. However, efforts to locate these intermediates ended in failure at the B3LYP/(LANL2DZ,6-31G(d)) theoretical level [17-20]. Other common methods including M06 [21], wB97xD [29], and B3LYP with the D3 version of Grimme's dispersion [30] also failed to locate these carbocationic intermediates.

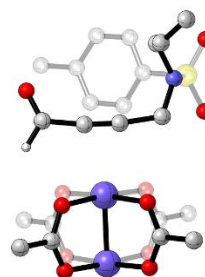
(2) The optimized structures of representative stable conformers (All the hydrogen atoms are omitted for clarity except the formyl C-H atom and the concerned hydrogen atoms in transition state).



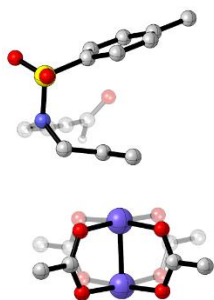
**[Rh]**



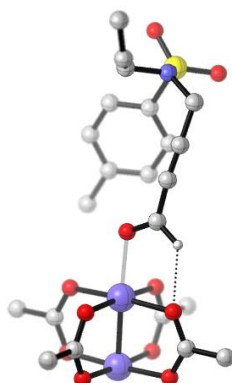
**1a**



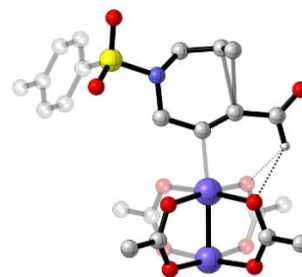
**I(a)-Yne**



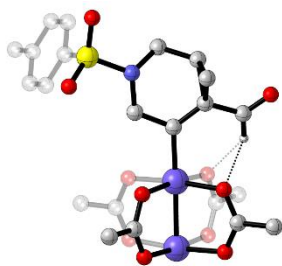
**I(a)-Ene**



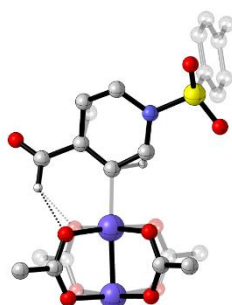
**I(a)-Ald**



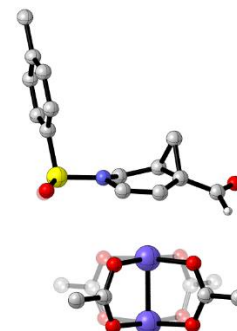
**I-TS-II(a)**



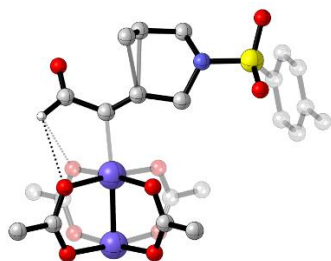
**II (a)**



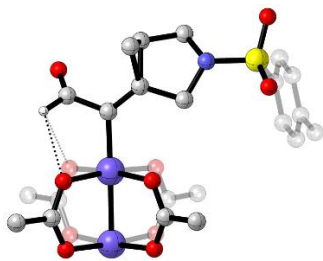
**II-TS-III(a)**



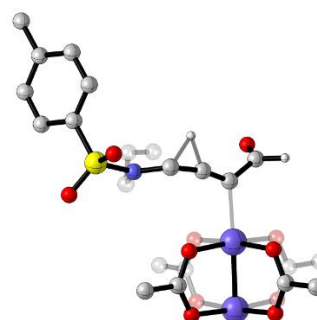
**III(a)**



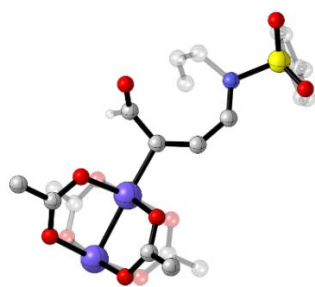
**I-TS-IV(a)**



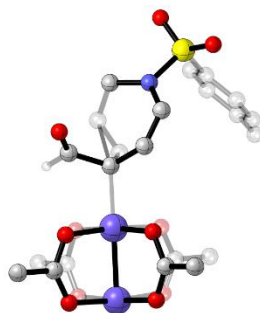
**IV(a)**



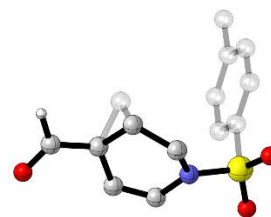
**I-TS-V(a)**



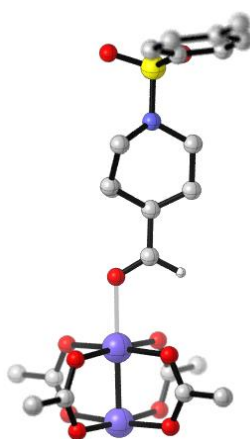
**V(a)**



**V-TS-III(a)**



**2a**



**VI(a)**

(3) Table of energies and other thermodynamic parameters.

**Table S3.**

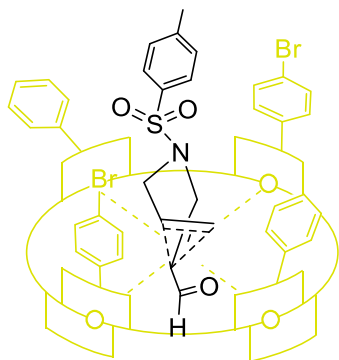
| Structures                             | E <sub>ele</sub> | E <sub>0</sub> | E           | H           | G           | E <sub>ele(sol)</sub> | E <sub>ele(gas)</sub> |
|----------------------------------------|------------------|----------------|-------------|-------------|-------------|-----------------------|-----------------------|
| <b>Rh<sub>2</sub>(OAc)<sub>4</sub></b> | -1133.12041      | -1132.90894    | -1132.88730 | -1132.88636 | -1132.96272 | -1134.95424           | -1134.93589           |
| <b>1a_conf1</b>                        | -1220.93591      | -1220.67136    | -1220.65127 | -1220.65032 | -1220.72462 | -1220.63436           | -1220.61245           |
| <b>1a_conf2</b>                        | -1220.92985      | -1220.66529    | -1220.64517 | -1220.64422 | -1220.71900 | -1220.62870           | -1220.60686           |
| <b>1a_conf3</b>                        | -1220.93348      | -1220.66892    | -1220.64884 | -1220.64789 | -1220.72159 | -1220.63425           | -1220.61292           |
| <b>I(a)-Yne_conf1</b>                  | -2354.07184      | -2353.59421    | -2353.55090 | -2353.54995 | -2353.67806 | -2355.61011           | -2355.57738           |
| <b>I(a)-Yne_conf2</b>                  | -2354.07563      | -2353.59781    | -2353.55462 | -2353.55368 | -2353.68079 | -2355.61465           | -2355.58493           |
| <b>I(a)-Yne_conf3</b>                  | -2354.07590      | -2353.59821    | -2353.55487 | -2353.55392 | -2353.68147 | -2355.61687           | -2355.58598           |
| <b>I(a)-Yne_conf4</b>                  | -2354.07229      | -2353.59487    | -2353.55148 | -2353.55054 | -2353.67863 | -2355.61273           | -2355.58182           |
| <b>I(a)-Yne_conf5</b>                  | -2354.07234      | -2353.59464    | -2353.55146 | -2353.55052 | -2353.67698 | -2355.61246           | -2355.58133           |
| <b>I(a)-Ene_conf1</b>                  | -2354.07802      | -2353.59965    | -2353.55676 | -2353.55582 | -2353.68256 | -2355.61901           | -2355.58706           |
| <b>I(a)-Ene_conf2</b>                  | -2354.07484      | -2353.59679    | -2353.55360 | -2353.55265 | -2353.68180 | -2355.61847           | -2355.58576           |
| <b>I(a)-Ald_conf1</b>                  | -2354.08027      | -2353.60182    | -2353.55894 | -2353.55799 | -2353.68477 | -2355.61138           | -2355.57908           |
| <b>I-TS-II(a)_conf1</b>                | -2354.05582      | -2353.57858    | -2353.53677 | -2353.53583 | -2353.65880 | -2355.59506           | -2355.56298           |
| <b>I-TS-II(a)_conf2</b>                | -2354.05494      | -2353.57788    | -2353.53602 | -2353.53508 | -2353.65868 | -2355.59315           | -2355.56087           |
| <b>I-TS-II(a)_conf3</b>                | -2354.05315      | -2353.57602    | -2353.53426 | -2353.53331 | -2353.65576 | -2355.59217           | -2355.55976           |
| <b>II(a)_conf1</b>                     | -2354.09315      | -2353.61234    | -2353.57151 | -2353.57057 | -2353.69132 | -2355.64382           | -2355.61000           |

|                    |             |             |             |             |             |             |             |
|--------------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| II(a)_conf2        | -2354.09200 | -2353.61125 | -2353.57052 | -2353.56958 | -2353.68915 | -2355.64082 | -2355.60707 |
| II-TS-III(a)_conf1 | -2354.06438 | -2353.58707 | -2353.54631 | -2353.54536 | -2353.66685 | -2355.61720 | -2355.58238 |
| II-TS-III(a)_conf2 | -2354.06414 | -2353.58693 | -2353.54612 | -2353.54518 | -2353.66774 | -2355.61692 | -2355.58197 |
| III(a)_conf1       | -2354.14388 | -2353.66166 | -2353.62095 | -2353.62001 | -2353.73910 | -2355.69092 | -2355.65980 |
| III(a)_conf2       | -2354.14223 | -2353.65991 | -2353.61924 | -2353.61829 | -2353.73681 | -2355.69268 | -2355.66192 |
| III(a)_conf3       | -2354.14387 | -2353.66177 | -2353.62096 | -2353.62001 | -2353.74077 | -2355.69092 | -2355.65979 |
| I-TS-IV(a)_conf1   | -2354.04851 | -2353.57106 | -2353.52916 | -2353.52821 | -2353.65134 | -2355.58716 | -2355.55357 |
| I-TS-IV(a)_conf2   | -2354.04748 | -2353.57002 | -2353.52821 | -2353.52727 | -2353.64984 | -2355.58419 | -2355.55086 |
| IV(a)_conf1        | -2354.08158 | -2353.60052 | -2353.55973 | -2353.55879 | -2353.67784 | -2355.63073 | -2355.59626 |
| IV(a)_conf2        | -2354.07999 | -2353.59899 | -2353.55814 | -2353.55720 | -2353.67759 | -2355.62742 | -2355.59322 |
| IV(a)_conf3        | -2354.07908 | -2353.59839 | -2353.55726 | -2353.55632 | -2353.67870 | -2355.62737 | -2355.59301 |
| I-TS-V(a)_conf1    | -2354.01272 | -2353.54046 | -2353.49755 | -2353.49660 | -2353.62398 | -2355.56023 | -2355.52553 |
| I-TS-V(a)_conf2    | -2354.01368 | -2353.54116 | -2353.49841 | -2353.49747 | -2353.62333 | -2355.55936 | -2355.52440 |
| I-TS-V(a)_conf3    | -2354.01137 | -2353.53875 | -2353.49595 | -2353.49501 | -2353.62149 | -2355.55429 | -2355.51894 |
| V(a)_conf1         | -2354.06074 | -2353.58352 | -2353.54069 | -2353.53974 | -2353.66812 | -2355.60121 | -2355.56402 |
| V(a)_conf2         | -2354.06700 | -2353.58875 | -2353.54626 | -2353.54531 | -2353.67176 | -2355.60710 | -2355.57195 |
| V(a)_conf3         | -2354.06862 | -2353.59017 | -2353.54777 | -2353.54683 | -2353.67230 | -2355.60694 | -2355.57117 |
| V-TS-III(a)_conf1  | -2354.04898 | -2353.57109 | -2353.52973 | -2353.52878 | -2353.65148 | -2355.59347 | -2355.55959 |
| V-TS-III(a)_conf2  | -2354.04990 | -2353.57172 | -2353.53042 | -2353.52948 | -2353.65174 | -2355.59172 | -2355.55782 |
| 2a_conf1           | -1220.99714 | -1220.72829 | -1220.71076 | -1220.70982 | -1220.77572 | -1220.70110 | -1220.67878 |
| 2a_conf2           | -1220.99656 | -1220.72813 | -1220.71038 | -1220.70944 | -1220.77670 | -1220.69877 | -1220.67721 |
| 2a_conf3           | -1220.99659 | -1220.72787 | -1220.71029 | -1220.70934 | -1220.77582 | -1220.70230 | -1220.68025 |
| 2a_conf4           | -1220.99484 | -1220.72619 | -1220.70860 | -1220.70766 | -1220.77421 | -1220.69865 | -1220.67648 |
| VI(a)_conf1        | -2354.04157 | -2353.56252 | -2353.52124 | -2353.52029 | -2353.64343 | -2355.58734 | -2355.54871 |

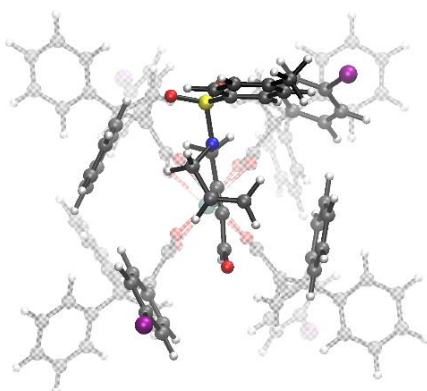
Notes:  $E_{\text{ele}}$ ,  $E_0$ ,  $E$ ,  $H$ , and  $G$  were the electronic energies, sum of electronic and zero-point energies, sum of electronic and thermal energies, sum of electronic and thermal enthalpies, and sum of electronic and thermal free energies, respectively, which were given at the B3LYP/(LANL2DZ,6-31G(d)) level.  $E_{\text{ele(sol)}}$  and  $E_{\text{ele(gas)}}$  were electronic energies at the M06/(SDD,6-311++G(d,p)) level with and without solvent correction, respectively.

## 10.2 Rate-determining transition states in chiral environment.

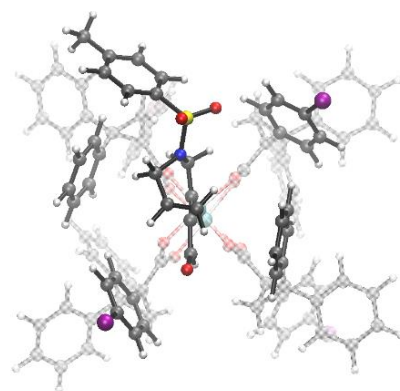
(1) The optimized structures of cyclopropanation transition state conformers



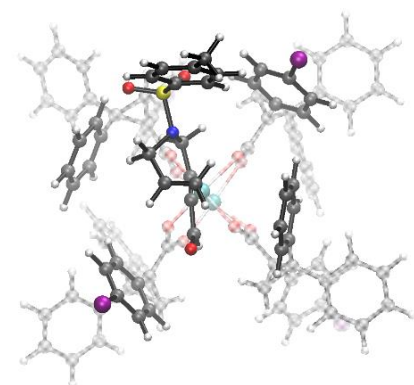
**(*R,R*)-I-TS-II(a)**



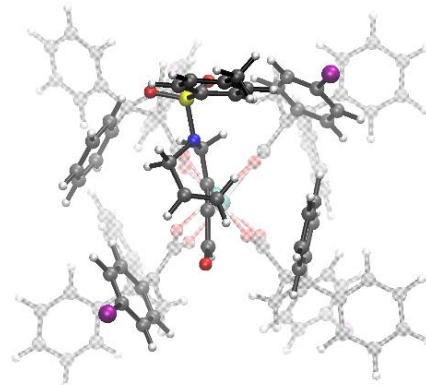
**Conf1:  $\Delta\Delta G_{\text{sol}} = 0.0$  kcal/mol  
( $\Delta\Delta H_{\text{sol}} = 0.0$  kcal/mol)**



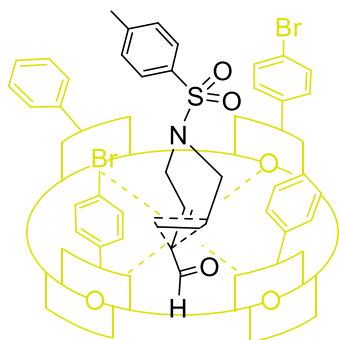
**Conf2: 0.1 (-1.0)**



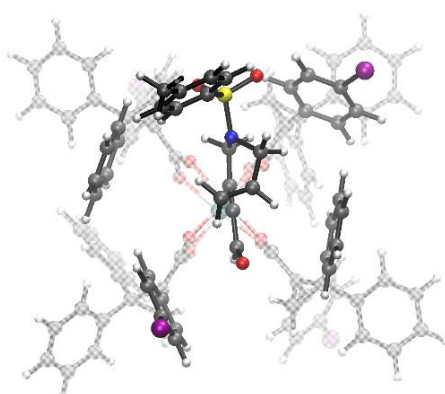
**Conf3: 1.1 (0.0)**



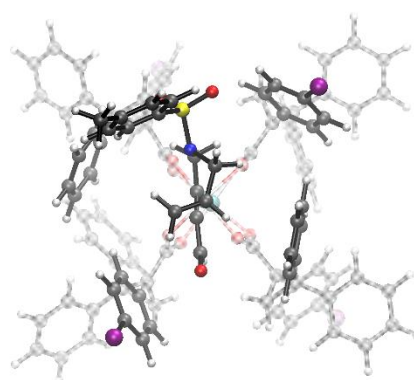
**Conf4: 1.4 (0.2)**



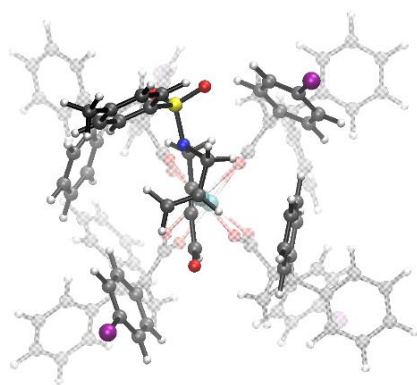
**(*S,S*)-I-TS-II(a)**



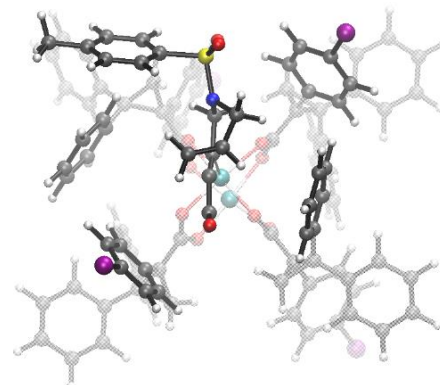
**Conf1: 1.4 (0.6)**



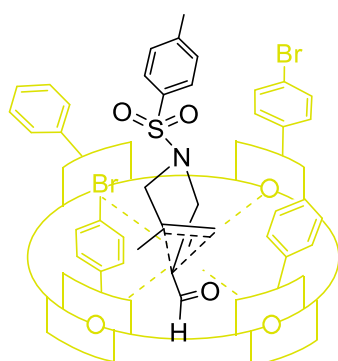
**Conf2: 1.5 (0.9)**



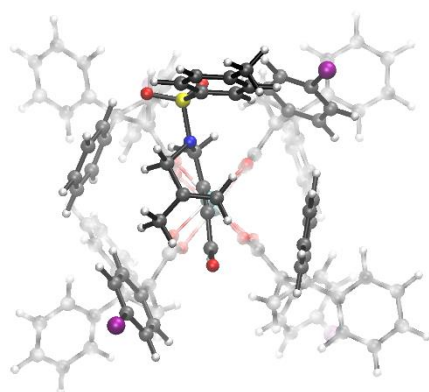
**Conf3: 1.6 (0.8)**



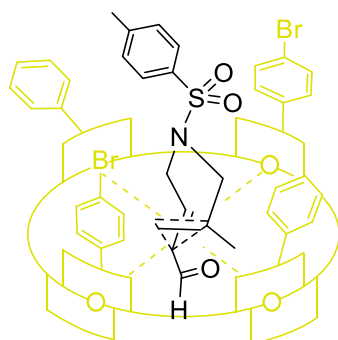
**Conf4: 2.4 (1.3)**



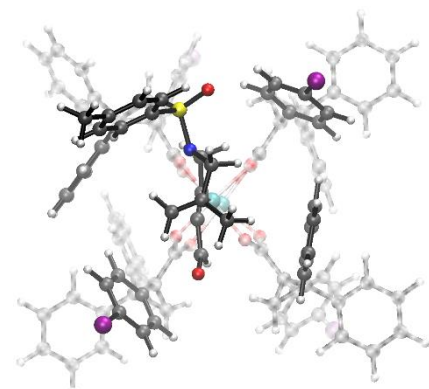
**(*R,R*)-I-TS-II(b)**



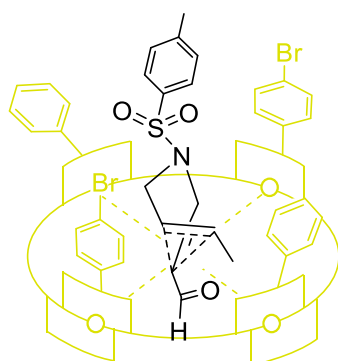
**Conf1: 0.0 (0.0)**



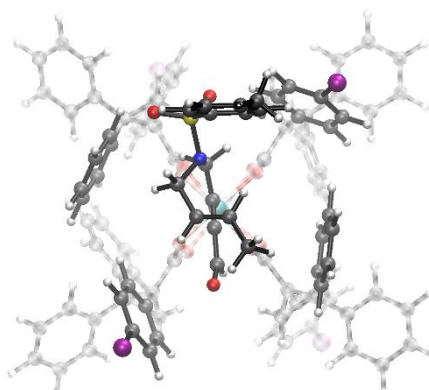
**(*S,S*)-I-TS-II(b)**



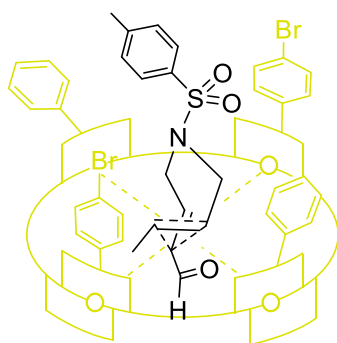
**Conf1: 1.0 (1.6)**



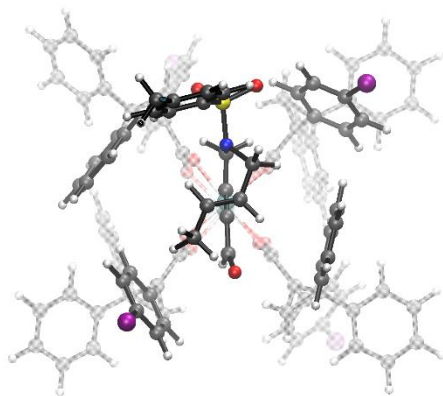
**(*R,R*)-I-TS-II(e)**



**Conf1: 0.0 (0.0)**



**(S,S)-I-TS-II(e)**



**Conf1: -0.1 (-0.9)**

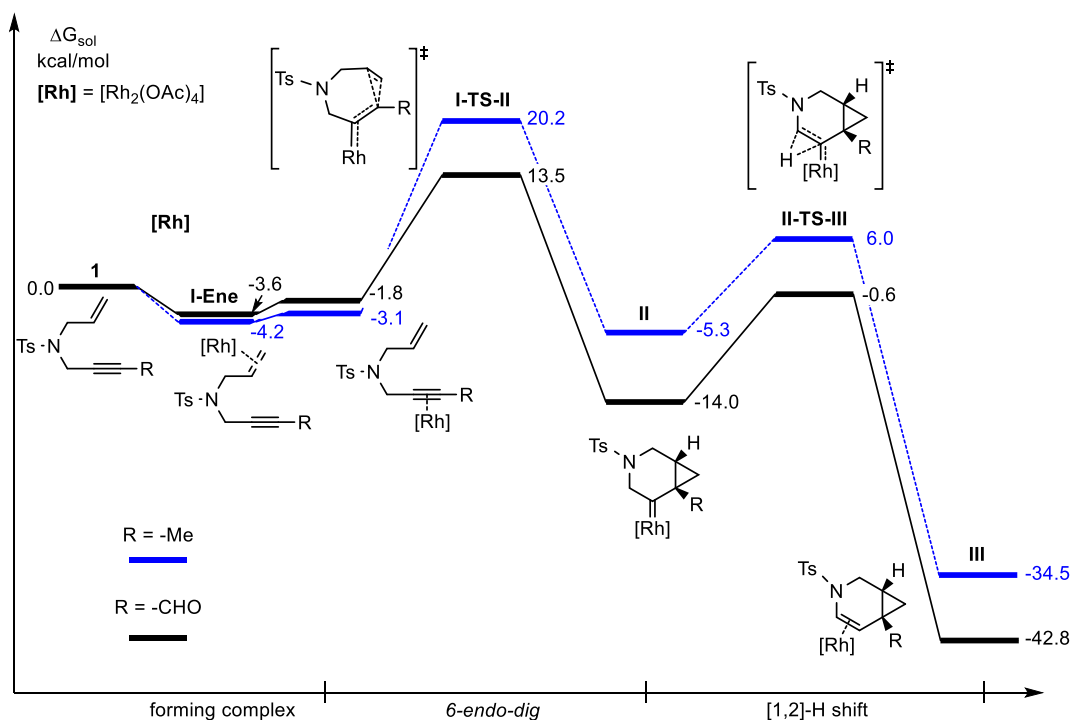
As the cyclopropanation step determines the stereochemistry, two cyclopropanation TSs in the real chiral catalyst  $\text{Rh}_2(\text{S-BTPCP})_4$  were calculated as well. The initial conformation was extracted from  $\text{Rh}_2(\text{R-BTPCP})_4$  (CCDC number: 830584) after mirror inversion. The substrate fits well in the pocket, where the alkyne group coordinates with the rhodium atom and the formyl hydrogen atom forms weak double hydrogen bonds with two carboxyl groups of the ligands. The substrate chain could rotate in a right-hand mode to give **(R,R)-2a**, corresponding to transition state **(R,R)-I-TS-II(a)**, or rotate in a left-hand mode to give **(S,S)-2a**, corresponding to transition state **(S,S)-I-TS-II(a)**. In **(R,R)-I-TS-II(a)**, the Ts group is apt to swing to the right, then forming weak C-H $\cdots$ Br hydrogen bond and C-H $\cdots$  $\pi$  interaction with ring D (ring of bromobenzene) of the ligand. Furthermore, the allylic CH<sub>2</sub> group has an extra C-H $\cdots$  $\pi$  interaction with ring C (ring of benzene). In **(S,S)-I-TS-II(a)**, the Ts group favors the left side to avoid steric repulsion with ring D on the right side, and forms some Van der Waals interaction with ring C. There is no obvious C-H $\cdots$  $\pi$  interaction for allylic CH<sub>2</sub> group. Even though to get exactly factors determining the enantioselectivity is complex, an approximate explanation can be extracted from the two transition states. DFT calculations show that transition state **(R,R)-I-TS-II(a)** is favored over **(S,S)-I-TS-II(a)** by 1.4 kcal/mol in Gibbs free energy ( $\Delta\Delta G_{\text{sol}}$ ), suggesting that **(R,R)** product was the major product. This is consistent with experimental confirmation that of the crystal structure of cyclopropanation product **2l**. The structure of **(R,R)-I-TS-II(a)** suggests that substituents at the terminal position of alkene group in the substrate will bring steric repulsion with the pocket phenyl ring A, possibly leading to a lower enantioselectivity. Our calculations show that, **(S,S)-I-TS-II(e)** is even more stable than **(R,R)-I-TS-II(e)**, by 0.1 kcal/mol in  $\Delta\Delta G_{\text{sol}}$  (**2e** in experiment, 25% *ee*). However, alkyl substituents at 2-position of the C=C double bond have less effects on enantioselectivity. It was found that the free energy in toluene of **(R,R)-I-TS-II(b)** is calculated to be lower than that of **(S,S)-I-TS-II(b)** by 1.0 kcal/mol, which is in consistence with the enantioselectivity 94% *ee* in experiment (**2b**). The free energy differences are a bit lower to explain 90 and 94% *ee* for **2a** and **2b**, respectively. However, even 95% *ee*, means the free energy difference at 2.0 kcal/mol at a reaction temperature 0 °C. As the real catalyst system is as large as 200 atoms, the energy difference within 1.0 kcal/mol should be acceptable considering the accuracy at the current theoretical level.

(2) Table of energies and other thermodynamic parameters of the cyclopropanation transition structures in chiral catalyst.

**Table S4.**

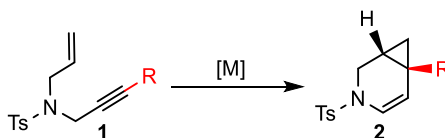
| Structures                      | $E_{\text{ele}}$ | $E_0$       | $E$         | $H$         | $G$         | $E_{\text{ele(sol)}}$ |
|---------------------------------|------------------|-------------|-------------|-------------|-------------|-----------------------|
| ( <i>R,R</i> )-I-TS-II(a)_conf1 | -5486.37908      | -5484.83471 | -5484.72478 | -5484.72383 | -5485.00562 | -5487.14304           |
| ( <i>R,R</i> )-I-TS-II(a)_conf2 | -5486.37572      | -5484.83103 | -5484.72128 | -5484.72034 | -5485.00032 | -5487.14476           |
| ( <i>R,R</i> )-I-TS-II(a)_conf3 | -5486.37934      | -5484.83452 | -5484.72477 | -5484.72383 | -5485.00389 | -5487.14325           |
| ( <i>R,R</i> )-I-TS-II(a)_conf4 | -5486.37926      | -5484.83453 | -5484.72475 | -5484.72381 | -5485.00370 | -5487.14295           |
| ( <i>S,S</i> )-I-TS-II(a)_conf1 | -5486.37856      | -5484.83392 | -5484.72409 | -5484.72314 | -5485.00366 | -5487.14232           |
| ( <i>S,S</i> )-I-TS-II(a)_conf2 | -5486.37863      | -5484.83390 | -5484.72407 | -5484.72313 | -5485.00388 | -5487.14192           |
| ( <i>S,S</i> )-I-TS-II(a)_conf3 | -5486.37862      | -5484.83391 | -5484.72409 | -5484.72314 | -5485.00370 | -5487.14193           |
| ( <i>S,S</i> )-I-TS-II(a)_conf4 | -5486.37749      | -5484.83247 | -5484.72278 | -5484.72184 | -5485.00184 | -5487.14140           |
| ( <i>R,R</i> )-I-TS-II(b)_conf1 | -5525.69903      | -5524.12693 | -5524.01532 | -5524.01437 | -5524.30015 | -5526.44322           |
| ( <i>S,S</i> )-I-TS-II(b)_conf1 | -5525.69834      | -5524.12617 | -5524.01455 | -5524.01360 | -5524.30030 | -5526.44081           |
| ( <i>R,R</i> )-I-TS-II(e)_conf1 | -5525.69827      | -5524.12549 | -5524.01394 | -5524.01300 | -5524.30078 | -5526.43920           |
| ( <i>S,S</i> )-I-TS-II(e)_conf1 | -5525.69768      | -5524.12552 | -5524.01382 | -5524.01287 | -5524.29928 | -5526.44024           |

### 10.3 Computational studies on different substrates.



**Scheme S2. Comparison of potential energy surfaces of substrates **1a** and **1y**.** The complex **I(y)-Yne** ( $R = -\text{Me}$ ) is more stable than **I(a)-Yne** ( $R = -\text{CHO}$ ) by -1.3 kcal/mol. However, the relative Gibbs free energy of transition state **I-TS-II(a)** ( $R = -\text{CHO}$ ) is much lower than that of **I-TS-II(y)** ( $R = -\text{Me}$ ) by -6.7 kcal/mol as electron-withdrawing group will activate the alkyne to facilitate the attack of the tethered alkene group.

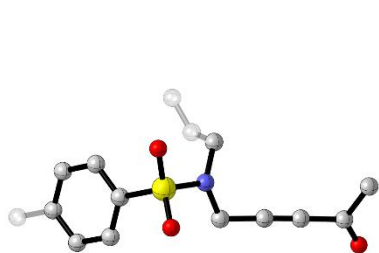
Table S5.



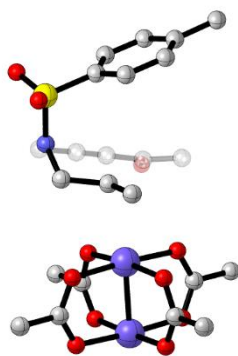
| 1   | -R                   | [M] = [Rh <sub>2</sub> (OAc) <sub>4</sub> ]  |                                                | [M] = AuCl                                   |
|-----|----------------------|----------------------------------------------|------------------------------------------------|----------------------------------------------|
|     |                      | I-TS-II ( $\Delta G_{\text{sol}}^\ddagger$ ) | II-TS-III ( $\Delta G_{\text{sol}}^\ddagger$ ) | I-TS-II ( $\Delta G_{\text{sol}}^\ddagger$ ) |
| 1a  | -CHO                 | 17.1                                         | 13.4                                           | 17.0                                         |
| 1w  | -COMe                | 25.2                                         | 9.9                                            | 16.6                                         |
| 1x  | -COPh                | 26.2                                         | 11.1                                           | 17.5                                         |
| 1v  | -CO <sub>2</sub> Me  | 26.6                                         | 15.4                                           | 19.3                                         |
| 1y  | -Me                  | 24.4                                         | 11.3                                           | 23.3                                         |
| 1z  | -Ph                  | 25.9                                         | 11.0                                           | 22.9                                         |
| 1u  | -CH <sub>2</sub> OH  | 18.3                                         | 12.0                                           | 21.1                                         |
| 1aa | -CH <sub>2</sub> F   | 19.9                                         | 10.3                                           | 20.2                                         |
| 1ab | -CH <sub>2</sub> OMe | 21.1                                         | 10.3                                           | 20.4                                         |
| 1ac | -H                   | 22.6                                         | 15.1                                           | 20.7                                         |

The free energy barrier of 6-*endo-dig* cyclization step under the catalysis of AuCl, where there was not steric repulsion between R group and catalyst, was compared with that under the catalysis of [Rh<sub>2</sub>(OAc)<sub>4</sub>]. Obviously, under the catalysis of AuCl, substrates with electron-withdrawing R groups, such as **1a**, **1w**, **1x**, and so on were more active than those with electron-donating groups in **1y** and **1z**.

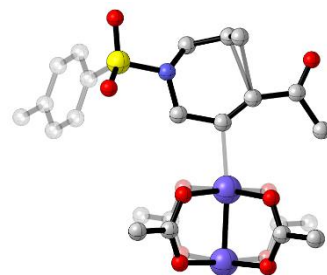
(1) The optimized structures of representative stable conformers.\*



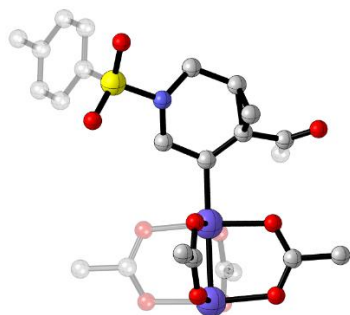
1w



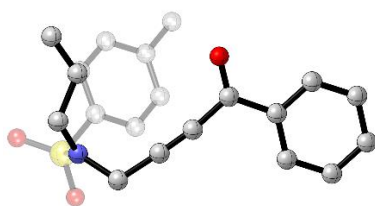
I(w)-Ene



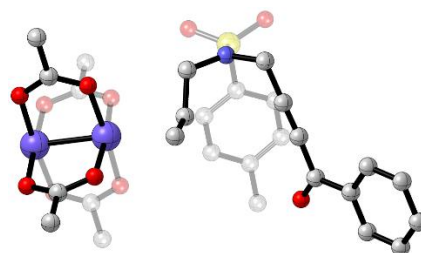
I-TS-II(w)



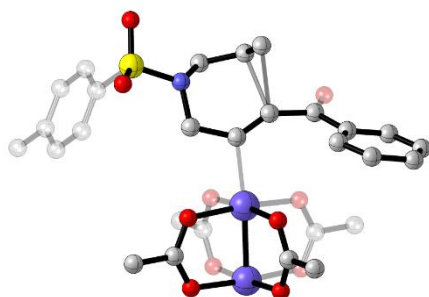
II(w)



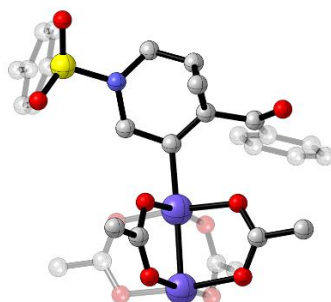
1x



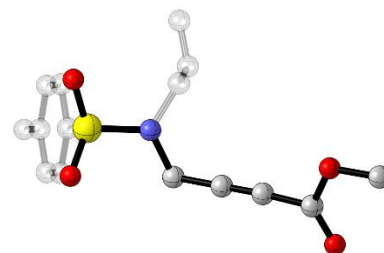
I(x)-Ene



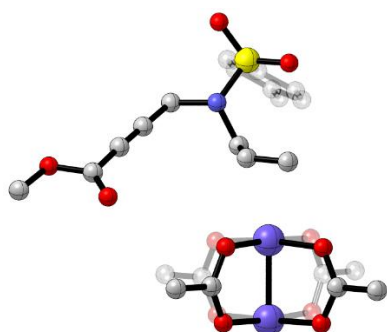
I-TS-II(x)



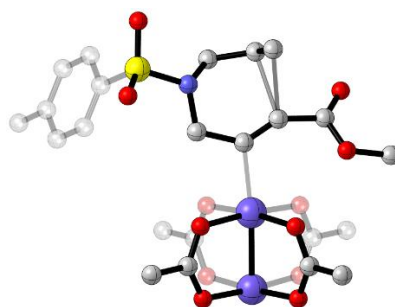
II(x)



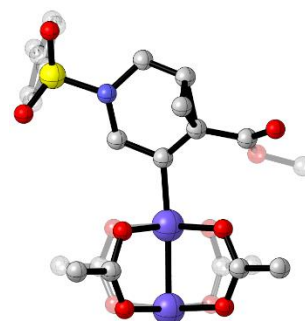
1v



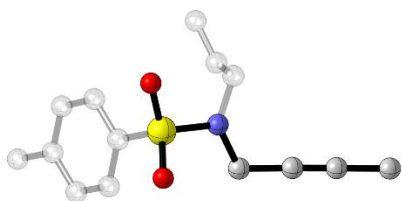
I(v)-Ene



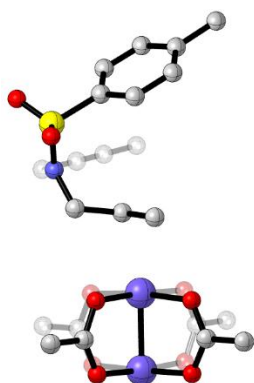
I-TS-II(v)



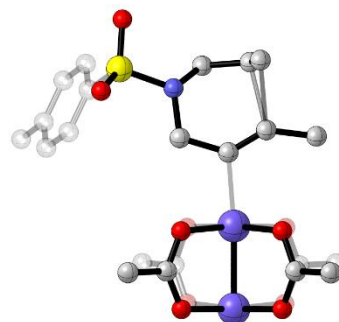
II(v)



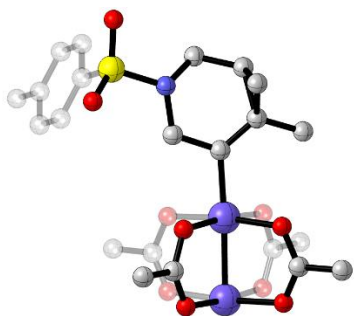
1y



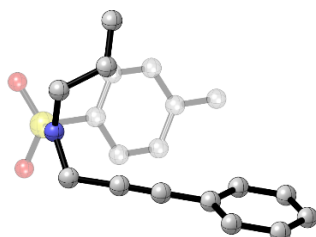
I(y)-Ene



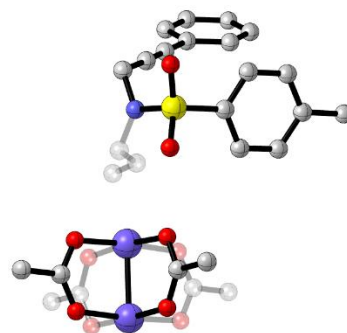
I-TS-II(y)



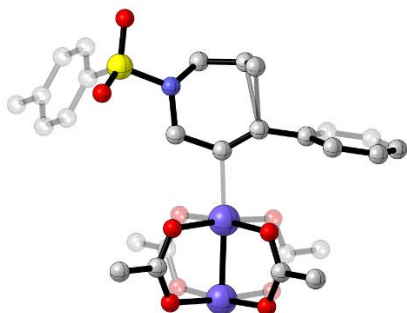
II(y)



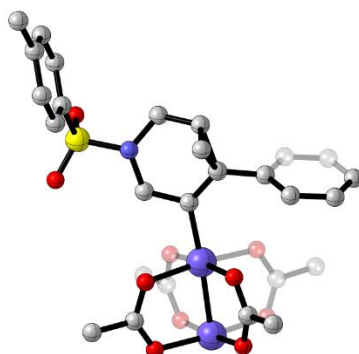
1z



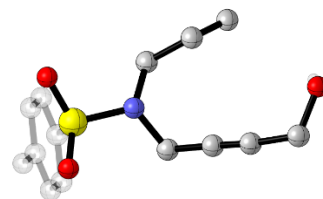
I(z)-Ene



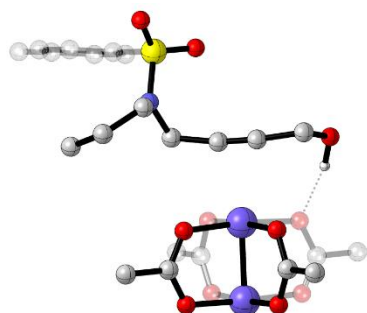
I-TS-II(z)



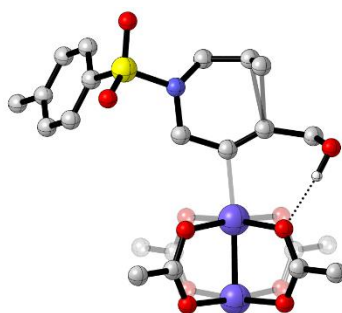
II(z)



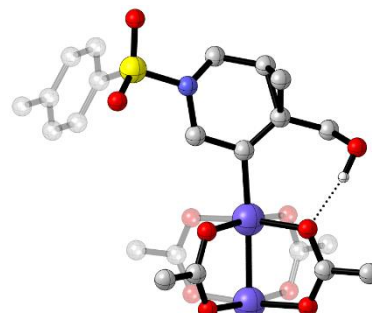
1u



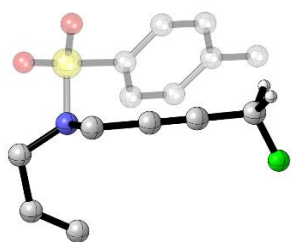
I(u)-Yne



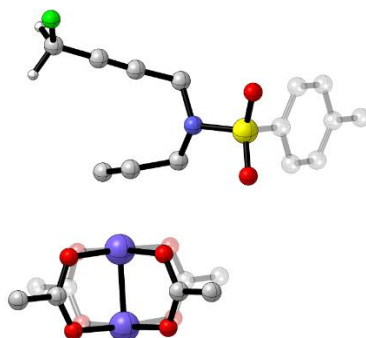
I-TS-II(u)



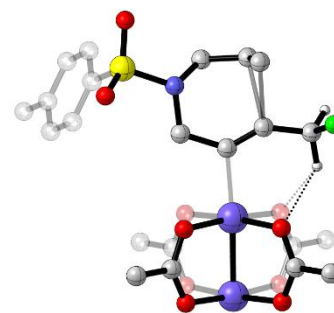
II(u)



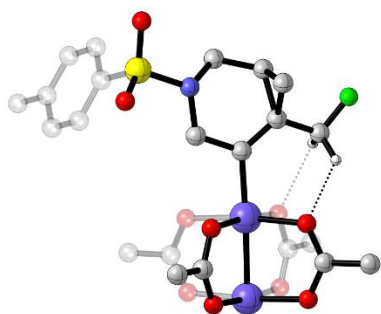
**1aa**



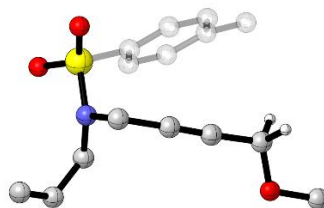
**I(aa)-Ene**



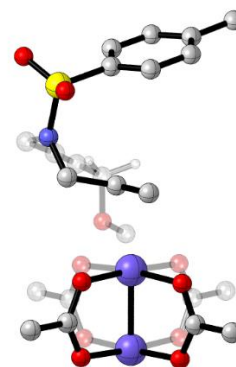
**I-TS-IIaa)**



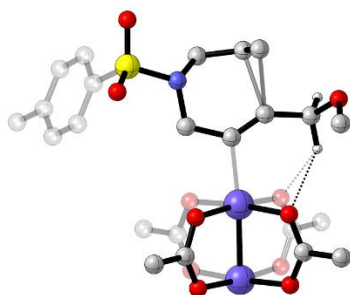
**II(aa)**



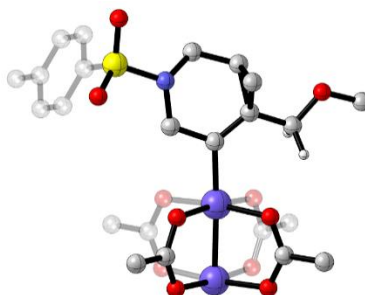
**1ab**



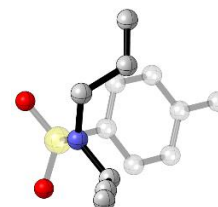
**I(ab)-Ene**



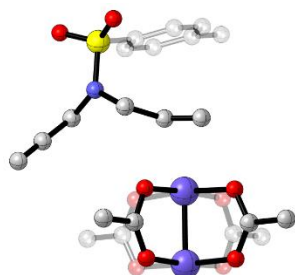
**I-TS-II(ab)**



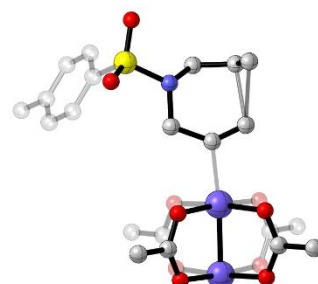
**II(ab)**



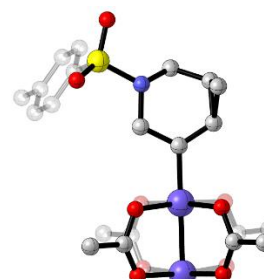
**1ac**



**I(ac)-Ene**



**I-TS-II(ac)**



**II(ac)**

\*)note: for all the metal-substrate complex, the alkene coordination mode is more stable than the alkyne coordination in all cases, but except the Rh-complex of 1,6-enynol **1u** (see the energy table S3 for detail).

(2) Table of energies and other thermodynamic parameters.

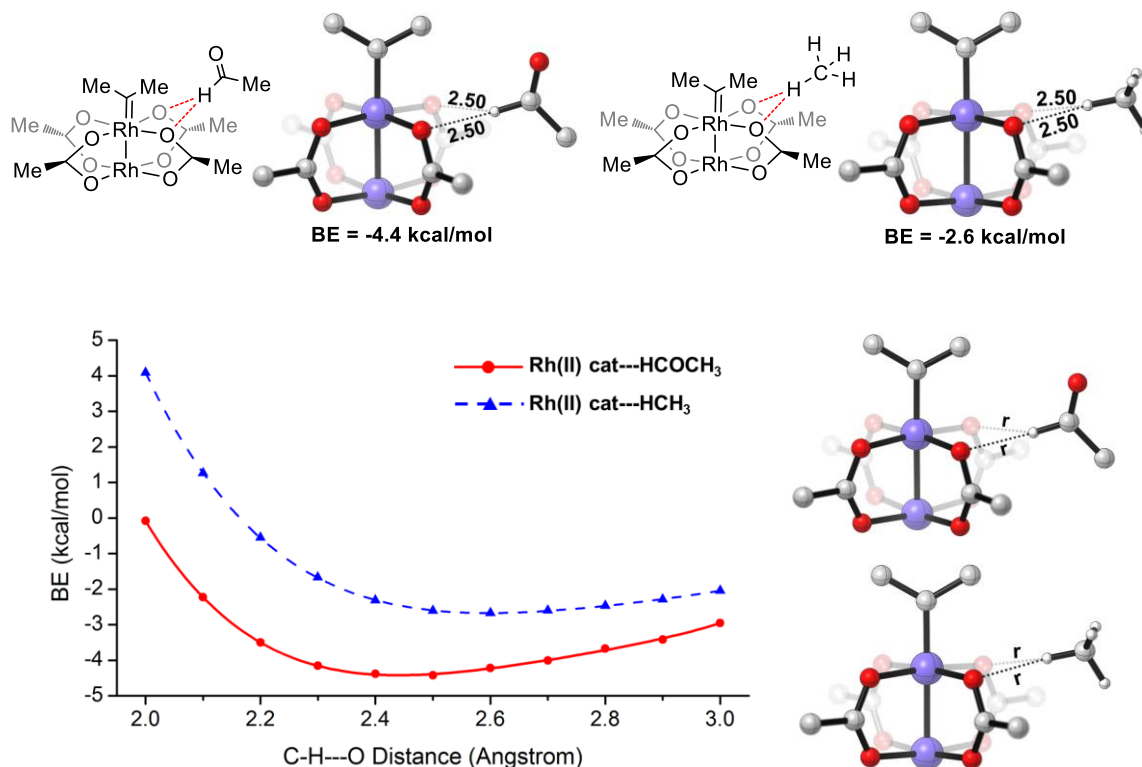
Table S6.

| Structures       | E <sub>ele</sub> | E <sub>0</sub> | E           | H           | G           | E <sub>ele(sol)</sub> |
|------------------|------------------|----------------|-------------|-------------|-------------|-----------------------|
| 1w_conf1         | -1260.25820      | -1259.96548    | -1259.94387 | -1259.94292 | -1260.02078 | -1259.93698           |
| I(w)-Yne_conf1   | -2393.39797      | -2392.89229    | -2392.84752 | -2392.84658 | -2392.97656 | -2394.91638           |
| I(w)-Ene_conf2   | -2393.40201      | -2392.89512    | -2392.85095 | -2392.85000 | -2392.97858 | -2394.92402           |
| I(w)-Ene_conf3   | -2393.40201      | -2392.89556    | -2392.85114 | -2392.85020 | -2392.98034 | -2394.92759           |
| I(w)-Yne_conf4   | -2393.39813      | -2392.89253    | -2392.84773 | -2392.84679 | -2392.97737 | -2394.91745           |
| I-TS-II(w)_conf1 | -2393.37315      | -2392.86688    | -2392.82400 | -2392.82306 | -2392.94748 | -2394.89153           |
| I-TS-II(w)_conf2 | -2393.37212      | -2392.86588    | -2392.82302 | -2392.82208 | -2392.94639 | -2394.88877           |
| II(w)_conf1      | -2393.40992      | -2392.90110    | -2392.85880 | -2392.85786 | -2392.98134 | -2394.94137           |
| 1x_conf1         | -1451.99604      | -1451.64935    | -1451.62499 | -1451.62405 | -1451.70972 | -1451.57569           |
| 1x_conf2         | -1451.99764      | -1451.65084    | -1451.62656 | -1451.62562 | -1451.71050 | -1451.57700           |
| I(x)-Ene_conf1   | -2585.14175      | -2584.58147    | -2584.53421 | -2584.53327 | -2584.67125 | -2586.56593           |
| I(x)-Ene_conf2   | -2585.13413      | -2584.57401    | -2584.52665 | -2584.52570 | -2584.66491 | -2586.55656           |
| I(x)-Yne_conf3   | -2585.13525      | -2584.57611    | -2584.52913 | -2584.52818 | -2584.66530 | -2586.55443           |
| I-TS-II(x)_conf1 | -2585.10443      | -2584.54498    | -2584.49900 | -2584.49805 | -2584.62949 | -2586.52870           |
| I-TS-II(x)_conf2 | -2585.10268      | -2584.54350    | -2584.49738 | -2584.49644 | -2584.62963 | -2586.52522           |
| II(x)_conf1      | -2585.14040      | -2584.57810    | -2584.53287 | -2584.53193 | -2584.66187 | -2586.57756           |
| 1v_conf1         | -1335.48511      | -1335.18645    | -1335.16402 | -1335.16308 | -1335.24304 | -1335.15774           |
| I(v)-Yne_conf1   | -2468.62363      | -2468.11247    | -2468.06674 | -2468.06579 | -2468.20009 | -2470.13712           |
| I(v)-Ene_conf2   | -2468.62794      | -2468.11563    | -2468.07024 | -2468.06930 | -2468.20253 | -2470.14196           |
| I-TS-II(v)_conf1 | -2468.59518      | -2468.08377    | -2468.03966 | -2468.03871 | -2468.16603 | -2470.10917           |
| I-TS-II(v)_conf2 | -2468.59399      | -2468.08289    | -2468.03862 | -2468.03767 | -2468.16644 | -2470.10534           |
| I-TS-II(v)_conf3 | -2468.59202      | -2468.08113    | -2468.03675 | -2468.03581 | -2468.16526 | -2470.10676           |
| II(v)_conf1      | -2468.63802      | -2468.12379    | -2468.08033 | -2468.07939 | -2468.20575 | -2470.16496           |
| II(v)_conf2      | -2468.63677      | -2468.12265    | -2468.07919 | -2468.07825 | -2468.20490 | -2470.16266           |
| 1y_conf1         | -1146.93920      | -1146.65591    | -1146.63610 | -1146.63515 | -1146.70902 | -1146.63882           |
| I(y)-Yne_conf1   | -2280.08130      | -2279.58468    | -2279.54194 | -2279.54100 | -2279.66617 | -2281.62160           |
| I(y)-Ene_conf2   | -2280.08165      | -2279.58478    | -2279.54191 | -2279.54097 | -2279.66929 | -2281.62418           |
| I(y)-Ene_conf3   | -2280.07869      | -2279.58194    | -2279.53908 | -2279.53814 | -2279.66698 | -2281.62244           |
| I-TS-II(y)_conf1 | -2280.04815      | -2279.55175    | -2279.51052 | -2279.50957 | -2279.63055 | -2281.59054           |
| II(y)_conf1      | -2280.08751      | -2279.58758    | -2279.54741 | -2279.54646 | -2279.66377 | -2281.63743           |
| 1z_conf1         | -1338.67704      | -1338.34000    | -1338.31762 | -1338.31668 | -1338.39586 | -1338.27802           |
| I(z)-Yne_conf1   | -2471.81428      | -2471.26463    | -2471.21883 | -2471.21789 | -2471.35111 | -2473.25678           |
| I(z)-Ene_conf2   | -2471.82105      | -2471.27042    | -2471.22501 | -2471.22406 | -2471.35745 | -2473.26552           |
| I-TS-II(z)_conf1 | -2471.77914      | -2471.22992    | -2471.18560 | -2471.18466 | -2471.31332 | -2473.22642           |
| I-TS-II(z)_conf2 | -2471.77588      | -2471.22670    | -2471.18242 | -2471.18148 | -2471.31023 | -2473.22186           |
| II(z)_conf1      | -2471.81409      | -2471.26158    | -2471.21833 | -2471.21739 | -2471.34222 | -2473.27026           |
| 1u_conf1         | -1222.13727      | -1221.84891    | -1221.82831 | -1221.82736 | -1221.90262 | -1221.84277           |
| I(u)-Ene_conf1   | -2355.28485      | -2354.78174    | -2354.73877 | -2354.73783 | -2354.86336 | -2356.83104           |
| I(u)-Yne_conf2   | -2355.28783      | -2354.78521    | -2354.74203 | -2354.74109 | -2354.86626 | -2356.83168           |
| I(u)-Yne_conf3   | -2355.28748      | -2354.78537    | -2354.74193 | -2354.74098 | -2354.86886 | -2356.83228           |
| I-TS-II(u)_conf1 | -2355.26228      | -2354.75972    | -2354.71803 | -2354.71709 | -2354.83860 | -2356.80813           |

|                   |             |             |             |             |             |             |
|-------------------|-------------|-------------|-------------|-------------|-------------|-------------|
| I-TS-II(u)_conf2  | -2355.26164 | -2354.75912 | -2354.71747 | -2354.71653 | -2354.83792 | -2356.80588 |
| II(u)_conf1       | -2355.30004 | -2354.79432 | -2354.75351 | -2354.75256 | -2354.87157 | -2356.85468 |
| 1aa_conf1         | -1246.15674 | -1245.88033 | -1245.86015 | -1245.85920 | -1245.93374 | -1245.86835 |
| 1aa_conf2         | -1246.15701 | -1245.88088 | -1245.86057 | -1245.85962 | -1245.93599 | -1245.86700 |
| 1aa_conf3         | -1246.15549 | -1245.87936 | -1245.85916 | -1245.85821 | -1245.93309 | -1245.86876 |
| 1aa_conf4         | -1246.15686 | -1245.88026 | -1245.86033 | -1245.85939 | -1245.93182 | -1245.86695 |
| I(aa)-Yne_conf1   | -2379.29012 | -2378.80069 | -2378.75723 | -2378.75629 | -2378.88363 | -2380.84467 |
| I(aa)-Ene_conf2   | -2379.29865 | -2378.80894 | -2378.76567 | -2378.76473 | -2378.89409 | -2380.85245 |
| I-TS-II(aa)_conf1 | -2379.27352 | -2378.78430 | -2378.74243 | -2378.74149 | -2378.86445 | -2380.82521 |
| II(aa)_conf1      | -2379.31092 | -2378.81819 | -2378.77732 | -2378.77638 | -2378.89646 | -2380.87129 |
| II(aa)_conf2      | -2379.31609 | -2378.82325 | -2378.78241 | -2378.78146 | -2378.90094 | -2380.87418 |
| 1ab_conf1         | -1261.44151 | -1261.12468 | -1261.10284 | -1261.10189 | -1261.17982 | -1261.11626 |
| 1ab_conf2         | -1261.44365 | -1261.12685 | -1261.10497 | -1261.10403 | -1261.18189 | -1261.11673 |
| 1ab_conf3         | -1261.44672 | -1261.12985 | -1261.10795 | -1261.10700 | -1261.18575 | -1261.12115 |
| 1ab_conf4         | -1261.43999 | -1261.12339 | -1261.10141 | -1261.10047 | -1261.17901 | -1261.11527 |
| I(ab)-Ene_conf1   | -2394.58245 | -2394.05178 | -2394.00722 | -2394.00627 | -2394.13586 | -2396.09939 |
| I(ab)-Yne_conf2   | -2394.58512 | -2394.05562 | -2394.01028 | -2394.00934 | -2394.14318 | -2396.09808 |
| I(ab)-Ene_conf3   | -2394.58855 | -2394.05816 | -2394.01315 | -2394.01220 | -2394.14574 | -2396.10571 |
| I(ab)Yne_conf4    | -2394.58786 | -2394.05841 | -2394.01292 | -2394.01198 | -2394.14755 | -2396.10174 |
| I-TS-II(ab)_conf1 | -2394.55962 | -2394.02996 | -2393.98629 | -2393.98534 | -2394.11196 | -2396.07366 |
| I-TS-II(ab)_conf2 | -2394.56120 | -2394.03114 | -2393.98755 | -2393.98661 | -2394.11346 | -2396.07697 |
| II(ab)_conf1      | -2394.60155 | -2394.06846 | -2394.02562 | -2394.02467 | -2394.14958 | -2396.12288 |
| II(ab)_conf2      | -2394.60161 | -2394.06840 | -2394.02563 | -2394.02468 | -2394.14885 | -2396.12286 |
| II(ab)_conf3      | -2394.59990 | -2394.06690 | -2394.02407 | -2394.02313 | -2394.14720 | -2396.12025 |
| II(ab)_conf4      | -2394.59982 | -2394.06689 | -2394.02399 | -2394.02305 | -2394.14764 | -2396.12023 |
| 1ac_conf1         | -1107.61299 | -1107.35840 | -1107.34052 | -1107.33957 | -1107.40694 | -1107.33515 |
| 1ac_conf2         | -1107.61391 | -1107.35936 | -1107.34148 | -1107.34054 | -1107.40758 | -1107.33633 |
| I(ac)-Yne_conf1   | -2240.75464 | -2240.28693 | -2240.24601 | -2240.24507 | -2240.36544 | -2242.31637 |
| I(ac)-Ene_conf2   | -2240.75788 | -2240.28979 | -2240.24890 | -2240.24795 | -2240.36987 | -2242.32385 |
| I(ac)-Ene_conf3   | -2240.75517 | -2240.28679 | -2240.24608 | -2240.24514 | -2240.36545 | -2242.32118 |
| II(ac)_conf1      | -2240.77568 | -2240.30392 | -2240.26505 | -2240.26411 | -2240.38135 | -2242.34591 |
| I-TS-II(ac)_conf1 | -2240.72617 | -2240.25867 | -2240.21880 | -2240.21785 | -2240.33757 | -2242.28839 |
| I-TS-II(ac)_conf2 | -2240.72617 | -2240.25861 | -2240.21879 | -2240.21784 | -2240.33699 | -2242.28838 |

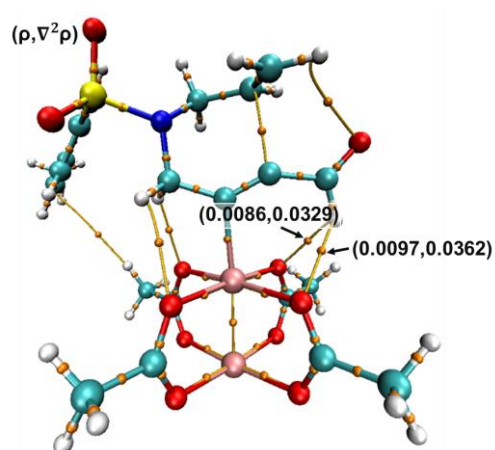
## 10.4 Analysis of C-H...O interaction.

### (1) Binding energies of R-H and Rh(II) carbene complex.

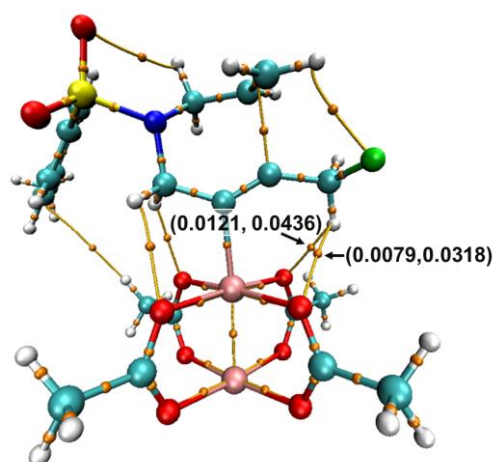


**Figure S2.** Dependence of binding energies (BEs) on the C-H...O distances. Both C-H...O distances were constrained to be equal during the optimization. BE of the complex was obtained through subtracting the energies of the isolated R-H species and Rh(II) catalyst from the energy of the complex, and corrected for BSSE. The energies were given at the M06/6-311++G(d,p)-SDD//B3LYP/6-31G(d)-Lanl2DZ theoretical level. During the optimization, all the heavy atoms of carbene, acetaldehyde, and methane were kept in the symmetry plane to avoid the unexpected interaction between substrate (acetaldehyde, or methane) and electrophilic carbene.

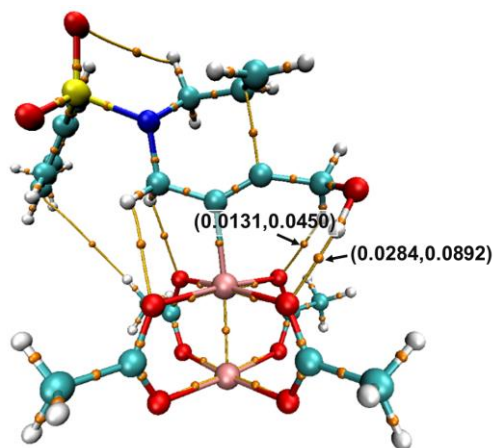
(2) QTAIM analysis of selected transition structures.



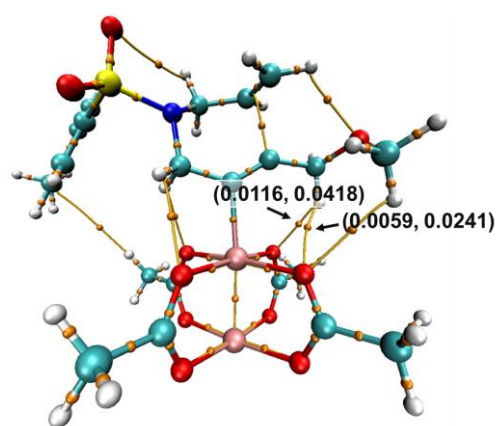
I-TS-II(a)



I-TS-II(aa)



I-TS-II(u)



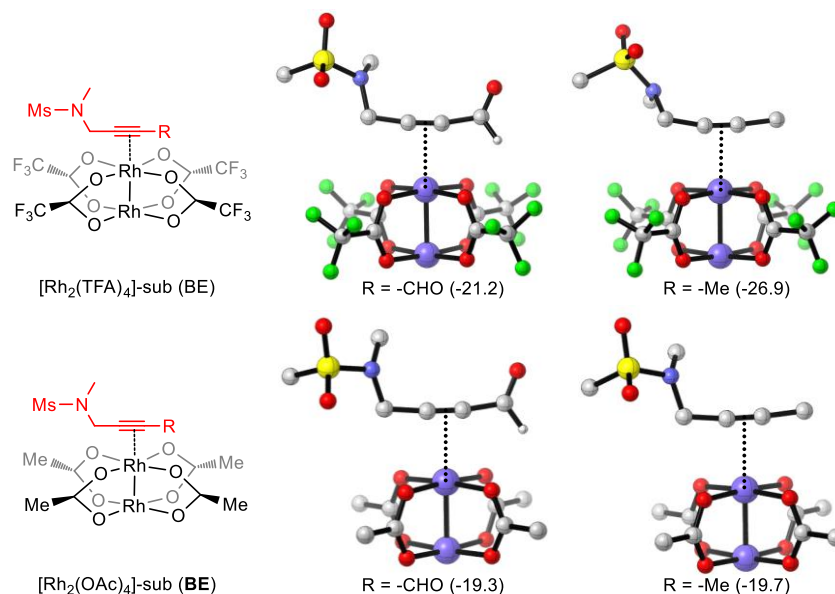
I-TS-II(ab)

**Figure S3.** QTAIM analysis of transition structures **I-TS-II** were performed by Multiwfn. The bond critical points were shown in orange dots, which supports attractive C-H...O interactions between –CHZ group and ligand oxygen atoms. Electron density and its Laplacian for selected BCPs are in a.u.

## 10.5 Analysis of the EWG activation on alkyne.

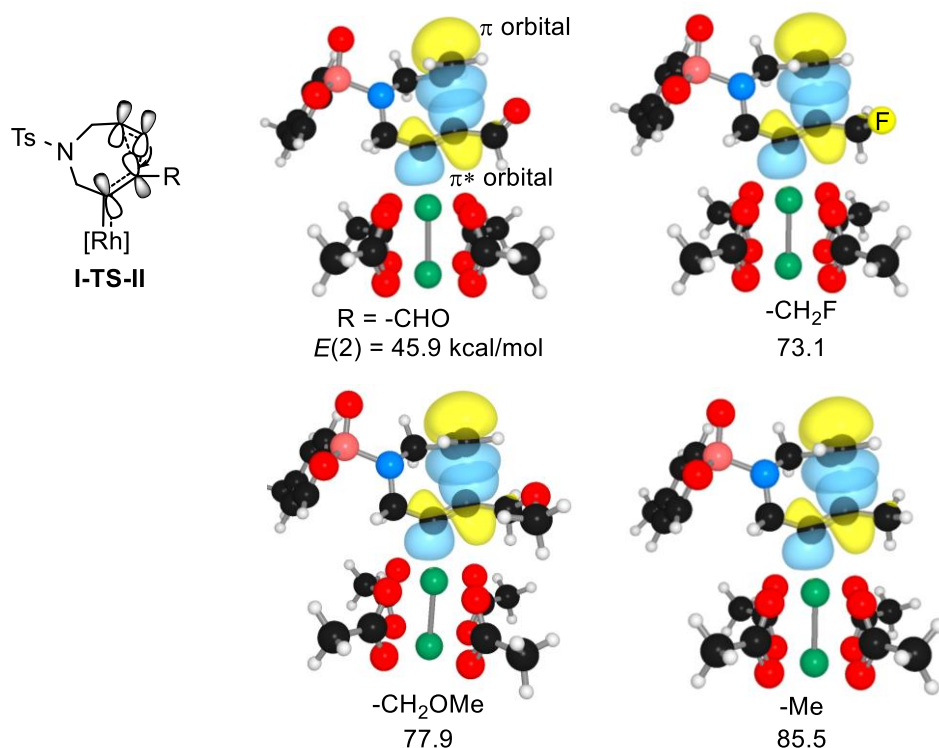
### (1) Substituent Effects on binding energies between catalyst and substrates.

The binding energy between  $[\text{Rh}_2(\text{TFA})_4]$  catalyst and alkynal ( $\text{R} = -\text{CHO}$ ) was calculated to be  $-21.2$  kcal/mol, much weaker than that between  $[\text{Rh}_2(\text{TFA})_4]$  catalyst and alkyne ( $\text{R} = -\text{Me}$ ). However, the binding energy difference between  $[\text{Rh}_2(\text{OAc})_4]$ -alkynal and  $[\text{Rh}_2(\text{OAc})_4]$ -alkyne is only  $0.4$  kcal/mol, because  $[\text{Rh}_2(\text{OAc})_4]$  is not as electron-poor as  $[\text{Rh}_2(\text{TFA})_4]$ . Therefore, the substituent effects on binding energy differences between  $[\text{Rh}_2(\text{OAc})_4]$  and different alkynes are small.



**Figure S4.** Binding energies (BE) between alkyne and Rh(II) catalyst. BE of the complexes were obtained through subtracting the energies of the isolated acetaldehyde and Rh(II) catalyst from the energy of the complex with counterpoise corrections at M06/(SDD, 6-311++G(d,p))/B3LYP/(LANL2DZ+f, 6-31G(d)) theoretical level.

(2) NBO analysis of the 6-*endo-dig* transition states [31].



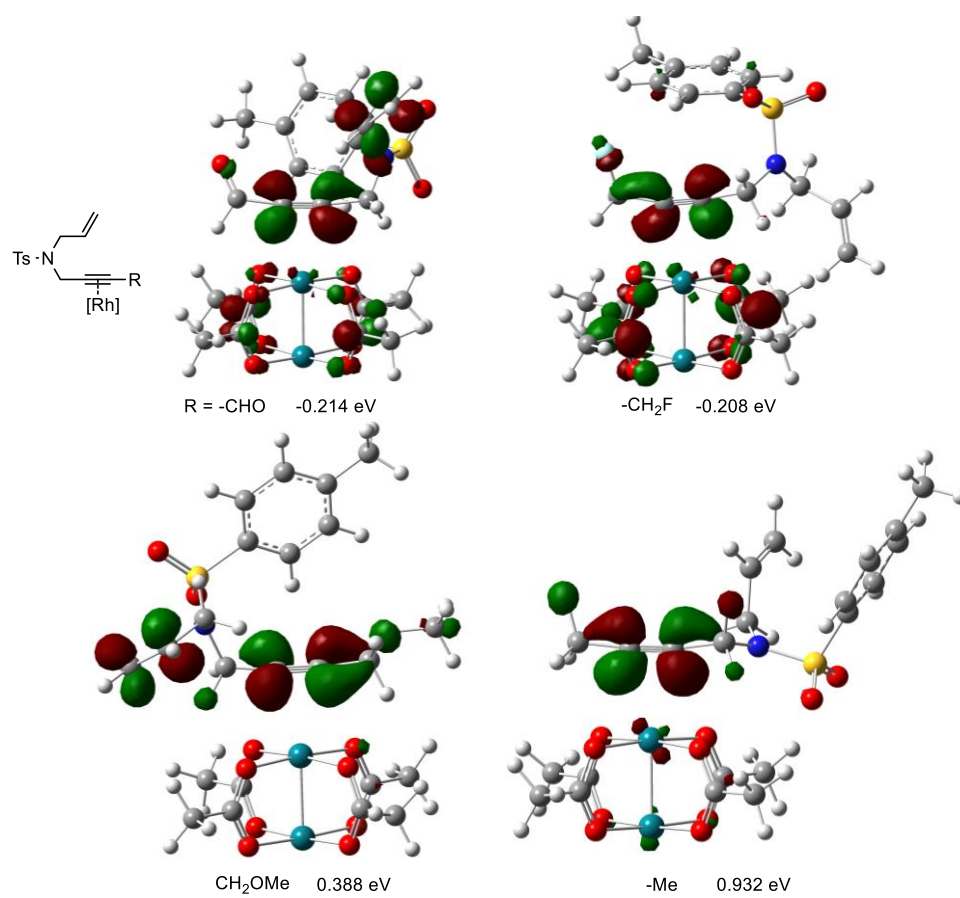
**Figure S5.**  $\pi(\text{C}=\text{C}) \rightarrow \pi^*(\text{C}\equiv\text{C}, \text{in plane})$  interactions in the 6-*endo-dig* transition states.

Natural bond orbital (NBO) analysis revealed that there were significant  $\pi(\text{C}=\text{C}) \rightarrow \pi^*(\text{C}\equiv\text{C}, \text{in plane})$  interactions in the cyclopropanation transition states (E(2) means second-order perturbation energies). Thus, EWG group may benefit this cyclopropanation step by decreasing the  $\pi^*(\text{C}\equiv\text{C}, \text{in plane})$  orbital energy.

**Table S7.** Second-order perturbation energies (E2) of I-TS-II calculated at B3LYP/LANL2DZ-6-31G(d) level.

| R                    | E(2) [kcal/mol]                                                                     |                                                                    |
|----------------------|-------------------------------------------------------------------------------------|--------------------------------------------------------------------|
|                      | $\pi(\text{C}=\text{C}) \rightarrow \pi^*(\text{C}\equiv\text{C}, \text{in plane})$ | $\pi(\text{C}\equiv\text{C}) \rightarrow \pi^*(\text{C}=\text{C})$ |
| -CHO                 | 45.86                                                                               | 5.74                                                               |
| -CH <sub>2</sub> F   | 73.10                                                                               | 11.41                                                              |
| -CH <sub>2</sub> OMe | 77.87                                                                               | 11.93                                                              |
| -Me                  | 85.48                                                                               | 14.24                                                              |

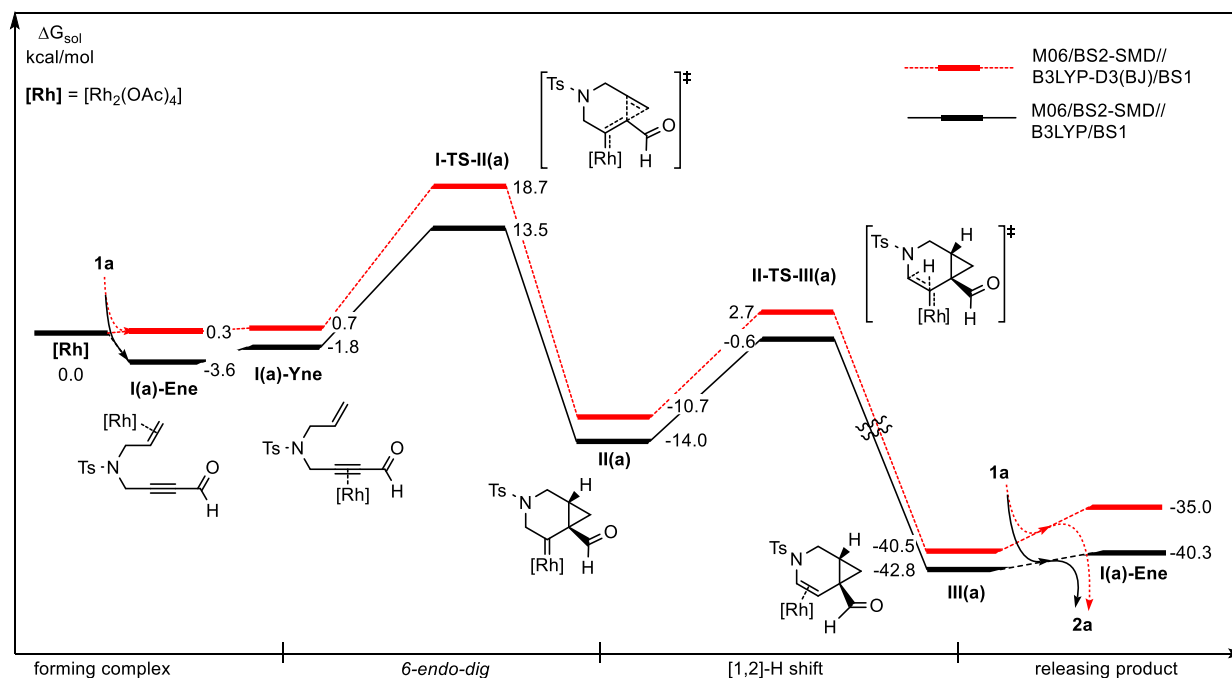
(3)  $\pi^*(\text{C}\equiv\text{C}, \text{ in plane})$  Orbital energies of the alkyne-coordinated complexes.



**Figure S6.**  $\pi^*(\text{C}\equiv\text{C}, \text{ in plane})$  orbital energies of the alkyne-coordinated complexes at B3LYP/LANL2DZ-6-31G(d) level.

## 10.6 Effect of empirical dispersion.

We have evaluated the effect of empirical dispersion and found that dispersion introduced by the D3 version of Grimme's dispersion with Becke-Johnson damping is not significant for the free energy barriers.



**Scheme S3. Comparison of potential energy surfaces: structures optimized with or without empirical dispersion.**

BS1: LANL2DZ basis set for rhodium (augmented with a 4f-function,  $\zeta_f(\text{Rh}) = 1.350$ ), and the 6-31G(d) basis set for the other atoms; BS2: SDD basis set for rhodium, and 6-311++G(d,p) for the other atoms.

## 10.7 Coordinates of all stationary points.

### **Rh<sub>2</sub>(OAc)<sub>4</sub>**

#### **0 imaginary frequency**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rh | -0.000001 | -0.000004 | 1.188079  |
| Rh | 0.000000  | -0.000001 | -1.188079 |
| O  | -1.451162 | 1.455126  | 1.133186  |
| O  | -1.453119 | 1.453239  | -1.134029 |
| O  | 1.451155  | 1.455136  | -1.133183 |
| O  | -1.451152 | -1.455141 | -1.133187 |
| O  | 1.453117  | -1.453244 | -1.134031 |
| O  | 1.451157  | -1.455139 | 1.133184  |
| O  | 1.453113  | 1.453242  | 1.134032  |
| O  | -1.453113 | -1.453252 | 1.134028  |
| C  | -1.864781 | -1.863020 | 0.000558  |
| C  | -1.864815 | 1.862979  | -0.000560 |
| C  | 1.864798  | 1.862996  | 0.000564  |
| C  | 1.864786  | -1.863014 | -0.000563 |
| C  | 2.961598  | -2.902761 | 0.002517  |
| C  | -2.961588 | -2.902772 | -0.002523 |
| C  | -2.961546 | 2.902811  | 0.002525  |
| C  | 2.961549  | 2.902807  | -0.002519 |
| H  | 2.837290  | 3.578939  | -0.851463 |
| H  | 3.928599  | 2.397668  | -0.111031 |
| H  | 2.963155  | 3.458404  | 0.937057  |
| H  | -2.963129 | 3.458424  | -0.937042 |
| H  | -2.837288 | 3.578928  | 0.851482  |
| H  | -3.928604 | 2.397685  | 0.111014  |
| H  | -3.928628 | -2.397576 | -0.110871 |
| H  | -2.837451 | -3.578820 | -0.851551 |
| H  | -2.963121 | -3.458466 | 0.936996  |
| H  | 2.963138  | -3.458449 | -0.937006 |
| H  | 2.837461  | -3.578814 | 0.851540  |
| H  | 3.928635  | -2.397561 | 0.110872  |

#### **1a\_conf1**

#### **0 imaginary frequency**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.749237 | 1.432066  | 0.594438  |
| H | 0.162507  | 1.324701  | 1.192839  |
| H | -1.601852 | 1.217622  | 1.252403  |
| N | -0.664671 | 0.448087  | -0.508348 |
| S | 0.052418  | -1.047293 | -0.077434 |
| O | -0.158733 | -1.925322 | -1.233518 |
| O | -0.363190 | -1.464905 | 1.267680  |
| C | 1.782699  | -0.588617 | 0.006379  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.452178  | -0.666934 | 1.226149  |
| C | 2.453365  | -0.212132 | -1.162087 |
| C | 3.811522  | -0.350330 | 1.274987  |
| H | 1.914533  | -0.977500 | 2.115649  |
| C | 3.806515  | 0.099267  | -1.093617 |
| H | 1.920416  | -0.169178 | -2.106147 |
| C | 4.507358  | 0.035867  | 0.123669  |
| H | 4.337756  | -0.408612 | 2.224257  |
| H | 4.332703  | 0.393213  | -1.998657 |
| C | 5.979855  | 0.366977  | 0.175180  |
| H | 6.356260  | 0.362871  | 1.202385  |
| H | 6.567816  | -0.359725 | -0.399405 |
| H | 6.181332  | 1.355271  | -0.255062 |
| C | -1.880651 | 0.326623  | -1.335045 |
| H | -2.048682 | 1.309032  | -1.790699 |
| H | -1.670289 | -0.382264 | -2.140783 |
| C | -3.092542 | -0.090123 | -0.619989 |
| C | -4.101801 | -0.427174 | -0.035971 |
| C | -0.825795 | 2.831158  | 0.045440  |
| H | 0.002340  | 3.129281  | -0.597081 |
| C | -1.815180 | 3.685173  | 0.310108  |
| H | -2.656022 | 3.407147  | 0.942081  |
| H | -1.818515 | 4.696414  | -0.087276 |
| C | -5.272688 | -0.859911 | 0.690918  |
| H | -5.059801 | -1.264577 | 1.700237  |
| O | -6.408088 | -0.797906 | 0.258247  |

#### **1a\_conf2**

#### **0 imaginary frequency**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.073541  | 1.736262  | -0.036597 |
| H | 1.796785  | 1.612576  | -0.854355 |
| H | 1.536013  | 2.373224  | 0.724585  |
| N | 0.843040  | 0.426954  | 0.637458  |
| S | 0.166317  | -0.809151 | -0.342223 |
| O | 0.532791  | -2.075321 | 0.303669  |
| O | 0.485775  | -0.567920 | -1.755792 |
| C | -1.596186 | -0.559992 | -0.134499 |
| C | -2.405936 | -0.537603 | -1.268484 |
| C | -2.150698 | -0.491781 | 1.146942  |
| C | -3.789246 | -0.431654 | -1.112878 |
| H | -1.955450 | -0.598287 | -2.253368 |
| C | -3.530121 | -0.383067 | 1.282260  |
| H | -1.509484 | -0.509527 | 2.021729  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.372024 | -0.352234 | 0.157224  |
| H | -4.423523 | -0.411662 | -1.995355 |
| H | -3.964330 | -0.321325 | 2.277290  |
| C | -5.868335 | -0.238695 | 0.326203  |
| H | -6.379514 | -0.197993 | -0.640234 |
| H | -6.269687 | -1.094956 | 0.882244  |
| H | -6.137503 | 0.663982  | 0.888124  |
| C | 1.986498  | -0.015496 | 1.460994  |
| H | 2.083088  | 0.708850  | 2.279592  |
| H | 1.731475  | -0.980626 | 1.906188  |
| C | 3.270363  | -0.135003 | 0.760222  |
| C | 4.338564  | -0.226587 | 0.191290  |
| C | -0.172039 | 2.408470  | -0.548714 |
| H | -0.650166 | 1.954710  | -1.413195 |
| C | -0.659043 | 3.539529  | -0.038178 |
| H | -0.198327 | 4.030401  | 0.817047  |
| H | -1.536562 | 4.022927  | -0.458897 |
| C | 5.587809  | -0.351158 | -0.523916 |
| H | 5.485000  | -0.355545 | -1.627090 |
| O | 6.675303  | -0.444879 | 0.013104  |

#### 1a\_conf3

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.374835 | -0.926472 | 1.192969  |
| H | -2.088880 | -1.935576 | 1.503849  |
| H | -3.472635 | -0.893103 | 1.200221  |
| N | -1.936038 | -0.783656 | -0.205662 |
| S | -0.746042 | -1.794971 | -0.839761 |
| O | -0.842658 | -1.648643 | -2.294613 |
| O | -0.916376 | -3.084691 | -0.166770 |
| C | 0.857786  | -1.156529 | -0.344475 |
| C | 1.425606  | -1.583930 | 0.858945  |
| C | 1.520263  | -0.236865 | -1.160108 |
| C | 2.658761  | -1.067045 | 1.251166  |
| H | 0.917497  | -2.327016 | 1.464387  |
| C | 2.754965  | 0.266438  | -0.753031 |
| H | 1.081456  | 0.065235  | -2.104502 |
| C | 3.342478  | -0.135769 | 0.455164  |
| H | 3.102837  | -1.400526 | 2.185927  |
| H | 3.275362  | 0.977863  | -1.389645 |
| C | 4.695780  | 0.389549  | 0.871359  |
| H | 4.777725  | 0.469386  | 1.960434  |
| H | 5.496884  | -0.281120 | 0.533432  |
| H | 4.893640  | 1.376209  | 0.440313  |

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -2.323084 | 0.416464 | -0.948618 |
| H | -2.311332 | 0.172020 | -2.015749 |
| H | -3.365910 | 0.636546 | -0.686139 |
| C | -1.503334 | 1.615196 | -0.725000 |
| C | -0.830212 | 2.616526 | -0.590924 |
| C | -1.825893 | 0.110748 | 2.139809  |
| H | -0.740451 | 0.184180 | 2.194547  |
| C | -2.589225 | 0.896824 | 2.899550  |
| H | -3.676091 | 0.846873 | 2.862360  |
| H | -2.161370 | 1.616130 | 3.592163  |
| C | 0.019075  | 3.765859 | -0.391564 |
| H | 0.984703  | 3.534941 | 0.102601  |
| O | -0.265126 | 4.900474 | -0.726096 |

#### I(a)-Yne\_conf1

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.386905 | 2.228271  | -0.990913 |
| H | -4.442216 | 2.028497  | -1.195287 |
| H | -2.808390 | 1.758196  | -1.798545 |
| N | -2.994788 | 1.556882  | 0.275516  |
| S | -4.226384 | 0.988824  | 1.283238  |
| O | -5.269856 | 2.012572  | 1.265823  |
| O | -3.569761 | 0.548945  | 2.516800  |
| C | -4.902722 | -0.473960 | 0.486408  |
| C | -4.285929 | -1.714600 | 0.675941  |
| C | -6.030220 | -0.357848 | -0.330249 |
| C | -4.796694 | -2.836402 | 0.026457  |
| H | -3.435535 | -1.801872 | 1.344114  |
| C | -6.527792 | -1.491668 | -0.971485 |
| H | -6.521333 | 0.603355  | -0.437251 |
| C | -5.921786 | -2.744924 | -0.807053 |
| H | -4.320888 | -3.802337 | 0.178397  |
| H | -7.407667 | -1.401891 | -1.603808 |
| C | -6.488638 | -3.974173 | -1.476761 |
| H | -5.701294 | -4.690663 | -1.733765 |
| H | -7.194731 | -4.491426 | -0.813707 |
| H | -7.029852 | -3.718536 | -2.393328 |
| C | -1.742430 | 0.792866  | 0.278907  |
| H | -1.616987 | 0.321600  | 1.257255  |
| H | -1.732175 | -0.001861 | -0.483444 |
| C | -0.588893 | 1.662776  | 0.037796  |
| C | 0.287333  | 2.483095  | -0.198680 |
| C | -3.148739 | 3.716930  | -0.968395 |
| H | -2.115954 | 4.044366  | -0.860372 |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | -4.126466 | 4.613161  | -1.094883 | O  | -3.201828 | -0.988901 | 2.167965  |
| H                            | -5.168435 | 4.315047  | -1.190485 | O  | -2.573341 | -1.942533 | -0.127411 |
| H                            | -3.922944 | 5.680436  | -1.094617 | C  | -4.889664 | -0.725515 | 0.168785  |
| C                            | 1.135096  | 3.628260  | -0.490057 | C  | -5.227781 | -1.012066 | -1.156804 |
| H                            | 2.216595  | 3.468045  | -0.366076 | C  | -5.854476 | -0.265351 | 1.067752  |
| O                            | 0.659733  | 4.691449  | -0.842288 | C  | -6.540413 | -0.818205 | -1.581459 |
| Rh                           | 1.569428  | 0.294629  | -0.025068 | H  | -4.476673 | -1.400296 | -1.836776 |
| Rh                           | 3.258879  | -1.407989 | 0.025772  | C  | -7.162894 | -0.076812 | 0.624243  |
| O                            | 2.805049  | 1.443391  | 1.166697  | H  | -5.584104 | -0.075730 | 2.101123  |
| O                            | 4.392488  | -0.174167 | 1.217851  | C  | -7.527003 | -0.345794 | -0.702877 |
| O                            | 2.351792  | -2.187728 | 1.700803  | H  | -6.804996 | -1.042608 | -2.611959 |
| O                            | 4.093956  | -0.548660 | -1.648907 | H  | -7.915097 | 0.280097  | 1.323426  |
| O                            | 2.053612  | -2.573065 | -1.169828 | C  | -8.952482 | -0.165657 | -1.168068 |
| O                            | 0.449374  | -0.972246 | -1.223304 | H  | -8.995063 | 0.151105  | -2.215509 |
| O                            | 0.745035  | -0.590038 | 1.653805  | H  | -9.512818 | -1.106731 | -1.089911 |
| O                            | 2.505699  | 1.067963  | -1.698288 | H  | -9.480432 | 0.579503  | -0.564505 |
| C                            | 3.548152  | 0.483714  | -2.147293 | C  | -1.823168 | 0.680079  | -1.016979 |
| C                            | 3.932388  | 0.966353  | 1.531694  | H  | -1.539559 | -0.310232 | -1.380541 |
| C                            | 1.313668  | -1.616073 | 2.157266  | H  | -2.535571 | 1.135630  | -1.723729 |
| C                            | 0.929196  | -2.113682 | -1.535742 | C  | -0.634601 | 1.538117  | -0.989800 |
| C                            | 0.081130  | -2.978915 | -2.441284 | C  | 0.272715  | 2.357370  | -1.001542 |
| C                            | 4.164062  | 1.058326  | -3.402740 | C  | -3.507493 | 2.772342  | 0.476150  |
| C                            | 4.777090  | 1.843247  | 2.427590  | H  | -4.552074 | 2.495110  | 0.334074  |
| C                            | 0.713773  | -2.175681 | 3.426912  | C  | -3.070208 | 3.964671  | 0.065771  |
| H                            | 0.884487  | -3.252884 | 3.482953  | H  | -2.030133 | 4.266936  | 0.175448  |
| H                            | -0.352488 | -1.947194 | 3.482759  | H  | -3.738600 | 4.684700  | -0.399710 |
| H                            | 1.208528  | -1.706532 | 4.285599  | C  | 1.137076  | 3.531238  | -1.065827 |
| H                            | 5.765514  | 1.404845  | 2.571568  | H  | 2.122864  | 3.370339  | -1.529503 |
| H                            | 4.279421  | 1.951440  | 3.397492  | O  | 0.776979  | 4.612612  | -0.643685 |
| H                            | 4.865707  | 2.842763  | 1.991680  | Rh | 1.589944  | 0.350054  | -0.297094 |
| H                            | 4.028071  | 2.141662  | -3.432834 | Rh | 3.236798  | -1.253222 | 0.388703  |
| H                            | 5.223255  | 0.799965  | -3.457813 | O  | 2.695070  | 1.791171  | 0.698654  |
| H                            | 3.656301  | 0.628514  | -4.274320 | O  | 4.264484  | 0.275718  | 1.309175  |
| H                            | 0.464442  | -4.000163 | -2.462743 | O  | 2.153971  | -1.563223 | 2.106664  |
| H                            | 0.104405  | -2.565043 | -3.455797 | O  | 4.233903  | -0.875999 | -1.379383 |
| H                            | -0.958987 | -2.968261 | -2.103687 | O  | 2.132181  | -2.720199 | -0.530495 |
| <b>I(a)-Yne_conf2</b>        |           |           |           | O  | 0.611154  | -1.202672 | -1.243397 |
| <b>0 imaginary frequency</b> |           |           |           | O  | 0.589852  | -0.056713 | 1.456295  |
| C                            | -2.625337 | 1.743807  | 1.139769  | O  | 2.707385  | 0.680395  | -2.006744 |
| H                            | -1.641464 | 2.170272  | 1.360965  | C  | 3.767691  | -0.009666 | -2.181080 |
| H                            | -3.045622 | 1.406177  | 2.090456  | C  | 3.776485  | 1.446471  | 1.282465  |
| N                            | -2.405438 | 0.532502  | 0.320659  | C  | 1.069851  | -0.917145 | 2.267366  |
| S                            | -3.183234 | -0.900131 | 0.704344  | C  | 1.058149  | -2.393210 | -1.122807 |
|                              |           |           |           | C  | 0.219211  | -3.489567 | -1.734248 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.514783  | 0.210398  | -3.477942 |
| C | 4.519770  | 2.529328  | 2.031709  |
| C | 0.279414  | -1.165592 | 3.530573  |
| H | 0.641376  | -2.062453 | 4.035901  |
| H | -0.783449 | -1.258001 | 3.289466  |
| H | 0.396705  | -0.305176 | 4.199799  |
| H | 5.567259  | 2.251268  | 2.161328  |
| H | 4.064502  | 2.650010  | 3.021769  |
| H | 4.434918  | 3.482938  | 1.505323  |
| H | 4.500657  | 1.269275  | -3.748081 |
| H | 5.541189  | -0.150432 | -3.392698 |
| H | 4.010304  | -0.346014 | -4.276575 |
| H | 0.692176  | -4.461827 | -1.589283 |
| H | 0.084001  | -3.296098 | -2.803540 |
| H | -0.770104 | -3.473332 | -1.265300 |

#### I(a)-Yne\_conf3

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.945276 | 2.114388  | 1.203127  |
| H | -3.876810 | 1.202612  | 1.817509  |
| H | -4.983344 | 2.246506  | 0.895294  |
| N | -3.154790 | 1.957678  | -0.041163 |
| S | -3.873422 | 1.061627  | -1.295976 |
| O | -2.938897 | 1.144158  | -2.423170 |
| O | -5.246945 | 1.559496  | -1.395053 |
| C | -3.958997 | -0.649633 | -0.767808 |
| C | -5.141576 | -1.133730 | -0.204169 |
| C | -2.836303 | -1.472393 | -0.902543 |
| C | -5.192517 | -2.456165 | 0.234588  |
| H | -6.010641 | -0.488544 | -0.134843 |
| C | -2.907885 | -2.788554 | -0.453937 |
| H | -1.925146 | -1.091514 | -1.351534 |
| C | -4.079021 | -3.300061 | 0.125746  |
| H | -6.113866 | -2.838587 | 0.666692  |
| H | -2.035089 | -3.428939 | -0.553826 |
| C | -4.126706 | -4.719033 | 0.639713  |
| H | -5.155119 | -5.087208 | 0.709972  |
| H | -3.564256 | -5.399610 | -0.008790 |
| H | -3.684086 | -4.784641 | 1.642339  |
| C | -1.696180 | 1.910484  | 0.069197  |
| H | -1.278780 | 1.734068  | -0.924420 |
| H | -1.339086 | 2.895353  | 0.392571  |
| C | -1.174567 | 0.900386  | 1.011222  |
| C | -0.864046 | 0.091176  | 1.876001  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.496293 | 3.306267  | 2.011322  |
| H  | -2.568719 | 3.197511  | 2.572860  |
| C  | -4.187988 | 4.442583  | 2.096619  |
| H  | -5.122419 | 4.583612  | 1.557842  |
| H  | -3.847800 | 5.273165  | 2.709403  |
| C  | -0.663862 | -0.855725 | 2.964632  |
| H  | 0.386997  | -1.090304 | 3.195810  |
| O  | -1.597497 | -1.338318 | 3.575893  |
| Rh | 1.184122  | 0.129341  | 0.329045  |
| Rh | 3.280342  | -0.237084 | -0.776849 |
| O  | 2.227889  | 0.207925  | 2.113914  |
| O  | 4.202767  | -0.146922 | 1.058799  |
| O  | 2.991661  | -2.258876 | -0.529353 |
| O  | 3.479535  | 1.800951  | -0.968184 |
| O  | 2.265787  | -0.299986 | -2.569190 |
| O  | 0.285214  | 0.028095  | -1.523705 |
| O  | 1.010328  | -1.922327 | 0.520154  |
| O  | 1.491537  | 2.156033  | 0.062689  |
| C  | 2.557022  | 2.549923  | -0.520793 |
| C  | 3.496494  | 0.060997  | 2.092641  |
| C  | 1.938190  | -2.663765 | 0.051634  |
| C  | 1.005463  | -0.150719 | -2.565484 |
| C  | 0.281065  | -0.208534 | -3.889819 |
| C  | 2.714268  | 4.042255  | -0.705574 |
| C  | 4.216334  | 0.173711  | 3.417311  |
| C  | 1.747508  | -4.159053 | 0.172587  |
| H  | 1.260400  | -4.528629 | -0.737755 |
| H  | 1.110455  | -4.396945 | 1.026831  |
| H  | 2.715843  | -4.655833 | 0.262957  |
| H  | 5.212448  | -0.266501 | 3.348409  |
| H  | 3.635677  | -0.311187 | 4.206117  |
| H  | 4.315157  | 1.233821  | 3.678416  |
| H  | 2.478651  | 4.560241  | 0.228340  |
| H  | 3.727890  | 4.283181  | -1.029100 |
| H  | 2.002248  | 4.386622  | -1.464175 |
| H  | 0.183600  | -1.256868 | -4.196173 |
| H  | 0.866154  | 0.306829  | -4.655779 |
| H  | -0.714765 | 0.229806  | -3.799646 |

#### I(a)-Yne\_conf4

##### 0 imaginary frequency

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -3.018280 | 2.404267 | 0.047278  |
| H | -4.022207 | 2.378797 | 0.487867  |
| H | -3.128171 | 2.823281 | -0.960629 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | -2.538180 | 1.012969  | -0.088767 |
| S  | -3.223217 | -0.169563 | 0.881889  |
| O  | -3.358262 | 0.419325  | 2.217638  |
| O  | -2.467599 | -1.403688 | 0.650053  |
| C  | -4.886650 | -0.437133 | 0.256868  |
| C  | -5.077181 | -1.271933 | -0.849237 |
| C  | -5.970362 | 0.201518  | 0.862406  |
| C  | -6.362145 | -1.450964 | -1.353678 |
| H  | -4.233300 | -1.790443 | -1.292665 |
| C  | -7.251064 | 0.009675  | 0.342830  |
| H  | -5.810889 | 0.819236  | 1.739664  |
| C  | -7.468625 | -0.814505 | -0.769061 |
| H  | -6.511610 | -2.102437 | -2.211374 |
| H  | -8.095889 | 0.504532  | 0.815347  |
| C  | -8.860773 | -1.044069 | -1.307401 |
| H  | -8.859400 | -1.125761 | -2.399662 |
| H  | -9.284747 | -1.977125 | -0.913280 |
| H  | -9.538957 | -0.232154 | -1.026843 |
| C  | -1.803715 | 0.622794  | -1.290400 |
| H  | -1.560901 | -0.441074 | -1.221783 |
| H  | -2.414681 | 0.784685  | -2.194824 |
| C  | -0.551645 | 1.370759  | -1.468322 |
| C  | 0.436727  | 2.042345  | -1.725278 |
| C  | -2.110779 | 3.266051  | 0.886851  |
| H  | -1.915092 | 2.887130  | 1.887463  |
| C  | -1.587886 | 4.419780  | 0.473318  |
| H  | -1.754697 | 4.802719  | -0.531388 |
| H  | -0.955750 | 5.022370  | 1.119348  |
| C  | 1.450356  | 3.003093  | -2.151724 |
| H  | 2.413234  | 2.563642  | -2.456727 |
| O  | 1.233375  | 4.197785  | -2.182440 |
| Rh | 1.555398  | 0.198450  | -0.411362 |
| Rh | 3.026135  | -1.302719 | 0.747274  |
| O  | 2.816526  | 1.738374  | 0.155143  |
| O  | 4.228704  | 0.306020  | 1.198498  |
| O  | 1.939277  | -0.968706 | 2.457742  |
| O  | 4.039154  | -1.572875 | -1.030806 |
| O  | 1.753112  | -2.844045 | 0.275346  |
| O  | 0.418374  | -1.453146 | -0.910168 |
| O  | 0.522162  | 0.414659  | 1.355247  |
| O  | 2.699154  | -0.097579 | -2.113371 |
| C  | 3.670826  | -0.923644 | -2.057018 |
| C  | 3.865588  | 1.464250  | 0.827180  |
| C  | 0.926628  | -0.200765 | 2.396359  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.726177  | -2.594231 | -0.426004 |
| C | -0.231803 | -3.726604 | -0.708474 |
| C | 4.432254  | -1.162097 | -3.342461 |
| C | 4.732113  | 2.632598  | 1.240665  |
| C | 0.142692  | 0.031531  | 3.666977  |
| H | 0.391563  | -0.727000 | 4.411089  |
| H | -0.929123 | 0.026998  | 3.452036  |
| H | 0.400431  | 1.019601  | 4.066432  |
| H | 5.749703  | 2.296775  | 1.448543  |
| H | 4.316447  | 3.074616  | 2.153869  |
| H | 4.729110  | 3.401307  | 0.464376  |
| H | 4.593119  | -0.215484 | -3.865228 |
| H | 5.385357  | -1.651920 | -3.136881 |
| H | 3.833786  | -1.806196 | -3.997031 |
| H | 0.172252  | -4.672130 | -0.344085 |
| H | -0.425983 | -3.789448 | -1.783841 |
| H | -1.180369 | -3.505454 | -0.207822 |

# I(a)-Yne\_conf5

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.578663 | 2.171301  | 0.742618  |
| H | -1.640977 | 2.712650  | 0.566119  |
| H | -2.696015 | 2.083021  | 1.823659  |
| N | -2.358815 | 0.812847  | 0.210692  |
| S | -3.129201 | -0.501007 | 0.919439  |
| O | -3.283760 | -0.162487 | 2.337424  |
| O | -2.399255 | -1.696722 | 0.486742  |
| C | -4.775901 | -0.627274 | 0.211431  |
| C | -4.958734 | -1.345252 | -0.973153 |
| C | -5.854747 | -0.002725 | 0.841207  |
| C | -6.232842 | -1.422646 | -1.533400 |
| H | -4.120238 | -1.856202 | -1.434541 |
| C | -7.121586 | -0.095916 | 0.269616  |
| H | -5.701200 | 0.534687  | 1.769932  |
| C | -7.332470 | -0.802450 | -0.923980 |
| H | -6.376250 | -1.982983 | -2.453985 |
| H | -7.962993 | 0.386257  | 0.761360  |
| C | -8.716479 | -0.919395 | -1.516989 |
| H | -8.676864 | -1.136343 | -2.589156 |
| H | -9.281178 | -1.730774 | -1.038979 |
| H | -9.291838 | 0.001847  | -1.376085 |
| C | -1.796742 | 0.637594  | -1.131377 |
| H | -1.549683 | -0.419719 | -1.260666 |
| H | -2.510875 | 0.928457  | -1.920227 |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | -0.573927 | 1.424268  | -1.335874 | H  | -1.339258 | -0.278580 | -0.425342 |
| C                            | 0.381065  | 2.140132  | -1.599970 | H  | -2.055518 | -1.479749 | -1.498708 |
| C                            | -3.737527 | 2.921328  | 0.134769  | N  | -2.503671 | -1.759238 | 0.528905  |
| H                            | -3.760987 | 2.986379  | -0.953429 | S  | -4.042736 | -2.317269 | 0.105527  |
| C                            | -4.685286 | 3.529430  | 0.848826  | O  | -4.621528 | -2.836610 | 1.347829  |
| H                            | -4.689449 | 3.495272  | 1.936711  | O  | -3.844151 | -3.151267 | -1.080299 |
| H                            | -5.485117 | 4.093789  | 0.377082  | C  | -5.026688 | -0.902234 | -0.394574 |
| C                            | 1.371940  | 3.122060  | -2.038929 | C  | -5.021572 | -0.493461 | -1.730735 |
| H                            | 2.279106  | 2.691689  | -2.493110 | C  | -5.783765 | -0.216744 | 0.558897  |
| O                            | 1.195462  | 4.317238  | -1.924752 | C  | -5.764223 | 0.625476  | -2.102707 |
| Rh                           | 1.616378  | 0.300084  | -0.384899 | H  | -4.469662 | -1.063191 | -2.470548 |
| Rh                           | 3.181966  | -1.173465 | 0.676664  | C  | -6.523194 | 0.896925  | 0.167232  |
| O                            | 2.821290  | 1.875735  | 0.205445  | H  | -5.811110 | -0.569464 | 1.584124  |
| O                            | 4.318470  | 0.472686  | 1.165746  | C  | -6.517483 | 1.343274  | -1.162535 |
| O                            | 2.123225  | -0.960021 | 2.423571  | H  | -5.766696 | 0.940570  | -3.143151 |
| O                            | 4.164776  | -1.326391 | -1.131413 | H  | -7.122291 | 1.424509  | 0.905433  |
| O                            | 1.974930  | -2.753389 | 0.163899  | C  | -7.292774 | 2.574081  | -1.567348 |
| O                            | 0.542335  | -1.378246 | -0.921452 | H  | -7.598091 | 2.529213  | -2.617697 |
| O                            | 0.627669  | 0.413273  | 1.416768  | H  | -8.191701 | 2.700932  | -0.955224 |
| O                            | 2.720630  | 0.111329  | -2.126772 | H  | -6.682390 | 3.478367  | -1.442485 |
| C                            | 3.735063  | -0.664283 | -2.124932 | C  | -2.310658 | -1.173269 | 1.857401  |
| C                            | 3.896901  | 1.625928  | 0.844645  | H  | -2.959679 | -1.704024 | 2.558758  |
| C                            | 1.079480  | -0.233186 | 2.419555  | H  | -1.270955 | -1.363006 | 2.154010  |
| C                            | 0.922035  | -2.525066 | -0.507182 | C  | -2.530429 | 0.279602  | 1.936028  |
| C                            | 0.027857  | -3.693770 | -0.843125 | C  | -2.670391 | 1.485133  | 1.990402  |
| C                            | 4.470612  | -0.820260 | -3.437618 | C  | -0.302041 | -2.175550 | -0.489795 |
| C                            | 4.720650  | 2.816906  | 1.279617  | H  | -0.098117 | -2.693530 | 0.444278  |
| C                            | 0.307812  | -0.099048 | 3.711578  | C  | 0.515802  | -2.374673 | -1.548938 |
| H                            | 0.657165  | -0.830513 | 4.441966  | H  | 0.312767  | -1.930896 | -2.519953 |
| H                            | -0.761470 | -0.226896 | 3.519643  | H  | 1.351582  | -3.063831 | -1.491448 |
| H                            | 0.455982  | 0.910181  | 4.112959  | C  | -2.876541 | 2.908492  | 2.080044  |
| H                            | 5.751976  | 2.516312  | 1.472808  | H  | -3.331499 | 3.253663  | 3.028861  |
| H                            | 4.294364  | 3.222754  | 2.204597  | O  | -2.587910 | 3.702411  | 1.201416  |
| H                            | 4.681970  | 3.602040  | 0.520784  | Rh | 1.742662  | -0.565535 | -0.361226 |
| H                            | 4.577951  | 0.151904  | -3.926217 | Rh | 3.358566  | 1.094993  | 0.300529  |
| H                            | 5.448528  | -1.276372 | -3.275954 | O  | 2.647355  | -0.540259 | -2.226892 |
| H                            | 3.881769  | -1.463127 | -4.102016 | O  | 4.159130  | 1.022486  | -1.587372 |
| H                            | 0.478511  | -4.629900 | -0.510541 | O  | 2.027445  | 2.541801  | -0.309667 |
| H                            | -0.148360 | -3.724951 | -1.923197 | O  | 4.600204  | -0.447088 | 0.880272  |
| H                            | -0.937679 | -3.541199 | -0.350450 | O  | 2.518602  | 1.114675  | 2.174819  |
| <b>I(a)-Ene_conf1</b>        |           |           |           | O  | 0.980783  | -0.439510 | 1.580365  |
| <b>0 imaginary frequency</b> |           |           |           | O  | 0.512041  | 0.983649  | -0.951016 |
| C                            | -1.569911 | -1.345455 | -0.530376 | O  | 3.076385  | -2.012549 | 0.266990  |
|                              |           |           |           | C  | 4.205194  | -1.645017 | 0.735818  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | 3.635481  | 0.237932  | -2.436501 | H  | -1.764356 | -2.325827 | -2.318467 |
| C                            | 0.907525  | 2.190377  | -0.793000 | H  | -3.520971 | -2.503178 | -2.312029 |
| C                            | 1.532207  | 0.357059  | 2.413510  | C  | -2.854769 | -0.525267 | -2.464595 |
| C                            | 0.943861  | 0.393065  | 3.807263  | C  | -3.051650 | 0.595387  | -2.889322 |
| C                            | 5.167729  | -2.745181 | 1.125429  | C  | -1.139574 | -0.315725 | 0.555302  |
| C                            | 4.213119  | 0.238237  | -3.834478 | H  | -1.406216 | 0.400995  | -0.217442 |
| C                            | -0.056834 | 3.277160  | -1.203403 | C  | -0.674447 | 0.130020  | 1.745972  |
| H                            | -0.881403 | 3.325921  | -0.481963 | H  | -0.456577 | -0.553893 | 2.562248  |
| H                            | -0.484734 | 3.041863  | -2.182356 | H  | -0.584731 | 1.190452  | 1.956983  |
| H                            | 0.450619  | 4.242740  | -1.234502 | C  | -3.329948 | 1.927472  | -3.371635 |
| H                            | 5.212753  | 0.676092  | -3.832907 | H  | -2.807508 | 2.208961  | -4.306647 |
| H                            | 3.566031  | 0.836585  | -4.486425 | O  | -4.084965 | 2.702855  | -2.812843 |
| H                            | 4.239586  | -0.779272 | -4.232552 | Rh | 1.397565  | 0.037879  | 0.377893  |
| H                            | 5.711018  | -3.073318 | 0.231304  | Rh | 3.664581  | 0.214100  | -0.419151 |
| H                            | 5.891369  | -2.376765 | 1.854925  | O  | 2.149244  | 0.475570  | 2.262693  |
| H                            | 4.622239  | -3.604298 | 1.522770  | O  | 4.279667  | 0.596778  | 1.500754  |
| H                            | -0.101621 | 0.714516  | 3.751503  | O  | 3.872405  | -1.806873 | -0.067469 |
| H                            | 1.506332  | 1.079261  | 4.441750  | O  | 3.327689  | 2.224161  | -0.720653 |
| H                            | 0.961320  | -0.612248 | 4.240780  | O  | 2.979329  | -0.169396 | -2.320410 |
| <b>I(a)-Ene_conf2</b>        |           |           |           | O  | 0.848733  | -0.396500 | -1.583774 |
| <b>0 imaginary frequency</b> |           |           |           | O  | 1.745086  | -1.972190 | 0.705476  |
| C                            | -1.408070 | -1.773225 | 0.241081  | O  | 1.180250  | 2.052406  | -0.007251 |
| H                            | -0.605514 | -2.165809 | -0.391363 | C  | 2.181317  | 2.703396  | -0.458672 |
| H                            | -1.419276 | -2.370517 | 1.155356  | C  | 3.402653  | 0.651347  | 2.416276  |
| N                            | -2.664222 | -2.017693 | -0.480135 | C  | 2.894585  | -2.451629 | 0.421968  |
| S                            | -4.115835 | -2.171676 | 0.375407  | C  | 1.744253  | -0.396542 | -2.492849 |
| O                            | -3.783005 | -2.905855 | 1.598401  | C  | 1.289509  | -0.727766 | -3.897841 |
| O                            | -5.081461 | -2.681315 | -0.603178 | C  | 1.983187  | 4.187790  | -0.671943 |
| C                            | -4.641815 | -0.530768 | 0.872783  | C  | 3.873616  | 0.953469  | 3.821711  |
| C                            | -5.212554 | 0.331083  | -0.068164 | C  | 3.114519  | -3.916246 | 0.729348  |
| C                            | -4.449893 | -0.122388 | 2.193718  | H  | 2.181947  | -4.474435 | 0.620941  |
| C                            | -5.564309 | 1.621395  | 0.316197  | H  | 3.449016  | -4.012416 | 1.769142  |
| H                            | -5.375802 | 0.001825  | -1.087398 | H  | 3.889424  | -4.327959 | 0.079781  |
| C                            | -4.826336 | 1.168032  | 2.565726  | H  | 4.957590  | 1.073523  | 3.845029  |
| H                            | -4.022108 | -0.810746 | 2.913993  | H  | 3.573079  | 0.141184  | 4.491232  |
| C                            | -5.379662 | 2.059855  | 1.636845  | H  | 3.390502  | 1.868696  | 4.179179  |
| H                            | -5.973815 | 2.299557  | -0.427144 | H  | 2.113199  | 4.705008  | 0.286008  |
| H                            | -4.683173 | 1.487720  | 3.594999  | H  | 2.720743  | 4.572409  | -1.378616 |
| C                            | -5.791511 | 3.453786  | 2.046677  | H  | 0.968934  | 4.387384  | -1.025993 |
| H                            | -6.875782 | 3.511136  | 2.210213  | H  | 1.404891  | -1.805492 | -4.064848 |
| H                            | -5.302171 | 3.760183  | 2.976571  | H  | 1.912287  | -0.205738 | -4.627512 |
| H                            | -5.542776 | 4.186364  | 1.271216  | H  | 0.237790  | -0.465175 | -4.031272 |
| C                            | -2.695107 | -1.890099 | -1.936436 |    |           |           |           |

**I(a)-Ald\_conf1****0 imaginary frequency**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 5.829181  | -1.286160 | 1.245362  |
| H  | 4.857653  | -0.974244 | 1.659781  |
| H  | 6.606013  | -0.644874 | 1.664712  |
| N  | 5.861265  | -1.071785 | -0.220820 |
| S  | 6.069348  | 0.538003  | -0.750203 |
| O  | 6.083387  | 0.458586  | -2.214473 |
| O  | 7.207042  | 1.050212  | 0.014907  |
| C  | 4.619272  | 1.464851  | -0.256300 |
| C  | 4.583745  | 2.065258  | 1.004058  |
| C  | 3.516534  | 1.535646  | -1.114455 |
| C  | 3.423243  | 2.724368  | 1.409151  |
| H  | 5.458935  | 2.035718  | 1.644205  |
| C  | 2.364702  | 2.190617  | -0.689630 |
| H  | 3.570897  | 1.091417  | -2.102386 |
| C  | 2.295093  | 2.786462  | 0.580598  |
| H  | 3.394431  | 3.197140  | 2.387520  |
| H  | 1.496555  | 2.228292  | -1.342516 |
| C  | 1.026345  | 3.464095  | 1.036127  |
| H  | 1.176118  | 3.997001  | 1.980650  |
| H  | 0.675174  | 4.188339  | 0.291120  |
| H  | 0.225268  | 2.728577  | 1.179874  |
| C  | 5.021206  | -1.939581 | -1.047780 |
| H  | 5.218667  | -1.693541 | -2.095919 |
| H  | 5.361698  | -2.971668 | -0.897442 |
| C  | 3.575499  | -1.864566 | -0.793360 |
| C  | 2.385663  | -1.755452 | -0.571301 |
| C  | 6.101407  | -2.725410 | 1.612120  |
| H  | 5.257296  | -3.413032 | 1.562717  |
| C  | 7.292268  | -3.174083 | 2.009510  |
| H  | 8.155889  | -2.516244 | 2.078318  |
| H  | 7.448425  | -4.214725 | 2.281092  |
| C  | 0.976872  | -1.559625 | -0.459643 |
| H  | 0.332990  | -2.138882 | -1.137527 |
| O  | 0.474086  | -0.756004 | 0.328900  |
| Rh | -1.752582 | -0.313976 | 0.132454  |
| Rh | -4.087962 | 0.140504  | -0.172876 |
| O  | -2.283536 | -1.758137 | 1.503297  |
| O  | -4.490967 | -1.323948 | 1.216645  |
| O  | -3.954039 | 1.525544  | 1.342378  |
| O  | -4.100848 | -1.278803 | -1.671893 |
| O  | -3.561907 | 1.581798  | -1.549218 |
| O  | -1.351460 | 1.161269  | -1.264527 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -1.742420 | 1.106687  | 1.628539  |
| O | -1.895764 | -1.713492 | -1.387693 |
| C | -3.027258 | -1.888182 | -1.956375 |
| C | -3.520052 | -1.952623 | 1.743171  |
| C | -2.834495 | 1.699317  | 1.917354  |
| C | -2.332576 | 1.783418  | -1.792336 |
| C | -1.988028 | 2.860241  | -2.798594 |
| C | -3.073478 | -2.913997 | -3.067465 |
| C | -3.861565 | -3.053983 | 2.722491  |
| C | -2.796382 | 2.675103  | 3.072773  |
| H | -3.590747 | 3.416976  | 2.970370  |
| H | -1.819711 | 3.160528  | 3.131509  |
| H | -2.956717 | 2.122568  | 4.006203  |
| H | -4.796732 | -2.824637 | 3.237760  |
| H | -3.049461 | -3.192499 | 3.439169  |
| H | -3.997289 | -3.991046 | 2.169417  |
| H | -2.733238 | -3.882880 | -2.687833 |
| H | -4.085853 | -3.004783 | -3.463176 |
| H | -2.388814 | -2.615659 | -3.868458 |
| H | -2.894344 | 3.320173  | -3.194655 |
| H | -1.403148 | 2.426153  | -3.616007 |
| H | -1.365672 | 3.622537  | -2.318270 |

**I-TS-II(a)\_conf1****1 imaginary frequency, value = -207.2233cm<sup>-1</sup>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.639777 | 0.881995  | 0.478271  |
| C | -0.414574 | 1.523488  | -0.058248 |
| C | -0.162918 | 2.671044  | -0.574692 |
| C | -2.179754 | 3.595567  | -1.086010 |
| C | -3.056388 | 2.372895  | -0.922015 |
| H | -1.954537 | 3.903476  | -2.104926 |
| H | -4.103368 | 2.685911  | -0.982390 |
| H | -2.869597 | 1.664137  | -1.742800 |
| H | -1.466402 | 0.630636  | 1.528424  |
| N | -2.836245 | 1.741579  | 0.383836  |
| S | -4.202039 | 1.191047  | 1.228138  |
| O | -3.717642 | 0.811085  | 2.555351  |
| O | -5.231082 | 2.214829  | 1.031125  |
| C | -4.751862 | -0.302787 | 0.399852  |
| C | -5.687916 | -0.215221 | -0.634783 |
| C | -4.220277 | -1.538290 | 0.779702  |
| C | -6.079352 | -1.376250 | -1.297868 |
| H | -6.118791 | 0.745457  | -0.896001 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -4.624538 | -2.689139 | 0.104080  |
| H  | -3.519523 | -1.595734 | 1.605668  |
| C  | -5.555706 | -2.628502 | -0.942803 |
| H  | -6.810322 | -1.310374 | -2.100061 |
| H  | -4.217308 | -3.651922 | 0.402925  |
| C  | -6.012985 | -3.883287 | -1.647614 |
| H  | -6.929305 | -4.278166 | -1.189247 |
| H  | -6.234760 | -3.691938 | -2.702764 |
| H  | -5.255860 | -4.672077 | -1.595224 |
| C  | -1.779316 | 4.374421  | -0.054026 |
| H  | -1.195333 | 5.268434  | -0.236566 |
| H  | -2.033750 | 4.114146  | 0.968434  |
| C  | 0.831847  | 3.492720  | -1.247938 |
| H  | 1.804747  | 2.973917  | -1.290460 |
| O  | 0.659134  | 4.599205  | -1.725831 |
| H  | -1.772068 | -0.066888 | -0.064890 |
| Rh | 3.135019  | -1.421992 | 0.144323  |
| Rh | 1.322947  | 0.186847  | -0.016761 |
| O  | 4.355941  | 0.130051  | 0.748869  |
| O  | 2.662286  | 1.633342  | 0.603568  |
| O  | 1.905534  | 0.533165  | -1.971162 |
| O  | 0.870799  | -0.268831 | 1.953236  |
| O  | 0.114314  | -1.384466 | -0.643339 |
| O  | 1.810109  | -2.881243 | -0.467919 |
| O  | 3.571620  | -1.002427 | -1.831281 |
| O  | 2.588773  | -1.744159 | 2.107226  |
| C  | 1.596476  | -1.112951 | 2.580583  |
| C  | 3.869676  | 1.294741  | 0.854695  |
| C  | 2.886266  | -0.134167 | -2.448878 |
| C  | 0.615445  | -2.555616 | -0.734028 |
| C  | -0.303603 | -3.647842 | -1.240092 |
| C  | 1.246783  | -1.351123 | 4.033726  |
| C  | 4.785389  | 2.395102  | 1.345561  |
| C  | 3.235569  | 0.133729  | -3.897252 |
| H  | 3.234349  | 1.210022  | -4.090649 |
| H  | 2.471765  | -0.318632 | -4.540111 |
| H  | 4.208360  | -0.295973 | -4.141092 |
| H  | 4.633280  | 3.303353  | 0.756099  |
| H  | 5.827485  | 2.075979  | 1.293123  |
| H  | 4.534666  | 2.630041  | 2.386379  |
| H  | 1.681364  | -0.547357 | 4.639597  |
| H  | 0.163314  | -1.325109 | 4.173456  |
| H  | 1.656423  | -2.304561 | 4.372041  |
| H  | -1.343401 | -3.419026 | -0.995803 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -0.010231 | -4.612066 | -0.819504 |
| H | -0.212488 | -3.709584 | -2.331089 |

# I-TS-II(a)\_conf2

1 imaginary frequency, value = -215.0201cm<sup>-1</sup>

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 1.625634  | 0.856370  | 0.723329  |
| C  | 0.548083  | 1.371704  | -0.158382 |
| C  | 0.460024  | 2.366987  | -0.966620 |
| C  | 2.245836  | 3.712980  | -0.509280 |
| C  | 2.707823  | 3.084980  | 0.784101  |
| H  | 1.727596  | 4.666637  | -0.431255 |
| H  | 3.672189  | 3.517405  | 1.070349  |
| H  | 1.994230  | 3.313721  | 1.589444  |
| H  | 1.819244  | -0.184965 | 0.444754  |
| N  | 2.878811  | 1.632611  | 0.623031  |
| S  | 4.188140  | 0.940695  | 1.480236  |
| O  | 5.248900  | 1.954427  | 1.465447  |
| O  | 3.722638  | 0.360620  | 2.746634  |
| C  | 4.654754  | -0.406713 | 0.398853  |
| C  | 4.348232  | -1.716956 | 0.762257  |
| C  | 5.350616  | -0.128171 | -0.781929 |
| C  | 4.732567  | -2.761133 | -0.081762 |
| H  | 3.829787  | -1.910090 | 1.695223  |
| C  | 5.725030  | -1.181277 | -1.609122 |
| H  | 5.604998  | 0.896113  | -1.034232 |
| C  | 5.421160  | -2.512664 | -1.275135 |
| H  | 4.499205  | -3.785085 | 0.198478  |
| H  | 6.268013  | -0.971253 | -2.527439 |
| C  | 5.848370  | -3.643205 | -2.180413 |
| H  | 6.941723  | -3.730050 | -2.213198 |
| H  | 5.448002  | -4.602970 | -1.840680 |
| H  | 5.507697  | -3.479096 | -3.209510 |
| C  | 2.531381  | 3.214980  | -1.735839 |
| H  | 2.211133  | 3.737973  | -2.628632 |
| H  | 3.084981  | 2.287727  | -1.841392 |
| C  | -0.441265 | 3.154326  | -1.795919 |
| H  | -1.452092 | 2.712932  | -1.803658 |
| O  | -0.169067 | 4.175207  | -2.401513 |
| H  | 1.236784  | 0.837603  | 1.751917  |
| Rh | -3.229834 | -1.254497 | 0.198301  |
| Rh | -1.290491 | 0.192730  | -0.029235 |
| O  | -3.461532 | -1.130163 | -1.849811 |
| O  | -1.645418 | 0.214089  | -2.068323 |
| O  | -2.568924 | 1.805422  | 0.175769  |

|                                                                |           |           |           |    |           |           |           |
|----------------------------------------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| O                                                              | -0.143355 | -1.526711 | -0.219298 | C  | 6.597874  | 0.152882  | -1.834573 |
| O                                                              | -1.083122 | 0.072322  | 2.029157  | H  | 4.567803  | -0.569015 | -1.959432 |
| O                                                              | -2.888684 | -1.287579 | 2.232394  | C  | 7.661176  | -0.042395 | 0.320156  |
| O                                                              | -4.373404 | 0.450344  | 0.419313  | H  | 6.452829  | -0.923787 | 1.888026  |
| O                                                              | -1.963601 | -2.869519 | -0.034105 | C  | 7.729109  | 0.347425  | -1.022419 |
| C                                                              | -0.722086 | -2.664384 | -0.182356 | H  | 6.638555  | 0.435009  | -2.883879 |
| C                                                              | -2.638418 | -0.447087 | -2.528422 | H  | 8.530534  | 0.086504  | 0.959692  |
| C                                                              | -3.815018 | 1.585681  | 0.363413  | C  | 8.982341  | 0.966582  | -1.593684 |
| C                                                              | -1.914024 | -0.627548 | 2.702117  | H  | 9.277037  | 0.477286  | -2.529130 |
| C                                                              | -1.716231 | -0.640600 | 4.202683  | H  | 8.828933  | 2.029447  | -1.820623 |
| C                                                              | 0.159486  | -3.886069 | -0.339057 | H  | 9.820702  | 0.893956  | -0.894561 |
| C                                                              | -2.821078 | -0.426228 | -4.030942 | C  | 2.994847  | 2.617719  | 0.098211  |
| C                                                              | -4.688523 | 2.805895  | 0.560258  | H  | 2.841253  | 3.658491  | -0.159185 |
| H                                                              | -4.397823 | 3.595374  | -0.137847 | H  | 3.322930  | 1.928456  | -0.672579 |
| H                                                              | -4.541274 | 3.189809  | 1.576419  | C  | 0.121065  | 3.238603  | 0.471849  |
| H                                                              | -5.740265 | 2.546744  | 0.428478  | H  | -0.967082 | 3.151400  | 0.316750  |
| H                                                              | -2.594161 | 0.566734  | -4.427205 | O  | 0.669768  | 4.308912  | 0.666309  |
| H                                                              | -3.838095 | -0.721651 | -4.294435 | H  | 0.995752  | -1.143513 | 1.297460  |
| H                                                              | -2.119002 | -1.135851 | -4.484280 | Rh | -3.834743 | -0.605980 | -0.375008 |
| H                                                              | -0.108780 | -4.407364 | -1.264213 | Rh | -1.560262 | 0.150474  | 0.021960  |
| H                                                              | 1.213370  | -3.604496 | -0.370397 | O  | -3.978339 | 0.854983  | -1.825923 |
| H                                                              | -0.023084 | -4.576561 | 0.489967  | O  | -1.861388 | 1.580457  | -1.444957 |
| H                                                              | -0.655508 | -0.756571 | 4.441311  | O  | -2.324235 | 1.467969  | 1.424163  |
| H                                                              | -2.300470 | -1.441851 | 4.657928  | O  | -0.962441 | -1.221968 | -1.409598 |
| H                                                              | -2.045261 | 0.320337  | 4.614822  | O  | -1.430802 | -1.322570 | 1.472027  |
| <b>I-TS-II(a)_conf3</b>                                        |           |           |           | O  | -3.554836 | -2.026461 | 1.094432  |
| <b>1 imaginary frequency, value = -234.8819cm<sup>-1</sup></b> |           |           |           | O  | -4.446980 | 0.753349  | 1.054917  |
| C                                                              | 1.409246  | -0.531883 | 0.480796  | O  | -3.090075 | -1.920700 | -1.779157 |
| C                                                              | 0.538968  | 0.662743  | 0.349260  | C  | -1.840545 | -1.947111 | -1.989470 |
| C                                                              | 0.757838  | 1.929522  | 0.430636  | C  | -2.988947 | 1.614506  | -2.046742 |
| C                                                              | 2.770985  | 2.184742  | 1.363106  | C  | -3.585372 | 1.475193  | 1.638260  |
| C                                                              | 3.035143  | 0.766902  | 1.819179  | C  | -2.435641 | -2.083143 | 1.685501  |
| H                                                              | 2.496860  | 2.905656  | 2.130440  | C  | -2.249812 | -3.154126 | 2.738841  |
| H                                                              | 4.070643  | 0.696849  | 2.170132  | C  | -1.322662 | -2.915246 | -3.031401 |
| H                                                              | 2.399346  | 0.516062  | 2.680074  | C  | -3.132925 | 2.648600  | -3.142994 |
| H                                                              | 1.333433  | -1.132713 | -0.428599 | C  | -4.077638 | 2.423373  | 2.710678  |
| N                                                              | 2.829358  | -0.181363 | 0.714997  | H  | -3.553602 | 3.380181  | 2.639546  |
| S                                                              | 3.897540  | -1.514644 | 0.686021  | H  | -3.855337 | 1.994554  | 3.694760  |
| O                                                              | 4.193713  | -1.965323 | 2.052677  | H  | -5.155489 | 2.569946  | 2.624023  |
| O                                                              | 3.341641  | -2.437514 | -0.306755 | H  | -2.664016 | 3.588496  | -2.840155 |
| C                                                              | 5.387416  | -0.769468 | 0.027276  | H  | -4.185871 | 2.805644  | -3.382748 |
| C                                                              | 5.430953  | -0.403526 | -1.322649 | H  | -2.614268 | 2.291348  | -4.040285 |
| C                                                              | 6.498210  | -0.603326 | 0.852590  | H  | -0.914677 | -2.351515 | -3.877587 |
|                                                                |           |           |           | H  | -0.506964 | -3.510563 | -2.610234 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -2.124852 | -3.566965 | -3.380470 |
| H | -1.497945 | -3.872841 | 2.394758  |
| H | -3.190735 | -3.673048 | 2.927115  |
| H | -1.874666 | -2.704171 | 3.662999  |

# II(a)\_conf1

## 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.577714 | 0.814667  | 0.474478  |
| C  | -0.356579 | 1.342244  | -0.183795 |
| C  | -0.364603 | 2.649244  | -0.767331 |
| C  | -1.770837 | 3.331627  | -1.010414 |
| C  | -2.981789 | 2.465290  | -0.731704 |
| H  | -1.781573 | 3.895978  | -1.939955 |
| H  | -3.856825 | 3.101045  | -0.574984 |
| H  | -3.176342 | 1.805880  | -1.594095 |
| H  | -1.313794 | 0.539700  | 1.503920  |
| N  | -2.745230 | 1.709507  | 0.499185  |
| S  | -4.100114 | 1.161804  | 1.359132  |
| O  | -3.571991 | 0.611597  | 2.607919  |
| O  | -5.063207 | 2.264278  | 1.329723  |
| C  | -4.788417 | -0.194362 | 0.409820  |
| C  | -5.742528 | 0.068429  | -0.578472 |
| C  | -4.344798 | -1.497799 | 0.647062  |
| C  | -6.242550 | -0.986584 | -1.337665 |
| H  | -6.102877 | 1.080699  | -0.728211 |
| C  | -4.857763 | -2.540710 | -0.123805 |
| H  | -3.628092 | -1.690230 | 1.438195  |
| C  | -5.809454 | -2.304807 | -1.125544 |
| H  | -6.988420 | -0.785114 | -2.102721 |
| H  | -4.518275 | -3.556421 | 0.062754  |
| C  | -6.383126 | -3.442370 | -1.936148 |
| H  | -7.369547 | -3.736828 | -1.554560 |
| H  | -6.514176 | -3.159446 | -2.986252 |
| H  | -5.739283 | -4.326473 | -1.898986 |
| C  | -0.967449 | 3.849710  | 0.082829  |
| H  | -0.388459 | 4.752109  | -0.085624 |
| H  | -1.241535 | 3.613822  | 1.104562  |
| C  | 0.711300  | 3.090710  | -1.724503 |
| H  | 1.422488  | 2.313303  | -2.033307 |
| O  | 0.756557  | 4.225215  | -2.162329 |
| Rh | 1.237133  | 0.122620  | -0.066018 |
| Rh | 3.190871  | -1.340188 | 0.237206  |
| O  | 0.090974  | -1.591701 | -0.267350 |
| O  | 1.893596  | -2.943408 | 0.021101  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 3.457998  | -1.274948 | -1.812414 |
| O | 2.798858  | -1.307214 | 2.268857  |
| O | 4.331266  | 0.377893  | 0.429182  |
| O | 2.523515  | 1.728002  | 0.164729  |
| O | 1.654835  | 0.076194  | -2.099783 |
| O | 0.972257  | 0.010876  | 1.983856  |
| C | 1.800535  | -0.662662 | 2.695163  |
| C | 0.663237  | -2.734467 | -0.168932 |
| C | 2.658729  | -0.602864 | -2.521013 |
| C | 3.772665  | 1.507928  | 0.356567  |
| C | 4.637401  | 2.739282  | 0.524586  |
| C | 1.544173  | -0.650714 | 4.187050  |
| C | -0.243388 | -3.944967 | -0.259087 |
| C | 2.884334  | -0.580563 | -4.018183 |
| H | 3.758227  | -1.178676 | -4.279930 |
| H | 3.025820  | 0.451889  | -4.354311 |
| H | 1.998498  | -0.972792 | -4.528401 |
| H | 0.293734  | -4.781455 | -0.711481 |
| H | -1.144602 | -3.712149 | -0.830234 |
| H | -0.539201 | -4.241305 | 0.754492  |
| H | 0.485900  | -0.840035 | 4.388095  |
| H | 2.166139  | -1.395724 | 4.685500  |
| H | 1.781595  | 0.342682  | 4.584233  |
| H | 5.693446  | 2.465618  | 0.519317  |
| H | 4.392733  | 3.224524  | 1.476095  |
| H | 4.426156  | 3.456543  | -0.273947 |
| H | -1.789037 | -0.143851 | -0.037722 |

# II(a)\_conf2

## 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.551952 | 0.954928  | 0.662646  |
| C | 0.362297 | 1.432398  | -0.086735 |
| C | 0.440697 | 2.629855  | -0.866869 |
| C | 1.673223 | 3.590236  | -0.595187 |
| C | 2.572827 | 3.197594  | 0.557768  |
| H | 1.377731 | 4.635515  | -0.646985 |
| H | 3.543773 | 3.688942  | 0.460762  |
| H | 2.122159 | 3.514715  | 1.511564  |
| H | 1.735007 | -0.083065 | 0.351049  |
| N | 2.784531 | 1.744982  | 0.500792  |
| S | 4.128040 | 1.153951  | 1.376009  |
| O | 5.155504 | 2.194412  | 1.267693  |
| O | 3.698044 | 0.651317  | 2.687122  |
| C | 4.610640 | -0.252479 | 0.380305  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 4.307270  | -1.542138 | 0.813972  |
| C  | 5.312581  | -0.037340 | -0.810408 |
| C  | 4.700848  | -2.629998 | 0.031085  |
| H  | 3.786612  | -1.687070 | 1.754449  |
| C  | 5.696681  | -1.132998 | -1.575428 |
| H  | 5.565362  | 0.972263  | -1.117381 |
| C  | 5.394699  | -2.445143 | -1.170918 |
| H  | 4.472577  | -3.637909 | 0.367979  |
| H  | 6.246925  | -0.971782 | -2.499306 |
| C  | 5.821850  | -3.621136 | -2.016353 |
| H  | 6.908235  | -3.626811 | -2.166224 |
| H  | 5.541561  | -4.571886 | -1.553478 |
| H  | 5.360504  | -3.582136 | -3.010863 |
| C  | 1.684980  | 2.830758  | -1.832878 |
| H  | 1.369737  | 3.326783  | -2.745342 |
| H  | 2.348049  | 1.978985  | -1.928544 |
| C  | -0.798449 | 3.327430  | -1.361867 |
| H  | -1.751192 | 2.922348  | -0.995609 |
| O  | -0.742018 | 4.303461  | -2.086605 |
| Rh | -1.225443 | 0.205327  | 0.038155  |
| Rh | -3.070140 | -1.415872 | 0.120587  |
| O  | -0.862314 | -0.243341 | 2.022923  |
| O  | -2.573195 | -1.735473 | 2.106204  |
| O  | -4.308350 | 0.140501  | 0.693389  |
| O  | -1.712258 | -2.868857 | -0.452926 |
| O  | -3.427504 | -0.968024 | -1.872154 |
| O  | -1.726688 | 0.537922  | -1.943440 |
| O  | -2.602249 | 1.638120  | 0.629667  |
| O  | -0.002737 | -1.377231 | -0.520728 |
| C  | -0.506954 | -2.549054 | -0.645907 |
| C  | -1.607637 | -1.101394 | 2.617413  |
| C  | -3.824346 | 1.298507  | 0.824397  |
| C  | -2.707288 | -0.110821 | -2.456621 |
| C  | -3.004323 | 0.193632  | -3.910065 |
| C  | 0.443400  | -3.636314 | -1.103182 |
| C  | -1.293249 | -1.344826 | 4.078217  |
| C  | -4.754413 | 2.414397  | 1.251239  |
| H  | -5.763580 | 2.030196  | 1.405724  |
| H  | -4.767869 | 3.195601  | 0.483944  |
| H  | -4.382543 | 2.869276  | 2.175010  |
| H  | -1.832167 | -2.221036 | 4.441785  |
| H  | -1.595517 | -0.467622 | 4.661457  |
| H  | -0.215937 | -1.474664 | 4.214784  |
| H  | 1.465151  | -3.414402 | -0.786910 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.119602  | -4.604636 | -0.715840 |
| H | 0.425813  | -3.682639 | -2.198618 |
| H | -3.896340 | -0.342473 | -4.236939 |
| H | -2.149159 | -0.103474 | -4.526691 |
| H | -3.143434 | 1.271283  | -4.041393 |
| H | 1.236240  | 0.883120  | 1.719634  |

## II-TS-III(a)\_ conf1

1 imaginary frequency, value = -905.3399cm<sup>-1</sup>

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.533555 | 0.880379  | 0.581230  |
| C  | -0.390657 | 1.358019  | -0.086125 |
| C  | -0.481993 | 2.703895  | -0.704467 |
| C  | -1.886619 | 3.320408  | -0.898110 |
| C  | -3.084842 | 2.462419  | -0.545617 |
| H  | -1.995090 | 3.894297  | -1.815839 |
| H  | -3.914295 | 3.091799  | -0.213373 |
| H  | -3.406280 | 1.900835  | -1.434191 |
| H  | -1.511588 | -0.120538 | 1.004783  |
| N  | -2.771627 | 1.529312  | 0.554400  |
| S  | -4.058203 | 0.911723  | 1.509754  |
| O  | -3.403294 | 0.174423  | 2.588370  |
| O  | -4.948839 | 2.045646  | 1.748134  |
| C  | -4.909312 | -0.254175 | 0.454562  |
| C  | -6.004092 | 0.174254  | -0.298456 |
| C  | -4.464668 | -1.579018 | 0.394074  |
| C  | -6.651269 | -0.738918 | -1.130327 |
| H  | -6.353340 | 1.197852  | -0.215702 |
| C  | -5.124542 | -2.473497 | -0.443234 |
| H  | -3.630563 | -1.905054 | 1.006289  |
| C  | -6.224657 | -2.070905 | -1.217956 |
| H  | -7.506671 | -0.411164 | -1.715142 |
| H  | -4.785171 | -3.505115 | -0.491260 |
| C  | -6.944775 | -3.062654 | -2.099382 |
| H  | -6.238384 | -3.693747 | -2.649810 |
| H  | -7.576829 | -3.731156 | -1.500535 |
| H  | -7.590898 | -2.560197 | -2.825372 |
| C  | -1.005181 | 3.889042  | 0.139235  |
| H  | -0.513668 | 4.832178  | -0.078615 |
| H  | -1.215556 | 3.691555  | 1.187523  |
| C  | 0.521985  | 3.087136  | -1.756328 |
| H  | 1.235105  | 2.303531  | -2.049819 |
| O  | 0.518178  | 4.187672  | -2.276306 |
| H  | -0.594470 | 1.417848  | 1.273686  |
| Rh | 3.280918  | -1.331239 | 0.135444  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rh | 1.319017  | 0.119923  | -0.039552 |
| O  | 4.439268  | 0.383722  | 0.119986  |
| O  | 2.617107  | 1.731462  | -0.029885 |
| O  | 1.518994  | -0.028698 | -2.102453 |
| O  | 1.249588  | 0.154553  | 2.027222  |
| O  | 0.145975  | -1.595790 | -0.004213 |
| O  | 1.973958  | -2.937928 | 0.132836  |
| O  | 3.339178  | -1.378249 | -1.931036 |
| O  | 3.079202  | -1.177174 | 2.193902  |
| C  | 2.140942  | -0.489240 | 2.685928  |
| C  | 3.876457  | 1.513956  | 0.046001  |
| C  | 2.471653  | -0.733212 | -2.587250 |
| C  | 0.728430  | -2.733044 | 0.077137  |
| C  | -0.181237 | -3.944106 | 0.138866  |
| C  | 2.052296  | -0.386741 | 4.194025  |
| C  | 4.759702  | 2.744114  | 0.061082  |
| C  | 2.549920  | -0.786645 | -4.099290 |
| H  | 2.667818  | 0.226892  | -4.496691 |
| H  | 1.614153  | -1.188890 | -4.501101 |
| H  | 3.387868  | -1.408666 | -4.417041 |
| H  | 4.470568  | 3.420398  | -0.748774 |
| H  | 5.808949  | 2.461749  | -0.036959 |
| H  | 4.615016  | 3.281002  | 1.005310  |
| H  | 2.336920  | 0.625448  | 4.503200  |
| H  | 1.022019  | -0.553499 | 4.521595  |
| H  | 2.722085  | -1.107869 | 4.664837  |
| H  | -0.586923 | -4.035790 | 1.153523  |
| H  | 0.377374  | -4.851178 | -0.097932 |
| H  | -1.021023 | -3.822021 | -0.550601 |

## II-TS-III(a)\_ conf2

1 imaginary frequency, value = -894.1585cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.477976 | 0.172873  | -0.923316 |
| C | -0.498960 | 0.995859  | -0.328662 |
| C | -0.916783 | 2.360980  | 0.076525  |
| C | -2.239797 | 2.916721  | -0.499132 |
| C | -2.971055 | 2.072933  | -1.523155 |
| H | -2.212754 | 3.980750  | -0.724056 |
| H | -4.046744 | 2.261760  | -1.464740 |
| H | -2.643790 | 2.340758  | -2.534871 |
| H | -1.190405 | -0.808970 | -1.292079 |
| N | -2.742591 | 0.631908  | -1.295601 |
| S | -3.934146 | -0.486793 | -1.820018 |
| O | -4.634250 | 0.152884  | -2.932400 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | -3.241984 | -1.767806 | -1.952752 |
| C  | -5.057118 | -0.582657 | -0.432457 |
| C  | -4.741526 | -1.412423 | 0.649356  |
| C  | -6.229152 | 0.174555  | -0.442870 |
| C  | -5.610192 | -1.463674 | 1.734968  |
| H  | -3.843643 | -2.021584 | 0.627945  |
| C  | -7.087052 | 0.106762  | 0.655407  |
| H  | -6.471861 | 0.786713  | -1.304756 |
| C  | -6.793447 | -0.706059 | 1.757901  |
| H  | -5.371641 | -2.109251 | 2.576532  |
| H  | -8.003183 | 0.691387  | 0.650531  |
| C  | -7.734378 | -0.792399 | 2.935440  |
| H  | -8.489863 | -0.001797 | 2.904585  |
| H  | -8.260948 | -1.755298 | 2.946590  |
| H  | -7.193396 | -0.710119 | 3.884870  |
| C  | -2.194238 | 2.538981  | 0.926893  |
| H  | -2.125123 | 3.337271  | 1.659495  |
| H  | -2.695199 | 1.631533  | 1.255710  |
| C  | 0.143493  | 3.398882  | 0.326143  |
| H  | 1.176187  | 3.095178  | 0.102759  |
| O  | -0.134063 | 4.518587  | 0.714169  |
| H  | -1.234384 | 0.032891  | 0.328267  |
| Rh | 3.553528  | -0.968027 | 0.335352  |
| Rh | 1.402056  | 0.137530  | -0.030668 |
| O  | 3.765605  | 0.212125  | 2.023931  |
| O  | 1.761882  | 1.229678  | 1.695363  |
| O  | 2.430053  | 1.556792  | -1.140788 |
| O  | 0.524105  | -1.365019 | 1.097066  |
| O  | 1.175636  | -1.048448 | -1.712591 |
| O  | 3.181740  | -2.060739 | -1.384816 |
| O  | 4.422374  | 0.516841  | -0.810086 |
| O  | 2.523278  | -2.378542 | 1.454538  |
| C  | 1.271855  | -2.282302 | 1.589426  |
| C  | 2.853546  | 1.031598  | 2.333466  |
| C  | 3.695945  | 1.434230  | -1.288814 |
| C  | 2.103666  | -1.876048 | -2.018947 |
| C  | 1.874422  | -2.691028 | -3.274708 |
| C  | 0.564655  | -3.344948 | 2.405740  |
| C  | 3.043947  | 1.854119  | 3.591231  |
| C  | 4.368496  | 2.499396  | -2.129890 |
| H  | 4.126863  | 3.490844  | -1.733975 |
| H  | 3.981928  | 2.452227  | -3.153656 |
| H  | 5.449504  | 2.353196  | -2.138787 |
| H  | 2.779769  | 2.898013  | 3.399878  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 4.074197  | 1.780186  | 3.942829  |
| H | 2.370442  | 1.480302  | 4.370983  |
| H | 0.015406  | -2.873862 | 3.227541  |
| H | -0.165033 | -3.865367 | 1.776154  |
| H | 1.284157  | -4.061903 | 2.803471  |
| H | 0.882102  | -3.150998 | -3.244731 |
| H | 2.643546  | -3.457848 | -3.378071 |
| H | 1.901954  | -2.027284 | -4.146009 |

### III(a)\_conf1

#### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.324389 | 0.288357  | 0.995836  |
| C | -0.602835 | 1.411002  | 1.292514  |
| C | -0.830378 | 2.678370  | 0.551993  |
| C | -1.715824 | 2.593524  | -0.679532 |
| C | -2.152309 | 1.221255  | -1.159153 |
| H | -1.416731 | 3.258151  | -1.486798 |
| H | -3.142899 | 1.281380  | -1.622705 |
| H | -1.441960 | 0.853811  | -1.905357 |
| H | -1.278626 | -0.606056 | 1.604234  |
| N | -2.220577 | 0.238107  | -0.057967 |
| S | -3.060135 | -1.225839 | -0.379358 |
| O | -2.948874 | -1.505799 | -1.811972 |
| O | -2.633217 | -2.180847 | 0.642550  |
| C | -4.758868 | -0.764768 | -0.050474 |
| C | -5.208986 | -0.716231 | 1.273345  |
| C | -5.614180 | -0.472178 | -1.112379 |
| C | -6.528845 | -0.358209 | 1.524803  |
| H | -4.538993 | -0.972261 | 2.087594  |
| C | -6.935459 | -0.114046 | -0.838526 |
| H | -5.253524 | -0.542804 | -2.132827 |
| C | -7.412789 | -0.050708 | 0.476213  |
| H | -6.884244 | -0.322924 | 2.551763  |
| H | -7.606220 | 0.112678  | -1.663122 |
| C | -8.848073 | 0.314714  | 0.769932  |
| H | -9.356326 | 0.695551  | -0.120852 |
| H | -9.410230 | -0.557872 | 1.126509  |
| H | -8.912355 | 1.080218  | 1.551736  |
| C | -2.270275 | 3.247568  | 0.533685  |
| H | -2.345952 | 4.331153  | 0.529552  |
| H | -3.003164 | 2.720349  | 1.138214  |
| C | 0.263245  | 3.695871  | 0.529051  |
| H | 1.147701  | 3.450097  | 1.148163  |
| O | 0.198306  | 4.737243  | -0.096882 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -0.066029 | 1.441042  | 2.235255  |
| Rh | 3.345796  | -0.866727 | -0.442846 |
| Rh | 1.264074  | 0.082673  | 0.326561  |
| O  | 4.286271  | 0.054323  | 1.143894  |
| O  | 2.348873  | 1.006087  | 1.840259  |
| O  | 1.639355  | 1.684331  | -0.927371 |
| O  | 1.039464  | -1.579278 | 1.534894  |
| O  | 0.345043  | -0.888640 | -1.244249 |
| O  | 2.306269  | -1.747817 | -1.986699 |
| O  | 3.633841  | 0.830300  | -1.582415 |
| O  | 2.950430  | -2.506562 | 0.741867  |
| C  | 1.905747  | -2.513639 | 1.461702  |
| C  | 3.602946  | 0.781594  | 1.926313  |
| C  | 2.735206  | 1.724888  | -1.583009 |
| C  | 1.050025  | -1.579389 | -2.055279 |
| C  | 0.321006  | -2.230999 | -3.208423 |
| C  | 1.641575  | -3.742173 | 2.303480  |
| C  | 4.329302  | 1.421724  | 3.089547  |
| C  | 2.953134  | 2.941043  | -2.455894 |
| H  | 2.429204  | 3.805004  | -2.040735 |
| H  | 2.547455  | 2.738540  | -3.454458 |
| H  | 4.020950  | 3.145731  | -2.558330 |
| H  | 3.892894  | 2.396240  | 3.321013  |
| H  | 5.392913  | 1.520628  | 2.864762  |
| H  | 4.218110  | 0.781949  | 3.973061  |
| H  | 1.392535  | -3.445586 | 3.326529  |
| H  | 0.775602  | -4.274617 | 1.894805  |
| H  | 2.509718  | -4.402978 | 2.300944  |
| H  | -0.753992 | -2.244390 | -3.022778 |
| H  | 0.702224  | -3.244395 | -3.359964 |
| H  | 0.524013  | -1.661731 | -4.123387 |

### III(a)\_conf2

#### 0 imaginary frequency

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 0.855981  | 1.858975 | -1.354643 |
| C | -0.340244 | 2.454841 | -1.068142 |
| C | -0.433496 | 3.482011 | -0.000056 |
| C | 0.770592  | 3.633689 | 0.909316  |
| C | 1.895147  | 2.618917 | 0.776333  |
| H | 0.527234  | 3.885091 | 1.939460  |
| H | 2.855299  | 3.082740 | 1.014483  |
| H | 1.707197  | 1.789385 | 1.465543  |
| H | 1.002571  | 1.262598 | -2.245552 |
| N | 1.991707  | 2.075773 | -0.593669 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| S  | 3.510288  | 1.516774  | -1.160108 |
| O  | 3.300279  | 1.209799  | -2.574601 |
| O  | 4.482608  | 2.514532  | -0.713565 |
| C  | 3.873932  | -0.011691 | -0.302878 |
| C  | 4.851743  | -0.019152 | 0.692480  |
| C  | 3.223825  | -1.187755 | -0.687697 |
| C  | 5.180790  | -1.227734 | 1.308040  |
| H  | 5.357014  | 0.901974  | 0.961205  |
| C  | 3.567843  | -2.382366 | -0.062365 |
| H  | 2.456599  | -1.163585 | -1.453119 |
| C  | 4.552426  | -2.424845 | 0.938881  |
| H  | 5.945915  | -1.240147 | 2.080108  |
| H  | 3.065390  | -3.300631 | -0.356403 |
| C  | 4.937605  | -3.736215 | 1.580971  |
| H  | 4.061486  | -4.371759 | 1.749545  |
| H  | 5.626376  | -4.299267 | 0.937506  |
| H  | 5.438411  | -3.581763 | 2.541718  |
| C  | 0.535221  | 4.695104  | -0.101462 |
| H  | 0.138922  | 5.644534  | 0.246423  |
| H  | 1.162332  | 4.737410  | -0.987599 |
| C  | -1.776828 | 3.820225  | 0.554889  |
| H  | -2.635035 | 3.434042  | -0.029770 |
| O  | -1.947465 | 4.511991  | 1.540901  |
| H  | -1.132784 | 2.388316  | -1.806714 |
| Rh | -2.145402 | -1.858560 | 0.413197  |
| Rh | -1.008688 | 0.144401  | -0.320210 |
| O  | -3.630204 | -1.444749 | -0.953220 |
| O  | -2.576656 | 0.442135  | -1.639747 |
| O  | -2.046152 | 1.147358  | 1.153155  |
| O  | -0.065347 | -1.026617 | -1.761792 |
| O  | 0.460741  | -0.283046 | 1.078553  |
| O  | -0.615612 | -2.159735 | 1.759787  |
| O  | -3.126300 | -0.725049 | 1.827124  |
| O  | -1.131212 | -2.897788 | -1.049840 |
| C  | -0.354825 | -2.268740 | -1.830121 |
| C  | -3.534588 | -0.401673 | -1.668474 |
| C  | -2.869973 | 0.515773  | 1.896943  |
| C  | 0.317961  | -1.304140 | 1.831951  |
| C  | 1.337679  | -1.484737 | 2.934739  |
| C  | 0.262557  | -3.055003 | -2.966921 |
| C  | -4.660197 | -0.109816 | -2.636477 |
| C  | -3.590837 | 1.319873  | 2.955818  |
| H  | -3.371543 | 2.383884  | 2.852568  |
| H  | -3.274727 | 0.973752  | 3.946012  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.667914 | 1.143180  | 2.877874  |
| H | -5.219750 | 0.764054  | -2.284117 |
| H | -5.334655 | -0.964272 | -2.708362 |
| H | -4.251012 | 0.135960  | -3.620649 |
| H | -0.424337 | -3.031452 | -3.821397 |
| H | 1.209309  | -2.611371 | -3.282670 |
| H | 0.401105  | -4.098184 | -2.674491 |
| H | 1.358972  | -2.525040 | 3.264838  |
| H | 1.046709  | -0.857633 | 3.786245  |
| H | 2.327064  | -1.167300 | 2.599516  |

### III(a)\_conf3

#### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.324439  | 0.286830  | -0.996073 |
| C | 0.604046  | 1.410528  | -1.291644 |
| C | 0.833194  | 2.676987  | -0.550045 |
| C | 1.718764  | 2.590088  | 0.681267  |
| C | 2.153757  | 1.216888  | 1.159631  |
| H | 1.420601  | 3.254420  | 1.489118  |
| H | 3.144520  | 1.275425  | 1.623037  |
| H | 1.443103  | 0.849588  | 1.905607  |
| H | 1.277701  | -0.606964 | -1.605304 |
| N | 2.220663  | 0.234659  | 0.057565  |
| S | 3.059464  | -1.230116 | 0.377054  |
| O | 2.947326  | -1.512663 | 1.809085  |
| O | 2.632750  | -2.183194 | -0.646738 |
| C | 4.758252  | -0.768099 | 0.049805  |
| C | 5.208419  | -0.715125 | -1.274051 |
| C | 5.614051  | -0.481343 | 1.112632  |
| C | 6.528377  | -0.357459 | -1.524243 |
| H | 4.538669  | -0.969563 | -2.089004 |
| C | 6.935877  | -0.123425 | 0.839946  |
| H | 5.254118  | -0.557928 | 2.132906  |
| C | 7.412383  | -0.052994 | -0.474488 |
| H | 6.884325  | -0.320917 | -2.550997 |
| H | 7.607712  | 0.096806  | 1.665405  |
| C | 8.842440  | 0.331354  | -0.769290 |
| H | 9.407068  | 0.513986  | 0.149669  |
| H | 9.356947  | -0.458555 | -1.329819 |
| H | 8.889895  | 1.241545  | -1.379741 |
| C | 2.273769  | 3.244468  | -0.531515 |
| H | 2.350767  | 4.327956  | -0.526530 |
| H | 3.005904  | 2.716832  | -1.136597 |
| C | -0.259162 | 3.695825  | -0.526202 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -1.143863 | 3.451755  | -1.145646 |
| O  | -0.192970 | 4.736548  | 0.100682  |
| H  | 0.067294  | 1.442093  | -2.234374 |
| Rh | -3.346395 | -0.865142 | 0.442474  |
| Rh | -1.264031 | 0.083242  | -0.326480 |
| O  | -4.285951 | 0.056016  | -1.144752 |
| O  | -2.347963 | 1.007013  | -1.840530 |
| O  | -1.638941 | 1.685276  | 0.927088  |
| O  | -1.039945 | -1.579080 | -1.534422 |
| O  | -0.345927 | -0.888170 | 1.244796  |
| O  | -2.307716 | -1.746490 | 1.986779  |
| O  | -3.634121 | 0.832356  | 1.581438  |
| O  | -2.951413 | -2.505489 | -0.741607 |
| C  | -1.906557 | -2.513131 | -1.461179 |
| C  | -3.602080 | 0.782941  | -1.927017 |
| C  | -2.735137 | 1.726597  | 1.582101  |
| C  | -1.051497 | -1.578273 | 2.055903  |
| C  | -0.323061 | -2.228418 | 3.210227  |
| C  | -1.642557 | -3.742009 | -2.302504 |
| C  | -4.327698 | 1.423353  | -3.090556 |
| C  | -2.953084 | 2.943242  | 2.454308  |
| H  | -2.427271 | 3.806444  | 2.039971  |
| H  | -2.549655 | 2.740407  | 3.453715  |
| H  | -4.020838 | 3.149311  | 2.554679  |
| H  | -3.893363 | 2.399516  | -3.319071 |
| H  | -5.392041 | 1.519029  | -2.867920 |
| H  | -4.212637 | 0.785801  | -3.975174 |
| H  | -2.510837 | -4.402632 | -2.299820 |
| H  | -1.393358 | -3.445823 | -3.325629 |
| H  | -0.776724 | -4.274480 | -1.893566 |
| H  | -0.514316 | -1.648912 | 4.121354  |
| H  | 0.750771  | -2.253982 | 3.018978  |
| H  | -0.713992 | -3.236332 | 3.372595  |

#### I-TS-IV(a)\_ conf1

1 imaginary frequency, value = -316.5858cm<sup>-1</sup>

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 1.862032  | 1.387001 | 0.520965  |
| C | 0.854352  | 2.172694 | -0.249911 |
| C | -0.338047 | 2.127665 | -0.724192 |
| C | 2.258872  | 3.436496 | -1.308866 |
| C | 3.388377  | 2.462030 | -1.087764 |
| H | 1.834534  | 3.527259 | -2.304378 |
| H | 3.368775  | 1.683695 | -1.865648 |
| H | 4.358197  | 2.967702 | -1.128334 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.746340  | 0.344437  | 0.187401  |
| N  | 3.207621  | 1.922893  | 0.260783  |
| S  | 4.514695  | 1.226108  | 1.066841  |
| O  | 5.666722  | 2.064771  | 0.731158  |
| O  | 4.060187  | 1.022454  | 2.442308  |
| C  | 4.780680  | -0.388111 | 0.334819  |
| C  | 4.130820  | -1.503688 | 0.869315  |
| C  | 5.625919  | -0.513493 | -0.771865 |
| C  | 4.328293  | -2.751796 | 0.279401  |
| H  | 3.502092  | -1.396436 | 1.746726  |
| C  | 5.807366  | -1.768048 | -1.349411 |
| H  | 6.151263  | 0.355172  | -1.154616 |
| C  | 5.165014  | -2.904934 | -0.835972 |
| H  | 3.832334  | -3.622955 | 0.700024  |
| H  | 6.466962  | -1.868516 | -2.207791 |
| C  | 5.400957  | -4.265615 | -1.446638 |
| H  | 6.298962  | -4.733670 | -1.022198 |
| H  | 4.560833  | -4.941603 | -1.258951 |
| H  | 5.550987  | -4.198461 | -2.529226 |
| C  | 1.747273  | 4.187857  | -0.292310 |
| C  | -1.080374 | 3.078971  | -1.570712 |
| H  | -2.117414 | 3.272994  | -1.248833 |
| O  | -0.610483 | 3.599659  | -2.568936 |
| H  | 1.658602  | 1.431258  | 1.592346  |
| Rh | -2.964745 | -1.479529 | 0.446735  |
| Rh | -1.519670 | 0.382842  | -0.144240 |
| O  | -3.798752 | -1.337355 | -1.436262 |
| O  | -2.433185 | 0.385891  | -2.001979 |
| O  | -3.004973 | 1.644913  | 0.558318  |
| O  | -0.133487 | -1.007589 | -0.810660 |
| O  | -0.708716 | 0.245666  | 1.763803  |
| O  | -2.048204 | -1.507017 | 2.297869  |
| O  | -4.333383 | -0.100994 | 1.144632  |
| O  | -1.506445 | -2.742425 | -0.296680 |
| C  | -0.436717 | -2.248410 | -0.760996 |
| C  | -3.365730 | -0.453975 | -2.236388 |
| C  | -4.068939 | 1.134419  | 1.049045  |
| C  | -1.147894 | -0.654241 | 2.557271  |
| C  | -0.549773 | -0.675816 | 3.948574  |
| C  | 0.579705  | -3.209333 | -1.341950 |
| C  | -4.027137 | -0.358550 | -3.595032 |
| C  | -5.094793 | 2.112875  | 1.581292  |
| H  | -5.260096 | 2.913278  | 0.854328  |
| H  | -4.710282 | 2.573988  | 2.498060  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -6.032853 | 1.601211  | 1.801616  |
| H | -4.740031 | 0.474335  | -3.587008 |
| H | -4.565554 | -1.280255 | -3.822436 |
| H | -3.279522 | -0.149110 | -4.364264 |
| H | 0.540868  | -3.149321 | -2.435809 |
| H | 1.588862  | -2.925867 | -1.030445 |
| H | 0.356073  | -4.232294 | -1.034315 |
| H | 0.512380  | -0.420480 | 3.913505  |
| H | -0.694707 | -1.654478 | 4.409799  |
| H | -1.055094 | 0.078064  | 4.563780  |
| H | 2.190534  | 4.178311  | 0.698565  |
| H | 0.931379  | 4.876889  | -0.479747 |

#### I-TS-IV(a)\_conf2

1 imaginary frequency, value = -324.5561cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.889557 | 1.046336  | -0.085277 |
| C | -0.903752 | 1.819136  | -0.890713 |
| C | 0.351867  | 1.908007  | -1.149790 |
| C | -2.067669 | 3.631948  | -1.044914 |
| C | -2.898529 | 3.266914  | 0.156666  |
| H | -1.336507 | 4.428946  | -0.945523 |
| H | -2.369138 | 3.555353  | 1.075944  |
| H | -3.865184 | 3.780166  | 0.148354  |
| H | -1.402101 | 0.847641  | 0.878403  |
| N | -3.142127 | 1.816215  | 0.066750  |
| S | -4.225922 | 1.186496  | 1.228198  |
| O | -3.501473 | 0.757906  | 2.432436  |
| O | -5.303369 | 2.176266  | 1.314881  |
| C | -4.820815 | -0.279701 | 0.394798  |
| C | -5.760026 | -0.151886 | -0.633252 |
| C | -4.361610 | -1.532552 | 0.800642  |
| C | -6.227428 | -1.299113 | -1.265991 |
| H | -6.122834 | 0.829747  | -0.919657 |
| C | -4.842754 | -2.671912 | 0.153197  |
| H | -3.649496 | -1.608425 | 1.615217  |
| C | -5.777679 | -2.575112 | -0.885474 |
| H | -6.958136 | -1.206718 | -2.065781 |
| H | -4.490615 | -3.651027 | 0.467382  |
| C | -6.312819 | -3.810280 | -1.569526 |
| H | -7.350499 | -4.005973 | -1.270195 |
| H | -6.308066 | -3.696584 | -2.659512 |
| H | -5.722893 | -4.696548 | -1.317583 |
| C | -2.184327 | 2.982705  | -2.238935 |
| C | 1.111087  | 2.879323  | -1.956442 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.886978  | 2.438360  | -2.604880 |
| O  | 0.931088  | 4.085258  | -1.901746 |
| H  | -2.108946 | 0.089032  | -0.567296 |
| Rh | 2.977257  | -1.442388 | 0.642793  |
| Rh | 1.561531  | 0.308406  | -0.269156 |
| O  | 4.330076  | 0.026410  | 1.163463  |
| O  | 3.022896  | 1.662690  | 0.284379  |
| O  | 2.527472  | 0.022417  | -2.082002 |
| O  | 0.700407  | 0.471459  | 1.606734  |
| O  | 0.194266  | -1.179315 | -0.765665 |
| O  | 1.538705  | -2.811503 | 0.061589  |
| O  | 3.858448  | -1.602628 | -1.218673 |
| O  | 2.003416  | -1.182714 | 2.449923  |
| C  | 1.094130  | -0.306096 | 2.543054  |
| C  | 4.066943  | 1.235029  | 0.881948  |
| C  | 3.459128  | -0.848885 | -2.155639 |
| C  | 0.487317  | -2.395878 | -0.509010 |
| C  | -0.515598 | -3.437915 | -0.961918 |
| C  | 0.413023  | -0.131837 | 3.883508  |
| C  | 5.066912  | 2.285145  | 1.317262  |
| C  | 4.159306  | -0.966291 | -3.493447 |
| H  | 4.821924  | -0.103377 | -3.627404 |
| H  | 3.425713  | -0.949731 | -4.304171 |
| H  | 4.753443  | -1.880548 | -3.535130 |
| H  | 5.143714  | 3.070996  | 0.561686  |
| H  | 6.041985  | 1.830132  | 1.500149  |
| H  | 4.713820  | 2.748036  | 2.246250  |
| H  | 0.805967  | 0.769203  | 4.368724  |
| H  | -0.662639 | 0.009964  | 3.744744  |
| H  | 0.608354  | -0.992661 | 4.525207  |
| H  | -1.535870 | -3.088202 | -0.781272 |
| H  | -0.338858 | -4.384827 | -0.448794 |
| H  | -0.403127 | -3.594336 | -2.041186 |
| H  | -2.949718 | 2.231235  | -2.404108 |
| H  | -1.561450 | 3.269437  | -3.078708 |

#### IV(a)\_conf1

0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.771864 | -1.496042 | 0.514856  |
| C | -0.868756 | -2.386399 | -0.340718 |
| C | 0.416185  | -2.001728 | -0.784997 |
| C | -1.837283 | -3.082013 | -1.428463 |
| C | -3.186517 | -2.420996 | -1.218688 |
| H | -1.440352 | -3.174431 | -2.432576 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -3.307891 | -1.587315 | -1.927770 |
| H  | -4.016507 | -3.121570 | -1.347060 |
| H  | -1.613057 | -0.447487 | 0.238936  |
| N  | -3.123426 | -1.980987 | 0.177986  |
| S  | -4.477369 | -1.369172 | 0.949381  |
| O  | -5.594345 | -2.203412 | 0.501115  |
| O  | -4.105757 | -1.239469 | 2.359131  |
| C  | -4.750253 | 0.284516  | 0.308341  |
| C  | -4.183708 | 1.381977  | 0.961516  |
| C  | -5.522719 | 0.460086  | -0.843644 |
| C  | -4.391782 | 2.661677  | 0.447558  |
| H  | -3.613177 | 1.233870  | 1.872152  |
| C  | -5.714715 | 1.745564  | -1.345812 |
| H  | -5.987284 | -0.396870 | -1.320011 |
| C  | -5.155988 | 2.864942  | -0.711316 |
| H  | -3.962433 | 3.517852  | 0.962265  |
| H  | -6.317890 | 1.883321  | -2.239864 |
| C  | -5.404594 | 4.257164  | -1.241015 |
| H  | -6.330567 | 4.674972  | -0.824200 |
| H  | -4.591015 | 4.939709  | -0.975210 |
| H  | -5.509696 | 4.258501  | -2.330905 |
| C  | -1.285102 | -3.898075 | -0.351555 |
| C  | 1.191441  | -2.860486 | -1.704555 |
| H  | 2.172011  | -3.187667 | -1.309474 |
| O  | 0.839783  | -3.114647 | -2.848398 |
| H  | -1.594947 | -1.617695 | 1.582600  |
| Rh | 2.855938  | 1.478820  | 0.591877  |
| Rh | 1.489248  | -0.390359 | -0.211232 |
| O  | 3.693204  | 1.564478  | -1.295810 |
| O  | 2.401136  | -0.144363 | -2.050679 |
| O  | 3.047766  | -1.629905 | 0.381323  |
| O  | 0.060615  | 1.009135  | -0.746826 |
| O  | 0.707827  | -0.488627 | 1.708957  |
| O  | 1.936004  | 1.278960  | 2.431206  |
| O  | 4.288347  | 0.104074  | 1.162231  |
| O  | 1.348457  | 2.742644  | -0.042578 |
| C  | 0.311656  | 2.254140  | -0.574396 |
| C  | 3.300773  | 0.756249  | -2.186392 |
| C  | 4.086647  | -1.121752 | 0.933494  |
| C  | 1.088884  | 0.355296  | 2.593790  |
| C  | 0.465325  | 0.201363  | 3.964961  |
| C  | -0.738606 | 3.215912  | -1.086725 |
| C  | 3.954601  | 0.831159  | -3.549475 |
| C  | 5.159674  | -2.106735 | 1.346420  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 5.476385  | -2.692406 | 0.477410  |
| H | 4.749988  | -2.806580 | 2.082334  |
| H | 6.015109  | -1.581096 | 1.772778  |
| H | 4.594311  | -0.047434 | -3.689868 |
| H | 4.559655  | 1.735240  | -3.632748 |
| H | 3.190265  | 0.808397  | -4.331257 |
| H | -0.722791 | 3.209469  | -2.182587 |
| H | -1.733758 | 2.892373  | -0.769241 |
| H | -0.532432 | 4.226552  | -0.730513 |
| H | -0.618378 | 0.081378  | 3.875737  |
| H | 0.701957  | 1.064445  | 4.589018  |
| H | 0.858561  | -0.704967 | 4.439104  |
| H | -1.924050 | -4.170048 | 0.484151  |
| H | -0.497577 | -4.603403 | -0.594710 |

#### IV(a)\_ conf2

#### 0 imaginary frequency

|   |            |           |           |
|---|------------|-----------|-----------|
| C | -1.658606  | 0.211064  | -0.629824 |
| C | -1.050937  | 1.609804  | -0.580468 |
| C | 0.322310   | 1.845866  | -0.325915 |
| C | -2.050963  | 2.494509  | 0.328670  |
| C | -3.042718  | 1.492691  | 0.878503  |
| H | -1.589499  | 3.207129  | 1.002555  |
| H | -2.718167  | 1.143914  | 1.867790  |
| H | -4.047684  | 1.923351  | 0.968463  |
| H | -1.078151  | -0.458814 | 0.005906  |
| N | -3.048752  | 0.415233  | -0.128977 |
| S | -3.857272  | -1.016465 | 0.301060  |
| O | -3.498805  | -1.988859 | -0.735237 |
| O | -3.640299  | -1.324542 | 1.723255  |
| C | -5.571291  | -0.543466 | 0.097352  |
| C | -6.362181  | -0.300861 | 1.220060  |
| C | -6.103088  | -0.455445 | -1.192679 |
| C | -7.701863  | 0.048051  | 1.042183  |
| H | -5.934688  | -0.397907 | 2.212356  |
| C | -7.440849  | -0.107703 | -1.349649 |
| H | -5.477487  | -0.667989 | -2.053262 |
| C | -8.261057  | 0.148576  | -0.238173 |
| H | -8.322725  | 0.238852  | 1.913851  |
| H | -7.860177  | -0.038655 | -2.350444 |
| C | -9.719360  | 0.493437  | -0.424840 |
| H | -10.316496 | -0.411497 | -0.598262 |
| H | -10.130295 | 0.993449  | 0.457659  |
| H | -9.868460  | 1.149127  | -1.289587 |

|                       |           |           |           |    |           |           |           |
|-----------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                     | -1.987941 | 2.730638  | -1.115356 | C  | 2.987938  | -1.504934 | 1.263457  |
| C                     | 0.858876  | 3.219752  | -0.258381 | H  | 0.823909  | -1.066146 | 1.731997  |
| H                     | 1.660261  | 3.426636  | -0.994055 | H  | 3.273847  | -0.552055 | 1.736917  |
| O                     | 0.534549  | 4.042862  | 0.587105  | H  | 3.317862  | -2.329023 | 1.901668  |
| H                     | -1.696013 | -0.195500 | -1.640173 | H  | 3.045672  | 0.108465  | -1.170945 |
| Rh                    | 3.516348  | -1.249048 | 0.101373  | N  | 3.555688  | -1.667313 | -0.080723 |
| Rh                    | 1.766428  | 0.457651  | -0.081449 | S  | 5.220657  | -1.788564 | -0.280232 |
| O                     | 4.356983  | -0.096560 | 1.595486  | O  | 5.686665  | -2.626676 | 0.826016  |
| O                     | 2.736833  | 1.485774  | 1.427922  | O  | 5.427883  | -2.144223 | -1.683505 |
| O                     | 2.979279  | 1.393792  | -1.483301 | C  | 5.878265  | -0.138789 | -0.031970 |
| O                     | 0.715666  | -0.610298 | 1.343770  | C  | 5.983411  | 0.734107  | -1.119228 |
| O                     | 0.950963  | -0.716032 | -1.585603 | C  | 6.255813  | 0.268671  | 1.250721  |
| O                     | 2.566732  | -2.299518 | -1.404221 | C  | 6.461733  | 2.026216  | -0.909599 |
| O                     | 4.592531  | -0.195176 | -1.315693 | H  | 5.718121  | 0.394216  | -2.114847 |
| O                     | 2.325172  | -2.201593 | 1.497605  | C  | 6.733085  | 1.564494  | 1.439822  |
| C                     | 1.210208  | -1.697083 | 1.811927  | H  | 6.200083  | -0.430682 | 2.078294  |
| C                     | 3.808899  | 0.994452  | 1.925267  | C  | 6.843164  | 2.462247  | 0.367904  |
| C                     | 4.108348  | 0.871117  | -1.788796 | H  | 6.548047  | 2.704880  | -1.754580 |
| C                     | 1.505242  | -1.827104 | -1.900279 | H  | 7.033298  | 1.881401  | 2.435583  |
| C                     | 0.795969  | -2.637325 | -2.964082 | C  | 7.394420  | 3.852616  | 0.576699  |
| C                     | 0.371612  | -2.404717 | 2.853469  | H  | 8.481414  | 3.869894  | 0.422085  |
| C                     | 4.469380  | 1.822305  | 3.006970  | H  | 6.955132  | 4.568001  | -0.126223 |
| C                     | 4.920500  | 1.619172  | -2.825048 | H  | 7.204280  | 4.211348  | 1.593412  |
| H                     | 5.077317  | 2.651560  | -2.496668 | C  | 0.951688  | -2.468917 | 0.047609  |
| H                     | 4.364527  | 1.654818  | -3.767942 | C  | 0.547268  | 0.831818  | -1.932498 |
| H                     | 5.881518  | 1.127688  | -2.982602 | H  | 0.301295  | 1.884622  | -1.702903 |
| H                     | 4.809270  | 2.771984  | 2.579909  | O  | 0.924025  | 0.474971  | -3.037816 |
| H                     | 5.318650  | 1.286036  | 3.432732  | H  | 2.844891  | -1.422860 | -2.052119 |
| H                     | 3.740079  | 2.058044  | 3.787851  | Rh | -3.967917 | 0.368103  | 0.532416  |
| H                     | 0.529535  | -1.919540 | 3.824095  | Rh | -1.648711 | 0.026519  | -0.201086 |
| H                     | -0.690459 | -2.323534 | 2.607087  | O  | -4.455197 | 0.707695  | -1.441860 |
| H                     | 0.671666  | -3.451113 | 2.932827  | O  | -2.312322 | 0.392596  | -2.121992 |
| H                     | -0.193009 | -2.930496 | -2.595072 | O  | -1.374158 | 2.062536  | 0.083062  |
| H                     | 1.374406  | -3.528024 | -3.213303 | O  | -2.133521 | -1.979958 | -0.416959 |
| H                     | 0.645787  | -2.024579 | -3.858504 | O  | -1.197723 | -0.300026 | 1.810278  |
| H                     | -2.793068 | 2.359199  | -1.743297 | O  | -3.347556 | 0.008231  | 2.470625  |
| H                     | -1.503710 | 3.640378  | -1.454797 | O  | -3.517659 | 2.373621  | 0.766420  |
| IV(a)_conf3           |           |           |           | O  | -4.278710 | -1.652165 | 0.249042  |
| 0 imaginary frequency |           |           |           | C  | -3.324083 | -2.375092 | -0.152220 |
| C                     | 2.746215  | -0.945925 | -1.075851 | C  | -3.550062 | 0.650701  | -2.323120 |
| C                     | 1.325453  | -1.035179 | -0.503135 | C  | -2.353615 | 2.780313  | 0.493241  |
| C                     | 0.279514  | -0.154823 | -0.853873 | C  | -2.129540 | -0.239301 | 2.688849  |
| C                     | 1.491431  | -1.526498 | 1.013755  | C  | -1.704044 | -0.484325 | 4.121921  |
|                       |           |           |           | C  | -3.587197 | -3.853015 | -0.347522 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.941406 | 0.904642  | -3.762577 |
| C | -2.060255 | 4.256243  | 0.662481  |
| H | -1.716996 | 4.674356  | -0.289402 |
| H | -1.252153 | 4.388661  | 1.389437  |
| H | -2.952368 | 4.785418  | 1.000068  |
| H | -3.357760 | 1.741529  | -4.159240 |
| H | -5.007325 | 1.125256  | -3.834395 |
| H | -3.700115 | 0.024162  | -4.366782 |
| H | -3.363681 | -4.131802 | -1.382297 |
| H | -2.922005 | -4.434222 | 0.299893  |
| H | -4.626451 | -4.088622 | -0.114608 |
| H | -1.203471 | -1.454972 | 4.199649  |
| H | -2.569368 | -0.459193 | 4.785489  |
| H | -0.984503 | 0.283429  | 4.426131  |
| H | 1.599714  | -3.238758 | -0.362891 |
| H | -0.112419 | -2.671524 | 0.053842  |

#### I-TS-V(a)\_ conf1

1 imaginary frequency, value = -1134.3398cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.346914 | 0.265667  | -0.952987 |
| H | -2.739171 | -0.281778 | -1.815080 |
| H | -1.258568 | 0.287382  | -1.041966 |
| N | -2.668133 | -0.569717 | 0.238094  |
| S | -3.976033 | -1.699074 | 0.169235  |
| O | -3.937288 | -2.408252 | 1.449198  |
| O | -3.836426 | -2.389626 | -1.111288 |
| C | -5.453478 | -0.699097 | 0.104788  |
| C | -6.064665 | -0.460325 | -1.128091 |
| C | -5.976477 | -0.170008 | 1.288206  |
| C | -7.208647 | 0.334583  | -1.169472 |
| H | -5.655512 | -0.899761 | -2.031259 |
| C | -7.119724 | 0.621462  | 1.223803  |
| H | -5.505466 | -0.388133 | 2.240979  |
| C | -7.752398 | 0.887966  | -0.001059 |
| H | -7.689009 | 0.524306  | -2.125769 |
| H | -7.531755 | 1.036251  | 2.140002  |
| C | -9.008463 | 1.723386  | -0.053975 |
| H | -9.112587 | 2.230195  | -1.018469 |
| H | -9.899105 | 1.096263  | 0.084087  |
| H | -9.018845 | 2.482034  | 0.735076  |
| C | -1.940932 | -0.486766 | 1.401619  |
| H | -2.127366 | 0.641988  | 2.195785  |
| H | -2.113735 | -1.288268 | 2.115859  |
| C | -0.933529 | 0.433932  | 1.625339  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.121676  | 1.165023  | 1.628691  |
| C  | -2.914270 | 1.660789  | -0.867798 |
| H  | -4.000295 | 1.744034  | -0.855226 |
| C  | -2.153583 | 2.756203  | -0.822577 |
| H  | -1.068999 | 2.702298  | -0.821639 |
| H  | -2.596410 | 3.747816  | -0.778247 |
| C  | 0.380525  | 2.488194  | 2.215537  |
| H  | 1.014067  | 2.463778  | 3.125346  |
| O  | -0.002491 | 3.536942  | 1.733434  |
| Rh | 1.748718  | 0.288732  | 0.460773  |
| Rh | 3.512668  | -0.647290 | -0.927143 |
| O  | 1.002159  | 1.189050  | -1.258792 |
| O  | 2.654800  | 0.314830  | -2.545818 |
| O  | 4.621911  | 1.046153  | -0.520101 |
| O  | 2.279722  | -2.278181 | -1.258403 |
| O  | 4.263233  | -1.546274 | 0.771001  |
| O  | 2.611196  | -0.682266 | 2.069423  |
| O  | 2.990628  | 1.907383  | 0.803132  |
| O  | 0.621696  | -1.402629 | 0.018274  |
| C  | 1.127629  | -2.304325 | -0.735045 |
| C  | 1.620917  | 1.021775  | -2.365873 |
| C  | 4.139282  | 1.932281  | 0.247844  |
| C  | 3.665365  | -1.375403 | 1.876405  |
| C  | 4.260088  | -2.039871 | 3.100911  |
| C  | 0.264647  | -3.521248 | -0.996495 |
| C  | 1.076587  | 1.770775  | -3.564607 |
| C  | 5.011404  | 3.128167  | 0.567633  |
| H  | 5.795681  | 3.239665  | -0.183270 |
| H  | 5.481290  | 2.974034  | 1.546260  |
| H  | 4.402744  | 4.033793  | 0.627580  |
| H  | 1.560838  | 2.753387  | -3.614004 |
| H  | 0.000034  | 1.928040  | -3.467326 |
| H  | 1.306931  | 1.230062  | -4.484959 |
| H  | 0.289386  | -4.172404 | -0.114726 |
| H  | -0.775483 | -3.225844 | -1.161075 |
| H  | 0.643408  | -4.078240 | -1.855136 |
| H  | 5.037521  | -2.748929 | 2.812206  |
| H  | 3.474201  | -2.547073 | 3.667949  |
| H  | 4.693937  | -1.272593 | 3.752034  |

#### I-TS-V(a)\_ conf2

1 imaginary frequency, value = -1085.6017cm<sup>-1</sup>

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.439502 | 1.600498 | 0.970781 |
| H | 3.217484 | 1.071864 | 1.532572 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.503440  | 1.052941  | 1.107483  |
| N  | 2.805091  | 1.456236  | -0.466110 |
| S  | 4.482519  | 1.495962  | -0.908517 |
| O  | 5.120297  | 2.559084  | -0.133638 |
| O  | 4.487311  | 1.494152  | -2.372673 |
| C  | 5.090998  | -0.072960 | -0.313624 |
| C  | 4.872613  | -1.226483 | -1.074170 |
| C  | 5.808609  | -0.118727 | 0.882487  |
| C  | 5.370489  | -2.440219 | -0.611295 |
| H  | 4.336771  | -1.169330 | -2.015828 |
| C  | 6.297211  | -1.346735 | 1.328484  |
| H  | 5.992397  | 0.792862  | 1.440763  |
| C  | 6.087517  | -2.521654 | 0.594752  |
| H  | 5.205930  | -3.340520 | -1.197656 |
| H  | 6.856002  | -1.389019 | 2.259499  |
| C  | 6.642057  | -3.843277 | 1.067957  |
| H  | 7.549307  | -4.108061 | 0.509475  |
| H  | 6.905513  | -3.811289 | 2.129280  |
| H  | 5.922103  | -4.655141 | 0.918513  |
| C  | 1.878213  | 1.634437  | -1.467560 |
| H  | 1.414483  | 2.924357  | -1.685049 |
| H  | 2.216892  | 1.368087  | -2.466085 |
| C  | 0.562060  | 2.002743  | -1.257748 |
| C  | -0.675389 | 2.147910  | -0.940709 |
| C  | 2.313503  | 3.033191  | 1.422258  |
| H  | 3.215227  | 3.637483  | 1.346700  |
| C  | 1.176463  | 3.543062  | 1.898545  |
| H  | 0.264585  | 2.955509  | 1.963103  |
| H  | 1.118060  | 4.575453  | 2.232315  |
| C  | -1.500272 | 3.370437  | -0.931246 |
| H  | -2.215923 | 3.436462  | -1.775417 |
| O  | -1.461038 | 4.216788  | -0.060401 |
| Rh | -1.691736 | 0.348141  | -0.288196 |
| Rh | -2.859362 | -1.637058 | 0.503016  |
| O  | -1.213943 | 0.743571  | 1.695425  |
| O  | -2.334776 | -1.090362 | 2.428625  |
| O  | -4.567712 | -0.488034 | 0.657933  |
| O  | -1.072801 | -2.658536 | 0.299252  |
| O  | -3.310664 | -2.051094 | -1.469083 |
| O  | -2.227934 | -0.196674 | -2.209859 |
| O  | -3.481831 | 1.361101  | -0.086977 |
| O  | 0.033837  | -0.814887 | -0.432369 |
| C  | -0.045053 | -2.051659 | -0.121066 |
| C  | -1.647774 | -0.041218 | 2.606079  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.511386 | 0.737265  | 0.338325  |
| C | -2.917411 | -1.257658 | -2.376469 |
| C | -3.326329 | -1.578037 | -3.799440 |
| C | 1.209737  | -2.881314 | -0.306690 |
| C | -1.330330 | 0.348188  | 4.035237  |
| C | -5.786017 | 1.547807  | 0.443942  |
| H | -5.570526 | 2.529408  | 0.874319  |
| H | -6.525532 | 1.018668  | 1.047287  |
| H | -6.193714 | 1.707613  | -0.560976 |
| H | -0.347714 | 0.822728  | 4.093595  |
| H | -1.375469 | -0.526189 | 4.687262  |
| H | -2.075342 | 1.076585  | 4.376643  |
| H | 1.193267  | -3.325532 | -1.309336 |
| H | 2.103705  | -2.260483 | -0.218704 |
| H | 1.233656  | -3.694103 | 0.422612  |
| H | -3.536906 | -2.644294 | -3.902757 |
| H | -2.546140 | -1.269233 | -4.499183 |
| H | -4.238113 | -1.019023 | -4.041195 |

# I-TS-V(a)\_ conf3

1 imaginary frequency, value = -1097.9531cm<sup>-1</sup>

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 2.182371 | -2.339850 | -0.967561 |
| H | 2.786238 | -2.315227 | -1.875233 |
| H | 1.208948 | -1.884550 | -1.176457 |
| N | 2.854779 | -1.414019 | -0.003956 |
| S | 4.601965 | -1.424534 | 0.077223  |
| O | 5.027636 | -2.021348 | -1.186524 |
| O | 4.997774 | -1.970459 | 1.376151  |
| C | 4.973826 | 0.323877  | 0.070733  |
| C | 5.497800 | 0.913543  | 1.220918  |
| C | 4.765373 | 1.067484  | -1.096408 |
| C | 5.804290 | 2.275359  | 1.201063  |
| H | 5.670831 | 0.312242  | 2.107068  |
| C | 5.075107 | 2.422743  | -1.093639 |
| H | 4.374723 | 0.590474  | -1.989296 |
| C | 5.598310 | 3.048755  | 0.052307  |
| H | 6.214094 | 2.740367  | 2.093599  |
| H | 4.916125 | 3.006700  | -1.996658 |
| C | 5.942774 | 4.518154  | 0.028358  |
| H | 6.788923 | 4.711370  | -0.642917 |
| H | 5.100256 | 5.117846  | -0.334961 |
| H | 6.215461 | 4.883151  | 1.022725  |
| C | 2.208507 | -0.960096 | 1.119482  |
| H | 1.918695 | -1.901030 | 2.102654  |

|                       |           |           |           |    |           |           |           |
|-----------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H                     | 2.726642  | -0.196764 | 1.698244  | C  | 3.132410  | -1.506436 | 1.105941  |
| C                     | 0.917475  | -1.307751 | 1.467562  | H  | 2.189127  | -0.992851 | 1.331897  |
| C                     | -0.343390 | -1.550940 | 1.546720  | H  | 3.919909  | -0.901482 | 1.575038  |
| C                     | 2.031286  | -3.754520 | -0.464507 | N  | 3.315689  | -1.410450 | -0.352504 |
| H                     | 1.263293  | -3.931061 | 0.287039  | S  | 5.001243  | -1.301592 | -0.926506 |
| C                     | 2.763090  | -4.768324 | -0.930080 | O  | 4.901235  | -1.267455 | -2.383291 |
| H                     | 3.533810  | -4.620093 | -1.683342 | O  | 5.728326  | -2.337610 | -0.207053 |
| H                     | 2.618128  | -5.783424 | -0.570455 | C  | 5.527372  | 0.296047  | -0.332039 |
| C                     | -1.018130 | -2.621337 | 2.305905  | C  | 6.326628  | 0.368310  | 0.810508  |
| H                     | -1.764427 | -2.270782 | 3.042861  | C  | 5.157329  | 1.447573  | -1.036376 |
| O                     | -0.822338 | -3.805683 | 2.103307  | C  | 6.747049  | 1.620791  | 1.258069  |
| Rh                    | -1.600678 | -0.215386 | 0.404031  | H  | 6.628572  | -0.540110 | 1.320706  |
| Rh                    | -3.059167 | 1.273843  | -0.851748 | C  | 5.586560  | 2.684963  | -0.570086 |
| O                     | -0.897207 | -0.923557 | -1.419611 | H  | 4.563094  | 1.373381  | -1.941001 |
| O                     | -2.280144 | 0.451108  | -2.582120 | C  | 6.382386  | 2.793465  | 0.583678  |
| O                     | -4.493392 | -0.210214 | -0.801676 | H  | 7.374850  | 1.684745  | 2.142546  |
| O                     | -1.528513 | 2.668836  | -0.818462 | H  | 5.307861  | 3.583440  | -1.114468 |
| O                     | -3.748994 | 1.996693  | 0.955149  | C  | 6.827118  | 4.147915  | 1.078698  |
| O                     | -2.396389 | 0.600210  | 2.130469  | H  | 7.565525  | 4.060435  | 1.880784  |
| O                     | -3.135622 | -1.600696 | 0.372534  | H  | 7.270723  | 4.739955  | 0.270149  |
| O                     | -0.155394 | 1.279126  | 0.340550  | H  | 5.976199  | 4.720876  | 1.468329  |
| C                     | -0.439012 | 2.380067  | -0.241385 | C  | 2.351729  | -1.098943 | -1.243550 |
| C                     | -1.392933 | -0.447172 | -2.498252 | H  | 2.762065  | -0.895084 | -2.229092 |
| C                     | -4.227839 | -1.304358 | -0.218463 | H  | 0.570586  | -0.324963 | -1.940289 |
| C                     | -3.288216 | 1.508737  | 2.030573  | C  | 0.979116  | -0.893208 | -1.103153 |
| C                     | -3.864012 | 2.027343  | 3.332023  | C  | 0.041807  | -1.269333 | -0.146447 |
| C                     | 0.636321  | 3.448576  | -0.210127 | C  | 3.143838  | -2.895030 | 1.694044  |
| C                     | -0.855823 | -1.023630 | -3.792482 | H  | 3.027029  | -2.895327 | 2.777584  |
| C                     | -5.290245 | -2.382893 | -0.238020 | C  | 3.267180  | -4.041766 | 1.033556  |
| H                     | -6.257575 | -1.960945 | -0.515725 | H  | 3.376101  | -4.081562 | -0.045303 |
| H                     | -5.349583 | -2.870115 | 0.738807  | H  | 3.248042  | -4.991751 | 1.557955  |
| H                     | -5.009306 | -3.146757 | -0.972193 | C  | 0.094759  | -2.449437 | 0.724190  |
| H                     | -1.003212 | -2.108387 | -3.800097 | H  | -0.052866 | -2.273318 | 1.807263  |
| H                     | 0.221578  | -0.838035 | -3.859999 | O  | 0.146114  | -3.578523 | 0.257349  |
| H                     | -1.359526 | -0.573975 | -4.649242 | Rh | -1.709414 | -0.247590 | -0.042997 |
| H                     | 0.684666  | 3.877198  | 0.797656  | Rh | -3.767152 | 1.092908  | 0.072960  |
| H                     | 1.613196  | 3.008417  | -0.430780 | O  | -1.917988 | -0.555513 | 2.000828  |
| H                     | 0.406399  | 4.242298  | -0.922928 | O  | -3.830433 | 0.668965  | 2.098681  |
| H                     | -4.329229 | 3.003026  | 3.180305  | O  | -2.583333 | 2.750409  | 0.452645  |
| H                     | -3.083674 | 2.087358  | 4.094787  | O  | -4.813577 | -0.646635 | -0.313308 |
| H                     | -4.628251 | 1.326084  | 3.687453  | O  | -3.555491 | 1.419074  | -1.961503 |
| V(a)_ conf1           |           |           |           | O  | -1.655244 | 0.180095  | -2.066174 |
| 0 imaginary frequency |           |           |           | O  | -0.673934 | 1.521684  | 0.332865  |
|                       |           |           |           | O  | -2.910448 | -1.884327 | -0.398426 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.178425 | -1.732005 | -0.456641 |
| C | -2.923229 | -0.048661 | 2.608826  |
| C | -1.328378 | 2.606969  | 0.502683  |
| C | -2.577564 | 0.908383  | -2.575984 |
| C | -2.472419 | 1.156927  | -4.066770 |
| C | -4.977092 | -2.989417 | -0.729300 |
| C | -3.020756 | -0.360611 | 4.088863  |
| C | -0.495974 | 3.836630  | 0.811735  |
| H | -1.117090 | 4.733350  | 0.788780  |
| H | 0.322591  | 3.924605  | 0.091057  |
| H | -0.050214 | 3.729543  | 1.807102  |
| H | -3.849401 | 0.186251  | 4.541038  |
| H | -2.081464 | -0.099365 | 4.586249  |
| H | -3.174879 | -1.436913 | 4.222649  |
| H | -4.744965 | -3.742797 | 0.030045  |
| H | -6.046044 | -2.771172 | -0.726695 |
| H | -4.683467 | -3.403864 | -1.699300 |
| H | -3.224707 | 1.879555  | -4.386288 |
| H | -2.621343 | 0.212850  | -4.602180 |
| H | -1.470589 | 1.520796  | -4.314816 |

#### V(a)\_ conf2

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.281482 | -1.955533 | -1.314095 |
| H | -4.183829 | -2.527360 | -1.547443 |
| H | -2.436867 | -2.644956 | -1.430618 |
| N | -3.356759 | -1.599517 | 0.112026  |
| S | -4.973850 | -1.696198 | 0.876590  |
| O | -4.719286 | -1.735289 | 2.314301  |
| O | -5.659186 | -2.772252 | 0.168085  |
| C | -5.741769 | -0.142592 | 0.466271  |
| C | -6.548663 | -0.056631 | -0.669049 |
| C | -5.533432 | 0.961474  | 1.300025  |
| C | -7.148222 | 1.164221  | -0.973947 |
| H | -6.717329 | -0.930877 | -1.287796 |
| C | -6.139304 | 2.169963  | 0.973554  |
| H | -4.928588 | 0.866614  | 2.195371  |
| C | -6.950363 | 2.293265  | -0.167451 |
| H | -7.783944 | 1.238364  | -1.851909 |
| H | -5.989149 | 3.031117  | 1.619470  |
| C | -7.588862 | 3.617351  | -0.509231 |
| H | -8.304921 | 3.519058  | -1.330088 |
| H | -8.116452 | 4.038032  | 0.354409  |
| H | -6.830924 | 4.350694  | -0.812329 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.329813 | -1.274439 | 0.916623  |
| H  | -2.658993 | -1.154562 | 1.945267  |
| H  | -0.494036 | -0.769158 | 1.673866  |
| C  | -0.957459 | -1.050561 | 0.730603  |
| C  | -0.086287 | -1.040227 | -0.352879 |
| C  | -3.129179 | -0.795400 | -2.263648 |
| H  | -3.033223 | -1.113985 | -3.301312 |
| C  | -3.083649 | 0.501555  | -1.962036 |
| H  | -3.158591 | 0.866756  | -0.941897 |
| H  | -2.959262 | 1.250892  | -2.737807 |
| C  | -0.223390 | -1.521019 | -1.723337 |
| H  | 0.033797  | -0.780194 | -2.500392 |
| O  | -0.451421 | -2.695291 | -2.011324 |
| Rh | 1.761323  | -0.225099 | -0.069830 |
| Rh | 3.929409  | 0.873347  | 0.299550  |
| O  | 1.610608  | 0.908493  | -1.805350 |
| O  | 3.618468  | 1.914619  | -1.463913 |
| O  | 2.929494  | 2.348900  | 1.351027  |
| O  | 4.788432  | -0.673298 | -0.773778 |
| O  | 4.088219  | -0.247325 | 2.032651  |
| O  | 2.075851  | -1.248557 | 1.697450  |
| O  | 0.922637  | 1.329885  | 1.034407  |
| O  | 2.781953  | -1.681942 | -1.116432 |
| C  | 4.051365  | -1.589864 | -1.240126 |
| C  | 2.557471  | 1.710280  | -2.118516 |
| C  | 1.676738  | 2.255408  | 1.492183  |
| C  | 3.159990  | -1.046727 | 2.346458  |
| C  | 3.341563  | -1.877219 | 3.600379  |
| C  | 4.716060  | -2.704129 | -2.021419 |
| C  | 2.367398  | 2.479709  | -3.410411 |
| C  | 0.976017  | 3.355687  | 2.265428  |
| H  | 1.705085  | 3.983578  | 2.779983  |
| H  | 0.275958  | 2.920383  | 2.984483  |
| H  | 0.396183  | 3.972571  | 1.569440  |
| H  | 3.204060  | 3.159908  | -3.576165 |
| H  | 1.430021  | 3.043792  | -3.368691 |
| H  | 2.290871  | 1.776556  | -4.246519 |
| H  | 4.274058  | -2.765725 | -3.020968 |
| H  | 5.790320  | -2.529467 | -2.097279 |
| H  | 4.528062  | -3.660597 | -1.522742 |
| H  | 4.142812  | -1.466465 | 4.216896  |
| H  | 3.600350  | -2.903038 | 3.313749  |
| H  | 2.405976  | -1.918277 | 4.164702  |

**V(a)\_ conf3****0 imaginary frequency**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.441291 | 1.220167  | -1.323307 |
| H  | -4.488346 | 1.220869  | -1.642133 |
| H  | -2.979632 | 0.319662  | -1.740769 |
| N  | -3.427836 | 1.089864  | 0.142303  |
| S  | -4.985166 | 1.392670  | 0.956234  |
| O  | -5.516743 | 2.603205  | 0.341244  |
| O  | -4.701079 | 1.296457  | 2.386014  |
| C  | -5.963126 | -0.005928 | 0.444071  |
| C  | -5.748718 | -1.250214 | 1.048067  |
| C  | -6.941685 | 0.168909  | -0.535510 |
| C  | -6.521381 | -2.332133 | 0.643288  |
| H  | -5.001333 | -1.364651 | 1.826196  |
| C  | -7.706645 | -0.931170 | -0.923513 |
| H  | -7.108277 | 1.148879  | -0.969606 |
| C  | -7.507660 | -2.193278 | -0.349340 |
| H  | -6.360606 | -3.302028 | 1.106655  |
| H  | -8.472289 | -0.803084 | -1.683634 |
| C  | -8.329764 | -3.384007 | -0.777660 |
| H  | -8.859130 | -3.825655 | 0.075015  |
| H  | -9.072927 | -3.109395 | -1.531549 |
| H  | -7.692307 | -4.168811 | -1.202722 |
| C  | -2.382911 | 0.759956  | 0.918358  |
| H  | -2.665366 | 0.752432  | 1.968164  |
| H  | -0.531809 | 0.238338  | 1.629639  |
| C  | -1.037995 | 0.431680  | 0.686395  |
| C  | -0.221988 | 0.309280  | -0.430828 |
| C  | -2.754006 | 2.454197  | -1.850281 |
| H  | -2.629560 | 2.439059  | -2.932427 |
| C  | -2.322996 | 3.496693  | -1.142416 |
| H  | -2.427632 | 3.552676  | -0.062806 |
| H  | -1.845038 | 4.341502  | -1.628676 |
| C  | -0.494345 | 0.377167  | -1.860302 |
| H  | 0.106670  | 1.129097  | -2.403003 |
| O  | -1.208688 | -0.422737 | -2.464164 |
| Rh | 1.762911  | -0.058162 | -0.116847 |
| Rh | 4.149365  | -0.420448 | 0.333907  |
| O  | 2.352458  | 1.366298  | -1.507694 |
| O  | 4.558803  | 1.021468  | -1.093295 |
| O  | 4.029117  | 1.050402  | 1.783596  |
| O  | 4.117400  | -1.865213 | -1.146067 |
| O  | 3.575837  | -1.837631 | 1.729092  |
| O  | 1.366744  | -1.489512 | 1.325246  |

|   |          |           |           |
|---|----------|-----------|-----------|
| O | 1.815251 | 1.375965  | 1.386662  |
| O | 1.910111 | -1.526486 | -1.562903 |
| C | 3.035738 | -2.099453 | -1.759548 |
| C | 3.599505 | 1.586807  | -1.690867 |
| C | 2.916712 | 1.615132  | 1.990850  |
| C | 2.345835 | -2.059997 | 1.919321  |
| C | 1.972495 | -3.119487 | 2.936435  |
| C | 3.050146 | -3.165182 | -2.835868 |
| C | 3.935720 | 2.636506  | -2.730656 |
| C | 2.865957 | 2.700091  | 3.048037  |
| H | 3.795851 | 2.721372  | 3.618375  |
| H | 2.015562 | 2.531690  | 3.715337  |
| H | 2.715791 | 3.670566  | 2.561892  |
| H | 5.016772 | 2.750325  | -2.822580 |
| H | 3.484236 | 3.592423  | -2.445224 |
| H | 3.508181 | 2.346822  | -3.696132 |
| H | 2.702265 | -2.736810 | -3.781170 |
| H | 4.054893 | -3.572965 | -2.956419 |
| H | 2.353589 | -3.965421 | -2.564851 |
| H | 2.847896 | -3.417105 | 3.515734  |
| H | 1.569738 | -3.994081 | 2.413264  |
| H | 1.188643 | -2.742158 | 3.599666  |

**V-TS-III(a)\_ conf1****1 imaginary frequency, value = -282.4740cm<sup>-1</sup>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.020708 | -2.346801 | -1.212469 |
| H | -3.942490 | -2.388720 | -1.800651 |
| H | -2.621148 | -3.371925 | -1.203606 |
| N | -3.362669 | -1.994977 | 0.161824  |
| S | -4.996375 | -1.581156 | 0.528322  |
| O | -5.155977 | -1.814000 | 1.961583  |
| O | -5.804405 | -2.269293 | -0.478197 |
| C | -5.110210 | 0.178044  | 0.225911  |
| C | -5.548810 | 0.633313  | -1.020244 |
| C | -4.743690 | 1.074899  | 1.233261  |
| C | -5.610803 | 2.005187  | -1.255123 |
| H | -5.855743 | -0.076800 | -1.780464 |
| C | -4.810662 | 2.442581  | 0.976406  |
| H | -4.430846 | 0.708435  | 2.205057  |
| C | -5.243438 | 2.929961  | -0.266249 |
| H | -5.956595 | 2.363702  | -2.221356 |
| H | -4.530314 | 3.143790  | 1.758110  |
| C | -5.346338 | 4.414467  | -0.521555 |
| H | -4.649235 | 4.979031  | 0.105617  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -5.138133 | 4.656937  | -1.568775 |
| H  | -6.357368 | 4.779601  | -0.297729 |
| C  | -2.403640 | -1.860921 | 1.159679  |
| H  | -2.831493 | -1.827258 | 2.154509  |
| H  | -0.517908 | -1.501830 | 1.927032  |
| C  | -1.065359 | -1.703167 | 1.007659  |
| C  | -0.244035 | -1.583937 | -0.175478 |
| C  | -2.007501 | -1.465115 | -1.880957 |
| H  | -1.617797 | -1.886285 | -2.807249 |
| C  | -1.490873 | -0.281538 | -1.448467 |
| H  | -1.886012 | 0.249381  | -0.591712 |
| H  | -0.769012 | 0.248191  | -2.058738 |
| C  | 0.078041  | -2.762586 | -1.032566 |
| H  | 0.549634  | -2.518429 | -2.001726 |
| O  | -0.056727 | -3.915833 | -0.660106 |
| Rh | 1.428201  | -0.299098 | -0.044473 |
| Rh | 3.430014  | 1.099517  | 0.196570  |
| O  | 2.714164  | -1.900887 | -0.306773 |
| O  | 4.563930  | -0.606905 | -0.061247 |
| O  | 3.377147  | 1.369009  | -1.856147 |
| O  | 3.357651  | 0.740172  | 2.227338  |
| O  | 2.158981  | 2.717871  | 0.438870  |
| O  | 0.301227  | 1.424912  | 0.246254  |
| O  | 1.516036  | 0.088838  | -2.086600 |
| O  | 1.515342  | -0.567905 | 2.009688  |
| C  | 2.444230  | -0.004572 | 2.685616  |
| C  | 3.977282  | -1.712135 | -0.252125 |
| C  | 2.467759  | 0.819529  | -2.537929 |
| C  | 0.907639  | 2.535741  | 0.427882  |
| C  | 0.032242  | 3.745582  | 0.688410  |
| C  | 2.437800  | -0.279072 | 4.174946  |
| C  | 4.835956  | -2.945920 | -0.434229 |
| C  | 2.494931  | 1.020341  | -4.039468 |
| H  | 3.244156  | 1.765485  | -4.310636 |
| H  | 1.507993  | 1.331741  | -4.395069 |
| H  | 2.736190  | 0.069118  | -4.526971 |
| H  | 4.593740  | -3.676250 | 0.344628  |
| H  | 5.894364  | -2.686191 | -0.385096 |
| H  | 4.609242  | -3.411947 | -1.398566 |
| H  | 2.649365  | -1.339999 | 4.347619  |
| H  | 3.190341  | 0.329248  | 4.678672  |
| H  | 1.446010  | -0.070834 | 4.587869  |
| H  | -0.956597 | 3.610695  | 0.244672  |
| H  | 0.510511  | 4.646580  | 0.297932  |

|   |           |          |          |
|---|-----------|----------|----------|
| H | -0.087679 | 3.867894 | 1.771524 |
|---|-----------|----------|----------|

# V-TS-III(a)\_conf2

1 imaginary frequency, value = -288.7386cm<sup>-1</sup>

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.068632 | -1.030359 | 1.487873  |
| H  | -3.723729 | -1.704700 | 2.051472  |
| H  | -3.371398 | 0.000927  | 1.727827  |
| N  | -3.293889 | -1.289772 | 0.067913  |
| S  | -4.887820 | -1.826182 | -0.358854 |
| O  | -5.283528 | -2.736482 | 0.715289  |
| O  | -4.803685 | -2.246477 | -1.755260 |
| C  | -5.903020 | -0.359892 | -0.255616 |
| C  | -5.955649 | 0.518616  | -1.342274 |
| C  | -6.617557 | -0.102346 | 0.916363  |
| C  | -6.724071 | 1.673971  | -1.237496 |
| H  | -5.421624 | 0.290842  | -2.258494 |
| C  | -7.382808 | 1.059885  | 0.998649  |
| H  | -6.592491 | -0.812808 | 1.735445  |
| C  | -7.441814 | 1.968216  | -0.067160 |
| H  | -6.772236 | 2.357768  | -2.080951 |
| H  | -7.948042 | 1.260576  | 1.905025  |
| C  | -8.244071 | 3.242013  | 0.042552  |
| H  | -9.019807 | 3.163461  | 0.810457  |
| H  | -7.596904 | 4.086814  | 0.312530  |
| H  | -8.726876 | 3.494408  | -0.907439 |
| C  | -2.487188 | -0.795389 | -0.948408 |
| H  | -2.869234 | -1.039732 | -1.932732 |
| H  | -0.725729 | -0.107502 | -1.784851 |
| C  | -1.260101 | -0.228077 | -0.844506 |
| C  | -0.461460 | 0.068750  | 0.322272  |
| C  | -1.668617 | -1.218539 | 1.984526  |
| H  | -1.517946 | -0.771735 | 2.966289  |
| C  | -0.596948 | -1.818602 | 1.391876  |
| H  | -0.674777 | -2.392137 | 0.477616  |
| H  | 0.338148  | -1.894521 | 1.933799  |
| C  | -0.863502 | 1.124721  | 1.296806  |
| H  | -0.272531 | 1.142432  | 2.230710  |
| O  | -1.697994 | 1.982131  | 1.055572  |
| Rh | 1.645678  | 0.078911  | 0.073847  |
| Rh | 4.067313  | 0.201882  | -0.290723 |
| O  | 1.710168  | 2.110758  | 0.481439  |
| O  | 3.948942  | 2.222159  | 0.120884  |
| O  | 4.297644  | -0.187995 | 1.730734  |
| O  | 3.684606  | 0.587963  | -2.281660 |

|   |          |           |           |
|---|----------|-----------|-----------|
| O | 4.025808 | -1.829968 | -0.687138 |
| O | 1.781618 | -1.947920 | -0.362623 |
| O | 2.056135 | -0.317389 | 2.072511  |
| O | 1.441050 | 0.479268  | -1.949980 |
| C | 2.483327 | 0.645564  | -2.672848 |
| C | 2.825675 | 2.729334  | 0.409525  |
| C | 3.278385 | -0.356697 | 2.456779  |
| C | 2.922945 | -2.447687 | -0.651877 |
| C | 2.934318 | -3.920386 | -1.008111 |
| C | 2.232062 | 0.946626  | -4.135887 |
| C | 2.776211 | 4.220051  | 0.672103  |
| C | 3.500161 | -0.633383 | 3.929991  |
| H | 4.566860 | -0.665318 | 4.155837  |
| H | 3.035029 | -1.586970 | 4.201077  |
| H | 3.018724 | 0.148629  | 4.526623  |
| H | 2.397555 | 4.726472  | -0.223385 |
| H | 3.774170 | 4.600155  | 0.897436  |
| H | 2.086591 | 4.436601  | 1.491894  |
| H | 1.687536 | 1.892853  | -4.223984 |
| H | 3.175413 | 1.013146  | -4.679644 |
| H | 1.602787 | 0.164092  | -4.571667 |
| H | 2.292828 | -4.481326 | -0.322910 |
| H | 3.953022 | -4.310593 | -0.981880 |
| H | 2.530422 | -4.046925 | -2.019312 |

## 2a\_conf1

### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.404425  | 0.194566  | 1.229029  |
| C | 2.511951  | -0.556304 | 1.177626  |
| C | 3.318742  | -0.665791 | -0.061135 |
| C | 2.679582  | -0.113489 | -1.336523 |
| C | 1.231334  | 0.333250  | -1.236967 |
| H | 2.888479  | -0.658248 | -2.256725 |
| H | 1.019915  | 1.109746  | -1.975239 |
| H | 0.587363  | -0.535054 | -1.446808 |
| H | 0.854671  | 0.367646  | 2.145381  |
| H | 2.867297  | -1.070592 | 2.062706  |
| N | 0.918733  | 0.886695  | 0.094606  |
| S | -0.542592 | 1.749457  | 0.238416  |
| O | -0.562866 | 2.267802  | 1.605902  |
| O | -0.600524 | 2.619988  | -0.935910 |
| C | -1.857637 | 0.540275  | 0.087163  |
| C | -2.391531 | 0.254324  | -1.171935 |
| C | -2.328023 | -0.113399 | 1.229632  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.395584 | -0.706459 | -1.281858 |
| H | -2.045505 | 0.799917  | -2.043315 |
| C | -3.331757 | -1.070153 | 1.099124  |
| H | -1.933580 | 0.147138  | 2.205786  |
| C | -3.875944 | -1.387895 | -0.154573 |
| H | -3.820465 | -0.922379 | -2.258975 |
| H | -3.706628 | -1.572028 | 1.987652  |
| C | -4.944446 | -2.446687 | -0.286596 |
| H | -5.574085 | -2.273486 | -1.165112 |
| H | -4.497097 | -3.443636 | -0.395644 |
| H | -5.590985 | -2.476000 | 0.596619  |
| C | 3.802199  | 0.644197  | -0.732869 |
| H | 4.765134  | 0.624926  | -1.237629 |
| H | 3.590299  | 1.552736  | -0.178139 |
| C | 4.228072  | -1.830370 | -0.198941 |
| H | 4.796693  | -1.856719 | -1.158606 |
| O | 4.380957  | -2.693858 | 0.639270  |

## 2a\_conf2

### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.791245  | 1.184235  | -1.023881 |
| C | 2.928305  | 0.491423  | -1.178422 |
| C | 3.254527  | -0.676682 | -0.323907 |
| C | 2.362236  | -0.886804 | 0.902601  |
| C | 1.341214  | 0.193103  | 1.210848  |
| H | 2.884884  | -1.262207 | 1.780191  |
| H | 0.477718  | -0.244998 | 1.722580  |
| H | 1.788803  | 0.933320  | 1.886316  |
| H | 1.502866  | 2.007282  | -1.664705 |
| H | 3.614393  | 0.770848  | -1.972313 |
| N | 0.860674  | 0.859484  | -0.015045 |
| S | -0.562196 | 1.783186  | 0.135434  |
| O | -0.603910 | 2.351663  | 1.485532  |
| O | -0.629888 | 2.628845  | -1.058166 |
| C | -1.843827 | 0.537613  | 0.031841  |
| C | -2.175609 | -0.000928 | -1.216247 |
| C | -2.503384 | 0.127782  | 1.189803  |
| C | -3.170929 | -0.968747 | -1.291098 |
| H | -1.669034 | 0.345764  | -2.111118 |
| C | -3.499061 | -0.846720 | 1.093848  |
| H | -2.249760 | 0.578132  | 2.143419  |
| C | -3.846949 | -1.409200 | -0.139713 |
| H | -3.434514 | -1.388056 | -2.259118 |
| H | -4.016570 | -1.168412 | 1.993921  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.932865 | -2.453332 | -0.244314 |
| H | -5.796080 | -2.070254 | -0.803043 |
| H | -4.577565 | -3.345332 | -0.773790 |
| H | -5.286603 | -2.764965 | 0.742928  |
| C | 2.224636  | -1.829948 | -0.232351 |
| H | 2.644200  | -2.824496 | -0.111327 |
| H | 1.367071  | -1.744739 | -0.893014 |
| C | 4.680115  | -1.080735 | -0.184841 |
| H | 5.401163  | -0.470368 | -0.772679 |
| O | 5.066490  | -2.003664 | 0.505774  |

#### 2a\_conf3

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.651086  | 0.824301  | -1.184131 |
| C | 2.493337  | -0.218650 | -1.157002 |
| C | 2.730786  | -1.003424 | 0.078893  |
| C | 2.215834  | -0.392219 | 1.387230  |
| C | 1.672591  | 1.025373  | 1.285813  |
| H | 2.830862  | -0.556012 | 2.272318  |
| H | 0.952874  | 1.232158  | 2.080328  |
| H | 2.506773  | 1.729063  | 1.409275  |
| H | 1.431140  | 1.392211  | -2.080183 |
| H | 3.041184  | -0.507414 | -2.046618 |
| N | 1.029274  | 1.294498  | -0.006939 |
| S | -0.517564 | 1.974045  | -0.081798 |
| O | -0.698689 | 2.703297  | 1.174666  |
| O | -0.607339 | 2.622973  | -1.389874 |
| C | -1.663993 | 0.595643  | -0.080299 |
| C | -1.936294 | -0.076178 | -1.277065 |
| C | -2.256249 | 0.192008  | 1.117361  |
| C | -2.801977 | -1.166138 | -1.260986 |
| H | -1.494021 | 0.267199  | -2.206131 |
| C | -3.123864 | -0.900668 | 1.112027  |
| H | -2.058408 | 0.743200  | 2.030347  |
| C | -3.406452 | -1.598829 | -0.069301 |
| H | -3.021429 | -1.684512 | -2.191303 |
| H | -3.595313 | -1.209706 | 2.041523  |
| C | -4.335613 | -2.789398 | -0.069589 |
| H | -5.087987 | -2.707537 | -0.862457 |
| H | -3.783422 | -3.721653 | -0.245153 |
| H | -4.860190 | -2.889273 | 0.885401  |
| C | 1.503084  | -1.569349 | 0.836701  |
| H | 1.622024  | -2.524975 | 1.342194  |
| H | 0.550572  | -1.432938 | 0.334385  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 3.960312 | -1.832821 | 0.145492  |
| H | 4.088914 | -2.382349 | 1.107873  |
| O | 4.773155 | -1.942717 | -0.747958 |

#### 2a\_conf4

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.767531 | 0.582630  | -1.313393 |
| C | -3.049991 | 0.252464  | -1.114759 |
| C | -3.503166 | -0.465213 | 0.101086  |
| C | -2.411357 | -1.100608 | 0.968477  |
| C | -1.006622 | -1.051827 | 0.384345  |
| H | -2.654303 | -2.054956 | 1.436229  |
| H | -0.264844 | -1.096815 | 1.186293  |
| H | -0.860308 | -1.933203 | -0.253435 |
| H | -1.428681 | 1.169503  | -2.157985 |
| H | -3.802215 | 0.505229  | -1.853595 |
| N | -0.742645 | 0.140979  | -0.434032 |
| S | 0.361184  | 1.296879  | 0.150837  |
| O | 0.339365  | 2.383342  | -0.830305 |
| O | 0.109930  | 1.560004  | 1.574605  |
| C | 1.920485  | 0.422117  | 0.038969  |
| C | 2.640296  | 0.151127  | 1.201150  |
| C | 2.423240  | 0.069846  | -1.218234 |
| C | 3.874452  | -0.494697 | 1.100056  |
| H | 2.238526  | 0.447913  | 2.163957  |
| C | 3.653294  | -0.572878 | -1.298897 |
| H | 1.859330  | 0.299930  | -2.116423 |
| C | 4.398825  | -0.865603 | -0.143447 |
| H | 4.438244  | -0.709156 | 2.004303  |
| H | 4.046819  | -0.850283 | -2.273837 |
| C | 5.739354  | -1.552078 | -0.253591 |
| H | 6.138329  | -1.814257 | 0.730810  |
| H | 5.668476  | -2.471656 | -0.846437 |
| H | 6.473680  | -0.905256 | -0.750132 |
| C | -3.098394 | 0.104006  | 1.485774  |
| H | -3.805046 | -0.019974 | 2.303047  |
| H | -2.579579 | 1.057011  | 1.468025  |
| C | -4.818715 | -1.149694 | 0.048068  |
| H | -5.096286 | -1.679279 | 0.989993  |
| O | -5.563992 | -1.150747 | -0.909251 |

#### VI(a)\_conf1

##### 0 imaginary frequency

|   |          |           |          |
|---|----------|-----------|----------|
| C | 4.227265 | -0.785652 | 1.324468 |
|---|----------|-----------|----------|

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.779091  | -0.585622 | 1.511535  |
| C  | 1.931212  | -0.918456 | 0.420682  |
| C  | 2.544224  | -1.032637 | -1.058105 |
| C  | 4.023891  | -0.705330 | -1.143070 |
| H  | 1.893395  | -0.568947 | -1.795840 |
| H  | 4.438247  | -1.152869 | -2.050446 |
| H  | 4.163365  | 0.387142  | -1.196706 |
| H  | 4.584016  | -1.467724 | 2.107524  |
| N  | 4.703357  | -1.294075 | 0.012019  |
| S  | 6.344500  | -1.673200 | -0.137560 |
| O  | 6.680279  | -2.410143 | 1.082363  |
| O  | 6.511279  | -2.248139 | -1.474655 |
| C  | 7.235869  | -0.117395 | -0.095580 |
| C  | 7.463419  | 0.580742  | -1.285331 |
| C  | 7.668990  | 0.397448  | 1.129366  |
| C  | 8.120359  | 1.808344  | -1.237843 |
| H  | 7.152148  | 0.152993  | -2.232533 |
| C  | 8.324633  | 1.627561  | 1.156339  |
| H  | 7.515024  | -0.171790 | 2.039886  |
| C  | 8.560108  | 2.351526  | -0.021075 |
| H  | 8.303035  | 2.350568  | -2.162352 |
| H  | 8.666000  | 2.027587  | 2.107790  |
| C  | 9.302419  | 3.666041  | 0.013191  |
| H  | 10.377365 | 3.512410  | -0.149848 |
| H  | 8.949655  | 4.346375  | -0.768935 |
| H  | 9.187478  | 4.167017  | 0.979646  |
| C  | 2.113520  | -2.264654 | -0.447685 |
| H  | 1.146563  | -2.675779 | -0.719969 |
| H  | 2.852944  | -2.952559 | -0.053818 |
| C  | 0.515779  | -0.484424 | 0.508490  |
| H  | 0.212130  | -0.039571 | 1.467363  |
| O  | -0.275837 | -0.597896 | -0.423979 |
| Rh | -2.448607 | -0.043384 | -0.145727 |
| Rh | -4.759916 | 0.495593  | 0.196133  |
| O  | -1.956544 | 1.682849  | 0.873868  |
| O  | -4.143285 | 2.203283  | 1.177425  |
| O  | -4.723113 | 1.516214  | -1.591680 |
| O  | -4.666024 | -0.557398 | 1.969508  |
| O  | -5.242483 | -1.240836 | -0.801026 |
| O  | -3.056427 | -1.749021 | -1.131939 |
| O  | -2.533052 | 1.018814  | -1.913168 |
| O  | -2.478779 | -1.061978 | 1.647701  |
| C  | -3.570917 | -1.103570 | 2.306025  |
| C  | -2.900126 | 2.424193  | 1.307382  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.635858 | 1.562000  | -2.247691 |
| C | -4.304964 | -1.971737 | -1.250765 |
| C | -4.708642 | -3.206361 | -2.027439 |
| C | -3.560251 | -1.904942 | 3.589657  |
| C | -2.489443 | 3.696511  | 2.016878  |
| C | -3.639830 | 2.330952  | -3.551682 |
| H | -4.623222 | 2.763829  | -3.740472 |
| H | -3.364787 | 1.659478  | -4.371592 |
| H | -2.885179 | 3.123036  | -3.510233 |
| H | -3.321261 | 4.093995  | 2.600832  |
| H | -2.192852 | 4.441879  | 1.269696  |
| H | -1.625705 | 3.506642  | 2.659376  |
| H | -2.590460 | -1.815585 | 4.085000  |
| H | -4.362532 | -1.573950 | 4.251716  |
| H | -3.720740 | -2.962540 | 3.348898  |
| H | -5.662744 | -3.589751 | -1.659367 |
| H | -3.932618 | -3.971545 | -1.959177 |
| H | -4.833564 | -2.935469 | -3.082600 |
| H | 4.689778  | 0.192225  | 1.562859  |

**(R,R)-I-TS-II(a)\_conf1**

**1 imaginary frequency, value = -219.6221cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -0.930175 | -4.283851 | -7.258147 |
| Br | -6.566680 | 6.650420  | -0.394841 |
| Br | 7.542899  | 2.804727  | -0.062258 |
| Br | -2.658083 | -1.213275 | 8.632865  |
| C  | 0.859040  | 1.643199  | 1.636964  |
| C  | 1.877981  | 2.347192  | 2.510037  |
| C  | 1.772742  | 1.970848  | 3.985011  |
| H  | 2.706172  | 1.761652  | 4.497096  |
| H  | 0.945526  | 1.323045  | 4.256824  |
| C  | 1.433205  | 3.380529  | 3.604668  |
| C  | -0.007964 | 3.829330  | 3.736682  |
| C  | -0.626368 | 3.736033  | 4.990080  |
| H  | -0.083672 | 3.290431  | 5.819964  |
| C  | -1.926335 | 4.203847  | 5.184499  |
| H  | -2.389458 | 4.117052  | 6.163901  |
| C  | -2.629360 | 4.777420  | 4.123427  |
| H  | -3.644445 | 5.136946  | 4.268976  |
| C  | -2.021699 | 4.878792  | 2.870384  |
| H  | -2.568267 | 5.301305  | 2.032222  |
| C  | -0.720709 | 4.411803  | 2.681790  |
| H  | -0.270348 | 4.467136  | 1.694109  |
| C  | 2.409643  | 4.491923  | 3.966247  |

|   |           |          |           |   |           |           |           |
|---|-----------|----------|-----------|---|-----------|-----------|-----------|
| C | 2.275925  | 5.760243 | 3.375897  | H | -2.837123 | 6.967556  | -6.305026 |
| H | 1.474336  | 5.936161 | 2.665215  | C | -1.997858 | 5.421770  | -5.065867 |
| C | 3.138821  | 6.804518 | 3.701487  | H | -2.534846 | 4.637179  | -5.589328 |
| H | 3.011951  | 7.773649 | 3.225870  | C | 0.554768  | 3.291404  | -3.615874 |
| C | 4.154531  | 6.611444 | 4.640787  | C | 1.087599  | 2.915560  | -4.857448 |
| H | 4.826535  | 7.425242 | 4.899305  | H | 0.425187  | 2.820850  | -5.713917 |
| C | 4.287934  | 5.365529 | 5.250872  | C | 2.453230  | 2.675342  | -5.009108 |
| H | 5.063457  | 5.201510 | 5.994518  | H | 2.844632  | 2.393291  | -5.983210 |
| C | 3.423455  | 4.319734 | 4.917718  | C | 3.310574  | 2.805533  | -3.914179 |
| H | 3.543119  | 3.366404 | 5.421701  | H | 4.377064  | 2.627944  | -4.027968 |
| C | 3.251584  | 2.469186 | 1.898737  | C | 2.789456  | 3.166655  | -2.670282 |
| C | 3.606674  | 3.584014 | 1.128791  | H | 3.442612  | 3.250198  | -1.807238 |
| H | 2.894367  | 4.390632 | 0.989590  | C | 1.422838  | 3.411353  | -2.524695 |
| C | 4.872242  | 3.693803 | 0.551465  | H | 1.029924  | 3.674284  | -1.546615 |
| H | 5.140642  | 4.573309 | -0.023775 | C | -2.548748 | -1.302742 | -1.127441 |
| C | 5.789107  | 2.658774 | 0.732194  | C | -3.531060 | -1.952601 | -2.087038 |
| C | 5.462970  | 1.526954 | 1.476104  | C | -4.885442 | -1.262209 | -2.137769 |
| H | 6.167339  | 0.712356 | 1.595426  | H | -5.374267 | -1.195481 | -3.104298 |
| C | 4.195356  | 1.447371 | 2.056875  | H | -4.988896 | -0.387379 | -1.505656 |
| H | 3.941411  | 0.561272 | 2.631880  | C | -4.828985 | -2.609907 | -1.489233 |
| C | -1.423595 | 2.062584 | -1.452849 | C | -5.019021 | -2.741059 | 0.007986  |
| C | -1.884662 | 3.089471 | -2.467761 | C | -4.337957 | -3.725527 | 0.736922  |
| C | -0.911628 | 3.664401 | -3.556346 | H | -3.605872 | -4.353668 | 0.237613  |
| C | -1.925087 | 2.620322 | -3.914963 | C | -4.593970 | -3.918084 | 2.094632  |
| H | -1.554172 | 1.620830 | -4.113914 | H | -4.066244 | -4.699239 | 2.636868  |
| H | -2.799389 | 2.902027 | -4.492115 | C | -5.536304 | -3.123586 | 2.751870  |
| C | -3.014297 | 3.961891 | -1.975609 | H | -5.741570 | -3.275768 | 3.808110  |
| C | -2.768144 | 5.070990 | -1.156127 | C | -6.218887 | -2.138316 | 2.037086  |
| H | -1.747504 | 5.322103 | -0.885643 | H | -6.956195 | -1.514563 | 2.535417  |
| C | -3.808539 | 5.870984 | -0.686710 | C | -5.964232 | -1.954298 | 0.677081  |
| H | -3.601193 | 6.736821 | -0.067213 | H | -6.508273 | -1.190396 | 0.129019  |
| C | -5.121640 | 5.549202 | -1.031928 | C | -5.470873 | -3.756524 | -2.251337 |
| C | -5.400432 | 4.445330 | -1.834243 | C | -4.870742 | -5.019659 | -2.351240 |
| H | -6.424119 | 4.198973 | -2.094361 | H | -3.883434 | -5.181525 | -1.931810 |
| C | -4.341900 | 3.662549 | -2.299664 | C | -5.517645 | -6.072514 | -2.998063 |
| H | -4.561574 | 2.799652 | -2.922580 | H | -5.027782 | -7.039898 | -3.071357 |
| C | -1.141123 | 5.098870 | -4.006364 | C | -6.785261 | -5.885523 | -3.552664 |
| C | -0.438157 | 6.144936 | -3.386098 | H | -7.288709 | -6.705599 | -4.057380 |
| H | 0.259686  | 5.917835 | -2.585524 | C | -7.398901 | -4.636609 | -3.453072 |
| C | -0.606870 | 7.466907 | -3.791828 | H | -8.387897 | -4.478117 | -3.875134 |
| H | -0.053905 | 8.257569 | -3.291335 | C | -6.745684 | -3.584791 | -2.808682 |
| C | -1.476628 | 7.775106 | -4.840846 | H | -7.237412 | -2.618964 | -2.728333 |
| H | -1.607956 | 8.805254 | -5.160467 | C | -2.915532 | -2.511997 | -3.344763 |
| C | -2.166678 | 6.745797 | -5.478846 | C | -1.982161 | -3.559136 | -3.275126 |

|   |           |           |           |    |           |           |           |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -1.693590 | -3.956416 | -2.308089 | C  | -0.435740 | -4.864558 | 0.984438  |
| C | -1.394036 | -4.085528 | -4.422098 | H  | -1.372951 | -4.532009 | 1.422249  |
| H | -0.680700 | -4.899414 | -4.348174 | O  | -0.552887 | 1.202634  | -1.817758 |
| C | -1.732479 | -3.554488 | -5.667870 | O  | -1.983016 | 2.105135  | -0.314952 |
| C | -2.640251 | -2.505144 | -5.770966 | O  | -1.306104 | -1.495329 | -1.353785 |
| H | -2.889965 | -2.086741 | -6.739699 | O  | -3.024096 | -0.576776 | -0.203172 |
| C | -3.222057 | -1.992966 | -4.607635 | O  | 0.526667  | -1.595819 | 1.070140  |
| H | -3.920970 | -1.167348 | -4.699683 | O  | -1.334869 | -1.071481 | 2.238139  |
| C | -0.229155 | -1.675046 | 2.096556  | O  | 1.289757  | 1.132442  | 0.547016  |
| C | 0.258929  | -2.507468 | 3.269551  | O  | -0.325832 | 1.549460  | 2.076902  |
| C | 0.810226  | -3.953553 | 3.010458  | Rh | 0.064996  | -0.236943 | -0.445645 |
| C | 1.747066  | -2.817552 | 3.277905  | Rh | -1.735879 | 0.519746  | 0.990632  |
| H | 2.328528  | -2.426441 | 2.450849  | C  | 2.879822  | -1.498648 | -0.718602 |
| H | 2.251815  | -2.791031 | 4.237815  | C  | 1.798894  | -0.996282 | -1.599668 |
| C | -0.440518 | -2.205426 | 4.573080  | C  | 1.623778  | -0.952760 | -2.868934 |
| C | 0.243280  | -1.620049 | 5.644533  | C  | 3.226076  | -2.288518 | -3.777634 |
| H | 1.297961  | -1.380763 | 5.548286  | C  | 3.669170  | -3.012772 | -2.528474 |
| C | -0.400398 | -1.322176 | 6.848553  | H  | 2.592276  | -2.846903 | -4.463220 |
| H | 0.147882  | -0.870717 | 7.668166  | H  | 4.541094  | -3.630339 | -2.773035 |
| C | -1.755474 | -1.610543 | 6.978375  | H  | 2.886284  | -3.703106 | -2.186229 |
| C | -2.469638 | -2.181347 | 5.924050  | H  | 3.234352  | -0.681739 | -0.085676 |
| H | -3.528158 | -2.392338 | 6.029458  | N  | 4.038722  | -2.062814 | -1.462712 |
| C | -1.809131 | -2.472124 | 4.732993  | S  | 5.277537  | -2.628537 | -0.428957 |
| H | -2.376368 | -2.890242 | 3.908514  | O  | 5.157428  | -4.080614 | -0.216466 |
| C | 0.625614  | -4.989973 | 4.105103  | O  | 5.280641  | -1.719396 | 0.723549  |
| C | 1.709171  | -5.390799 | 4.897119  | C  | 6.740531  | -2.342318 | -1.417942 |
| H | 2.682115  | -4.931011 | 4.748798  | C  | 7.166301  | -1.028813 | -1.644888 |
| C | 1.563025  | -6.385998 | 5.866200  | C  | 7.460939  | -3.429280 | -1.910643 |
| H | 2.419454  | -6.680885 | 6.466929  | C  | 8.320492  | -0.814411 | -2.389346 |
| C | 0.326223  | -7.000526 | 6.058795  | H  | 6.612686  | -0.191140 | -1.233554 |
| H | 0.208806  | -7.772714 | 6.814238  | C  | 8.616496  | -3.192273 | -2.657994 |
| C | -0.760543 | -6.616952 | 5.269362  | H  | 7.126506  | -4.439217 | -1.698893 |
| H | -1.729236 | -7.089679 | 5.408698  | C  | 9.061474  | -1.889398 | -2.911140 |
| C | -0.609197 | -5.626160 | 4.300813  | H  | 8.657346  | 0.204863  | -2.560594 |
| H | -1.460877 | -5.344383 | 3.689457  | H  | 9.182645  | -4.036068 | -3.043790 |
| C | 0.772897  | -4.575767 | 1.631725  | C  | 10.309158 | -1.633943 | -3.722303 |
| C | 1.969651  | -4.989967 | 1.031587  | H  | 11.017235 | -1.003044 | -3.172077 |
| H | 2.919434  | -4.775805 | 1.513144  | H  | 10.072509 | -1.111101 | -4.657502 |
| C | 1.961196  | -5.685473 | -0.179651 | H  | 10.818446 | -2.567091 | -3.980588 |
| H | 2.905458  | -5.995575 | -0.618266 | C  | 3.653184  | -1.054648 | -4.131727 |
| C | 0.750096  | -5.984872 | -0.807111 | H  | 3.324981  | -0.606066 | -5.061278 |
| H | 0.737523  | -6.543108 | -1.739825 | H  | 4.316439  | -0.488575 | -3.486732 |
| C | -0.447823 | -5.568237 | -0.220600 | C  | 0.682564  | -0.716511 | -3.954087 |
| H | -1.396452 | -5.804030 | -0.697101 | H  | -0.281975 | -0.357350 | -3.560467 |

|   |          |           |           |
|---|----------|-----------|-----------|
| O | 0.879931 | -0.894897 | -5.141583 |
| H | 2.425295 | -2.246067 | -0.054931 |

**(R,R)-I-TS-II(a)\_conf2**

**1 imaginary frequency, value = -202.5339cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -2.441125 | 7.048756  | -4.371365 |
| Br | 7.454261  | 2.480945  | 4.940235  |
| Br | 3.002397  | -5.113157 | -5.753542 |
| Br | -2.717022 | -4.393166 | 7.234526  |
| C  | 1.267217  | -2.097245 | 0.313299  |
| C  | 1.761319  | -3.519604 | 0.144418  |
| C  | 1.050333  | -4.515763 | 1.056088  |
| H  | 0.737775  | -5.451081 | 0.603188  |
| H  | 0.348902  | -4.096758 | 1.770739  |
| C  | 2.506915  | -4.263433 | 1.308907  |
| C  | 2.907416  | -3.558224 | 2.589178  |
| C  | 2.513385  | -4.113048 | 3.813211  |
| H  | 1.878487  | -4.995517 | 3.818551  |
| C  | 2.924108  | -3.548685 | 5.021734  |
| H  | 2.603308  | -3.993093 | 5.960297  |
| C  | 3.741885  | -2.417322 | 5.023272  |
| H  | 4.060704  | -1.972491 | 5.962110  |
| C  | 4.143772  | -1.857041 | 3.808679  |
| H  | 4.763981  | -0.965240 | 3.795948  |
| C  | 3.732138  | -2.426603 | 2.603798  |
| H  | 4.023419  | -1.960061 | 1.666664  |
| C  | 3.507585  | -5.345496 | 0.924417  |
| C  | 4.875406  | -5.036388 | 0.835186  |
| H  | 5.208602  | -4.023477 | 1.038863  |
| C  | 5.817539  | -6.010107 | 0.510976  |
| H  | 6.868270  | -5.739532 | 0.445941  |
| C  | 5.417062  | -7.328275 | 0.280170  |
| H  | 6.150410  | -8.090022 | 0.030054  |
| C  | 4.066697  | -7.656167 | 0.385308  |
| H  | 3.738565  | -8.679555 | 0.222967  |
| C  | 3.124937  | -6.675108 | 0.705881  |
| H  | 2.083133  | -6.964617 | 0.796173  |
| C  | 2.059591  | -3.919242 | -1.278528 |
| C  | 3.324245  | -3.688657 | -1.834389 |
| H  | 4.103643  | -3.240162 | -1.226657 |
| C  | 3.614182  | -4.045670 | -3.151105 |
| H  | 4.604025  | -3.877792 | -3.561469 |
| C  | 2.613930  | -4.624137 | -3.932917 |
| C  | 1.338895  | -4.847338 | -3.416653 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.557945  | -5.264066 | -4.040964 |
| C | 1.077860  | -4.499168 | -2.090023 |
| H | 0.084858  | -4.676165 | -1.684870 |
| C | 2.546401  | 1.478993  | 0.102511  |
| C | 3.834019  | 2.240573  | -0.132585 |
| C | 4.496717  | 2.328422  | -1.552857 |
| C | 3.718221  | 3.484377  | -1.003270 |
| H | 2.748011  | 3.678012  | -1.447929 |
| H | 4.243234  | 4.369495  | -0.659422 |
| C | 4.724883  | 2.306615  | 1.084561  |
| C | 5.550937  | 1.229500  | 1.430907  |
| H | 5.570879  | 0.345367  | 0.801365  |
| C | 6.360748  | 1.271112  | 2.564711  |
| H | 7.006912  | 0.435490  | 2.811122  |
| C | 6.336587  | 2.407650  | 3.374174  |
| C | 5.518167  | 3.490807  | 3.062884  |
| H | 5.502473  | 4.368735  | 3.699438  |
| C | 4.719817  | 3.429442  | 1.918885  |
| H | 4.077652  | 4.273311  | 1.681623  |
| C | 6.014187  | 2.419176  | -1.602654 |
| C | 6.777936  | 1.248950  | -1.743957 |
| H | 6.274884  | 0.288902  | -1.811549 |
| C | 8.167913  | 1.300159  | -1.821379 |
| H | 8.734668  | 0.378754  | -1.926900 |
| C | 8.830184  | 2.529410  | -1.772454 |
| H | 9.914066  | 2.572021  | -1.835680 |
| C | 8.084679  | 3.700854  | -1.651748 |
| H | 8.583979  | 4.665904  | -1.625832 |
| C | 6.691033  | 3.644520  | -1.569395 |
| H | 6.133102  | 4.572172  | -1.491695 |
| C | 3.945201  | 1.604780  | -2.763945 |
| C | 3.786019  | 2.338087  | -3.948770 |
| H | 3.977119  | 3.408112  | -3.941970 |
| C | 3.401191  | 1.711293  | -5.134202 |
| H | 3.292892  | 2.298745  | -6.042400 |
| C | 3.166863  | 0.334530  | -5.151931 |
| H | 2.876867  | -0.161902 | -6.074349 |
| C | 3.309517  | -0.403524 | -3.975340 |
| H | 3.113211  | -1.470965 | -3.972258 |
| C | 3.699462  | 0.227166  | -2.792493 |
| H | 3.787474  | -0.359097 | -1.882309 |
| C | -0.700148 | 2.773366  | 0.923269  |
| C | -1.043792 | 4.250259  | 1.029398  |
| C | -0.250149 | 4.983293  | 2.098886  |

|   |           |           |           |    |           |           |           |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 0.058866  | 6.001025  | 1.883990  | C  | -2.699092 | -4.447736 | 4.355853  |
| H | 0.480055  | 4.383061  | 2.629005  | H  | -2.501071 | -5.507662 | 4.472132  |
| C | -1.704953 | 4.757770  | 2.369861  | C  | -2.849126 | -3.629801 | 5.471671  |
| C | -2.143313 | 3.787815  | 3.450052  | C  | -3.091307 | -2.262807 | 5.329166  |
| C | -3.404256 | 3.176530  | 3.388615  | H  | -3.194584 | -1.630253 | 6.203993  |
| H | -4.047803 | 3.358055  | 2.533178  | C  | -3.192943 | -1.718383 | 4.051264  |
| C | -3.859449 | 2.360781  | 4.424773  | H  | -3.354052 | -0.650939 | 3.948166  |
| H | -4.849192 | 1.914313  | 4.363117  | C  | -5.787759 | -2.102493 | 1.684936  |
| C | -3.059169 | 2.139459  | 5.548318  | C  | -6.482862 | -3.279560 | 1.378545  |
| H | -3.415482 | 1.513011  | 6.361785  | H  | -6.122175 | -3.924588 | 0.582185  |
| C | -1.803659 | 2.743701  | 5.622766  | C  | -7.639746 | -3.636469 | 2.075554  |
| H | -1.172546 | 2.585730  | 6.493226  | H  | -8.160214 | -4.555786 | 1.819625  |
| C | -1.354909 | 3.562557  | 4.585198  | C  | -8.124290 | -2.817433 | 3.094628  |
| H | -0.380119 | 4.033739  | 4.663130  | H  | -9.021678 | -3.093973 | 3.641201  |
| C | -2.594065 | 5.987992  | 2.313433  | C  | -7.445155 | -1.637142 | 3.406158  |
| C | -3.811292 | 6.015911  | 1.619060  | H  | -7.812614 | -0.990249 | 4.198359  |
| H | -4.114151 | 5.159152  | 1.026898  | C  | -6.293435 | -1.283453 | 2.705566  |
| C | -4.633215 | 7.142882  | 1.657440  | H  | -5.781478 | -0.359192 | 2.954609  |
| H | -5.567559 | 7.145118  | 1.102282  | C  | -4.850424 | -0.484132 | 0.009512  |
| C | -4.256924 | 8.263882  | 2.398970  | C  | -5.318845 | -0.681525 | -1.296594 |
| H | -4.896793 | 9.141643  | 2.427586  | H  | -5.379000 | -1.690315 | -1.695340 |
| C | -3.050938 | 8.247983  | 3.101168  | C  | -5.726766 | 0.397088  | -2.083586 |
| H | -2.747136 | 9.112472  | 3.685680  | H  | -6.097645 | 0.216763  | -3.089464 |
| C | -2.230198 | 7.120474  | 3.056243  | C  | -5.679622 | 1.695655  | -1.571935 |
| H | -1.296971 | 7.112879  | 3.613349  | H  | -6.014730 | 2.536279  | -2.173824 |
| C | -1.368989 | 4.931004  | -0.276582 | C  | -5.206750 | 1.902398  | -0.274262 |
| C | -2.456871 | 4.500996  | -1.054368 | H  | -5.175340 | 2.907936  | 0.137428  |
| H | -3.052531 | 3.658586  | -0.721445 | C  | -4.788262 | 0.823892  | 0.506789  |
| C | -2.778025 | 5.118936  | -2.260004 | H  | -4.406487 | 1.004236  | 1.507787  |
| H | -3.627276 | 4.776654  | -2.841820 | O  | 1.698424  | 1.417849  | -0.850776 |
| C | -1.995467 | 6.182359  | -2.712363 | O  | 2.381604  | 0.992783  | 1.263765  |
| C | -0.898241 | 6.619414  | -1.977138 | O  | -0.954096 | 2.190536  | -0.185435 |
| H | -0.283943 | 7.436536  | -2.338851 | O  | -0.140892 | 2.233382  | 1.924632  |
| C | -0.594505 | 5.988610  | -0.767463 | O  | -1.781744 | -0.729365 | -0.048303 |
| H | 0.269326  | 6.334657  | -0.208614 | O  | -1.357391 | -0.497337 | 2.160392  |
| C | -2.019950 | -0.960563 | 1.184873  | O  | 0.953134  | -1.463662 | -0.752324 |
| C | -3.154791 | -1.914200 | 1.524868  | O  | 1.137548  | -1.658019 | 1.495483  |
| C | -4.566760 | -1.686291 | 0.883516  | Rh | -0.062136 | 0.354129  | -0.560983 |
| C | -3.661266 | -2.766823 | 0.377574  | Rh | 0.515433  | 0.274318  | 1.789756  |
| H | -3.177250 | -2.618077 | -0.580079 | C  | -1.364112 | -0.969970 | -3.082572 |
| H | -3.918843 | -3.795903 | 0.604252  | C  | -0.678612 | 0.292152  | -2.693780 |
| C | -3.060413 | -2.517898 | 2.905644  | C  | -0.428833 | 1.388723  | -3.308920 |
| C | -2.803652 | -3.882078 | 3.082484  | C  | -1.725974 | 1.408259  | -5.183043 |
| H | -2.673605 | -4.526265 | 2.217872  | C  | -2.646989 | 0.259184  | -4.833471 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -2.128523 | 2.413108  | -5.072607 |
| H | -3.260135 | 0.026998  | -5.709406 |
| H | -3.322903 | 0.548782  | -4.016946 |
| H | -0.654845 | -1.797352 | -2.990699 |
| N | -1.878660 | -0.934491 | -4.464548 |
| S | -2.233766 | -2.393327 | -5.227484 |
| O | -1.164479 | -3.317315 | -4.843789 |
| O | -2.514990 | -2.052706 | -6.623885 |
| C | -3.759729 | -3.031684 | -4.522632 |
| C | -4.989589 | -2.626018 | -5.047594 |
| C | -3.703382 | -3.943990 | -3.465682 |
| C | -6.167187 | -3.121762 | -4.488950 |
| H | -5.021701 | -1.960205 | -5.903505 |
| C | -4.890503 | -4.436751 | -2.926117 |
| H | -2.740938 | -4.283053 | -3.097984 |
| C | -6.139591 | -4.027619 | -3.418249 |
| H | -7.123890 | -2.813590 | -4.903031 |
| H | -4.846260 | -5.161378 | -2.116563 |
| C | -7.417603 | -4.543745 | -2.801202 |
| H | -7.340822 | -5.608420 | -2.554753 |
| H | -8.270590 | -4.411096 | -3.473693 |
| H | -7.646051 | -4.009245 | -1.869533 |
| C | -0.502033 | 1.239233  | -5.733766 |
| H | 0.100437  | 2.096720  | -6.005825 |
| H | -0.097347 | 0.245607  | -5.895148 |
| C | 0.095610  | 2.744384  | -3.205076 |
| H | 0.477845  | 2.935406  | -2.190009 |
| O | 0.117247  | 3.587514  | -4.081458 |
| H | -2.171011 | -1.138009 | -2.354551 |

**(R,R)-I-TS-II(a)\_conf3**

**1 imaginary frequency, value = -220.8747cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | 0.085780  | 5.316718  | -6.620052 |
| Br | 6.891347  | -6.101906 | -1.643482 |
| Br | -7.327607 | -3.289544 | 0.065810  |
| Br | 3.241394  | 0.298728  | 8.505088  |
| C  | -0.627404 | -1.883524 | 1.470466  |
| C  | -1.529861 | -2.766685 | 2.307870  |
| C  | -1.343961 | -2.578444 | 3.810318  |
| H  | -2.249390 | -2.506964 | 4.403955  |
| H  | -0.543448 | -1.912174 | 4.115451  |
| C  | -0.938238 | -3.897360 | 3.223766  |
| C  | 0.537462  | -4.241486 | 3.207638  |
| C  | 1.229803  | -4.269515 | 4.424996  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.711336  | -3.989910 | 5.338671  |
| C | 2.571929  | -4.646923 | 4.478373  |
| H | 3.091406  | -4.656695 | 5.432971  |
| C | 3.244161  | -5.005997 | 3.308654  |
| H | 4.291284  | -5.294328 | 3.344383  |
| C | 2.563271  | -4.985273 | 2.089810  |
| H | 3.082862  | -5.239857 | 1.170586  |
| C | 1.220190  | -4.610390 | 2.042375  |
| H | 0.711226  | -4.566567 | 1.083066  |
| C | -1.807335 | -5.119708 | 3.488998  |
| C | -1.586221 | -6.304160 | 2.765294  |
| H | -0.791775 | -6.337366 | 2.026385  |
| C | -2.352068 | -7.445581 | 2.993974  |
| H | -2.158177 | -8.345942 | 2.416632  |
| C | -3.355126 | -7.437771 | 3.965898  |
| H | -3.950774 | -8.327933 | 4.148942  |
| C | -3.574717 | -6.277109 | 4.705635  |
| H | -4.341850 | -6.256538 | 5.475299  |
| C | -2.807766 | -5.133586 | 4.469879  |
| H | -2.994603 | -4.250889 | 5.071943  |
| C | -2.934002 | -2.910010 | 1.774896  |
| C | -3.282624 | -3.956572 | 0.911865  |
| H | -2.541113 | -4.700767 | 0.640853  |
| C | -4.578315 | -4.079828 | 0.408371  |
| H | -4.839591 | -4.907832 | -0.241797 |
| C | -5.533104 | -3.126240 | 0.759669  |
| C | -5.215999 | -2.062372 | 1.601663  |
| H | -5.952281 | -1.309243 | 1.855813  |
| C | -3.917061 | -1.969739 | 2.105637  |
| H | -3.669336 | -1.137999 | 2.759137  |
| C | 1.422164  | -1.787888 | -1.799047 |
| C | 1.864897  | -2.652966 | -2.961944 |
| C | 0.848335  | -3.158596 | -4.044946 |
| C | 1.769732  | -2.014400 | -4.340000 |
| H | 1.326331  | -1.026000 | -4.388429 |
| H | 2.614590  | -2.165315 | -5.003944 |
| C | 3.077376  | -3.499596 | -2.657490 |
| C | 2.958793  | -4.710125 | -1.962826 |
| H | 1.977496  | -5.059073 | -1.657472 |
| C | 4.076817  | -5.486377 | -1.662083 |
| H | 3.967372  | -6.430039 | -1.138655 |
| C | 5.339536  | -5.037832 | -2.051287 |
| C | 5.491914  | -3.832840 | -2.733014 |
| H | 6.477163  | -3.489070 | -3.028626 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.357098  | -3.075704 | -3.031121 | C | 4.883403  | 6.788789  | -2.468221 |
| H | 4.478150  | -2.133835 | -3.559467 | H | 4.334077  | 7.718933  | -2.348799 |
| C | 1.123793  | -4.511528 | -4.681930 | C | 6.103832  | 6.778367  | -3.146443 |
| C | 0.535798  | -5.668626 | -4.144831 | H | 6.510978  | 7.699014  | -3.555524 |
| H | -0.106218 | -5.585740 | -3.272748 | C | 6.794782  | 5.575474  | -3.294283 |
| C | 0.746661  | -6.918770 | -4.722246 | H | 7.748339  | 5.553109  | -3.815401 |
| H | 0.283091  | -7.798556 | -4.283548 | C | 6.265001  | 4.394643  | -2.771281 |
| C | 1.543500  | -7.041148 | -5.863301 | H | 6.816355  | 3.464924  | -2.883772 |
| H | 1.707165  | -8.014919 | -6.316733 | C | 2.486755  | 3.137031  | -3.173286 |
| C | 2.118435  | -5.899433 | -6.418796 | C | 1.505639  | 4.097628  | -2.879027 |
| H | 2.730503  | -5.976028 | -7.313649 | H | 1.276823  | 4.331210  | -1.844992 |
| C | 1.908392  | -4.648203 | -5.833595 | C | 0.795263  | 4.743300  | -3.887490 |
| H | 2.354402  | -3.772712 | -6.294502 | H | 0.045772  | 5.487360  | -3.639776 |
| C | -0.636772 | -2.876395 | -3.957662 | C | 1.057975  | 4.421855  | -5.220137 |
| C | -1.280834 | -2.378125 | -5.099320 | C | 2.011402  | 3.462495  | -5.546034 |
| H | -0.690642 | -2.130910 | -5.977853 | H | 2.202550  | 3.206474  | -6.582224 |
| C | -2.664942 | -2.207767 | -5.125167 | C | 2.716110  | 2.828186  | -4.518727 |
| H | -3.143007 | -1.826980 | -6.024126 | H | 3.450998  | 2.074481  | -4.784551 |
| C | -3.429603 | -2.534061 | -4.002828 | C | 0.303003  | 1.414532  | 2.258452  |
| H | -4.509765 | -2.412415 | -4.020164 | C | -0.142450 | 2.055481  | 3.562049  |
| C | -2.797911 | -3.019899 | -2.856456 | C | -0.796008 | 3.481351  | 3.528459  |
| H | -3.378979 | -3.257823 | -1.971032 | C | -1.641632 | 2.260453  | 3.710270  |
| C | -1.412777 | -3.191930 | -2.836461 | H | -2.259009 | 1.933670  | 2.881405  |
| H | -0.933734 | -3.552019 | -1.930274 | H | -2.070514 | 2.086112  | 4.691158  |
| C | 2.372853  | 1.595917  | -1.142789 | C | 0.670003  | 1.639688  | 4.765626  |
| C | 3.234499  | 2.444542  | -2.061684 | C | 0.096592  | 0.907767  | 5.811594  |
| C | 4.618999  | 1.867676  | -2.314176 | H | -0.952669 | 0.632433  | 5.770354  |
| H | 5.028474  | 1.975858  | -3.313278 | C | 0.845113  | 0.506666  | 6.921421  |
| H | 4.827895  | 0.920965  | -1.828709 | H | 0.380573  | -0.058183 | 7.722234  |
| C | 4.535269  | 3.099152  | -1.467697 | C | 2.194926  | 0.838904  | 6.981158  |
| C | 4.846493  | 3.023275  | 0.012949  | C | 2.800768  | 1.556089  | 5.948655  |
| C | 4.166411  | 3.829007  | 0.935959  | H | 3.856159  | 1.801230  | 5.996600  |
| H | 3.345959  | 4.456000  | 0.599234  | C | 2.036622  | 1.948526  | 4.852504  |
| C | 4.534517  | 3.845081  | 2.281357  | H | 2.520870  | 2.481290  | 4.041676  |
| H | 4.005065  | 4.491750  | 2.977196  | C | -0.596359 | 4.383901  | 4.733144  |
| C | 5.589196  | 3.047348  | 2.731399  | C | -1.662747 | 4.651566  | 5.601253  |
| H | 5.880736  | 3.062081  | 3.778172  | H | -2.624506 | 4.175317  | 5.431756  |
| C | 6.270767  | 2.237046  | 1.822387  | C | -1.512940 | 5.533202  | 6.673878  |
| H | 7.094485  | 1.612917  | 2.158553  | H | -2.355417 | 5.726243  | 7.332881  |
| C | 5.904364  | 2.231209  | 0.475600  | C | -0.289533 | 6.164820  | 6.896043  |
| H | 6.449656  | 1.604959  | -0.224681 | H | -0.168978 | 6.848358  | 7.732105  |
| C | 5.038882  | 4.389243  | -2.091944 | C | 0.779879  | 5.912279  | 6.033621  |
| C | 4.360310  | 5.607198  | -1.943684 | H | 1.738204  | 6.398303  | 6.196750  |
| H | 3.408143  | 5.633667  | -1.424500 | C | 0.624628  | 5.035006  | 4.961605  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.463187  | 4.851386  | 4.297189  |
| C  | -0.903405 | 4.276074  | 2.244798  |
| C  | -2.167686 | 4.658518  | 1.776775  |
| H  | -3.061895 | 4.300357  | 2.278548  |
| C  | -2.298517 | 5.507201  | 0.675252  |
| H  | -3.292626 | 5.787888  | 0.338842  |
| C  | -1.161398 | 5.995287  | 0.028202  |
| H  | -1.257742 | 6.672771  | -0.816474 |
| C  | 0.103737  | 5.613944  | 0.483111  |
| H  | 0.995383  | 5.997343  | -0.007333 |
| C  | 0.230739  | 4.757149  | 1.577239  |
| H  | 1.219553  | 4.459187  | 1.914472  |
| O  | 0.484811  | -0.943280 | -1.998644 |
| O  | 2.059157  | -1.935866 | -0.711324 |
| O  | 1.106810  | 1.725679  | -1.258276 |
| O  | 2.961773  | 0.786187  | -0.365387 |
| O  | -0.527631 | 1.403748  | 1.288763  |
| O  | 1.455544  | 0.886584  | 2.237342  |
| O  | -1.167360 | -1.283747 | 0.479054  |
| O  | 0.575889  | -1.749111 | 1.845880  |
| Rh | -0.109659 | 0.276635  | -0.419918 |
| Rh | 1.835861  | -0.521456 | 0.782702  |
| C  | -3.009272 | 1.366746  | -0.343248 |
| C  | -1.966718 | 1.049272  | -1.348207 |
| C  | -1.880274 | 1.178046  | -2.621041 |
| C  | -3.609096 | 2.522547  | -3.243448 |
| C  | -4.002439 | 3.047701  | -1.883441 |
| H  | -3.055830 | 3.205703  | -3.884531 |
| H  | -4.920590 | 3.636985  | -1.987878 |
| H  | -3.234845 | 3.733969  | -1.500484 |
| H  | -3.273271 | 0.456976  | 0.201030  |
| N  | -4.245684 | 1.945607  | -0.934528 |
| S  | -5.444336 | 2.289489  | 0.235164  |
| O  | -5.396049 | 3.707406  | 0.629264  |
| O  | -5.317301 | 1.242360  | 1.256004  |
| C  | -6.950921 | 2.033149  | -0.695171 |
| C  | -7.318432 | 0.731866  | -1.055039 |
| C  | -7.757271 | 3.124562  | -1.014036 |
| C  | -8.502288 | 0.536540  | -1.756805 |
| H  | -6.696539 | -0.112924 | -0.778069 |
| C  | -8.941255 | 2.907178  | -1.721954 |
| H  | -7.465955 | 4.121083  | -0.699790 |
| C  | -9.330374 | 1.618266  | -2.105070 |
| H  | -8.792978 | -0.474150 | -2.032137 |

|   |            |          |           |
|---|------------|----------|-----------|
| H | -9.573661  | 3.754663 | -1.973235 |
| C | -10.613047 | 1.382801 | -2.866208 |
| H | -11.292257 | 0.730815 | -2.303462 |
| H | -10.419132 | 0.891161 | -3.827307 |
| H | -11.138616 | 2.320810 | -3.068155 |
| C | -3.991029  | 1.320756 | -3.733885 |
| H | -3.703106  | 1.020293 | -4.733787 |
| H | -4.576693  | 0.633350 | -3.132856 |
| C | -1.003738  | 1.142476 | -3.783104 |
| H | 0.008539   | 0.815613 | -3.495554 |
| O | -1.294918  | 1.442343 | -4.925986 |
| H | -2.551247  | 2.053592 | 0.380560  |

**(R,R)-I-TS-II(a)\_conf4**

**1 imaginary frequency, value = -219.9959cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -0.548346 | -4.969578 | -6.848165 |
| Br | -6.734783 | 6.438902  | -0.838294 |
| Br | 7.432189  | 3.012268  | -0.125728 |
| Br | -2.584164 | -0.651511 | 8.680487  |
| C  | 0.772314  | 1.745072  | 1.557150  |
| C  | 1.750284  | 2.532322  | 2.405375  |
| C  | 1.638112  | 2.235270  | 3.897760  |
| H  | 2.572493  | 2.093664  | 4.430973  |
| H  | 0.834580  | 1.569920  | 4.197136  |
| C  | 1.248074  | 3.606564  | 3.434470  |
| C  | -0.212565 | 3.999843  | 3.522746  |
| C  | -0.844709 | 3.951551  | 4.771812  |
| H  | -0.295269 | 3.579811  | 5.633020  |
| C  | -2.167200 | 4.369867  | 4.922324  |
| H  | -2.640443 | 4.319075  | 5.899417  |
| C  | -2.879530 | 4.847419  | 3.820671  |
| H  | -3.911914 | 5.167721  | 3.932248  |
| C  | -2.258442 | 4.903459  | 2.571384  |
| H  | -2.810816 | 5.249954  | 1.702801  |
| C  | -0.934804 | 4.487018  | 2.426877  |
| H  | -0.472733 | 4.504755  | 1.443203  |
| C  | 2.171439  | 4.776782  | 3.745241  |
| C  | 1.985147  | 6.007073  | 3.091865  |
| H  | 1.180952  | 6.110873  | 2.370040  |
| C  | 2.798416  | 7.103890  | 3.369012  |
| H  | 2.631554  | 8.041630  | 2.845243  |
| C  | 3.815195  | 7.003529  | 4.321576  |
| H  | 4.448237  | 7.858615  | 4.542433  |
| C  | 3.999977  | 5.796584  | 4.993500  |

|   |           |          |           |   |           |           |           |
|---|-----------|----------|-----------|---|-----------|-----------|-----------|
| H | 4.776948  | 5.704619 | 5.747954  | H | 2.879305  | 2.155382  | -6.052321 |
| C | 3.185309  | 4.697847 | 4.708873  | C | 3.299289  | 2.697599  | -4.003490 |
| H | 3.344117  | 3.776964 | 5.259968  | H | 4.371963  | 2.543810  | -4.090503 |
| C | 3.128692  | 2.668181 | 1.807170  | C | 2.747788  | 3.114209  | -2.790377 |
| C | 3.469791  | 3.760111 | 0.999328  | H | 3.384061  | 3.265196  | -1.923958 |
| H | 2.743329  | 4.545940 | 0.820784  | C | 1.372727  | 3.327677  | -2.679426 |
| C | 4.739966  | 3.873957 | 0.432177  | H | 0.956406  | 3.633102  | -1.723603 |
| H | 4.996837  | 4.736102 | -0.173823 | C | -2.483148 | -1.442336 | -1.120641 |
| C | 5.675031  | 2.865386 | 0.661314  | C | -3.416846 | -2.189154 | -2.055049 |
| C | 5.363914  | 1.756682 | 1.445475  | C | -4.771998 | -1.521525 | -2.240235 |
| H | 6.082696  | 0.961537 | 1.603064  | H | -5.202695 | -1.541558 | -3.236098 |
| C | 4.092003  | 1.673645 | 2.015562  | H | -4.920094 | -0.598698 | -1.690383 |
| H | 3.848950  | 0.805369 | 2.621687  | C | -4.737895 | -2.802142 | -1.467028 |
| C | -1.454850 | 1.945980 | -1.588475 | C | -5.016780 | -2.784813 | 0.021084  |
| C | -1.926368 | 2.909046 | -2.659372 | C | -4.263867 | -3.554425 | 0.916615  |
| C | -0.950053 | 3.456419 | -3.759168 | H | -3.396330 | -4.100812 | 0.557414  |
| C | -1.927944 | 2.367895 | -4.081812 | C | -4.608285 | -3.620591 | 2.266783  |
| H | -1.525272 | 1.370953 | -4.222985 | H | -4.019647 | -4.235300 | 2.943727  |
| H | -2.799351 | 2.594760 | -4.687206 | C | -5.709518 | -2.909295 | 2.748044  |
| C | -3.087084 | 3.773217 | -2.229242 | H | -5.979337 | -2.961067 | 3.799379  |
| C | -2.884384 | 4.924350 | -1.457178 | C | -6.462521 | -2.132904 | 1.865700  |
| H | -1.875804 | 5.213449 | -1.179454 | H | -7.321281 | -1.573635 | 2.227447  |
| C | -3.953131 | 5.718055 | -1.044194 | C | -6.120251 | -2.077433 | 0.514000  |
| H | -3.779260 | 6.616220 | -0.461517 | H | -6.717836 | -1.478904 | -0.168284 |
| C | -5.250960 | 5.347368 | -1.398103 | C | -5.312093 | -4.035560 | -2.142243 |
| C | -5.486768 | 4.201577 | -2.153973 | C | -4.735540 | -5.302430 | -1.969956 |
| H | -6.498804 | 3.917329 | -2.420903 | H | -3.828129 | -5.404185 | -1.383464 |
| C | -4.400304 | 3.425767 | -2.563595 | C | -5.307546 | -6.436097 | -2.545237 |
| H | -4.586373 | 2.530041 | -3.150043 | H | -4.837152 | -7.405783 | -2.405062 |
| C | -1.209727 | 4.859140 | -4.285880 | C | -6.477951 | -6.327921 | -3.299582 |
| C | -0.557672 | 5.956922 | -3.700617 | H | -6.923902 | -7.211272 | -3.748496 |
| H | 0.121692  | 5.793075 | -2.869274 | C | -7.069966 | -5.076607 | -3.468804 |
| C | -0.752990 | 7.250342 | -4.179830 | H | -7.985516 | -4.978598 | -4.046310 |
| H | -0.239615 | 8.082676 | -3.705425 | C | -6.490759 | -3.943316 | -2.894208 |
| C | -1.598515 | 7.476766 | -5.268830 | H | -6.969001 | -2.976377 | -3.023879 |
| H | -1.750281 | 8.484535 | -5.645638 | C | -2.740274 | -2.860481 | -3.223712 |
| C | -2.237553 | 6.395034 | -5.872250 | C | -1.832627 | -3.909955 | -3.010284 |
| H | -2.888215 | 6.552987 | -6.728368 | H | -1.609771 | -4.230597 | -1.998262 |
| C | -2.042520 | 5.100003 | -5.385414 | C | -1.184311 | -4.536285 | -4.071495 |
| H | -2.538835 | 4.272548 | -5.882236 | H | -0.489748 | -5.348676 | -3.886307 |
| C | 0.526729  | 3.121987 | -3.775202 | C | -1.436906 | -4.105134 | -5.374808 |
| C | 1.090337  | 2.691590 | -4.985024 | C | -2.319123 | -3.057563 | -5.620172 |
| H | 0.445154  | 2.530095 | -5.844669 | H | -2.501572 | -2.717531 | -6.633459 |
| C | 2.464229  | 2.481161 | -5.101933 | C | -2.962436 | -2.444698 | -4.541053 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.641881 | -1.621971 | -4.742646 |
| C | -0.213786 | -1.571295 | 2.162737  |
| C | 0.293212  | -2.307012 | 3.393078  |
| C | 0.861005  | -3.762869 | 3.232241  |
| C | 1.784466  | -2.599053 | 3.409537  |
| H | 2.353828  | -2.254755 | 2.554035  |
| H | 2.297942  | -2.506109 | 4.360562  |
| C | -0.398691 | -1.915938 | 4.677442  |
| C | 0.298303  | -1.282005 | 5.712642  |
| H | 1.356497  | -1.066753 | 5.602045  |
| C | -0.335557 | -0.904179 | 6.899289  |
| H | 0.224266  | -0.416473 | 7.689815  |
| C | -1.694999 | -1.159685 | 7.049566  |
| C | -2.422748 | -1.776876 | 6.031370  |
| H | -3.484547 | -1.962192 | 6.151122  |
| C | -1.771722 | -2.147477 | 4.857271  |
| H | -2.349392 | -2.600490 | 4.059428  |
| C | 0.712572  | -4.720050 | 4.401765  |
| C | 1.840420  | -5.113238 | 5.134200  |
| H | 2.812409  | -4.696283 | 4.885451  |
| C | 1.737095  | -6.044307 | 6.169707  |
| H | 2.626764  | -6.334922 | 6.722295  |
| C | 0.498864  | -6.600079 | 6.491046  |
| H | 0.414554  | -7.321700 | 7.299082  |
| C | -0.632424 | -6.221957 | 5.764465  |
| H | -1.602921 | -6.647326 | 6.006073  |
| C | -0.523987 | -5.295144 | 4.728633  |
| H | -1.412317 | -5.011844 | 4.173185  |
| C | 0.818366  | -4.485083 | 1.902780  |
| C | 2.015093  | -4.850424 | 1.271894  |
| H | 2.967197  | -4.533611 | 1.687473  |
| C | 2.005815  | -5.633224 | 0.115000  |
| H | 2.951155  | -5.906903 | -0.345455 |
| C | 0.795703  | -6.070913 | -0.426808 |
| H | 0.785500  | -6.697084 | -1.315339 |
| C | -0.403579 | -5.708593 | 0.192469  |
| H | -1.351466 | -6.055010 | -0.212606 |
| C | -0.390864 | -4.919716 | 1.343460  |
| H | -1.329672 | -4.644377 | 1.815661  |
| O | -0.556569 | 1.092943  | -1.899004 |
| O | -2.031773 | 2.028391  | -0.461364 |
| O | -1.229892 | -1.605690 | -1.310594 |
| O | -3.002867 | -0.674771 | -0.255843 |
| O | 0.556379  | -1.520411 | 1.145414  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | -1.348226 | -1.011764 | 2.246704  |
| O  | 1.236478  | 1.203742  | 0.496056  |
| O  | -0.413322 | 1.622187  | 1.988412  |
| Rh | 0.078652  | -0.256608 | -0.447626 |
| Rh | -1.771318 | 0.508480  | 0.916641  |
| C  | 2.943580  | -1.419789 | -0.615618 |
| C  | 1.856034  | -1.011481 | -1.535380 |
| C  | 1.693759  | -1.049581 | -2.806366 |
| C  | 3.344404  | -2.387680 | -3.616648 |
| C  | 3.791392  | -3.022027 | -2.321213 |
| H  | 2.733819  | -3.004794 | -4.272425 |
| H  | 4.681611  | -3.629903 | -2.520086 |
| H  | 3.022368  | -3.710647 | -1.945757 |
| H  | 3.268331  | -0.550675 | -0.038515 |
| N  | 4.125467  | -1.999828 | -1.311372 |
| S  | 5.351964  | -2.486651 | -0.223310 |
| O  | 5.235021  | -3.922176 | 0.084295  |
| O  | 5.331682  | -1.503649 | 0.866631  |
| C  | 6.828247  | -2.255882 | -1.206572 |
| C  | 7.248952  | -0.956620 | -1.511744 |
| C  | 7.562146  | -3.367303 | -1.618165 |
| C  | 8.412072  | -0.782578 | -2.252668 |
| H  | 6.684144  | -0.098236 | -1.163255 |
| C  | 8.726726  | -3.170716 | -2.363302 |
| H  | 7.230868  | -4.363905 | -1.346531 |
| C  | 9.167212  | -1.883701 | -2.693612 |
| H  | 8.744704  | 0.225747  | -2.486013 |
| H  | 9.303182  | -4.033596 | -2.686465 |
| C  | 10.426261 | -1.671584 | -3.499652 |
| H  | 10.922557 | -2.619690 | -3.726828 |
| H  | 11.139818 | -1.037884 | -2.959447 |
| H  | 10.207498 | -1.170260 | -4.450633 |
| C  | 3.742896  | -1.167027 | -4.042770 |
| H  | 3.413459  | -0.786385 | -5.001754 |
| H  | 4.382476  | -0.542973 | -3.427839 |
| C  | 0.758334  | -0.905470 | -3.912226 |
| H  | -0.223662 | -0.563958 | -3.547026 |
| O  | 0.976373  | -1.136759 | -5.086889 |
| H  | 2.505542  | -2.132854 | 0.094926  |

**(S,S)-I-TS-II(a)\_conf1**

**1 imaginary frequency, value = -217.9986cm<sup>-1</sup>**

|    |           |          |           |
|----|-----------|----------|-----------|
| Br | -4.299964 | 5.672716 | -4.608353 |
| Br | 8.858371  | 3.098374 | -0.271133 |

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Br | -0.608784 | -7.028736 | -4.015367 | H | 1.547647  | 2.653434  | -3.541092 |
| Br | 1.603126  | -1.860583 | 8.693578  | H | 3.178694  | 3.410978  | -3.859375 |
| C  | 1.398784  | -2.088701 | 0.494923  | C | 4.611780  | 1.968527  | -2.013599 |
| C  | 1.722848  | -3.563226 | 0.616216  | C | 5.584106  | 0.984532  | -1.792784 |
| C  | 1.649837  | -4.085617 | 2.047728  | H | 5.363330  | -0.051096 | -2.031574 |
| H  | 1.146378  | -5.036369 | 2.188326  | C | 6.839778  | 1.307385  | -1.280749 |
| H  | 1.458013  | -3.347713 | 2.820260  | H | 7.588109  | 0.536654  | -1.130391 |
| C  | 2.997590  | -4.050783 | 1.392090  | C | 7.125532  | 2.638114  | -0.972929 |
| C  | 4.029735  | -3.077129 | 1.923609  | C | 6.176285  | 3.638115  | -1.170203 |
| C  | 4.394646  | -3.157349 | 3.273496  | H | 6.404960  | 4.669405  | -0.924316 |
| H  | 3.889210  | -3.869663 | 3.920690  | C | 4.927286  | 3.292483  | -1.690205 |
| C  | 5.393329  | -2.334951 | 3.796167  | H | 4.186009  | 4.073190  | -1.837593 |
| H  | 5.657163  | -2.410197 | 4.847833  | C | 4.401449  | 1.111136  | -4.866511 |
| C  | 6.047463  | -1.417756 | 2.971563  | C | 5.097065  | -0.104533 | -4.972590 |
| H  | 6.821830  | -0.771677 | 3.376303  | H | 4.714232  | -0.985004 | -4.464939 |
| C  | 5.694642  | -1.331424 | 1.623220  | C | 6.259850  | -0.205599 | -5.733108 |
| H  | 6.180792  | -0.606134 | 0.976956  | H | 6.780906  | -1.157485 | -5.794532 |
| C  | 4.697251  | -2.157927 | 1.105133  | C | 6.750622  | 0.908115  | -6.419207 |
| H  | 4.409221  | -2.057298 | 0.061977  | H | 7.656250  | 0.830850  | -7.014586 |
| C  | 3.629523  | -5.365136 | 0.953700  | C | 6.060842  | 2.116569  | -6.338954 |
| C  | 4.725345  | -5.356664 | 0.074110  | H | 6.422322  | 2.988796  | -6.877290 |
| H  | 5.113020  | -4.408897 | -0.286526 | C | 4.897206  | 2.214600  | -5.571861 |
| C  | 5.339800  | -6.540905 | -0.327337 | H | 4.369848  | 3.162641  | -5.539217 |
| H  | 6.183718  | -6.502577 | -1.011341 | C | 2.107510  | 0.156976  | -4.528237 |
| C  | 4.881486  | -7.769823 | 0.153258  | C | 1.329674  | 0.471987  | -5.651759 |
| H  | 5.361252  | -8.694531 | -0.155638 | H | 1.404809  | 1.463489  | -6.090414 |
| C  | 3.809145  | -7.794383 | 1.043008  | C | 0.473666  | -0.471663 | -6.220050 |
| H  | 3.448762  | -8.740434 | 1.438531  | H | -0.112050 | -0.206726 | -7.096492 |
| C  | 3.192859  | -6.604668 | 1.438931  | C | 0.381513  | -1.752082 | -5.668892 |
| H  | 2.370246  | -6.654841 | 2.144644  | H | -0.268756 | -2.498598 | -6.118780 |
| C  | 1.166937  | -4.419896 | -0.494015 | C | 1.139343  | -2.072292 | -4.540067 |
| C  | 1.899615  | -4.643016 | -1.666315 | H | 1.064358  | -3.058085 | -4.091404 |
| H  | 2.894786  | -4.222077 | -1.766263 | C | 1.997099  | -1.125287 | -3.977635 |
| C  | 1.386077  | -5.418844 | -2.706021 | H | 2.566547  | -1.383827 | -3.089522 |
| H  | 1.975477  | -5.602216 | -3.598079 | C | -0.125673 | 2.973960  | 0.348836  |
| C  | 0.106817  | -5.960494 | -2.580363 | C | -0.429654 | 4.448322  | 0.134757  |
| C  | -0.656891 | -5.743860 | -1.434449 | C | 0.745139  | 5.364519  | 0.431661  |
| H  | -1.661248 | -6.143099 | -1.356233 | H | 0.876326  | 6.234602  | -0.203392 |
| C  | -0.112729 | -4.981412 | -0.397873 | H | 1.662838  | 4.865665  | 0.720748  |
| H  | -0.707281 | -4.814448 | 0.496640  | C | -0.398253 | 5.397063  | 1.397964  |
| C  | 2.297135  | 1.087469  | -1.488089 | C | -0.236033 | 4.841006  | 2.799730  |
| C  | 3.247003  | 1.607180  | -2.548386 | C | -1.359225 | 4.443054  | 3.540053  |
| C  | 3.118404  | 1.179443  | -4.052337 | H | -2.344836 | 4.488630  | 3.087433  |
| C  | 2.622187  | 2.517592  | -3.596360 | C | -1.236444 | 4.019559  | 4.863711  |

|   |           |           |           |    |           |           |           |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -2.125384 | 3.734296  | 5.421226  | C  | -3.949504 | -0.777474 | 5.001757  |
| C | 0.018127  | 3.987075  | 5.477463  | C  | -4.682133 | -1.881464 | 5.455722  |
| H | 0.115619  | 3.668203  | 6.511842  | H  | -4.774801 | -2.761375 | 4.825544  |
| C | 1.142895  | 4.383852  | 4.753469  | C  | -5.309125 | -1.864489 | 6.703874  |
| H | 2.124659  | 4.370326  | 5.219266  | H  | -5.873228 | -2.733081 | 7.033615  |
| C | 1.013970  | 4.809999  | 3.430559  | C  | -5.214575 | -0.738407 | 7.520810  |
| H | 1.898587  | 5.124994  | 2.886616  | H  | -5.698482 | -0.724061 | 8.493649  |
| C | -1.255134 | 6.650668  | 1.374272  | C  | -4.494349 | 0.373083  | 7.076133  |
| C | -2.655104 | 6.616519  | 1.316575  | H  | -4.414970 | 1.257408  | 7.703042  |
| H | -3.166806 | 5.666503  | 1.207316  | C  | -3.874309 | 0.353687  | 5.828164  |
| C | -3.404109 | 7.792821  | 1.370811  | H  | -3.325131 | 1.227106  | 5.490151  |
| H | -4.488264 | 7.741791  | 1.314271  | C  | -4.050949 | 0.157422  | 2.675421  |
| C | -2.766566 | 9.028409  | 1.491298  | C  | -5.135870 | -0.333304 | 1.934667  |
| H | -3.350028 | 9.944196  | 1.532110  | H  | -5.363094 | -1.395274 | 1.959346  |
| C | -1.373174 | 9.077306  | 1.556956  | C  | -5.927152 | 0.528008  | 1.173177  |
| H | -0.863765 | 10.032445 | 1.654705  | H  | -6.778986 | 0.132190  | 0.625069  |
| C | -0.628239 | 7.899132  | 1.498347  | C  | -5.646768 | 1.895687  | 1.137714  |
| H | 0.456036  | 7.945379  | 1.559205  | H  | -6.272167 | 2.570147  | 0.558561  |
| C | -1.357945 | 4.749072  | -1.016078 | C  | -4.559486 | 2.389356  | 1.860982  |
| C | -2.660752 | 4.222465  | -1.042513 | H  | -4.336309 | 3.453243  | 1.846604  |
| H | -2.996094 | 3.579595  | -0.236499 | C  | -3.765237 | 1.527128  | 2.619214  |
| C | -3.530542 | 4.488295  | -2.097012 | H  | -2.916565 | 1.925052  | 3.168611  |
| H | -4.534023 | 4.076335  | -2.095636 | O  | 1.093511  | 0.834409  | -1.833369 |
| C | -3.097471 | 5.288417  | -3.155498 | O  | 2.761273  | 0.992543  | -0.311069 |
| C | -1.807936 | 5.810175  | -3.170034 | O  | -0.876763 | 2.130918  | -0.248415 |
| H | -1.470256 | 6.420973  | -4.000023 | O  | 0.878253  | 2.683511  | 1.066537  |
| C | -0.950216 | 5.532988  | -2.101728 | O  | -1.419220 | -0.480539 | 1.203501  |
| H | 0.056360  | 5.937905  | -2.131455 | O  | 0.047670  | 0.314924  | 2.727901  |
| C | -0.997814 | -0.323518 | 2.398653  | O  | 0.591155  | -1.753423 | -0.438748 |
| C | -1.774308 | -0.997649 | 3.516245  | O  | 1.891445  | -1.302030 | 1.357073  |
| C | -3.322805 | -0.774993 | 3.618743  | Rh | -0.236633 | 0.163042  | -0.388261 |
| C | -2.771256 | -2.063045 | 3.092594  | Rh | 1.448451  | 0.703794  | 1.267405  |
| H | -2.862410 | -2.262559 | 2.031249  | C  | -2.443594 | -1.752838 | -1.313555 |
| H | -2.846064 | -2.941560 | 3.724545  | C  | -1.836804 | -0.472619 | -1.752473 |
| C | -0.971601 | -1.206252 | 4.778785  | C  | -2.032353 | 0.303772  | -2.757347 |
| C | -0.612074 | -2.491717 | 5.199751  | C  | -3.224698 | -0.908627 | -4.260049 |
| H | -0.920256 | -3.357091 | 4.620616  | C  | -3.150542 | -2.279497 | -3.624127 |
| C | 0.147778  | -2.698355 | 6.354110  | H  | -2.582688 | -0.735613 | -5.120842 |
| H | 0.413956  | -3.702779 | 6.664771  | H  | -3.832577 | -2.954286 | -4.153965 |
| C | 0.559521  | -1.595687 | 7.096462  | H  | -2.142179 | -2.699284 | -3.739032 |
| C | 0.228911  | -0.300169 | 6.696788  | H  | -2.844606 | -1.619298 | -0.307969 |
| H | 0.563212  | 0.554103  | 7.275313  | N  | -3.533367 | -2.211747 | -2.204506 |
| C | -0.530665 | -0.115494 | 5.543975  | S  | -4.404563 | -3.544100 | -1.601237 |
| H | -0.762997 | 0.895261  | 5.226679  | O  | -3.884792 | -4.810097 | -2.139291 |

|   |            |           |           |
|---|------------|-----------|-----------|
| O | -4.480057  | -3.338303 | -0.149409 |
| C | -6.020613  | -3.276829 | -2.325322 |
| C | -6.786700  | -2.180704 | -1.913306 |
| C | -6.514278  | -4.190286 | -3.254722 |
| C | -8.052877  | -1.999177 | -2.457852 |
| H | -6.393696  | -1.488360 | -1.175466 |
| C | -7.788874  | -3.990745 | -3.790165 |
| H | -5.910566  | -5.044083 | -3.543386 |
| C | -8.574398  | -2.898357 | -3.405161 |
| H | -8.652634  | -1.148893 | -2.141815 |
| H | -8.177195  | -4.700054 | -4.516370 |
| C | -9.954148  | -2.685775 | -3.980483 |
| H | -10.720634 | -2.735306 | -3.197223 |
| H | -10.040015 | -1.699469 | -4.452223 |
| H | -10.195695 | -3.441599 | -4.733527 |
| C | -4.110769  | 0.044769  | -3.885085 |
| H | -4.151199  | 0.992345  | -4.408401 |
| H | -4.786788  | -0.124553 | -3.053781 |
| C | -1.554409  | 1.485654  | -3.460906 |
| H | -0.754382  | 1.980271  | -2.885526 |
| O | -1.941390  | 1.903737  | -4.536067 |
| H | -1.632948  | -2.493835 | -1.244989 |

**(S,S)-I-TS-II(a)\_conf2**

**1 imaginary frequency, value = -221.8064cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -4.263304 | 5.233484  | -5.139891 |
| Br | 8.720242  | 3.401929  | -0.262641 |
| Br | -0.390421 | -7.336986 | -3.459989 |
| Br | 1.359627  | -1.093220 | 8.896956  |
| C  | 1.414222  | -2.019816 | 0.690966  |
| C  | 1.769715  | -3.472632 | 0.932314  |
| C  | 1.679955  | -3.881904 | 2.399217  |
| H  | 1.194752  | -4.829939 | 2.606683  |
| H  | 1.456251  | -3.088847 | 3.105606  |
| C  | 3.039749  | -3.866481 | 1.768108  |
| C  | 4.037655  | -2.827687 | 2.237781  |
| C  | 4.381271  | -2.793187 | 3.595199  |
| H  | 3.882695  | -3.466443 | 4.287925  |
| C  | 5.349793  | -1.906469 | 4.067201  |
| H  | 5.597561  | -1.892742 | 5.125349  |
| C  | 5.994249  | -1.038978 | 3.183332  |
| H  | 6.744762  | -0.342761 | 3.547903  |
| C  | 5.662756  | -1.067277 | 1.827152  |
| H  | 6.141384  | -0.381470 | 1.133893  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.695859  | -1.957889 | 1.360025  |
| H | 4.424224  | -1.947429 | 0.307696  |
| C | 3.711553  | -5.195413 | 1.447407  |
| C | 4.836813  | -5.226503 | 0.606119  |
| H | 5.219516  | -4.298779 | 0.192184  |
| C | 5.486125  | -6.423193 | 0.310165  |
| H | 6.352232  | -6.415424 | -0.346593 |
| C | 5.033936  | -7.624520 | 0.860986  |
| H | 5.540679  | -8.558632 | 0.634445  |
| C | 3.932066  | -7.608381 | 1.714105  |
| H | 3.575196  | -8.531528 | 2.163280  |
| C | 3.281111  | -6.406814 | 2.004280  |
| H | 2.435799  | -6.425234 | 2.684024  |
| C | 1.256910  | -4.426647 | -0.117319 |
| C | 2.024507  | -4.734292 | -1.247358 |
| H | 3.016768  | -4.308440 | -1.354924 |
| C | 1.549771  | -5.600609 | -2.232613 |
| H | 2.165539  | -5.847348 | -3.090936 |
| C | 0.274392  | -6.148597 | -2.096491 |
| C | -0.522752 | -5.851513 | -0.992040 |
| H | -1.524101 | -6.256700 | -0.907652 |
| C | -0.016890 | -4.998819 | -0.007866 |
| H | -0.636413 | -4.769466 | 0.855395  |
| C | 2.289597  | 1.027897  | -1.504235 |
| C | 3.252661  | 1.493780  | -2.577879 |
| C | 3.190877  | 0.932083  | -4.041381 |
| C | 2.634011  | 2.285708  | -3.721007 |
| H | 1.554150  | 2.384691  | -3.714782 |
| H | 3.168436  | 3.173424  | -4.042721 |
| C | 4.584205  | 1.954021  | -2.035193 |
| C | 5.590142  | 1.034398  | -1.711823 |
| H | 5.421471  | -0.025045 | -1.876422 |
| C | 6.814010  | 1.451450  | -1.190971 |
| H | 7.589767  | 0.729047  | -0.960914 |
| C | 7.032381  | 2.813021  | -0.977610 |
| C | 6.048121  | 3.751560  | -1.278384 |
| H | 6.224609  | 4.807844  | -1.106485 |
| C | 4.832467  | 3.311662  | -1.806212 |
| H | 4.063479  | 4.044570  | -2.034999 |
| C | 4.502663  | 0.837051  | -4.805319 |
| C | 5.232449  | -0.363019 | -4.791442 |
| H | 4.853704  | -1.211361 | -4.228970 |
| C | 6.424007  | -0.490470 | -5.501884 |
| H | 6.970983  | -1.429162 | -5.470065 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 6.910181  | 0.579506  | -6.257343 | H | 0.258856  | 8.037042  | 1.003544  |
| H | 7.837962  | 0.481618  | -6.814333 | C | -1.425059 | 4.627663  | -1.399190 |
| C | 6.187238  | 1.770556  | -6.296131 | C | -2.716542 | 4.073823  | -1.429166 |
| H | 6.545298  | 2.607818  | -6.889471 | H | -3.067269 | 3.484346  | -0.589555 |
| C | 4.994924  | 1.895589  | -5.578662 | C | -3.555609 | 4.245437  | -2.527303 |
| H | 4.443243  | 2.828285  | -5.638228 | H | -4.550886 | 3.814070  | -2.527809 |
| C | 2.228389  | -0.161040 | -4.456975 | C | -3.102606 | 4.977246  | -3.626187 |
| C | 1.487158  | 0.027420  | -5.632566 | C | -1.822820 | 5.522730  | -3.637209 |
| H | 1.554245  | 0.976568  | -6.157591 | H | -1.469166 | 6.079897  | -4.497723 |
| C | 0.678363  | -0.988310 | -6.142368 | C | -0.995768 | 5.339790  | -2.525359 |
| H | 0.120786  | -0.821666 | -7.060355 | H | 0.003515  | 5.762495  | -2.552724 |
| C | 0.597629  | -2.215177 | -5.478914 | C | -1.060424 | -0.168789 | 2.409010  |
| H | -0.015162 | -3.018271 | -5.881435 | C | -1.855091 | -0.766104 | 3.556970  |
| C | 1.318515  | -2.408775 | -4.298285 | C | -3.410920 | -0.572264 | 3.592371  |
| H | 1.251176  | -3.351613 | -3.764526 | C | -2.815510 | -1.885928 | 3.192840  |
| C | 2.129589  | -1.390191 | -3.794588 | H | -2.866384 | -2.172943 | 2.149085  |
| H | 2.671639  | -1.550570 | -2.866985 | H | -2.894860 | -2.711494 | 3.892074  |
| C | -0.210217 | 2.983134  | 0.135246  | C | -1.090823 | -0.846491 | 4.857237  |
| C | -0.530970 | 4.431254  | -0.199954 | C | -0.732434 | -2.081562 | 5.409455  |
| C | 0.619570  | 5.387246  | 0.064424  | H | -1.012889 | -3.001991 | 4.906257  |
| H | 0.759701  | 6.210932  | -0.628076 | C | -0.009580 | -2.168111 | 6.602293  |
| H | 1.534298  | 4.926331  | 0.418157  | H | 0.255961  | -3.135106 | 7.015516  |
| C | -0.555150 | 5.471947  | 0.988869  | C | 0.366221  | -0.994970 | 7.249559  |
| C | -0.433206 | 5.024441  | 2.433015  | C | 0.035645  | 0.252549  | 6.718724  |
| C | -1.576991 | 4.669458  | 3.163645  | H | 0.341159  | 1.161964  | 7.224529  |
| H | -2.546776 | 4.668946  | 2.675939  | C | -0.686582 | 0.317279  | 5.529549  |
| C | -1.495345 | 4.349310  | 4.519048  | H | -0.918994 | 1.290175  | 5.110546  |
| H | -2.399935 | 4.096411  | 5.066911  | C | -4.083731 | -0.477378 | 4.950242  |
| C | -0.262204 | 4.380131  | 5.175058  | C | -4.821253 | -1.553615 | 5.459791  |
| H | -0.197243 | 4.143244  | 6.233758  | H | -4.883172 | -2.478577 | 4.893522  |
| C | 0.882812  | 4.734075  | 4.460606  | C | -5.491793 | -1.451920 | 6.680894  |
| H | 1.848201  | 4.768053  | 4.958462  | H | -6.058728 | -2.300516 | 7.054904  |
| C | 0.795109  | 5.056435  | 3.105266  | C | -5.436895 | -0.267287 | 7.414452  |
| H | 1.694990  | 5.339371  | 2.568748  | H | -5.954731 | -0.186894 | 8.366386  |
| C | -1.427682 | 6.706823  | 0.845683  | C | -4.712316 | 0.816868  | 6.913146  |
| C | -2.823957 | 6.647392  | 0.739203  | H | -4.663354 | 1.746050  | 7.474891  |
| H | -3.319442 | 5.684480  | 0.677365  | C | -4.048501 | 0.712753  | 5.692087  |
| C | -3.589330 | 7.813269  | 0.686030  | H | -3.495643 | 1.565527  | 5.310231  |
| H | -4.669902 | 7.742024  | 0.593875  | C | -4.126177 | 0.262163  | 2.552240  |
| C | -2.972524 | 9.063745  | 0.745140  | C | -5.160951 | -0.318238 | 1.804887  |
| H | -3.568729 | 9.971199  | 0.702427  | H | -5.357200 | -1.382448 | 1.898864  |
| C | -1.583232 | 9.138197  | 0.857727  | C | -5.941369 | 0.457069  | 0.945750  |
| H | -1.090010 | 10.105411 | 0.908500  | H | -6.754206 | -0.007160 | 0.392265  |
| C | -0.821732 | 7.970279  | 0.906657  | C | -5.700485 | 1.826710  | 0.818417  |

|    |            |           |           |
|----|------------|-----------|-----------|
| H  | -6.318188  | 2.435035  | 0.162782  |
| C  | -4.662305  | 2.408696  | 1.548352  |
| H  | -4.469393  | 3.475104  | 1.461576  |
| C  | -3.879019  | 1.632623  | 2.404461  |
| H  | -3.067662  | 2.097693  | 2.957268  |
| O  | 1.099466   | 0.725186  | -1.855853 |
| O  | 2.729409   | 1.023240  | -0.314018 |
| O  | -0.932744  | 2.083011  | -0.411686 |
| O  | 0.780018   | 2.767481  | 0.897135  |
| O  | -1.447988  | -0.429317 | 1.220514  |
| O  | -0.035415  | 0.514648  | 2.710924  |
| O  | 0.622108   | -1.773603 | -0.282897 |
| O  | 1.867896   | -1.159737 | 1.502863  |
| Rh | -0.249669  | 0.124877  | -0.392693 |
| Rh | 1.387279   | 0.822060  | 1.252838  |
| C  | -2.415806  | -1.887250 | -1.201242 |
| C  | -1.804152  | -0.648481 | -1.741089 |
| C  | -1.965882  | 0.016458  | -2.829586 |
| C  | -3.040985  | -1.362101 | -4.254647 |
| C  | -2.973617  | -2.660634 | -3.480822 |
| H  | -2.352161  | -1.256821 | -5.089885 |
| H  | -3.606986  | -3.403848 | -3.978269 |
| H  | -1.950904  | -3.060375 | -3.494073 |
| H  | -2.877757  | -1.655611 | -0.240321 |
| N  | -3.443237  | -2.462398 | -2.099887 |
| S  | -4.310288  | -3.758285 | -1.415312 |
| O  | -3.724098  | -5.052961 | -1.793462 |
| O  | -4.475822  | -3.412837 | 0.001987  |
| C  | -5.888434  | -3.620830 | -2.249966 |
| C  | -6.714787  | -2.523816 | -1.982366 |
| C  | -6.297171  | -4.635001 | -3.114279 |
| C  | -7.954628  | -2.444025 | -2.606597 |
| H  | -6.389609  | -1.753585 | -1.290151 |
| C  | -7.546041  | -4.536739 | -3.731607 |
| H  | -5.650012  | -5.488129 | -3.287435 |
| C  | -8.389311  | -3.445356 | -3.493006 |
| H  | -8.602440  | -1.595283 | -2.400915 |
| H  | -7.869303  | -5.325634 | -4.405728 |
| C  | -9.732827  | -3.333229 | -4.172905 |
| H  | -10.524775 | -3.096514 | -3.453123 |
| H  | -9.729023  | -2.531770 | -4.922802 |
| H  | -10.003917 | -4.262924 | -4.681844 |
| C  | -3.977311  | -0.407514 | -4.035737 |
| H  | -4.009484  | 0.481029  | -4.654377 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.700522 | -0.514888 | -3.234356 |
| C | -1.482902 | 1.141046  | -3.618636 |
| H | -0.716263 | 1.702554  | -3.060030 |
| O | -1.833692 | 1.452560  | -4.741378 |
| H | -1.599450 | -2.598997 | -1.007521 |

**(S,S)-I-TS-II(a)\_conf3**

**1 imaginary frequency, value = -222.3849cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | 4.332254  | -5.236119 | -5.083627 |
| Br | -8.708468 | -3.422000 | -0.337214 |
| Br | 0.387875  | 7.324605  | -3.483155 |
| Br | -1.459594 | 1.123240  | 8.873061  |
| C  | -1.427401 | 2.015812  | 0.673194  |
| C  | -1.791752 | 3.467761  | 0.906160  |
| C  | -1.715849 | 3.882843  | 2.372258  |
| H  | -1.237091 | 4.834103  | 2.580005  |
| H  | -1.493978 | 3.093617  | 3.083508  |
| C  | -3.070315 | 3.858550  | 1.730121  |
| C  | -4.067315 | 2.816740  | 2.195068  |
| C  | -4.421387 | 2.784497  | 3.549841  |
| H  | -3.931087 | 3.461711  | 4.244610  |
| C  | -5.389803 | 1.894949  | 4.016731  |
| H  | -5.645722 | 1.883022  | 5.072957  |
| C  | -6.023730 | 1.022410  | 3.130234  |
| H  | -6.774185 | 0.324059  | 3.490827  |
| C  | -5.681754 | 1.048382  | 1.776602  |
| H  | -6.152166 | 0.358744  | 1.081510  |
| C  | -4.714919 | 1.941718  | 1.314596  |
| H  | -4.434807 | 1.929377  | 0.264510  |
| C  | -3.745602 | 5.183271  | 1.399532  |
| C  | -4.862250 | 5.206781  | 0.546660  |
| H  | -5.235869 | 4.276190  | 0.130859  |
| C  | -5.514542 | 6.399489  | 0.241367  |
| H  | -6.373756 | 6.385908  | -0.424287 |
| C  | -5.074189 | 7.604272  | 0.794241  |
| H  | -5.583297 | 8.535302  | 0.560427  |
| C  | -3.981208 | 7.595589  | 1.658823  |
| H  | -3.633768 | 8.521506  | 2.109688  |
| C  | -3.327113 | 6.397990  | 1.958282  |
| H  | -2.488929 | 6.422018  | 2.646666  |
| C  | -1.274651 | 4.420074  | -0.142866 |
| C  | -2.033696 | 4.719132  | -1.280957 |
| H  | -3.022797 | 4.287818  | -1.395686 |
| C  | -1.554465 | 5.583530  | -2.265731 |

|   |           |           |           |   |           |            |           |
|---|-----------|-----------|-----------|---|-----------|------------|-----------|
| H | -2.163844 | 5.823584  | -3.130492 | C | 0.222312  | -2.981759  | 0.146269  |
| C | -0.283022 | 6.138362  | -2.120744 | C | 0.551662  | -4.429739  | -0.181319 |
| C | 0.505802  | 5.849798  | -1.008110 | C | -0.597589 | -5.389091  | 0.076412  |
| H | 1.504399  | 6.260194  | -0.916597 | H | -0.728456 | -6.215980  | -0.614096 |
| C | -0.004586 | 4.998810  | -0.024811 | H | -1.517278 | -4.930484  | 0.420194  |
| H | 0.608496  | 4.776049  | 0.844749  | C | 0.569284  | -5.466180  | 1.011493  |
| C | -2.269876 | -1.040219 | -1.522144 | C | 0.433725  | -5.013799  | 2.452902  |
| C | -3.220748 | -1.513110 | -2.603606 | C | 1.570870  | -4.656391  | 3.192686  |
| C | -3.144762 | -0.958638 | -4.069140 | H | 2.545086  | -4.658058  | 2.713910  |
| C | -2.587687 | -2.309110 | -3.736042 | C | 1.477017  | -4.331306  | 4.546120  |
| H | -1.507716 | -2.405330 | -3.717187 | H | 2.376682  | -4.076657  | 5.101228  |
| H | -3.116317 | -3.199777 | -4.059129 | C | 0.237944  | -4.359470  | 5.190973  |
| C | -4.556867 | -1.973873 | -2.072835 | H | 0.163380  | -4.118775  | 6.248181  |
| C | -5.567358 | -1.054671 | -1.762664 | C | -0.900573 | -4.715828  | 4.467401  |
| H | -5.398533 | 0.004492  | -1.929010 | H | -1.870459 | -4.747870  | 4.956571  |
| C | -6.795797 | -1.471785 | -1.252745 | C | -0.800645 | -5.043182  | 3.114108  |
| H | -7.574857 | -0.749758 | -1.032884 | H | -1.695674 | -5.328055  | 2.570603  |
| C | -7.014334 | -2.832977 | -1.037074 | C | 1.446978  | -6.698760  | 0.880286  |
| C | -6.025737 | -3.771037 | -1.324811 | C | 2.843762  | -6.635536  | 0.783197  |
| H | -6.202405 | -4.827007 | -1.151185 | H | 3.336763  | -5.671426  | 0.720330  |
| C | -4.805463 | -3.331102 | -1.841832 | C | 3.612998  | -7.799325  | 0.740586  |
| H | -4.033204 | -4.063674 | -2.060421 | H | 4.693958  | -7.725186  | 0.655534  |
| C | -4.448571 | -0.871522 | -4.847599 | C | 2.999608  | -9.051395  | 0.801165  |
| C | -5.183157 | 0.325708  | -4.846242 | H | 3.598847  | -9.957200  | 0.766667  |
| H | -4.814254 | 1.177489  | -4.282432 | C | 1.609802  | -9.129590  | 0.904566  |
| C | -6.366944 | 0.445974  | -5.570780 | H | 1.119174  | -10.098068 | 0.956368  |
| H | -6.917904 | 1.382612  | -5.548594 | C | 0.844467  | -7.963806  | 0.942895  |
| C | -6.840273 | -0.628553 | -6.327938 | H | -0.236565 | -8.033402  | 1.032594  |
| H | -7.761979 | -0.536214 | -6.895857 | C | 1.457090  | -4.626801  | -1.371833 |
| C | -6.112409 | -1.816940 | -6.354131 | C | 2.746477  | -4.067642  | -1.392248 |
| H | -6.460438 | -2.657698 | -6.948496 | H | 3.087002  | -3.473363  | -0.551825 |
| C | -4.927915 | -1.934739 | -5.622630 | C | 3.596253  | -4.240170  | -2.481966 |
| H | -4.371957 | -2.865462 | -5.672638 | H | 4.589691  | -3.804640  | -2.475173 |
| C | -2.181550 | 0.135681  | -4.479860 | C | 3.156372  | -4.978278  | -3.581953 |
| C | -1.426357 | -0.055990 | -5.645956 | C | 1.878965  | -5.529030  | -3.602547 |
| H | -1.483585 | -1.008219 | -6.166528 | H | 1.535504  | -6.091096  | -4.464010 |
| C | -0.616169 | 0.960461  | -6.152161 | C | 1.041018  | -5.345093  | -2.499033 |
| H | -0.047545 | 0.791234  | -7.062868 | H | 0.043770  | -5.772050  | -2.533779 |
| C | -0.548295 | 2.191329  | -5.494706 | C | 1.038597  | 0.179846   | 2.419002  |
| H | 0.065480  | 2.994888  | -5.894789 | C | 1.819010  | 0.784460   | 3.572877  |
| C | -1.283092 | 2.388181  | -4.323218 | C | 3.374962  | 0.596218   | 3.625491  |
| H | -1.225753 | 3.334190  | -3.793874 | C | 2.779237  | 1.906458   | 3.215190  |
| C | -2.095312 | 1.368794  | -3.823042 | H | 2.840315  | 2.190334   | 2.171127  |
| H | -2.648144 | 1.531629  | -2.902262 | H | 2.847940  | 2.734608   | 3.912506  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 1.040031  | 0.867491  | 4.864219  |
| C  | 0.667666  | 2.103631  | 5.404670  |
| H  | 0.948384  | 3.022683  | 4.899068  |
| C  | -0.069743 | 2.192895  | 6.588358  |
| H  | -0.346064 | 3.160686  | 6.992549  |
| C  | -0.446056 | 1.021331  | 7.238214  |
| C  | -0.101510 | -0.227277 | 6.718945  |
| H  | -0.407445 | -1.135489 | 7.226641  |
| C  | 0.635128  | -0.294692 | 5.538798  |
| H  | 0.878381  | -1.268596 | 5.128376  |
| C  | 4.033433  | 0.507757  | 4.990765  |
| C  | 4.759563  | 1.588809  | 5.506435  |
| H  | 4.823223  | 2.512932  | 4.938991  |
| C  | 5.416651  | 1.493019  | 6.735323  |
| H  | 5.974884  | 2.345299  | 7.114014  |
| C  | 5.359538  | 0.309596  | 7.470651  |
| H  | 5.866875  | 0.233811  | 8.428597  |
| C  | 4.646461  | -0.779363 | 6.963279  |
| H  | 4.596031  | -1.707716 | 7.526267  |
| C  | 3.996060  | -0.681111 | 5.734547  |
| H  | 3.452234  | -1.537579 | 5.348025  |
| C  | 4.103523  | -0.239066 | 2.595289  |
| C  | 5.144004  | 0.342353  | 1.856660  |
| H  | 5.336465  | 1.407322  | 1.949961  |
| C  | 5.934704  | -0.432824 | 1.006879  |
| H  | 6.751470  | 0.032341  | 0.459985  |
| C  | 5.698762  | -1.803419 | 0.880501  |
| H  | 6.324274  | -2.411558 | 0.232138  |
| C  | 4.655284  | -2.386532 | 1.601924  |
| H  | 4.466027  | -3.453639 | 1.515787  |
| C  | 3.861615  | -1.610568 | 2.448514  |
| H  | 3.046218  | -2.076682 | 2.994450  |
| O  | -1.077700 | -0.733716 | -1.863296 |
| O  | -2.720992 | -1.034232 | -0.336200 |
| O  | 0.946593  | -2.080270 | -0.396045 |
| O  | -0.776237 | -2.767927 | 0.897772  |
| O  | 1.436412  | 0.438698  | 1.233562  |
| O  | 0.014146  | -0.507761 | 2.713006  |
| O  | -0.625115 | 1.770105  | -0.292466 |
| O  | -1.884552 | 1.156349  | 1.483769  |
| Rh | 0.255220  | -0.124670 | -0.388880 |
| Rh | -1.394372 | -0.824364 | 1.243114  |
| C  | 2.420115  | 1.894825  | -1.181988 |
| C  | 1.819508  | 0.651544  | -1.723850 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.995828  | -0.016692 | -2.808094 |
| C | 3.081312  | 1.360502  | -4.226177 |
| C | 2.999640  | 2.661902  | -3.458434 |
| H | 2.402919  | 1.248986  | -5.069093 |
| H | 3.635460  | 3.405753  | -3.951823 |
| H | 1.975526  | 3.057371  | -3.484690 |
| H | 2.872771  | 1.668594  | -0.215362 |
| N | 3.454681  | 2.471037  | -2.071621 |
| S | 4.309195  | 3.772813  | -1.382539 |
| O | 3.720906  | 5.063697  | -1.770276 |
| O | 4.462543  | 3.432251  | 0.037311  |
| C | 5.895963  | 3.639925  | -2.201410 |
| C | 6.307884  | 4.652685  | -3.065886 |
| C | 6.725074  | 2.548065  | -1.921601 |
| C | 7.562868  | 4.558017  | -3.671216 |
| H | 5.658293  | 5.502026  | -3.248312 |
| C | 7.971016  | 2.471782  | -2.534034 |
| H | 6.397283  | 1.779192  | -1.229092 |
| C | 8.409051  | 3.471596  | -3.420488 |
| H | 7.888650  | 5.345824  | -4.345393 |
| H | 8.621003  | 1.627063  | -2.318884 |
| C | 9.759133  | 3.363085  | -4.087855 |
| H | 9.764628  | 2.561021  | -4.837109 |
| H | 10.031988 | 4.293173  | -4.595141 |
| H | 10.545173 | 3.129387  | -3.360673 |
| C | 4.018998  | 0.410841  | -3.992066 |
| H | 4.062447  | -0.480108 | -4.606537 |
| H | 4.731901  | 0.524923  | -3.182463 |
| C | 1.526681  | -1.146564 | -3.597940 |
| H | 0.754983  | -1.708167 | -3.046465 |
| O | 1.892885  | -1.462071 | -4.714633 |
| H | 1.598802  | 2.603812  | -0.999471 |

**(S,S)-I-TS-II(a)\_conf4**

**1 imaginary frequency, value = -206.4570cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -5.216801 | 5.547907  | -3.673911 |
| Br | 7.129551  | 4.727401  | 3.558697  |
| Br | 2.462133  | -4.892217 | -6.160970 |
| Br | 0.763722  | -5.522256 | 6.775023  |
| C  | 1.741606  | -1.820017 | 0.079863  |
| C  | 2.480043  | -3.115791 | -0.182966 |
| C  | 2.258642  | -4.170058 | 0.897759  |
| H  | 2.060321  | -5.179529 | 0.552960  |
| H  | 1.676025  | -3.861055 | 1.759345  |

|   |          |           |           |   |           |           |           |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.636540 | -3.594965 | 0.768215  | C | 5.867364  | 4.216464  | 2.197594  |
| C | 4.152092 | -2.719486 | 1.892540  | C | 4.713789  | 4.974195  | 2.010643  |
| C | 4.199474 | -3.249555 | 3.188062  | H | 4.519842  | 5.842287  | 2.631106  |
| H | 3.810082 | -4.247998 | 3.370375  | C | 3.812402  | 4.599391  | 1.012217  |
| C | 4.734880 | -2.512326 | 4.245086  | H | 2.910338  | 5.188669  | 0.871508  |
| H | 4.757547 | -2.941729 | 5.243283  | C | 4.807661  | 3.809150  | -2.667213 |
| C | 5.235165 | -1.228460 | 4.020273  | C | 5.870791  | 2.921757  | -2.902303 |
| H | 5.647787 | -0.648895 | 4.841732  | H | 5.693257  | 1.851263  | -2.856309 |
| C | 5.195422 | -0.690572 | 2.732115  | C | 7.145620  | 3.390273  | -3.212378 |
| H | 5.560454 | 0.316058  | 2.549012  | H | 7.951405  | 2.681589  | -3.384957 |
| C | 4.661930 | -1.433075 | 1.678392  | C | 7.386314  | 4.763122  | -3.308604 |
| H | 4.607244 | -0.989946 | 0.687467  | H | 8.379244  | 5.130557  | -3.552862 |
| C | 4.737606 | -4.456386 | 0.163212  | C | 6.336859  | 5.655571  | -3.097087 |
| C | 5.962966 | -3.872460 | -0.201186 | H | 6.504665  | 6.726107  | -3.180996 |
| H | 6.115523 | -2.809541 | -0.043210 | C | 5.060890  | 5.181594  | -2.781748 |
| C | 6.996420 | -4.635447 | -0.740889 | H | 4.257698  | 5.897115  | -2.637743 |
| H | 7.931493 | -4.153924 | -1.015379 | C | 2.947567  | 2.320305  | -3.446960 |
| C | 6.837415 | -6.011661 | -0.918535 | C | 2.407785  | 2.877159  | -4.615566 |
| H | 7.643211 | -6.609336 | -1.335827 | H | 2.254514  | 3.951590  | -4.671382 |
| C | 5.636054 | -6.610061 | -0.543035 | C | 2.084554  | 2.074920  | -5.709875 |
| H | 5.498989 | -7.681804 | -0.660740 | H | 1.681848  | 2.531017  | -6.610711 |
| C | 4.600930 | -5.840382 | -0.006807 | C | 2.293869  | 0.694670  | -5.649985 |
| H | 3.684316 | -6.339159 | 0.289142  | H | 2.063253  | 0.066094  | -6.506644 |
| C | 2.487307 | -3.556085 | -1.625623 | C | 2.811345  | 0.126653  | -4.483596 |
| C | 3.520644 | -3.179264 | -2.492973 | H | 2.961618  | -0.946428 | -4.417959 |
| H | 4.346873 | -2.583638 | -2.118753 | C | 3.137349  | 0.934693  | -3.392608 |
| C | 3.526086 | -3.577951 | -3.830139 | H | 3.527816  | 0.476873  | -2.488052 |
| H | 4.346293 | -3.300082 | -4.483611 | C | -1.085301 | 2.534428  | 1.068058  |
| C | 2.466443 | -4.345842 | -4.313792 | C | -1.738560 | 3.892061  | 1.231601  |
| C | 1.412006 | -4.719784 | -3.482548 | C | -0.879942 | 4.922588  | 1.952257  |
| H | 0.575179 | -5.290916 | -3.866409 | H | -0.903356 | 5.937026  | 1.567387  |
| C | 1.438266 | -4.326050 | -2.142881 | H | 0.091145  | 4.576692  | 2.289890  |
| H | 0.613589 | -4.616435 | -1.497753 | C | -2.085767 | 4.405279  | 2.672761  |
| C | 2.095592 | 1.981438  | -0.396261 | C | -1.889720 | 3.528823  | 3.892103  |
| C | 3.041945 | 3.073930  | -0.852120 | C | -2.543993 | 2.300724  | 4.042499  |
| C | 3.420809 | 3.264178  | -2.361929 | H | -3.140601 | 1.903211  | 3.226651  |
| C | 2.416660 | 4.165059  | -1.710402 | C | -2.414354 | 1.565884  | 5.221518  |
| H | 1.378021 | 4.025656  | -1.989229 | H | -2.928248 | 0.612615  | 5.320400  |
| H | 2.691000 | 5.187817  | -1.474154 | C | -1.627666 | 2.045895  | 6.270159  |
| C | 4.042998 | 3.482738  | 0.201794  | H | -1.526900 | 1.472590  | 7.187816  |
| C | 5.206461 | 2.734657  | 0.422705  | C | -0.969351 | 3.269086  | 6.128805  |
| H | 5.406100 | 1.860729  | -0.189159 | H | -0.351997 | 3.653531  | 6.936442  |
| C | 6.123660 | 3.094166  | 1.408908  | C | -1.103721 | 4.003307  | 4.950221  |
| H | 7.028204 | 2.514325  | 1.557276  | H | -0.593211 | 4.957577  | 4.848475  |

|   |           |           |           |    |           |           |           |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -3.279469 | 5.331563  | 2.820038  | C  | -5.350104 | -3.662939 | 5.410553  |
| C | -4.583720 | 4.816168  | 2.865552  | H  | -5.319827 | -3.370964 | 6.456885  |
| H | -4.739131 | 3.747522  | 2.755721  | C  | -4.565201 | -2.978884 | 4.481521  |
| C | -5.680792 | 5.654487  | 3.053662  | H  | -3.928016 | -2.169269 | 4.820486  |
| H | -6.682597 | 5.233434  | 3.078090  | C  | -4.546258 | -1.357399 | 1.574877  |
| C | -5.495919 | 7.030250  | 3.212064  | C  | -5.029605 | -1.288224 | 0.262004  |
| H | -6.350766 | 7.684600  | 3.359679  | H  | -4.799300 | -2.082665 | -0.439878 |
| C | -4.204359 | 7.554618  | 3.184018  | C  | -5.829606 | -0.222995 | -0.157800 |
| H | -4.044788 | 8.621610  | 3.315902  | H  | -6.197715 | -0.202273 | -1.180235 |
| C | -3.107834 | 6.711002  | 2.990264  | C  | -6.168580 | 0.794920  | 0.733779  |
| H | -2.107223 | 7.133453  | 2.984622  | H  | -6.807431 | 1.614971  | 0.416439  |
| C | -2.588834 | 4.322165  | 0.062753  | C  | -5.689378 | 0.741909  | 2.045757  |
| C | -3.792821 | 3.660764  | -0.221878 | H  | -5.957189 | 1.518492  | 2.757640  |
| H | -4.119757 | 2.840287  | 0.408010  | C  | -4.886024 | -0.321006 | 2.458299  |
| C | -4.573268 | 4.018200  | -1.318510 | H  | -4.544552 | -0.358276 | 3.487797  |
| H | -5.502653 | 3.497400  | -1.522249 | O  | 1.128131  | 1.663069  | -1.166838 |
| C | -4.143247 | 5.050094  | -2.154175 | O  | 2.305222  | 1.499070  | 0.759454  |
| C | -2.947760 | 5.718210  | -1.907084 | O  | -1.431520 | 1.850755  | 0.043514  |
| H | -2.611235 | 6.508282  | -2.568832 | O  | -0.211931 | 2.192716  | 1.920299  |
| C | -2.181552 | 5.347095  | -0.798530 | O  | -1.526173 | -1.169502 | 0.334340  |
| H | -1.244088 | 5.865341  | -0.618628 | O  | -0.750813 | -0.740770 | 2.412864  |
| C | -1.454016 | -1.397692 | 1.588093  | O  | 1.102311  | -1.308218 | -0.903240 |
| C | -2.223088 | -2.597421 | 2.134602  | O  | 1.752346  | -1.365110 | 1.263190  |
| C | -3.794577 | -2.577365 | 2.069551  | Rh | -0.243700 | 0.245973  | -0.511355 |
| C | -2.989448 | -3.402771 | 1.109716  | Rh | 0.800720  | 0.408141  | 1.666766  |
| H | -2.893135 | -3.072720 | 0.082703  | C  | -1.419323 | -1.513192 | -2.786129 |
| H | -3.023987 | -4.479618 | 1.237552  | C  | -1.204566 | -0.075077 | -2.474843 |
| C | -1.515839 | -3.305778 | 3.267584  | C  | -1.388230 | 1.014824  | -3.125814 |
| C | -1.082788 | -4.630139 | 3.127256  | C  | -1.597786 | 0.396806  | -5.326640 |
| H | -1.258916 | -5.163503 | 2.198539  | C  | -1.176062 | -1.048545 | -5.211364 |
| C | -0.410221 | -5.295274 | 4.155876  | H  | -0.865649 | 1.081149  | -5.749760 |
| H | -0.086044 | -6.321987 | 4.025245  | H  | -1.354535 | -1.564558 | -6.159687 |
| C | -0.159550 | -4.620395 | 5.346789  | H  | -0.097750 | -1.105010 | -5.010176 |
| C | -0.565877 | -3.296104 | 5.515485  | H  | -2.130970 | -1.912984 | -2.057483 |
| H | -0.358906 | -2.772932 | 6.442725  | N  | -1.933526 | -1.732918 | -4.153849 |
| C | -1.235503 | -2.650392 | 4.478605  | S  | -2.535790 | -3.287205 | -4.476920 |
| H | -1.522568 | -1.613185 | 4.605898  | O  | -2.472826 | -3.460161 | -5.931766 |
| C | -4.572229 | -3.340775 | 3.127172  | O  | -1.910531 | -4.258088 | -3.567631 |
| C | -5.396758 | -4.403508 | 2.730922  | C  | -4.261740 | -3.167366 | -4.005053 |
| H | -5.424336 | -4.692990 | 1.683466  | C  | -4.720413 | -3.857899 | -2.882662 |
| C | -6.185906 | -5.088279 | 3.655753  | C  | -5.140154 | -2.422854 | -4.796419 |
| H | -6.816198 | -5.909213 | 3.323734  | C  | -6.071345 | -3.780690 | -2.542464 |
| C | -6.164297 | -4.720375 | 5.001774  | H  | -4.027632 | -4.454824 | -2.299466 |
| H | -6.773435 | -5.254291 | 5.726015  | C  | -6.484620 | -2.353814 | -4.439349 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.779447 | -1.917500 | -5.686539 |
| C | -6.972648 | -3.028405 | -3.309293 |
| H | -6.431731 | -4.317738 | -1.668459 |
| H | -7.169430 | -1.774012 | -5.052906 |
| C | -8.436583 | -2.973950 | -2.942408 |
| H | -8.952508 | -3.892311 | -3.251587 |
| H | -8.573272 | -2.873959 | -1.860221 |
| H | -8.941585 | -2.133849 | -3.428909 |
| C | -2.833064 | 0.854856  | -5.014611 |
| H | -3.084573 | 1.899152  | -5.155172 |
| H | -3.591695 | 0.186450  | -4.620011 |
| C | -1.189408 | 2.458582  | -3.131364 |
| H | -0.870152 | 2.810465  | -2.137412 |
| O | -1.341661 | 3.212635  | -4.074040 |
| H | -0.471851 | -2.043626 | -2.621744 |

**(R,R)-I-TS-II(b)\_conf1**

**1 imaginary frequency, value = -217.3663cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -0.729254 | -5.786438 | -6.199885 |
| Br | -6.839492 | 6.148502  | -1.844851 |
| Br | 7.444678  | 3.098116  | -0.462745 |
| Br | -2.859007 | 0.503204  | 8.652508  |
| C  | 0.750891  | 1.998130  | 1.284142  |
| C  | 1.722581  | 2.903016  | 2.014352  |
| C  | 1.592964  | 2.826589  | 3.532879  |
| H  | 2.519020  | 2.758306  | 4.094152  |
| H  | 0.781053  | 2.216002  | 3.914827  |
| C  | 1.215848  | 4.118087  | 2.871194  |
| C  | -0.242662 | 4.528453  | 2.886571  |
| C  | -0.885093 | 4.670175  | 4.123142  |
| H  | -0.345108 | 4.426490  | 5.034614  |
| C  | -2.205196 | 5.115715  | 4.198397  |
| H  | -2.686376 | 5.213555  | 5.167992  |
| C  | -2.904726 | 5.430328  | 3.031878  |
| H  | -3.935098 | 5.771369  | 3.085466  |
| C  | -2.273066 | 5.296682  | 1.793775  |
| H  | -2.815493 | 5.516130  | 0.878628  |
| C  | -0.952037 | 4.853634  | 1.724173  |
| H  | -0.482117 | 4.722999  | 0.752875  |
| C  | 2.145738  | 5.315734  | 3.017690  |
| C  | 1.960649  | 6.448206  | 2.206141  |
| H  | 1.151979  | 6.459593  | 1.482090  |
| C  | 2.781564  | 7.567514  | 2.327383  |
| H  | 2.614810  | 8.427195  | 1.683419  |

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 3.805716  | 7.590252 | 3.276856  |
| H | 4.444737  | 8.463475 | 3.375966  |
| C | 3.990095  | 6.483271 | 4.103286  |
| H | 4.772879  | 6.488507 | 4.857299  |
| C | 3.167549  | 5.361383 | 3.975211  |
| H | 3.327452  | 4.522221 | 4.643745  |
| C | 3.106644  | 2.956353 | 1.416716  |
| C | 3.446439  | 3.921982 | 0.460568  |
| H | 2.711800  | 4.660518 | 0.157008  |
| C | 4.724980  | 3.973774 | -0.095789 |
| H | 4.980212  | 4.741315 | -0.818442 |
| C | 5.671630  | 3.028926 | 0.298590  |
| C | 5.361396  | 2.041878 | 1.231621  |
| H | 6.090416  | 1.294110 | 1.520310  |
| C | 4.079382  | 2.019487 | 1.785045  |
| H | 3.838480  | 1.245593 | 2.508274  |
| C | -1.467012 | 1.713426 | -1.867447 |
| C | -1.935766 | 2.496778 | -3.077544 |
| C | -0.952125 | 2.896995 | -4.233446 |
| C | -1.905187 | 1.753498 | -4.404850 |
| H | -1.480709 | 0.755747 | -4.394568 |
| H | -2.771485 | 1.870478 | -5.047422 |
| C | -3.118919 | 3.391152 | -2.794464 |
| C | -2.949671 | 4.649802 | -2.203365 |
| H | -1.950386 | 5.000769 | -1.966293 |
| C | -4.039965 | 5.471073 | -1.921198 |
| H | -3.892083 | 6.450213 | -1.478567 |
| C | -5.325486 | 5.021032 | -2.224372 |
| C | -5.528004 | 3.769719 | -2.801536 |
| H | -6.530693 | 3.425521 | -3.030481 |
| C | -4.420509 | 2.966876 | -3.082402 |
| H | -4.580723 | 1.989024 | -3.528527 |
| C | -1.227934 | 4.203928 | -4.960068 |
| C | -0.585232 | 5.381584 | -4.543776 |
| H | 0.100792  | 5.346176 | -3.702569 |
| C | -0.797637 | 6.590474 | -5.202739 |
| H | -0.290822 | 7.487560 | -4.856648 |
| C | -1.651369 | 6.649070 | -6.307119 |
| H | -1.816544 | 7.590383 | -6.824108 |
| C | -2.281385 | 5.485030 | -6.743886 |
| H | -2.938397 | 5.511169 | -7.609290 |
| C | -2.069335 | 4.275617 | -6.077180 |
| H | -2.560263 | 3.381126 | -6.446949 |
| C | 0.529336  | 2.588697 | -4.180772 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.119477  | 2.001253  | -5.309136 | C | -2.519052 | -3.791175 | -5.143295 |
| H | 0.491971  | 1.712185  | -6.148096 | H | -2.789136 | -3.619561 | -6.179379 |
| C | 2.496784  | 1.791043  | -5.370881 | C | -3.124454 | -3.052058 | -4.122791 |
| H | 2.932300  | 1.337796  | -6.257598 | H | -3.862853 | -2.304421 | -4.395302 |
| C | 3.308748  | 2.165549  | -4.298049 | C | -0.260579 | -1.191951 | 2.387482  |
| H | 4.383692  | 2.009747  | -4.342908 | C | 0.224192  | -1.749224 | 3.714937  |
| C | 2.731220  | 2.742235  | -3.165406 | C | 0.824943  | -3.197619 | 3.767491  |
| H | 3.349306  | 3.018531  | -2.317037 | C | 1.720865  | -1.999928 | 3.811199  |
| C | 1.352768  | 2.955603  | -3.110308 | H | 2.309347  | -1.765041 | 2.931655  |
| H | 0.915983  | 3.387909  | -2.214379 | H | 2.202054  | -1.762289 | 4.753840  |
| C | -2.499769 | -1.567862 | -0.879403 | C | -0.514500 | -1.211893 | 4.917489  |
| C | -3.443812 | -2.453467 | -1.674911 | C | 0.129575  | -0.414013 | 5.869787  |
| C | -4.824457 | -1.848964 | -1.876732 | H | 1.182107  | -0.173999 | 5.754399  |
| H | -5.308754 | -2.015893 | -2.833415 | C | -0.551522 | 0.097937  | 6.977488  |
| H | -4.966636 | -0.860849 | -1.454090 | H | -0.033069 | 0.712175  | 7.705610  |
| C | -4.721915 | -3.018271 | -0.947900 | C | -1.904460 | -0.189329 | 7.129684  |
| C | -4.927636 | -2.828949 | 0.541737  | C | -2.579676 | -0.970200 | 6.190643  |
| C | -4.274255 | -3.655069 | 1.466927  | H | -3.637020 | -1.179857 | 6.310070  |
| H | -3.558500 | -4.392897 | 1.116807  | C | -1.882180 | -1.472840 | 5.095134  |
| C | -4.543802 | -3.557413 | 2.832155  | H | -2.419776 | -2.056448 | 4.355859  |
| H | -4.038593 | -4.221449 | 3.529636  | C | 0.647284  | -3.992866 | 5.048921  |
| C | -5.473280 | -2.625416 | 3.300202  | C | 1.732092  | -4.207366 | 5.908738  |
| H | -5.690514 | -2.552613 | 4.362516  | H | 2.697797  | -3.768513 | 5.674146  |
| C | -6.129109 | -1.796497 | 2.389205  | C | 1.595731  | -4.989943 | 7.057497  |
| H | -6.857170 | -1.069430 | 2.738908  | H | 2.452637  | -5.143123 | 7.708308  |
| C | -5.860907 | -1.902961 | 1.023540  | C | 0.367560  | -5.574175 | 7.365651  |
| H | -6.386156 | -1.258926 | 0.324519  | H | 0.257542  | -6.180504 | 8.260645  |
| C | -5.311130 | -4.327596 | -1.444182 | C | -0.720234 | -5.375304 | 6.512105  |
| C | -4.648770 | -5.555091 | -1.302907 | H | -1.682251 | -5.826199 | 6.741154  |
| H | -3.645919 | -5.582110 | -0.890453 | C | -0.578564 | -4.597186 | 5.364416  |
| C | -5.253113 | -6.746834 | -1.703618 | H | -1.431010 | -4.456113 | 4.707222  |
| H | -4.715825 | -7.685057 | -1.592998 | C | 0.841147  | -4.094667 | 2.549030  |
| C | -6.538617 | -6.736056 | -2.247862 | C | 2.065128  | -4.586666 | 2.075494  |
| H | -7.008710 | -7.664419 | -2.560715 | H | 2.994967  | -4.242894 | 2.519310  |
| C | -7.213536 | -5.522787 | -2.387036 | C | 2.108914  | -5.524990 | 1.041944  |
| H | -8.216793 | -5.500017 | -2.804506 | H | 3.072899  | -5.891049 | 0.699620  |
| C | -6.603254 | -4.332629 | -1.988553 | C | 0.924139  | -5.993010 | 0.469616  |
| H | -7.141212 | -3.393933 | -2.091530 | H | 0.952611  | -6.739112 | -0.320519 |
| C | -2.794041 | -3.250885 | -2.777622 | C | -0.300524 | -5.501487 | 0.929249  |
| C | -1.810632 | -4.208283 | -2.479059 | H | -1.228967 | -5.866527 | 0.496519  |
| H | -1.504003 | -4.358875 | -1.449743 | C | -0.341006 | -4.556091 | 1.955062  |
| C | -1.199824 | -4.958940 | -3.480214 | H | -1.299110 | -4.171651 | 2.293889  |
| H | -0.452736 | -5.704027 | -3.227736 | O | -0.556050 | 0.833886  | -2.032560 |
| C | -1.563320 | -4.746059 | -4.811231 | O | -2.060947 | 1.960330  | -0.773329 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | -1.247592 | -1.746672 | -1.059670 |
| O  | -3.016686 | -0.683092 | -0.133269 |
| O  | 0.511185  | -1.308129 | 1.376971  |
| O  | -1.382567 | -0.601173 | 2.385312  |
| O  | 1.227196  | 1.285077  | 0.336005  |
| O  | -0.443582 | 1.959168  | 1.706796  |
| Rh | 0.062854  | -0.289515 | -0.391147 |
| Rh | -1.792672 | 0.682537  | 0.828954  |
| C  | 2.895826  | -1.532667 | -0.323079 |
| C  | 1.857787  | -1.219297 | -1.333532 |
| C  | 1.736572  | -1.371276 | -2.598683 |
| C  | 3.500946  | -2.982187 | -3.156904 |
| C  | 3.871321  | -3.342623 | -1.732446 |
| H  | 4.776036  | -3.961683 | -1.761966 |
| H  | 3.088256  | -3.977010 | -1.291221 |
| H  | 3.184548  | -0.610985 | 0.187219  |
| N  | 4.120482  | -2.162329 | -0.887728 |
| S  | 5.338072  | -2.409407 | 0.289075  |
| O  | 5.296635  | -3.789675 | 0.800994  |
| O  | 5.227605  | -1.282690 | 1.223849  |
| C  | 6.830515  | -2.235441 | -0.682190 |
| C  | 7.177539  | -0.977003 | -1.185792 |
| C  | 7.651608  | -3.343878 | -0.883058 |
| C  | 8.356181  | -0.843362 | -1.910350 |
| H  | 6.543700  | -0.115777 | -1.002462 |
| C  | 8.829889  | -3.189203 | -1.616451 |
| H  | 7.375131  | -4.303747 | -0.460218 |
| C  | 9.198696  | -1.945022 | -2.141329 |
| H  | 8.631140  | 0.135165  | -2.295658 |
| H  | 9.474024  | -4.050083 | -1.775800 |
| C  | 10.472367 | -1.778005 | -2.934978 |
| H  | 11.041262 | -2.711244 | -2.983020 |
| H  | 11.118093 | -1.011214 | -2.490472 |
| H  | 10.258874 | -1.461157 | -3.963400 |
| C  | 3.741069  | -1.746222 | -3.661988 |
| H  | 3.483492  | -1.508395 | -4.686974 |
| H  | 4.265402  | -0.999947 | -3.077326 |
| C  | 0.815106  | -1.354211 | -3.725969 |
| H  | -0.184725 | -1.026557 | -3.398633 |
| O  | 1.054130  | -1.659174 | -4.879755 |
| H  | 2.424224  | -2.180525 | 0.427495  |
| C  | 2.912766  | -4.102277 | -3.968885 |
| H  | 2.026344  | -4.522386 | -3.478483 |
| H  | 2.625197  | -3.768820 | -4.966651 |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 3.642004 | -4.919771 | -4.061036 |
|---|----------|-----------|-----------|

**(S,S)-I-TS-II(b)\_conf1**

**1 imaginary frequency, value = -227.4637cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -4.331006 | 6.519965  | -2.983889 |
| Br | 8.933022  | 2.808300  | -0.188800 |
| Br | -2.075118 | -6.307969 | -4.687850 |
| Br | 2.043470  | -4.054518 | 7.718067  |
| C  | 1.145112  | -2.313172 | 0.049400  |
| C  | 1.253222  | -3.822818 | -0.034991 |
| C  | 1.242733  | -4.506836 | 1.328930  |
| H  | 0.615610  | -5.387344 | 1.421681  |
| H  | 1.240338  | -3.852905 | 2.194728  |
| C  | 2.510193  | -4.576459 | 0.531458  |
| C  | 3.717822  | -3.819392 | 1.045315  |
| C  | 4.198218  | -4.112295 | 2.327945  |
| H  | 3.662972  | -4.828042 | 2.946634  |
| C  | 5.348578  | -3.495045 | 2.820538  |
| H  | 5.700963  | -3.732863 | 3.820764  |
| C  | 6.040548  | -2.573512 | 2.032347  |
| H  | 6.933146  | -2.085820 | 2.414811  |
| C  | 5.573051  | -2.277140 | 0.750448  |
| H  | 6.091333  | -1.545145 | 0.137465  |
| C  | 4.423727  | -2.898601 | 0.261586  |
| H  | 4.052393  | -2.636929 | -0.725942 |
| C  | 2.897655  | -5.898578 | -0.118852 |
| C  | 3.942738  | -5.936937 | -1.058063 |
| H  | 4.469028  | -5.021423 | -1.308949 |
| C  | 4.332537  | -7.132044 | -1.659269 |
| H  | 5.142736  | -7.128266 | -2.383928 |
| C  | 3.694633  | -8.329016 | -1.326170 |
| H  | 3.999423  | -9.262847 | -1.790660 |
| C  | 2.669729  | -8.311803 | -0.381863 |
| H  | 2.170907  | -9.235327 | -0.099782 |
| C  | 2.278997  | -7.110741 | 0.214906  |
| H  | 1.487856  | -7.134556 | 0.956477  |
| C  | 0.461034  | -4.448126 | -1.156253 |
| C  | 1.041426  | -4.700764 | -2.405152 |
| H  | 2.090874  | -4.477410 | -2.565978 |
| C  | 0.302187  | -5.260302 | -3.448410 |
| H  | 0.771699  | -5.471066 | -4.403370 |
| C  | -1.046876 | -5.548196 | -3.245551 |
| C  | -1.660604 | -5.297078 | -2.019018 |
| H  | -2.716156 | -5.497271 | -1.877140 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.894653 | -4.756853 | -0.983294 | H | 2.394185  | 4.502432  | 0.952503  |
| H | -1.370563 | -4.562051 | -0.025603 | C | 0.578569  | 5.165954  | 2.039797  |
| C | 2.337030  | 1.041978  | -1.533293 | C | 0.967579  | 4.449376  | 3.315341  |
| C | 3.276456  | 1.659487  | -2.551504 | C | 0.095672  | 3.574334  | 3.973654  |
| C | 3.128476  | 1.382363  | -4.088284 | H | -0.852556 | 3.309855  | 3.514333  |
| C | 2.667347  | 2.681010  | -3.498172 | C | 0.444128  | 3.015815  | 5.203954  |
| H | 1.595852  | 2.831019  | -3.425889 | H | -0.246854 | 2.341149  | 5.703831  |
| H | 3.241690  | 3.583897  | -3.677068 | C | 1.672435  | 3.318299  | 5.794536  |
| C | 4.654810  | 1.937618  | -2.000337 | H | 1.942796  | 2.882359  | 6.752541  |
| C | 5.614606  | 0.922035  | -1.901474 | C | 2.551946  | 4.184465  | 5.142190  |
| H | 5.375291  | -0.077261 | -2.250434 | H | 3.512748  | 4.425849  | 5.589153  |
| C | 6.879013  | 1.169086  | -1.370238 | C | 2.198025  | 4.746759  | 3.915466  |
| H | 7.617035  | 0.376327  | -1.312793 | H | 2.882972  | 5.427666  | 3.416723  |
| C | 7.187152  | 2.453095  | -0.919087 | C | -0.155605 | 6.466088  | 2.316565  |
| C | 6.251161  | 3.481678  | -0.993432 | C | -1.423021 | 6.458740  | 2.918724  |
| H | 6.497050  | 4.475910  | -0.636646 | H | -1.896387 | 5.510919  | 3.155312  |
| C | 4.992409  | 3.213011  | -1.535440 | C | -2.080871 | 7.648905  | 3.222768  |
| H | 4.261366  | 4.015396  | -1.587834 | H | -3.065231 | 7.617533  | 3.682662  |
| C | 4.404071  | 1.351526  | -4.914440 | C | -1.479016 | 8.877673  | 2.940253  |
| C | 5.032807  | 0.122188  | -5.173134 | H | -1.990909 | 9.806223  | 3.177946  |
| H | 4.599831  | -0.791835 | -4.776933 | C | -0.213653 | 8.900646  | 2.355460  |
| C | 6.191337  | 0.053359  | -5.943710 | H | 0.271438  | 9.848985  | 2.139320  |
| H | 6.660064  | -0.910417 | -6.124764 | C | 0.440113  | 7.704915  | 2.048296  |
| C | 6.744308  | 1.215549  | -6.487374 | H | 1.431489  | 7.741215  | 1.606086  |
| H | 7.646445  | 1.163988  | -7.090778 | C | -0.896108 | 4.915434  | -0.155064 |
| C | 6.121330  | 2.440513  | -6.254575 | C | -2.246542 | 4.672655  | 0.138201  |
| H | 6.532315  | 3.352059  | -6.680507 | H | -2.511855 | 4.091753  | 1.015152  |
| C | 4.962182  | 2.505904  | -5.477267 | C | -3.262891 | 5.142587  | -0.689671 |
| H | 4.489368  | 3.470442  | -5.322583 | H | -4.301671 | 4.947659  | -0.445983 |
| C | 2.082303  | 0.441892  | -4.646712 | C | -2.929124 | 5.863377  | -1.837111 |
| C | 1.367781  | 0.859154  | -5.779729 | C | -1.599214 | 6.109832  | -2.164055 |
| H | 1.526711  | 1.861886  | -6.167982 | H | -1.345799 | 6.657845  | -3.064636 |
| C | 0.477595  | 0.000285  | -6.422850 | C | -0.594261 | 5.632408  | -1.317965 |
| H | -0.054044 | 0.339811  | -7.308159 | H | 0.441689  | 5.819736  | -1.585083 |
| C | 0.279939  | -1.294286 | -5.934109 | C | -0.840665 | -0.570697 | 2.380034  |
| H | -0.403690 | -1.973253 | -6.437770 | C | -1.615946 | -1.321830 | 3.455683  |
| C | 0.972939  | -1.714101 | -4.797417 | C | -3.052182 | -0.806015 | 3.846144  |
| H | 0.812429  | -2.709877 | -4.397238 | C | -2.876064 | -2.023366 | 2.991261  |
| C | 1.872246  | -0.854146 | -4.163559 | H | -3.109565 | -1.967911 | 1.935616  |
| H | 2.397678  | -1.193570 | -3.275598 | H | -3.112856 | -2.978020 | 3.448875  |
| C | 0.319443  | 2.863231  | 0.732814  | C | -0.738366 | -1.977894 | 4.497622  |
| C | 0.187145  | 4.373315  | 0.743145  | C | -0.730475 | -3.368952 | 4.659784  |
| C | 1.507185  | 5.120828  | 0.866460  | H | -1.363862 | -3.991464 | 4.035972  |
| H | 1.623479  | 6.016866  | 0.265596  | C | 0.085002  | -3.993402 | 5.607459  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 0.071612  | -5.072357 | 5.717011  |
| C  | 0.915413  | -3.211700 | 6.404577  |
| C  | 0.943197  | -1.824027 | 6.260131  |
| H  | 1.600482  | -1.221377 | 6.877406  |
| C  | 0.121469  | -1.220488 | 5.311047  |
| H  | 0.168963  | -0.145051 | 5.185967  |
| C  | -3.545162 | -1.038431 | 5.263530  |
| C  | -4.685933 | -1.829403 | 5.462751  |
| H  | -5.163068 | -2.299262 | 4.606667  |
| C  | -5.220980 | -2.013185 | 6.738343  |
| H  | -6.106227 | -2.630566 | 6.867152  |
| C  | -4.621490 | -1.406566 | 7.843096  |
| H  | -5.032440 | -1.551397 | 8.838576  |
| C  | -3.487112 | -0.614326 | 7.658990  |
| H  | -3.007989 | -0.141197 | 8.512077  |
| C  | -2.957422 | -0.429999 | 6.381255  |
| H  | -2.067637 | 0.178302  | 6.259163  |
| C  | -3.621138 | 0.463912  | 3.246217  |
| C  | -4.553236 | 0.411994  | 2.200865  |
| H  | -4.810189 | -0.543673 | 1.754236  |
| C  | -5.170509 | 1.575994  | 1.736577  |
| H  | -5.899642 | 1.513565  | 0.932059  |
| C  | -4.874609 | 2.812372  | 2.310879  |
| H  | -5.370802 | 3.714553  | 1.962603  |
| C  | -3.944357 | 2.876372  | 3.351667  |
| H  | -3.715936 | 3.829165  | 3.822741  |
| C  | -3.325046 | 1.714007  | 3.810713  |
| H  | -2.624160 | 1.777191  | 4.637188  |
| O  | 1.093884  | 0.971002  | -1.819029 |
| O  | 2.861468  | 0.682098  | -0.435126 |
| O  | -0.582715 | 2.214446  | 0.100861  |
| O  | 1.331066  | 2.354029  | 1.302366  |
| O  | -1.360072 | -0.495082 | 1.215938  |
| O  | 0.296744  | -0.111143 | 2.700444  |
| O  | 0.339299  | -1.744071 | -0.764474 |
| O  | 1.804518  | -1.727270 | 0.959533  |
| Rh | -0.217439 | 0.235875  | -0.375065 |
| Rh | 1.635280  | 0.310338  | 1.185109  |
| C  | -2.717609 | -1.235089 | -1.381582 |
| C  | -1.999990 | 0.031319  | -1.670008 |
| C  | -2.196187 | 1.017563  | -2.467268 |
| C  | -3.847841 | 0.120257  | -4.080505 |
| C  | -3.879269 | -1.310202 | -3.572994 |
| H  | -4.728762 | -1.824803 | -4.038596 |

|   |            |           |           |
|---|------------|-----------|-----------|
| H | -2.979505  | -1.847408 | -3.908455 |
| H | -2.920945  | -1.279657 | -0.311470 |
| N | -4.001861  | -1.370552 | -2.110170 |
| S | -5.011519  | -2.599790 | -1.500609 |
| O | -4.761685  | -3.883878 | -2.172540 |
| O | -4.901691  | -2.507470 | -0.038254 |
| C | -6.632105  | -2.034064 | -2.010079 |
| C | -7.190326  | -0.903144 | -1.404577 |
| C | -7.341625  | -2.762531 | -2.963712 |
| C | -8.465550  | -0.495713 | -1.779099 |
| H | -6.635599  | -0.362122 | -0.644977 |
| C | -8.620759  | -2.336786 | -3.327856 |
| H | -6.899932  | -3.652141 | -3.399886 |
| C | -9.199922  | -1.201898 | -2.748173 |
| H | -8.904664  | 0.381197  | -1.309702 |
| H | -9.177528  | -2.901873 | -4.070742 |
| C | -10.580931 | -0.739006 | -3.145852 |
| H | -10.544356 | 0.248399  | -3.622796 |
| H | -11.050035 | -1.433188 | -3.849194 |
| H | -11.236194 | -0.649373 | -2.271303 |
| C | -4.288187  | 1.147240  | -3.307825 |
| H | -4.285879  | 2.162278  | -3.686941 |
| H | -4.752019  | 0.955020  | -2.348091 |
| C | -1.593298  | 2.217412  | -3.031293 |
| H | -0.651011  | 2.453216  | -2.509558 |
| O | -2.015607  | 2.895140  | -3.949931 |
| H | -2.031125  | -2.063835 | -1.613464 |
| C | -3.344080  | 0.305974  | -5.482087 |
| H | -3.983826  | -0.246599 | -6.185219 |
| H | -3.331052  | 1.359860  | -5.764699 |
| H | -2.329486  | -0.095439 | -5.590637 |

**(R,R)-I-TS-II(e)\_conf1**

**1 imaginary frequency, value = -226.7243 cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -0.782013 | -6.532188 | -5.395642 |
| Br | -7.572583 | 5.029251  | -2.174835 |
| Br | 7.391504  | 3.107828  | -1.050714 |
| Br | -2.397221 | 1.629065  | 8.621482  |
| C  | 0.752383  | 2.199578  | 0.978538  |
| C  | 1.728276  | 3.201805  | 1.562605  |
| C  | 1.632395  | 3.320623  | 3.080647  |
| H  | 2.570629  | 3.336987  | 3.625330  |
| H  | 0.838595  | 2.753218  | 3.555546  |
| C  | 1.221136  | 4.511483  | 2.268034  |

|   |           |          |           |   |           |           |           |
|---|-----------|----------|-----------|---|-----------|-----------|-----------|
| C | -0.244699 | 4.893665 | 2.258016  | C | -5.976179 | 2.764044  | -2.957090 |
| C | -0.873575 | 5.177007 | 3.476944  | H | -6.928463 | 2.266312  | -3.104191 |
| H | -0.317181 | 5.058417 | 4.403195  | C | -4.777783 | 2.092585  | -3.208817 |
| C | -2.200896 | 5.605079 | 3.516186  | H | -4.815598 | 1.060766  | -3.547650 |
| H | -2.671611 | 5.814014 | 4.473226  | C | -1.834501 | 3.546603  | -5.332376 |
| C | -2.921045 | 5.761299 | 2.330292  | C | -1.324945 | 4.827933  | -5.063988 |
| H | -3.956724 | 6.089087 | 2.356835  | H | -0.606402 | 4.957976  | -4.259653 |
| C | -2.302512 | 5.486279 | 1.109105  | C | -1.711594 | 5.930329  | -5.822858 |
| H | -2.860337 | 5.585176 | 0.182221  | H | -1.305880 | 6.911694  | -5.591185 |
| C | -0.975013 | 5.058975 | 1.075041  | C | -2.610583 | 5.774859  | -6.881096 |
| H | -0.512794 | 4.819959 | 0.120615  | H | -2.911648 | 6.632813  | -7.476005 |
| C | 2.133339  | 5.731572 | 2.236613  | C | -3.109864 | 4.506272  | -7.171294 |
| C | 1.884323  | 6.768397 | 1.320717  | H | -3.799975 | 4.367243  | -7.999339 |
| H | 1.036421  | 6.694067 | 0.647318  | C | -2.723543 | 3.403953  | -6.404601 |
| C | 2.692588  | 7.902620 | 1.273199  | H | -3.115324 | 2.424551  | -6.659394 |
| H | 2.474899  | 8.685839 | 0.551586  | C | 0.140916  | 2.256657  | -4.481639 |
| C | 3.768349  | 8.038541 | 2.153274  | C | 0.768949  | 1.732501  | -5.621669 |
| H | 4.397327  | 8.924008 | 2.121144  | H | 0.158466  | 1.361646  | -6.441067 |
| C | 4.017856  | 7.028556 | 3.080707  | C | 2.159281  | 1.702112  | -5.724201 |
| H | 4.842662  | 7.122384 | 3.782273  | H | 2.624153  | 1.310376  | -6.625606 |
| C | 3.208567  | 5.890811 | 3.121264  | C | 2.947820  | 2.185185  | -4.676217 |
| H | 3.424536  | 5.129680 | 3.863157  | H | 4.032129  | 2.164824  | -4.750200 |
| C | 3.097999  | 3.190872 | 0.931478  | C | 2.333542  | 2.698071  | -3.533240 |
| C | 3.420146  | 4.051073 | -0.125701 | H | 2.935410  | 3.058524  | -2.705352 |
| H | 2.682750  | 4.760862 | -0.485703 | C | 0.940606  | 2.741766  | -3.441712 |
| C | 4.685748  | 4.035597 | -0.713468 | H | 0.478557  | 3.137031  | -2.541846 |
| H | 4.927371  | 4.722800 | -1.517155 | C | -2.435113 | -1.740479 | -0.532554 |
| C | 5.636301  | 3.129289 | -0.245946 | C | -3.374386 | -2.764058 | -1.147516 |
| C | 5.344061  | 2.246186 | 0.791500  | C | -4.796639 | -2.258689 | -1.329334 |
| H | 6.075740  | 1.526355 | 1.138529  | H | -5.330848 | -2.577415 | -2.218305 |
| C | 4.075307  | 2.290795 | 1.373332  | H | -4.967523 | -1.229967 | -1.033790 |
| H | 3.847631  | 1.600271 | 2.180623  | C | -4.572509 | -3.286772 | -0.264907 |
| C | -1.646393 | 1.392406 | -1.998633 | C | -4.699202 | -2.911257 | 1.198371  |
| C | -2.254299 | 1.959737 | -3.267543 | C | -3.993171 | -3.619015 | 2.181526  |
| C | -1.368867 | 2.365015 | -4.498007 | H | -3.299250 | -4.400453 | 1.887003  |
| C | -2.164600 | 1.094308 | -4.513145 | C | -4.187588 | -3.353554 | 3.537228  |
| H | -1.608040 | 0.168195 | -4.424092 | H | -3.643443 | -3.929985 | 4.281714  |
| H | -3.057328 | 1.028749 | -5.126597 | C | -5.093865 | -2.368636 | 3.937777  |
| C | -3.539104 | 2.716025 | -3.024601 | H | -5.254119 | -2.166490 | 4.993507  |
| C | -3.526424 | 4.040928 | -2.570046 | C | -5.802057 | -1.656702 | 2.968958  |
| H | -2.577924 | 4.544579 | -2.414866 | H | -6.513842 | -0.890960 | 3.265653  |
| C | -4.710009 | 4.732096 | -2.318611 | C | -5.608627 | -1.930759 | 1.614005  |
| H | -4.685422 | 5.762013 | -1.979318 | H | -6.175386 | -1.375879 | 0.872509  |
| C | -5.929946 | 4.083847 | -2.515079 | C | -5.117534 | -4.676283 | -0.546334 |

|   |           |           |           |    |           |           |           |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -4.368838 | -5.841544 | -0.330905 | H  | -1.139798 | -4.896655 | 7.505790  |
| H | -3.331411 | -5.766683 | -0.023331 | C  | -0.134599 | -3.837162 | 5.927449  |
| C | -4.931902 | -7.102659 | -0.528706 | H  | -1.019983 | -3.801624 | 5.300414  |
| H | -4.328528 | -7.991573 | -0.364526 | C  | 1.135588  | -3.671585 | 2.998870  |
| C | -6.260167 | -7.224093 | -0.940307 | C  | 2.347233  | -4.183270 | 2.515332  |
| H | -6.697930 | -8.206489 | -1.095277 | H  | 3.287842  | -3.764086 | 2.860472  |
| C | -7.019583 | -6.072774 | -1.153052 | C  | 2.366008  | -5.235439 | 1.597188  |
| H | -8.056058 | -6.152324 | -1.470469 | H  | 3.321438  | -5.608262 | 1.239490  |
| C | -6.451032 | -4.813486 | -0.957619 | C  | 1.167821  | -5.801408 | 1.156654  |
| H | -7.052956 | -3.922600 | -1.117064 | H  | 1.177608  | -6.634100 | 0.457857  |
| C | -2.751887 | -3.667506 | -2.183064 | C  | -0.045428 | -5.294190 | 1.629284  |
| C | -1.677386 | -4.507525 | -1.845548 | H  | -0.983336 | -5.734490 | 1.299355  |
| H | -1.280192 | -4.491880 | -0.836778 | C  | -0.061488 | -4.233983 | 2.536507  |
| C | -1.091313 | -5.351177 | -2.785584 | H  | -1.012005 | -3.837281 | 2.882110  |
| H | -0.266455 | -5.996657 | -2.502974 | O  | -0.697170 | 0.543828  | -2.102934 |
| C | -1.576514 | -5.357338 | -4.094153 | O  | -2.168617 | 1.777546  | -0.908603 |
| C | -2.627051 | -4.524879 | -4.466583 | O  | -1.185457 | -1.894266 | -0.746418 |
| H | -2.992973 | -4.523047 | -5.487422 | O  | -2.957381 | -0.780261 | 0.110971  |
| C | -3.202512 | -3.686281 | -3.507993 | O  | 0.677428  | -1.050821 | 1.499463  |
| H | -4.014697 | -3.034817 | -3.814932 | O  | -1.204674 | -0.312716 | 2.507065  |
| C | -0.054541 | -0.846523 | 2.525808  | O  | 1.202338  | 1.406477  | 0.082738  |
| C | 0.512589  | -1.212359 | 3.886725  | O  | -0.416789 | 2.171153  | 1.467799  |
| C | 1.154715  | -2.628957 | 4.095272  | Rh | 0.084039  | -0.304784 | -0.362210 |
| C | 2.017851  | -1.416349 | 3.939608  | Rh | -1.751051 | 0.741397  | 0.827914  |
| H | 2.558983  | -1.286370 | 3.009357  | C  | 2.983299  | -1.396466 | -0.292861 |
| H | 2.534811  | -1.047018 | 4.818917  | C  | 1.870425  | -1.285621 | -1.265284 |
| C | -0.183113 | -0.536899 | 5.044516  | C  | 1.693519  | -1.711093 | -2.462132 |
| C | 0.480799  | 0.402377  | 5.841673  | C  | 3.354813  | -3.066963 | -2.984973 |
| H | 1.518331  | 0.649615  | 5.638696  | C  | 3.807704  | -3.361850 | -1.567561 |
| C | -0.161671 | 1.047698  | 6.901784  | H  | 2.746538  | -3.830380 | -3.466154 |
| H | 0.371419  | 1.770712  | 7.509471  | H  | 4.693445  | -4.004581 | -1.610339 |
| C | -1.495709 | 0.750983  | 7.163236  | H  | 3.038031  | -3.925973 | -1.025253 |
| C | -2.189870 | -0.172186 | 6.380076  | H  | 3.297168  | -0.397062 | 0.017079  |
| H | -3.232573 | -0.390235 | 6.583560  | N  | 4.155500  | -2.123975 | -0.846153 |
| C | -1.530844 | -0.806296 | 5.329788  | S  | 5.436068  | -2.287003 | 0.269101  |
| H | -2.084636 | -1.502215 | 4.709141  | O  | 5.417052  | -3.616097 | 0.901994  |
| C | 1.058650  | -3.254780 | 5.475286  | O  | 5.392990  | -1.079453 | 1.103594  |
| C | 2.188206  | -3.333561 | 6.300023  | C  | 6.871838  | -2.219677 | -0.797813 |
| H | 3.130247  | -2.910914 | 5.962166  | C  | 7.226703  | -1.004974 | -1.393949 |
| C | 2.126499  | -3.961547 | 7.546049  | C  | 7.638971  | -3.367798 | -0.990688 |
| H | 3.016908  | -4.011747 | 8.167328  | C  | 8.357644  | -0.955533 | -2.201602 |
| C | 0.929763  | -4.523980 | 7.988928  | H  | 6.636133  | -0.111668 | -1.219825 |
| H | 0.877984  | -5.009631 | 8.959624  | C  | 8.768837  | -3.298197 | -1.807913 |
| C | -0.201786 | -4.460562 | 7.172317  | H  | 7.357875  | -4.292823 | -0.498911 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 9.145557  | -2.098217 | -2.423319 |
| H | 8.637542  | -0.010933 | -2.661074 |
| H | 9.368710  | -4.191315 | -1.963120 |
| C | 10.383022 | -2.019030 | -3.285072 |
| H | 11.195887 | -1.503685 | -2.757213 |
| H | 10.192584 | -1.458863 | -4.207430 |
| H | 10.745880 | -3.014153 | -3.559669 |
| C | 3.910927  | -2.085497 | -3.746522 |
| H | 4.563978  | -1.376489 | -3.238982 |
| C | 0.717412  | -1.867686 | -3.529352 |
| H | -0.208689 | -1.320162 | -3.288537 |
| O | 0.847400  | -2.510953 | -4.554477 |
| H | 2.580999  | -1.898408 | 0.596115  |
| C | 3.725440  | -1.890671 | -5.214022 |
| H | 3.096169  | -2.661037 | -5.660483 |
| H | 3.272466  | -0.911895 | -5.417640 |
| H | 4.710423  | -1.886837 | -5.702726 |

**(S,S)-I-TS-II(e)\_conf1**

**1 imaginary frequency, value = -230.6448 cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -5.851035 | 5.076998  | -3.327425 |
| Br | 8.299433  | 4.261582  | -1.196262 |
| Br | -0.317035 | -6.989868 | -4.088189 |
| Br | 3.095971  | -2.315845 | 8.183701  |
| C  | 1.698771  | -1.903106 | 0.262384  |
| C  | 2.200021  | -3.332521 | 0.291396  |
| C  | 2.372879  | -3.884784 | 1.703394  |
| H  | 1.998255  | -4.888007 | 1.877951  |
| H  | 2.203779  | -3.186940 | 2.517130  |
| C  | 3.611934  | -3.685010 | 0.883283  |
| C  | 4.586701  | -2.607132 | 1.312298  |
| C  | 5.133643  | -2.672561 | 2.600090  |
| H  | 4.803648  | -3.454096 | 3.279790  |
| C  | 6.090625  | -1.748039 | 3.020253  |
| H  | 6.498182  | -1.814095 | 4.025627  |
| C  | 6.518736  | -0.741132 | 2.153049  |
| H  | 7.259297  | -0.015438 | 2.478388  |
| C  | 5.983030  | -0.668261 | 0.865526  |
| H  | 6.291626  | 0.124559  | 0.190098  |
| C  | 5.028698  | -1.596908 | 0.449453  |
| H  | 4.595423  | -1.509481 | -0.543457 |
| C  | 4.326380  | -4.908743 | 0.324191  |
| C  | 5.323594  | -4.750649 | -0.653499 |
| H  | 5.577911  | -3.753940 | -1.000187 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 6.009262  | -5.847215 | -1.171948 |
| H | 6.773517  | -5.692730 | -1.929320 |
| C | 5.724743  | -7.136060 | -0.714996 |
| H | 6.260642  | -7.992449 | -1.115121 |
| C | 4.752684  | -7.308439 | 0.268726  |
| H | 4.527514  | -8.302429 | 0.646335  |
| C | 4.064484  | -6.206585 | 0.782434  |
| H | 3.324448  | -6.373062 | 1.557862  |
| C | 1.602486  | -4.230681 | -0.762918 |
| C | 2.214534  | -4.384736 | -2.012813 |
| H | 3.149681  | -3.875063 | -2.220459 |
| C | 1.659296  | -5.205179 | -2.995600 |
| H | 2.157409  | -5.333282 | -3.950705 |
| C | 0.457553  | -5.861721 | -2.731610 |
| C | -0.188137 | -5.716114 | -1.504655 |
| H | -1.137215 | -6.204431 | -1.318361 |
| C | 0.398424  | -4.907203 | -0.528643 |
| H | -0.101426 | -4.795953 | 0.430197  |
| C | 1.967643  | 1.398455  | -1.697365 |
| C | 2.709632  | 2.044159  | -2.849999 |
| C | 2.467747  | 1.603041  | -4.336660 |
| C | 1.856168  | 2.864113  | -3.806915 |
| H | 0.785881  | 2.853118  | -3.632339 |
| H | 2.256943  | 3.823732  | -4.116199 |
| C | 4.067541  | 2.582156  | -2.468030 |
| C | 5.180981  | 1.736514  | -2.381000 |
| H | 5.073260  | 0.682238  | -2.615445 |
| C | 6.433342  | 2.222144  | -2.008739 |
| H | 7.289769  | 1.558218  | -1.961568 |
| C | 6.573458  | 3.577108  | -1.706055 |
| C | 5.483294  | 4.441430  | -1.771418 |
| H | 5.599458  | 5.492310  | -1.529786 |
| C | 4.239584  | 3.934342  | -2.153631 |
| H | 3.389128  | 4.609257  | -2.198700 |
| C | 3.648342  | 1.700544  | -5.290275 |
| C | 4.470866  | 0.581083  | -5.498548 |
| H | 4.257295  | -0.343707 | -4.970654 |
| C | 5.544719  | 0.630330  | -6.384633 |
| H | 6.167828  | -0.249355 | -6.523409 |
| C | 5.815746  | 1.801293  | -7.096930 |
| H | 6.651388  | 1.841150  | -7.790283 |
| C | 4.996965  | 2.914493  | -6.915192 |
| H | 5.186636  | 3.828843  | -7.471317 |
| C | 3.923710  | 2.862218  | -6.022121 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 3.292254  | 3.737837  | -5.910445 | H | -5.396988 | 3.738040  | -0.695539 |
| C | 1.545897  | 0.460730  | -4.709262 | C | -4.310182 | 4.852022  | -2.191742 |
| C | 0.611950  | 0.676904  | -5.732746 | C | -3.085020 | 5.385581  | -2.580096 |
| H | 0.514261  | 1.670148  | -6.162655 | H | -2.986989 | 5.912570  | -3.522640 |
| C | -0.183356 | -0.364237 | -6.210696 | C | -1.981027 | 5.228752  | -1.737223 |
| H | -0.894891 | -0.173697 | -7.009926 | H | -1.026593 | 5.641582  | -2.050301 |
| C | -0.056692 | -1.645122 | -5.667755 | C | -0.600146 | -0.481855 | 2.527721  |
| H | -0.661850 | -2.465089 | -6.046826 | C | -1.132102 | -1.294267 | 3.701181  |
| C | 0.860028  | -1.869293 | -4.638227 | C | -2.662393 | -1.182217 | 4.055495  |
| H | 0.955868  | -2.856044 | -4.196392 | C | -2.124517 | -2.384054 | 3.342667  |
| C | 1.656577  | -0.824432 | -4.166012 | H | -2.344187 | -2.516999 | 2.290582  |
| H | 2.352447  | -1.011207 | -3.352923 | H | -2.076667 | -3.307689 | 3.909519  |
| C | -0.384865 | 2.949556  | 0.507366  | C | -0.117590 | -1.540236 | 4.794085  |
| C | -0.889088 | 4.374671  | 0.389086  | C | 0.290665  | -2.839030 | 5.121958  |
| C | 0.203030  | 5.433816  | 0.412060  | H | -0.125133 | -3.689331 | 4.590946  |
| H | 0.091251  | 6.273769  | -0.265601 | C | 1.237562  | -3.080826 | 6.120890  |
| H | 1.215873  | 5.063090  | 0.526127  | H | 1.536116  | -4.095809 | 6.359561  |
| C | -0.701534 | 5.353865  | 1.602018  | C | 1.793236  | -2.001607 | 6.800931  |
| C | -0.143508 | 4.873380  | 2.924382  | C | 1.420392  | -0.693480 | 6.489378  |
| C | -0.782428 | 3.888600  | 3.687019  | H | 1.866066  | 0.143894  | 7.015127  |
| H | -1.644159 | 3.366148  | 3.281004  | C | 0.473731  | -0.473667 | 5.491646  |
| C | -0.309030 | 3.553920  | 4.956197  | H | 0.210901  | 0.546087  | 5.235597  |
| H | -0.822788 | 2.793271  | 5.539170  | C | -3.087834 | -1.380911 | 5.499461  |
| C | 0.816766  | 4.191369  | 5.480884  | C | -3.940088 | -2.448271 | 5.816688  |
| H | 1.184595  | 3.929652  | 6.469346  | H | -4.239223 | -3.140807 | 5.034262  |
| C | 1.467210  | 5.167368  | 4.723564  | C | -4.416140 | -2.627667 | 7.116172  |
| H | 2.346800  | 5.668807  | 5.118541  | H | -5.076033 | -3.462511 | 7.337439  |
| C | 0.985941  | 5.506788  | 3.458845  | C | -4.046195 | -1.738564 | 8.126250  |
| H | 1.489482  | 6.275782  | 2.878716  | H | -4.411003 | -1.877930 | 9.140307  |
| C | -1.734438 | 6.452294  | 1.784666  | C | -3.200711 | -0.669784 | 7.823741  |
| C | -2.959241 | 6.187907  | 2.416379  | H | -2.901145 | 0.026096  | 8.602948  |
| H | -3.183401 | 5.178348  | 2.746528  | C | -2.729979 | -0.491823 | 6.522413  |
| C | -3.889868 | 7.202172  | 2.633084  | H | -2.063599 | 0.336944  | 6.308212  |
| H | -4.834538 | 6.971078  | 3.118463  | C | -3.567300 | -0.212461 | 3.323243  |
| C | -3.610953 | 8.510722  | 2.230940  | C | -4.459386 | -0.665048 | 2.341754  |
| H | -4.335599 | 9.302459  | 2.400491  | H | -4.448132 | -1.708694 | 2.041354  |
| C | -2.391950 | 8.791458  | 1.615390  | C | -5.375845 | 0.208909  | 1.752378  |
| H | -2.156484 | 9.806673  | 1.306772  | H | -6.064706 | -0.164089 | 0.998139  |
| C | -1.463951 | 7.770522  | 1.396285  | C | -5.424275 | 1.548909  | 2.137601  |
| H | -0.513260 | 8.009808  | 0.928738  | H | -6.151152 | 2.223701  | 1.692821  |
| C | -2.081506 | 4.551419  | -0.516918 | C | -4.539285 | 2.011097  | 3.115215  |
| C | -3.326678 | 4.008724  | -0.164792 | H | -4.577234 | 3.048090  | 3.439838  |
| H | -3.428876 | 3.448161  | 0.758339  | C | -3.620971 | 1.138095  | 3.698687  |
| C | -4.439937 | 4.156157  | -0.988639 | H | -2.954672 | 1.506540  | 4.472601  |

|    |            |           |           |
|----|------------|-----------|-----------|
| O  | 0.763284   | 1.022579  | -1.894172 |
| O  | 2.590600   | 1.326407  | -0.593562 |
| O  | -1.112116  | 2.039466  | -0.019228 |
| O  | 0.734860   | 2.764670  | 1.071464  |
| O  | -1.158972  | -0.649488 | 1.392481  |
| O  | 0.394911   | 0.273565  | 2.746078  |
| O  | 0.743637   | -1.641008 | -0.546895 |
| O  | 2.209890   | -1.084300 | 1.083914  |
| Rh | -0.280337  | 0.168438  | -0.316005 |
| Rh | 1.539906   | 0.857036  | 1.127098  |
| C  | -2.396524  | -1.942169 | -1.020112 |
| C  | -1.975418  | -0.605757 | -1.499660 |
| C  | -2.340808  | 0.140154  | -2.476991 |
| C  | -3.647198  | -1.043189 | -3.807797 |
| C  | -3.300667  | -2.420121 | -3.264798 |
| H  | -3.160255  | -0.753924 | -4.736938 |
| H  | -3.933745  | -3.164705 | -3.759047 |
| H  | -2.261429  | -2.675980 | -3.507585 |
| H  | -2.697209  | -1.863544 | 0.024625  |
| N  | -3.527037  | -2.481266 | -1.810327 |
| S  | -4.151441  | -3.938776 | -1.195353 |
| O  | -3.505228  | -5.106495 | -1.812308 |
| O  | -4.139114  | -3.778462 | 0.265358  |
| C  | -5.845750  | -3.896576 | -1.774684 |
| C  | -6.759862  | -3.030970 | -1.164928 |
| C  | -6.244300  | -4.758570 | -2.795522 |
| C  | -8.079805  | -3.022628 | -1.603156 |
| H  | -6.439732  | -2.387588 | -0.351771 |
| C  | -7.573094  | -4.734065 | -3.223575 |
| H  | -5.525633  | -5.442459 | -3.234439 |
| C  | -8.507868  | -3.870991 | -2.639110 |
| H  | -8.794553  | -2.352897 | -1.131070 |
| H  | -7.887085  | -5.402660 | -4.020916 |
| C  | -9.949868  | -3.864212 | -3.086992 |
| H  | -10.323769 | -2.842126 | -3.215283 |
| H  | -10.078359 | -4.394944 | -4.035070 |
| H  | -10.593661 | -4.352139 | -2.343821 |
| C  | -4.724540  | -0.336569 | -3.366020 |
| H  | -5.213785  | -0.701032 | -2.463691 |
| C  | -2.063344  | 1.393283  | -3.162575 |
| H  | -1.386791  | 2.023312  | -2.561595 |
| O  | -2.481316  | 1.742447  | -4.250902 |
| H  | -1.517183  | -2.602504 | -1.060466 |
| C  | -5.321106  | 0.872755  | -4.005169 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | -5.296181 | 1.735292 | -3.327072 |
| H | -4.810830 | 1.153462 | -4.926508 |
| H | -6.382553 | 0.677081 | -4.215528 |

1w\_conf1

0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.972436  | 1.659136  | -0.203662 |
| H | 2.051600  | 1.676398  | -0.405455 |
| H | 0.757182  | 2.482725  | 0.479093  |
| N | 0.739428  | 0.403559  | 0.534250  |
| S | -0.578194 | 0.284375  | 1.585091  |
| O | -0.788566 | 1.636468  | 2.105567  |
| O | -0.284643 | -0.855833 | 2.457874  |
| C | -2.030213 | -0.163993 | 0.626564  |
| C | -2.312437 | -1.513178 | 0.395431  |
| C | -2.868327 | 0.835576  | 0.127085  |
| C | -3.433569 | -1.855526 | -0.358702 |
| H | -1.679281 | -2.282415 | 0.824567  |
| C | -3.987857 | 0.474016  | -0.618901 |
| H | -2.649911 | 1.876787  | 0.333716  |
| C | -4.287942 | -0.871855 | -0.876648 |
| H | -3.654573 | -2.904982 | -0.537323 |
| H | -4.643393 | 1.251096  | -1.004437 |
| C | -5.521617 | -1.252285 | -1.660253 |
| H | -5.396109 | -2.216530 | -2.163279 |
| H | -6.394252 | -1.339775 | -0.999414 |
| H | -5.762972 | -0.500032 | -2.418491 |
| C | 1.263204  | -0.849313 | -0.028633 |
| H | 1.032544  | -1.649039 | 0.682357  |
| H | 0.775839  | -1.108624 | -0.982532 |
| C | 2.711571  | -0.806789 | -0.228800 |
| C | 3.908767  | -0.798709 | -0.421975 |
| C | 0.207442  | 1.821124  | -1.494236 |
| H | 0.270918  | 1.000803  | -2.209624 |
| C | -0.486996 | 2.914530  | -1.811309 |
| H | -0.567818 | 3.757229  | -1.127288 |
| H | -0.993590 | 3.014004  | -2.767526 |
| C | 5.349358  | -0.804901 | -0.637991 |
| O | 5.893207  | -1.722780 | -1.228008 |
| C | 6.103741  | 0.387059  | -0.084193 |
| H | 5.723926  | 1.316334  | -0.526135 |
| H | 5.951861  | 0.460616  | 0.999432  |
| H | 7.167773  | 0.278315  | -0.304999 |

**I(w)-Yne\_conf1****0 imaginary frequency**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.997773 | 2.265585  | 0.404589  |
| H  | -4.088875 | 2.275943  | 0.533772  |
| H  | -2.785240 | 2.826872  | -0.510494 |
| N  | -2.549693 | 0.869906  | 0.164538  |
| S  | -3.364772 | -0.366706 | 0.947927  |
| O  | -3.570444 | 0.086859  | 2.326323  |
| O  | -2.651182 | -1.610086 | 0.640652  |
| C  | -4.987784 | -0.482025 | 0.185463  |
| C  | -5.144311 | -1.223205 | -0.989935 |
| C  | -6.074142 | 0.185846  | 0.756153  |
| C  | -6.396207 | -1.280540 | -1.597897 |
| H  | -4.302649 | -1.766782 | -1.406610 |
| C  | -7.319876 | 0.116785  | 0.132996  |
| H  | -5.944941 | 0.728636  | 1.686341  |
| C  | -7.502241 | -0.613439 | -1.049577 |
| H  | -6.519467 | -1.860509 | -2.509318 |
| H  | -8.166275 | 0.633811  | 0.578437  |
| C  | -8.862955 | -0.711728 | -1.697257 |
| H  | -8.782908 | -0.843789 | -2.781230 |
| H  | -9.422656 | -1.571020 | -1.304634 |
| H  | -9.464047 | 0.183010  | -1.505551 |
| C  | -1.865862 | 0.559367  | -1.095108 |
| H  | -1.584308 | -0.496901 | -1.086551 |
| H  | -2.521879 | 0.737461  | -1.965168 |
| C  | -0.656331 | 1.365825  | -1.280907 |
| C  | 0.280334  | 2.121518  | -1.491516 |
| C  | -2.320330 | 2.922667  | 1.579655  |
| H  | -2.554151 | 2.495205  | 2.551642  |
| C  | -1.496813 | 3.964842  | 1.469097  |
| H  | -1.212618 | 4.385805  | 0.507325  |
| H  | -1.041433 | 4.418491  | 2.345698  |
| C  | 1.146648  | 3.271308  | -1.795537 |
| O  | 0.954239  | 4.326421  | -1.217803 |
| Rh | 1.541145  | 0.145362  | -0.368568 |
| Rh | 3.010251  | -1.406213 | 0.723221  |
| O  | 2.848274  | 1.648127  | 0.184389  |
| O  | 4.247641  | 0.172780  | 1.184747  |
| O  | 1.967162  | -1.095354 | 2.464295  |
| O  | 3.982722  | -1.662155 | -1.078150 |
| O  | 1.711063  | -2.921306 | 0.245341  |
| O  | 0.364109  | -1.483249 | -0.866865 |
| O  | 0.557350  | 0.340780  | 1.422741  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 2.635690  | -0.155444 | -2.107868 |
| C | 3.594706  | -0.997575 | -2.087203 |
| C | 3.900373  | 1.343901  | 0.837696  |
| C | 0.965413  | -0.310476 | 2.439260  |
| C | 0.671050  | -2.641878 | -0.425554 |
| C | -0.300290 | -3.758015 | -0.725504 |
| C | 4.314904  | -1.239110 | -3.396001 |
| C | 4.793617  | 2.488935  | 1.258935  |
| C | 0.192625  | -0.110281 | 3.721873  |
| H | 0.513362  | -0.828841 | 4.477722  |
| H | -0.879088 | -0.209879 | 3.526516  |
| H | 0.368046  | 0.907231  | 4.088824  |
| H | 5.808332  | 2.132074  | 1.444828  |
| H | 4.398964  | 2.920815  | 2.186135  |
| H | 4.791534  | 3.272240  | 0.497458  |
| H | 4.463747  | -0.294167 | -3.925216 |
| H | 5.271658  | -1.733479 | -3.220216 |
| H | 3.693791  | -1.881917 | -4.030551 |
| H | 0.092184  | -4.713347 | -0.374298 |
| H | -0.489790 | -3.803388 | -1.802823 |
| H | -1.248795 | -3.532770 | -0.227055 |
| C | 2.195380  | 3.077359  | -2.861288 |
| H | 2.830127  | 2.221260  | -2.614532 |
| H | 1.708878  | 2.850154  | -3.818769 |
| H | 2.786090  | 3.991094  | -2.956679 |

**I(w)-Ene\_conf2****0 imaginary frequency**

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.835265 | 0.401210  | -0.655634 |
| H | 1.529974 | 0.461582  | 0.393572  |
| H | 2.139360 | -0.628608 | -0.855584 |
| N | 2.973203 | 1.329311  | -0.861804 |
| S | 4.326251 | 0.747218  | -1.691765 |
| O | 5.188160 | 1.909721  | -1.918724 |
| O | 3.802527 | -0.073623 | -2.783141 |
| C | 5.184541 | -0.345483 | -0.554161 |
| C | 4.914286 | -1.715900 | -0.570635 |
| C | 6.093819 | 0.191177  | 0.363667  |
| C | 5.548741 | -2.545977 | 0.353321  |
| H | 4.236525 | -2.124383 | -1.312509 |
| C | 6.715985 | -0.653373 | 1.279725  |
| H | 6.327268 | 1.250467  | 0.340136  |
| C | 6.452904 | -2.031861 | 1.292835  |
| H | 5.342187 | -3.613208 | 0.338973  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 7.424807  | -0.237023 | 1.991455  |
| C  | 7.156115  | -2.939229 | 2.274138  |
| H  | 6.623751  | -3.887495 | 2.396993  |
| H  | 8.172706  | -3.174298 | 1.932528  |
| H  | 7.247186  | -2.469019 | 3.259358  |
| C  | 3.229541  | 2.318318  | 0.199076  |
| H  | 3.552550  | 1.830460  | 1.134305  |
| H  | 4.043457  | 2.965719  | -0.141267 |
| C  | 2.037848  | 3.123958  | 0.463196  |
| C  | 1.018783  | 3.735087  | 0.700347  |
| C  | 0.675180  | 0.781987  | -1.543345 |
| H  | 0.353983  | 1.817695  | -1.474899 |
| C  | 0.110443  | -0.037811 | -2.458801 |
| H  | 0.464002  | -1.055143 | -2.602083 |
| H  | -0.647907 | 0.318271  | -3.147668 |
| C  | -0.243369 | 4.407709  | 0.966841  |
| O  | -0.667247 | 4.528450  | 2.106541  |
| Rh | -1.450536 | -0.295634 | -0.526159 |
| Rh | -3.269899 | -0.972527 | 0.902895  |
| O  | -0.507754 | -2.068985 | -0.041181 |
| O  | -2.216836 | -2.696461 | 1.313125  |
| O  | -2.350804 | -0.032494 | 2.478796  |
| O  | -4.153211 | -1.894015 | -0.705292 |
| O  | -4.224288 | 0.782487  | 0.402393  |
| O  | -2.506432 | 1.442082  | -0.926045 |
| O  | -0.621593 | 0.595776  | 1.159641  |
| O  | -2.462431 | -1.252828 | -2.071133 |
| C  | -3.571177 | -1.834713 | -1.831496 |
| C  | -1.087236 | -2.873216 | 0.763665  |
| C  | -1.240220 | 0.546429  | 2.277600  |
| C  | -3.655441 | 1.595174  | -0.388327 |
| C  | -4.396409 | 2.876980  | -0.700494 |
| C  | -4.248866 | -2.503608 | -3.007242 |
| C  | -0.346818 | -4.154149 | 1.081943  |
| C  | -0.588139 | 1.250050  | 3.444945  |
| H  | -1.143808 | 1.055403  | 4.363453  |
| H  | -0.558488 | 2.328026  | 3.250030  |
| H  | 0.445257  | 0.905281  | 3.552115  |
| H  | -0.920373 | -4.765266 | 1.780110  |
| H  | 0.630598  | -3.914388 | 1.513132  |
| H  | -0.170048 | -4.712916 | 0.157068  |
| H  | -3.547752 | -3.185586 | -3.497911 |
| H  | -5.135922 | -3.047551 | -2.679608 |
| H  | -4.534714 | -1.742545 | -3.741309 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | -5.473559 | 2.696423 | -0.694865 |
| H | -4.080520 | 3.280346 | -1.664799 |
| H | -4.173212 | 3.615399 | 0.078588  |
| C | -1.001133 | 4.894835 | -0.248909 |
| H | -0.343451 | 5.440602 | -0.934035 |
| H | -1.393160 | 4.022750 | -0.789424 |
| H | -1.832118 | 5.529141 | 0.068545  |

# I(w)-Ene\_conf3

## 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.364044 | -1.892159 | -0.492868 |
| H  | -0.577378 | -1.902302 | -1.253832 |
| H  | -1.343887 | -2.857511 | 0.016424  |
| N  | -2.634963 | -1.783461 | -1.224336 |
| S  | -4.073545 | -2.290284 | -0.504881 |
| O  | -3.703697 | -3.392641 | 0.385079  |
| O  | -5.026843 | -2.455450 | -1.606348 |
| C  | -4.694463 | -0.958073 | 0.527358  |
| C  | -5.463012 | 0.058638  | -0.044756 |
| C  | -4.405743 | -0.953446 | 1.893831  |
| C  | -5.929850 | 1.094373  | 0.762684  |
| H  | -5.708419 | 0.028548  | -1.100717 |
| C  | -4.883397 | 0.088700  | 2.686349  |
| H  | -3.830575 | -1.764840 | 2.325365  |
| C  | -5.649596 | 1.127414  | 2.137096  |
| H  | -6.532517 | 1.883627  | 0.319980  |
| H  | -4.664183 | 0.090936  | 3.751330  |
| C  | -6.193485 | 2.231804  | 3.012156  |
| H  | -6.359764 | 3.151527  | 2.442102  |
| H  | -7.156445 | 1.942909  | 3.453729  |
| H  | -5.513006 | 2.459988  | 3.839186  |
| C  | -2.693785 | -0.973257 | -2.443491 |
| H  | -1.860863 | -1.286718 | -3.086484 |
| H  | -3.614739 | -1.235062 | -2.973220 |
| C  | -2.616908 | 0.482023  | -2.252039 |
| C  | -2.533989 | 1.683255  | -2.101128 |
| C  | -1.103001 | -0.764980 | 0.485999  |
| H  | -1.425072 | 0.223814  | 0.172550  |
| C  | -0.579101 | -0.937561 | 1.722201  |
| H  | -0.300606 | -1.922727 | 2.087894  |
| H  | -0.497740 | -0.114349 | 2.424239  |
| C  | -2.404733 | 3.112762  | -1.858568 |
| O  | -2.413725 | 3.919638  | -2.772991 |
| Rh | 1.421324  | -0.241766 | 0.417520  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| Rh                           | 3.648524  | 0.361574  | -0.275841 | C  | -4.984365 | -1.173168 | -1.180757 |
| O                            | 1.895169  | -2.204502 | -0.000564 | C  | -5.944540 | -0.145179 | 0.799040  |
| O                            | 3.977068  | -1.628909 | -0.696234 | C  | -6.237378 | -1.153000 | -1.788966 |
| O                            | 2.942481  | 0.662540  | -2.181434 | H  | -4.128700 | -1.603437 | -1.690325 |
| O                            | 4.293776  | 0.055209  | 1.647741  | C  | -7.191971 | -0.139738 | 0.176915  |
| O                            | 3.190275  | 2.314792  | 0.196539  | H  | -5.822915 | 0.232144  | 1.807808  |
| O                            | 1.068825  | 1.765350  | 0.788565  | C  | -7.359581 | -0.638104 | -1.122598 |
| O                            | 0.859012  | 0.022241  | -1.568862 | H  | -6.348258 | -1.552985 | -2.794017 |
| O                            | 2.195612  | -0.455265 | 2.334276  | H  | -8.051270 | 0.256562  | 0.712157  |
| C                            | 3.442136  | -0.271341 | 2.529874  | C  | -8.719525 | -0.653470 | -1.779419 |
| C                            | 3.057092  | -2.470939 | -0.459677 | H  | -8.647440 | -0.458454 | -2.854849 |
| C                            | 1.721009  | 0.423419  | -2.421238 | H  | -9.203034 | -1.632019 | -1.659240 |
| C                            | 2.023157  | 2.596242  | 0.607019  | H  | -9.385612 | 0.096233  | -1.340818 |
| C                            | 1.723120  | 4.053935  | 0.879393  | C  | -1.821007 | 0.740872  | -0.944009 |
| C                            | 3.936812  | -0.458475 | 3.947128  | H  | -1.546108 | -0.286418 | -1.199616 |
| C                            | 3.368325  | -3.928915 | -0.713973 | H  | -2.528950 | 1.110328  | -1.705370 |
| C                            | 1.237763  | 0.601786  | -3.843223 | C  | -0.616680 | 1.572190  | -1.018675 |
| H                            | 1.923061  | 1.243984  | -4.399001 | C  | 0.324334  | 2.345422  | -1.117977 |
| H                            | 0.228571  | 1.021369  | -3.849290 | C  | -3.818841 | 2.817573  | 0.586477  |
| H                            | 1.202983  | -0.378376 | -4.333934 | H  | -3.840088 | 3.014733  | -0.485830 |
| H                            | 4.157454  | -4.023346 | -1.462324 | C  | -4.773825 | 3.325854  | 1.365945  |
| H                            | 2.468934  | -4.461500 | -1.031363 | H  | -4.781333 | 3.157346  | 2.441226  |
| H                            | 3.719819  | -4.383749 | 0.219762  | H  | -5.576879 | 3.937828  | 0.964169  |
| H                            | 3.670876  | -1.459969 | 4.299770  | C  | 1.223393  | 3.504724  | -1.254291 |
| H                            | 5.017565  | -0.319179 | 3.997372  | O  | 1.169841  | 4.400017  | -0.432779 |
| H                            | 3.439987  | 0.263369  | 4.603892  | Rh | 1.611787  | 0.266070  | -0.296380 |
| H                            | 2.637502  | 4.579812  | 1.161340  | Rh | 3.100240  | -1.409584 | 0.559115  |
| H                            | 0.967361  | 4.150619  | 1.661977  | O  | 2.901884  | 1.686339  | 0.470810  |
| H                            | 1.332645  | 4.514333  | -0.036046 | O  | 4.317843  | 0.098348  | 1.251956  |
| C                            | -2.246110 | 3.504568  | -0.402791 | O  | 2.044743  | -1.375293 | 2.319833  |
| H                            | -3.083250 | 3.113821  | 0.188516  | O  | 4.085409  | -1.379705 | -1.250305 |
| H                            | -1.327604 | 3.062345  | 0.004838  | O  | 1.826059  | -2.853670 | -0.147495 |
| H                            | -2.205228 | 4.593353  | -0.321295 | O  | 0.461501  | -1.284577 | -1.041442 |
| <b>I(w)-Yne_conf4</b>        |           |           |           | O  | 0.627314  | 0.193013  | 1.504470  |
| <b>0 imaginary frequency</b> |           |           |           | O  | 2.712554  | 0.235282  | -2.056147 |
| C                            | -2.655309 | 2.007799  | 1.101589  | C  | 3.695697  | -0.573853 | -2.149486 |
| H                            | -1.722646 | 2.576353  | 1.003519  | C  | 3.955002  | 1.303597  | 1.078962  |
| H                            | -2.779633 | 1.779869  | 2.161322  | C  | 1.035828  | -0.606120 | 2.410687  |
| N                            | -2.413915 | 0.732590  | 0.399419  | C  | 0.792202  | -2.492451 | -0.790013 |
| S                            | -3.222760 | -0.655054 | 0.887548  | C  | -0.136336 | -3.568632 | -1.297835 |
| O                            | -3.424630 | -0.520289 | 2.333150  | C  | 4.477276  | -0.545177 | -3.444887 |
| O                            | -2.487945 | -1.788110 | 0.315655  | C  | 4.832205  | 2.382560  | 1.672672  |
| C                            | -4.844014 | -0.660177 | 0.112385  | C  | 0.251308  | -0.618526 | 3.701738  |
|                              |           |           |           | H  | 0.597370  | -1.424057 | 4.351159  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -0.814875 | -0.734146 | 3.484050  |
| H | 0.383109  | 0.342709  | 4.211150  |
| H | 5.879542  | 2.073132  | 1.648773  |
| H | 4.545433  | 2.531116  | 2.720450  |
| H | 4.692799  | 3.325988  | 1.141462  |
| H | 5.114379  | 0.346948  | -3.458450 |
| H | 5.108270  | -1.431254 | -3.530135 |
| H | 3.793076  | -0.479177 | -4.295008 |
| H | 0.280506  | -4.557697 | -1.102716 |
| H | -0.300406 | -3.436067 | -2.372186 |
| H | -1.101658 | -3.457822 | -0.794168 |
| C | 2.132574  | 3.511947  | -2.458204 |
| H | 2.715894  | 2.586107  | -2.493892 |
| H | 1.529848  | 3.549429  | -3.375020 |
| H | 2.784685  | 4.387059  | -2.412776 |

#### I-TS-II(w)\_conf1

1 imaginary frequency, value = -249.8363 cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.563907 | 0.950947  | 0.351310  |
| C | -0.348444 | 1.692924  | -0.105425 |
| C | -0.202698 | 2.924402  | -0.478944 |
| C | -2.247335 | 3.757931  | -0.833039 |
| C | -3.101105 | 2.514334  | -0.811016 |
| H | -2.071648 | 4.239511  | -1.790521 |
| H | -4.154962 | 2.810798  | -0.791335 |
| H | -2.933867 | 1.918263  | -1.721052 |
| H | -1.367756 | 0.562756  | 1.353263  |
| N | -2.805079 | 1.743952  | 0.394986  |
| S | -4.094866 | 1.078189  | 1.263210  |
| O | -3.530653 | 0.636567  | 2.539206  |
| O | -5.176334 | 2.064303  | 1.184784  |
| C | -4.629944 | -0.385216 | 0.372719  |
| C | -5.637997 | -0.277166 | -0.589524 |
| C | -4.023770 | -1.616116 | 0.637462  |
| C | -6.029364 | -1.412782 | -1.295314 |
| H | -6.122661 | 0.678186  | -0.760620 |
| C | -4.428992 | -2.741576 | -0.079234 |
| H | -3.263972 | -1.692131 | 1.407768  |
| C | -5.434067 | -2.660017 | -1.054051 |
| H | -6.817409 | -1.331434 | -2.039983 |
| H | -3.964913 | -3.701897 | 0.131884  |
| C | -5.893588 | -3.890909 | -1.798480 |
| H | -5.107351 | -4.651254 | -1.841703 |
| H | -6.761816 | -4.346010 | -1.303693 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -6.193885 | -3.650709 | -2.823818 |
| C  | -1.797013 | 4.350522  | 0.304035  |
| H  | -1.252366 | 5.284442  | 0.254096  |
| H  | -2.022441 | 3.924522  | 1.275562  |
| C  | 0.675562  | 3.928818  | -1.127395 |
| O  | 0.240340  | 4.982409  | -1.568698 |
| H  | -1.670371 | 0.082964  | -0.316709 |
| Rh | 2.915106  | -1.670752 | 0.204039  |
| Rh | 1.308086  | 0.146938  | -0.028807 |
| O  | 4.173507  | -0.346752 | 1.157171  |
| O  | 2.683587  | 1.352811  | 0.949497  |
| O  | 2.169301  | 0.516271  | -1.887509 |
| O  | 0.575153  | -0.415408 | 1.827103  |
| O  | 0.059742  | -1.228030 | -0.961384 |
| O  | 1.573609  | -2.906526 | -0.761100 |
| O  | 3.699149  | -1.138796 | -1.625733 |
| O  | 2.054819  | -2.121219 | 2.022767  |
| C  | 1.098990  | -1.403897 | 2.443289  |
| C  | 3.795936  | 0.850894  | 1.327057  |
| C  | 3.160745  | -0.191747 | -2.272048 |
| C  | 0.460595  | -2.428785 | -1.131865 |
| C  | -0.482228 | -3.351931 | -1.875112 |
| C  | 0.540232  | -1.718942 | 3.813836  |
| C  | 4.754776  | 1.792518  | 2.024576  |
| C  | 3.755794  | 0.160492  | -3.619290 |
| H  | 4.359516  | 1.070163  | -3.518584 |
| H  | 2.959806  | 0.368025  | -4.339420 |
| H  | 4.394136  | -0.648571 | -3.977970 |
| H  | 5.174758  | 2.489029  | 1.289595  |
| H  | 5.567648  | 1.233421  | 2.490458  |
| H  | 4.220339  | 2.383768  | 2.773371  |
| H  | 1.094294  | -1.139738 | 4.562079  |
| H  | -0.512173 | -1.433267 | 3.875744  |
| H  | 0.668744  | -2.779662 | 4.039329  |
| H  | -1.517537 | -3.144247 | -1.592190 |
| H  | -0.229440 | -4.394829 | -1.675404 |
| H  | -0.385408 | -3.166994 | -2.951464 |
| C  | 2.139553  | 3.578039  | -1.224793 |
| H  | 2.539088  | 3.299113  | -0.246046 |
| H  | 2.270479  | 2.703336  | -1.869020 |
| H  | 2.662794  | 4.443905  | -1.636679 |

#### I-TS-II(w)\_conf2

1 imaginary frequency, value = -251.9071 cm<sup>-1</sup>

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.550979 | 0.885472  | -0.675884 |
| C  | -0.498579 | 1.561868  | 0.143681  |
| C  | -0.521828 | 2.678729  | 0.800053  |
| C  | -2.348139 | 3.792905  | 0.129064  |
| C  | -2.752407 | 3.008318  | -1.089177 |
| H  | -1.913589 | 4.776415  | -0.025096 |
| H  | -3.731610 | 3.353880  | -1.437603 |
| H  | -2.035304 | 3.175688  | -1.907004 |
| H  | -1.707191 | -0.113959 | -0.258007 |
| N  | -2.852814 | 1.585921  | -0.740298 |
| S  | -4.061776 | 0.713117  | -1.576377 |
| O  | -5.175514 | 1.653215  | -1.750532 |
| O  | -3.490697 | 0.011058  | -2.733524 |
| C  | -4.528025 | -0.519264 | -0.365140 |
| C  | -4.226591 | -1.858971 | -0.601307 |
| C  | -5.240075 | -0.129387 | 0.773947  |
| C  | -4.634604 | -2.819139 | 0.327625  |
| H  | -3.693380 | -2.139255 | -1.503222 |
| C  | -5.634389 | -1.098875 | 1.689244  |
| H  | -5.490888 | 0.915146  | 0.927698  |
| C  | -5.338552 | -2.457672 | 1.482607  |
| H  | -4.408128 | -3.866368 | 0.144358  |
| H  | -6.188622 | -0.801261 | 2.576113  |
| C  | -5.788571 | -3.497160 | 2.481090  |
| H  | -5.432237 | -3.259332 | 3.490464  |
| H  | -6.883424 | -3.548869 | 2.530276  |
| H  | -5.418797 | -4.492695 | 2.218458  |
| C  | -2.590283 | 3.366071  | 1.396501  |
| H  | -2.345264 | 3.996404  | 2.241297  |
| H  | -3.081936 | 2.416160  | 1.573511  |
| C  | 0.266902  | 3.734609  | 1.482452  |
| O  | -0.205275 | 4.832260  | 1.740970  |
| H  | -1.133578 | 0.738284  | -1.680977 |
| Rh | 3.040765  | -1.504844 | -0.216111 |
| Rh | 1.288847  | 0.171439  | 0.021669  |
| O  | 3.482243  | -1.234763 | 1.779001  |
| O  | 1.811291  | 0.279011  | 2.033623  |
| O  | 2.716103  | 1.582682  | -0.517170 |
| O  | 0.009807  | -1.392848 | 0.510694  |
| O  | 0.907165  | -0.114475 | -1.996589 |
| O  | 2.509971  | -1.705808 | -2.197981 |
| O  | 4.338417  | 0.011523  | -0.736232 |
| O  | 1.655578  | -2.939897 | 0.305719  |
| C  | 0.465615  | -2.584463 | 0.555444  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.779466  | -0.433868 | 2.464226  |
| C | 3.906844  | 1.201289  | -0.781232 |
| C | 1.581214  | -0.976241 | -2.656566 |
| C | 1.236896  | -1.111573 | -4.123891 |
| C | -0.502647 | -3.670155 | 0.975724  |
| C | 3.123642  | -0.283612 | 3.931481  |
| C | 4.890955  | 2.287711  | -1.160649 |
| H | 5.157165  | 2.861573  | -0.265300 |
| H | 4.430809  | 2.978598  | -1.872410 |
| H | 5.796459  | 1.851049  | -1.584779 |
| H | 3.598036  | 0.691266  | 4.093247  |
| H | 3.810637  | -1.070975 | 4.245384  |
| H | 2.211401  | -0.311613 | 4.534127  |
| H | -0.337637 | -3.900706 | 2.034781  |
| H | -1.535209 | -3.340441 | 0.845795  |
| H | -0.312517 | -4.580962 | 0.402488  |
| H | 0.152719  | -1.186958 | -4.247613 |
| H | 1.731181  | -1.984102 | -4.553697 |
| H | 1.566934  | -0.211168 | -4.654231 |
| C | 1.693014  | 3.389647  | 1.830691  |
| H | 1.731010  | 2.479876  | 2.435867  |
| H | 2.261605  | 3.172251  | 0.921591  |
| H | 2.120920  | 4.240914  | 2.364769  |

# II(w)\_conf1

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.643012 | 0.431275  | 0.273986  |
| C | -0.433060 | 1.082211  | -0.307534 |
| C | -0.470571 | 2.490980  | -0.596226 |
| C | -1.797461 | 3.273364  | -0.338700 |
| C | -3.046304 | 2.452574  | -0.093689 |
| H | -1.924186 | 4.124187  | -1.004483 |
| H | -3.791165 | 3.058733  | 0.427909  |
| H | -3.474049 | 2.128077  | -1.057957 |
| H | -1.351710 | -0.238398 | 1.084871  |
| N | -2.705136 | 1.318693  | 0.763519  |
| S | -3.961836 | 0.595341  | 1.640397  |
| O | -3.319630 | -0.377066 | 2.525410  |
| O | -4.780419 | 1.698305  | 2.147560  |
| C | -4.948010 | -0.312746 | 0.449015  |
| C | -6.028473 | 0.319085  | -0.174524 |
| C | -4.610421 | -1.631285 | 0.132514  |
| C | -6.765861 | -0.378998 | -1.127776 |
| H | -6.297002 | 1.332003  | 0.106029  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -5.360509 | -2.312976 | -0.825379 |
| H  | -3.789030 | -2.119418 | 0.646328  |
| C  | -6.445522 | -1.702003 | -1.469375 |
| H  | -7.610304 | 0.108426  | -1.609086 |
| H  | -5.102677 | -3.340140 | -1.070436 |
| C  | -7.274132 | -2.456711 | -2.481455 |
| H  | -8.198279 | -2.836146 | -2.026031 |
| H  | -7.567105 | -1.813776 | -3.318579 |
| H  | -6.730158 | -3.316150 | -2.885204 |
| C  | -0.750920 | 3.369433  | 0.682674  |
| H  | -0.100887 | 4.238779  | 0.683062  |
| H  | -0.872537 | 2.837180  | 1.618991  |
| C  | 0.420945  | 3.185811  | -1.624485 |
| O  | 0.771225  | 4.339185  | -1.446167 |
| Rh | 1.245738  | -0.028918 | -0.168697 |
| Rh | 3.315214  | -1.231331 | 0.385890  |
| O  | 0.243392  | -1.835765 | 0.019009  |
| O  | 2.159619  | -2.946912 | 0.526762  |
| O  | 3.571149  | -1.569982 | -1.636462 |
| O  | 2.947039  | -0.834621 | 2.378706  |
| O  | 4.309901  | 0.576806  | 0.197946  |
| O  | 2.396306  | 1.677211  | -0.327988 |
| O  | 1.639194  | -0.494281 | -2.150728 |
| O  | 1.030213  | 0.271456  | 1.873978  |
| C  | 1.906763  | -0.189475 | 2.688163  |
| C  | 0.913877  | -2.883413 | 0.326742  |
| C  | 2.703333  | -1.145817 | -2.448813 |
| C  | 3.657486  | 1.613880  | -0.111171 |
| C  | 4.420800  | 2.916697  | -0.220153 |
| C  | 1.655139  | 0.095243  | 4.153140  |
| C  | 0.111103  | -4.160340 | 0.468267  |
| C  | 2.920364  | -1.412182 | -3.923486 |
| H  | 3.786236  | -2.059431 | -4.069731 |
| H  | 3.081583  | -0.462466 | -4.445426 |
| H  | 2.026385  | -1.875096 | -4.352356 |
| H  | 0.773917  | -5.010860 | 0.633543  |
| H  | -0.490809 | -4.321816 | -0.431425 |
| H  | -0.577846 | -4.063727 | 1.314660  |
| H  | 0.612624  | -0.121272 | 4.402799  |
| H  | 2.327688  | -0.497140 | 4.775382  |
| H  | 1.827931  | 1.159855  | 4.347630  |
| H  | 5.345219  | 2.756241  | -0.781760 |
| H  | 4.699911  | 3.249704  | 0.786021  |
| H  | 3.810205  | 3.686260  | -0.695336 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.995887 | -0.227492 | -0.548373 |
| C | 0.665356  | 2.466654  | -2.929140 |
| H | 1.113001  | 1.481624  | -2.777562 |
| H | -0.298822 | 2.307903  | -3.433017 |
| H | 1.300883  | 3.087027  | -3.564954 |

# 1x\_conf1

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.214645 | -0.926109 | 1.252355  |
| H | 0.833877  | -0.678973 | 1.465165  |
| H | -0.284523 | -2.013319 | 1.188947  |
| N | -0.471095 | -0.387419 | -0.097561 |
| S | -1.684663 | -1.068917 | -1.055118 |
| O | -1.742025 | -2.480141 | -0.669619 |
| O | -1.391615 | -0.641545 | -2.426183 |
| C | -3.254629 | -0.317391 | -0.609593 |
| C | -3.658328 | 0.860138  | -1.245117 |
| C | -4.061109 | -0.916572 | 0.360892  |
| C | -4.871422 | 1.446220  | -0.887849 |
| H | -3.044328 | 1.294331  | -2.027016 |
| C | -5.273190 | -0.319695 | 0.700233  |
| H | -3.745351 | -1.841091 | 0.830003  |
| C | -5.697216 | 0.868454  | 0.086860  |
| H | -5.186762 | 2.361443  | -1.382839 |
| H | -5.903956 | -0.787147 | 1.452494  |
| C | -7.027611 | 1.488923  | 0.441429  |
| H | -7.025696 | 2.569768  | 0.267276  |
| H | -7.834635 | 1.061209  | -0.168192 |
| H | -7.285568 | 1.312312  | 1.490942  |
| C | -0.093732 | 1.005624  | -0.377038 |
| H | -0.347067 | 1.211286  | -1.421892 |
| H | -0.659398 | 1.717293  | 0.245062  |
| C | 1.340347  | 1.232621  | -0.192370 |
| C | 2.524679  | 1.436205  | -0.032227 |
| C | -1.099172 | -0.397660 | 2.354292  |
| H | -1.177953 | 0.685945  | 2.444356  |
| C | -1.734994 | -1.176897 | 3.229991  |
| H | -1.673350 | -2.262215 | 3.176774  |
| H | -2.332509 | -0.762458 | 4.037507  |
| C | 3.935902  | 1.739519  | 0.171533  |
| O | 4.280783  | 2.880715  | 0.456115  |
| C | 4.909219  | 0.619396  | 0.025215  |
| C | 4.510109  | -0.667860 | -0.363318 |
| C | 6.264574  | 0.879443  | 0.284043  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 5.456737 | -1.683760 | -0.490292 |
| H | 3.462992 | -0.866793 | -0.571237 |
| C | 7.206175 | -0.136842 | 0.158727  |
| H | 6.550955 | 1.883118  | 0.580908  |
| C | 6.803229 | -1.419895 | -0.228617 |
| H | 5.144658 | -2.678832 | -0.794555 |
| H | 8.254221 | 0.066080  | 0.361079  |
| H | 7.539992 | -2.212757 | -0.327368 |

# 1x\_conf2

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.182760 | -2.372142 | 1.177808  |
| H | -1.675626 | -3.338107 | 1.310303  |
| H | -3.254440 | -2.554095 | 1.287019  |
| N | -1.933211 | -2.000203 | -0.228414 |
| S | -2.943699 | -0.898830 | -1.009844 |
| O | -4.257712 | -1.061513 | -0.385065 |
| O | -2.726686 | -1.119793 | -2.444327 |
| C | -2.375662 | 0.766260  | -0.654845 |
| C | -1.413132 | 1.352988  | -1.479031 |
| C | -2.902556 | 1.460813  | 0.436824  |
| C | -0.967584 | 2.642413  | -1.193280 |
| H | -1.036383 | 0.815706  | -2.342531 |
| C | -2.447405 | 2.749190  | 0.704387  |
| H | -3.661042 | 0.998140  | 1.057015  |
| C | -1.473717 | 3.359382  | -0.100679 |
| H | -0.218324 | 3.101208  | -1.833607 |
| H | -2.856564 | 3.292194  | 1.552968  |
| C | -1.006682 | 4.765696  | 0.190494  |
| H | -0.058549 | 4.985419  | -0.310099 |
| H | -1.741647 | 5.504485  | -0.155466 |
| H | -0.868729 | 4.926070  | 1.265456  |
| C | -0.662415 | -2.362266 | -0.855530 |
| H | -0.522468 | -3.446296 | -0.734800 |
| H | -0.757535 | -2.182600 | -1.930365 |
| C | 0.517811  | -1.674998 | -0.312036 |
| C | 1.471361  | -1.121103 | 0.194042  |
| C | -1.708497 | -1.395883 | 2.228648  |
| H | -0.673946 | -1.063237 | 2.165838  |
| C | -2.488737 | -0.972244 | 3.224111  |
| H | -3.527656 | -1.285949 | 3.310717  |
| H | -2.116196 | -0.301384 | 3.993522  |
| C | 2.508509  | -0.417473 | 0.933420  |
| O | 2.249715  | 0.030177  | 2.046529  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 3.849533 | -0.272561 | 0.301897  |
| C | 4.123428 | -0.782296 | -0.975402 |
| C | 4.857595 | 0.394216  | 1.016164  |
| C | 5.391991 | -0.627369 | -1.532733 |
| H | 3.341419 | -1.297446 | -1.525602 |
| C | 6.122623 | 0.547427  | 0.457749  |
| H | 4.623651 | 0.780219  | 2.002973  |
| C | 6.391270 | 0.036691  | -0.817264 |
| H | 5.601362 | -1.023203 | -2.522507 |
| H | 6.901907 | 1.063167  | 1.011936  |
| H | 7.380046 | 0.156979  | -1.251939 |

# I(x)-Ene\_conf1

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.510805  | -0.241032 | -2.228444 |
| H | -0.084592 | -1.156226 | -2.219824 |
| H | 0.114632  | 0.398432  | -3.027302 |
| N | 1.880913  | -0.627119 | -2.595243 |
| S | 2.410045  | -2.218282 | -2.361158 |
| O | 3.615732  | -2.351375 | -3.184979 |
| O | 1.233229  | -3.065688 | -2.570816 |
| C | 2.906945  | -2.374016 | -0.646944 |
| C | 1.934501  | -2.533978 | 0.343802  |
| C | 4.260460  | -2.273236 | -0.317718 |
| C | 2.331996  | -2.560024 | 1.679509  |
| H | 0.885933  | -2.624811 | 0.078498  |
| C | 4.635621  | -2.305944 | 1.022526  |
| H | 5.000380  | -2.174768 | -1.104104 |
| C | 3.680169  | -2.428478 | 2.041263  |
| H | 1.578507  | -2.675289 | 2.454597  |
| H | 5.687416  | -2.220735 | 1.283523  |
| C | 4.096406  | -2.377529 | 3.490603  |
| H | 3.324890  | -2.790810 | 4.147998  |
| H | 5.025793  | -2.931500 | 3.663078  |
| H | 4.273749  | -1.337705 | 3.794252  |
| C | 2.886351  | 0.417070  | -2.801184 |
| H | 3.682392  | -0.003504 | -3.424010 |
| H | 2.409220  | 1.210706  | -3.391000 |
| C | 3.478765  | 0.996734  | -1.585159 |
| C | 3.991060  | 1.451805  | -0.583385 |
| C | 0.394041  | 0.462393  | -0.894118 |
| H | 0.887665  | -0.015765 | -0.051810 |
| C | -0.212784 | 1.658533  | -0.710804 |
| H | -0.666979 | 2.198516  | -1.538460 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -0.191633 | 2.163930  | 0.248737  |
| C  | 4.565836  | 1.925347  | 0.666731  |
| O  | 4.375164  | 1.301565  | 1.706342  |
| Rh | -2.059431 | 0.106909  | -0.073978 |
| Rh | -4.166612 | -0.833822 | 0.623740  |
| O  | -2.892080 | 0.389086  | -1.943336 |
| O  | -4.891265 | -0.441742 | -1.265097 |
| O  | -3.524161 | -2.675858 | -0.027191 |
| O  | -4.755167 | 1.033861  | 1.241726  |
| O  | -3.319260 | -1.169259 | 2.472557  |
| O  | -1.353459 | -0.231683 | 1.834921  |
| O  | -1.511502 | -1.823523 | -0.607107 |
| O  | -2.805439 | 1.949413  | 0.538543  |
| C  | -3.967892 | 2.011974  | 1.057065  |
| C  | -4.110199 | 0.058003  | -2.132126 |
| C  | -2.350032 | -2.781142 | -0.494037 |
| C  | -2.127151 | -0.785929 | 2.684261  |
| C  | -1.582258 | -0.976993 | 4.082751  |
| C  | -4.457009 | 3.385240  | 1.461838  |
| C  | -4.658162 | 0.255297  | -3.528233 |
| C  | -1.889165 | -4.151326 | -0.935636 |
| H  | -1.691677 | -4.763304 | -0.047588 |
| H  | -0.979539 | -4.079593 | -1.534573 |
| H  | -2.686411 | -4.642471 | -1.500307 |
| H  | -5.748284 | 0.304567  | -3.505326 |
| H  | -4.359535 | -0.597138 | -4.149799 |
| H  | -4.240756 | 1.160557  | -3.975627 |
| H  | -4.798295 | 3.918873  | 0.567066  |
| H  | -5.290898 | 3.302011  | 2.160951  |
| H  | -3.640474 | 3.961678  | 1.903930  |
| H  | -1.931863 | -0.151568 | 4.714025  |
| H  | -0.490620 | -0.970046 | 4.075397  |
| H  | -1.961239 | -1.908716 | 4.509431  |
| C  | 5.378835  | 3.175777  | 0.625448  |
| C  | 5.594809  | 3.882596  | -0.566236 |
| C  | 5.937130  | 3.648083  | 1.823825  |
| C  | 6.359774  | 5.048219  | -0.559693 |
| H  | 5.162675  | 3.515559  | -1.492279 |
| C  | 6.699706  | 4.811763  | 1.828025  |
| H  | 5.757313  | 3.086131  | 2.734461  |
| C  | 6.911981  | 5.513486  | 0.636034  |
| H  | 6.525130  | 5.592931  | -1.485007 |
| H  | 7.130111  | 5.175565  | 2.756923  |
| H  | 7.507907  | 6.422298  | 0.640518  |

# I(x)-Ene\_conf2

## 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.712815 | -1.046761 | -0.159442 |
| H  | -0.193544 | -0.875533 | -1.102436 |
| H  | -0.690392 | -2.124058 | 0.043221  |
| N  | -2.124118 | -0.662836 | -0.366640 |
| S  | -2.476704 | 0.522741  | -1.547821 |
| O  | -3.839853 | 0.272034  | -2.006489 |
| O  | -1.346663 | 0.480239  | -2.481258 |
| C  | -2.464329 | 2.119743  | -0.726583 |
| C  | -1.252106 | 2.804652  | -0.584902 |
| C  | -3.657975 | 2.658108  | -0.239454 |
| C  | -1.243890 | 4.037563  | 0.062616  |
| H  | -0.335710 | 2.378281  | -0.981268 |
| C  | -3.624813 | 3.894991  | 0.405988  |
| H  | -4.596300 | 2.127679  | -0.363100 |
| C  | -2.426323 | 4.602558  | 0.566888  |
| H  | -0.304418 | 4.574002  | 0.173369  |
| H  | -4.552043 | 4.315426  | 0.786796  |
| C  | -2.406516 | 5.954860  | 1.239133  |
| H  | -1.505062 | 6.087051  | 1.847432  |
| H  | -2.417075 | 6.762867  | 0.495628  |
| H  | -3.278404 | 6.094064  | 1.885879  |
| C  | -2.950471 | -0.756770 | 0.852946  |
| H  | -2.714276 | -1.734802 | 1.292625  |
| H  | -2.650484 | -0.000890 | 1.597341  |
| C  | -4.395951 | -0.648284 | 0.663360  |
| C  | -5.596608 | -0.495197 | 0.616592  |
| C  | -0.019703 | -0.293183 | 0.956208  |
| H  | -0.070739 | 0.792221  | 0.906050  |
| C  | 0.575927  | -0.873625 | 2.025152  |
| H  | 0.602988  | -1.954212 | 2.143373  |
| H  | 0.984258  | -0.283168 | 2.839099  |
| C  | -6.991936 | -0.104376 | 0.472929  |
| O  | -7.269088 | 1.088351  | 0.382424  |
| Rh | 2.505457  | -0.467067 | 0.498135  |
| Rh | 4.677542  | -0.337167 | -0.526824 |
| O  | 2.246909  | -2.278031 | -0.462842 |
| O  | 4.308660  | -2.162935 | -1.401970 |
| O  | 3.820334  | 0.590790  | -2.149214 |
| O  | 5.475314  | -1.279612 | 1.114527  |
| O  | 4.923843  | 1.485896  | 0.409042  |
| O  | 2.889724  | 1.346031  | 1.406281  |

|                              |            |           |           |    |           |           |           |
|------------------------------|------------|-----------|-----------|----|-----------|-----------|-----------|
| O                            | 1.782935   | 0.535603  | -1.167209 | C  | -6.213129 | -0.920145 | 0.146791  |
| O                            | 3.431992   | -1.451282 | 2.079305  | C  | -5.451344 | 1.008287  | -1.119557 |
| C                            | 4.692920   | -1.636225 | 2.048032  | C  | -7.047398 | -1.273236 | -0.907464 |
| C                            | 3.190485   | -2.727684 | -1.196469 | H  | -6.184328 | -1.514164 | 1.054377  |
| C                            | 2.573458   | 0.824533  | -2.128107 | C  | -6.294545 | 0.636836  | -2.169708 |
| C                            | 4.000768   | 1.925150  | 1.161986  | H  | -4.837697 | 1.900792  | -1.180253 |
| C                            | 4.229042   | 3.273182  | 1.810447  | C  | -7.101294 | -0.503202 | -2.082666 |
| C                            | 5.299196   | -2.350774 | 3.235872  | H  | -7.671929 | -2.159159 | -0.819699 |
| C                            | 2.933421   | -4.044168 | -1.895051 | H  | -6.326943 | 1.248421  | -3.067811 |
| C                            | 1.965601   | 1.524929  | -3.321026 | C  | -8.022498 | -0.898299 | -3.212289 |
| H                            | 2.062646   | 2.608895  | -3.183435 | H  | -7.867605 | -1.943370 | -3.505817 |
| H                            | 0.905739   | 1.276590  | -3.405727 | H  | -9.074619 | -0.800263 | -2.916262 |
| H                            | 2.507113   | 1.252562  | -4.229768 | H  | -7.865688 | -0.272397 | -4.095870 |
| H                            | 3.859430   | -4.443118 | -2.311784 | C  | -2.165666 | -0.409148 | 0.306057  |
| H                            | 2.213769   | -3.883868 | -2.705967 | H  | -1.718291 | -1.395168 | 0.146906  |
| H                            | 2.490313   | -4.758526 | -1.195669 | H  | -2.657714 | -0.129501 | -0.631554 |
| H                            | 4.869536   | -3.355045 | 3.313717  | C  | -1.090286 | 0.549123  | 0.616184  |
| H                            | 6.382595   | -2.420703 | 3.129427  | C  | -0.249964 | 1.372819  | 0.948026  |
| H                            | 5.046894   | -1.813675 | 4.155646  | C  | -2.505743 | -2.568930 | 2.547795  |
| H                            | 5.266624   | 3.354754  | 2.143841  | H  | -3.414206 | -3.149841 | 2.388792  |
| H                            | 3.544777   | 3.420315  | 2.647878  | C  | -1.321872 | -3.177773 | 2.635913  |
| H                            | 4.055662   | 4.059885  | 1.066952  | H  | -0.401454 | -2.613803 | 2.768602  |
| C                            | -8.027665  | -1.172393 | 0.443023  | H  | -1.233267 | -4.259858 | 2.574952  |
| C                            | -7.686460  | -2.531092 | 0.502854  | C  | 0.410726  | 2.550959  | 1.539285  |
| C                            | -9.377002  | -0.796652 | 0.346729  | O  | 0.624924  | 2.569055  | 2.741239  |
| C                            | -8.684180  | -3.504251 | 0.467323  | Rh | 1.412971  | -0.334571 | -0.006106 |
| H                            | -6.641039  | -2.817492 | 0.570349  | Rh | 3.327352  | -1.555869 | -0.797982 |
| C                            | -10.370633 | -1.769621 | 0.313794  | O  | 2.729119  | 1.164624  | 0.526765  |
| H                            | -9.617639  | 0.260315  | 0.298029  | O  | 4.522276  | 0.014480  | -0.239172 |
| C                            | -10.025248 | -3.124620 | 0.373901  | O  | 3.522331  | -2.353894 | 1.086969  |
| H                            | -8.417007  | -4.556381 | 0.510162  | O  | 3.044638  | -0.684104 | -2.642504 |
| H                            | -11.414482 | -1.477525 | 0.239671  | O  | 2.079746  | -3.101232 | -1.333519 |
| H                            | -10.802615 | -3.883621 | 0.346100  | O  | 0.264197  | -1.955587 | -0.616443 |
| <b>I(x)-Yne_conf3</b>        |            |           |           | O  | 1.696970  | -1.231234 | 1.832279  |
| <b>0 imaginary frequency</b> |            |           |           | O  | 1.244532  | 0.479021  | -1.898626 |
| C                            | -2.695864  | -1.079431 | 2.654621  | C  | 2.087038  | 0.136250  | -2.793417 |
| H                            | -3.454635  | -0.842927 | 3.404320  | C  | 3.975431  | 1.024301  | 0.305395  |
| H                            | -1.760220  | -0.586541 | 2.949194  | C  | 2.687976  | -2.018340 | 1.986256  |
| N                            | -3.179416  | -0.534862 | 1.362620  | C  | 0.835054  | -2.975012 | -1.130184 |
| S                            | -4.354097  | 0.699187  | 1.397286  | C  | -0.065409 | -4.120320 | -1.536182 |
| O                            | -3.758207  | 1.995715  | 1.050480  | C  | 1.931974  | 0.785163  | -4.151179 |
| O                            | -5.093782  | 0.517914  | 2.650176  | C  | 4.876824  | 2.148740  | 0.760158  |
| C                            | -5.411867  | 0.220428  | 0.029139  | C  | 2.896043  | -2.613063 | 3.361432  |
|                              |            |           |           | H  | 2.854948  | -3.705264 | 3.296616  |

|                                                                 |           |           |           |    |           |           |           |
|-----------------------------------------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H                                                               | 2.141147  | -2.251270 | 4.060802  | H  | -4.094376 | -0.690726 | 1.779081  |
| H                                                               | 3.894012  | -2.344939 | 3.722661  | C  | -6.310231 | -1.378400 | -0.734892 |
| H                                                               | 5.792614  | 2.165268  | 0.165908  | H  | -7.187242 | 0.115202  | -2.019361 |
| H                                                               | 5.146342  | 1.981978  | 1.809769  | H  | -5.274398 | -2.594456 | 0.713762  |
| H                                                               | 4.351442  | 3.103874  | 0.693146  | C  | -7.063954 | -2.532617 | -1.351511 |
| H                                                               | 2.189538  | 1.847251  | -4.071533 | H  | -6.496810 | -3.466334 | -1.279824 |
| H                                                               | 2.587457  | 0.308437  | -4.881392 | H  | -8.021795 | -2.692824 | -0.838976 |
| H                                                               | 0.889790  | 0.721151  | -4.477294 | H  | -7.287140 | -2.348093 | -2.407368 |
| H                                                               | -0.718350 | -4.387549 | -0.699815 | C  | -0.768193 | 4.322639  | -0.146976 |
| H                                                               | 0.526811  | -4.982928 | -1.844709 | H  | 0.022816  | 5.040929  | -0.332910 |
| H                                                               | -0.705374 | -3.801473 | -2.366342 | H  | -1.157436 | 4.243411  | 0.861863  |
| C                                                               | 0.724800  | 3.697314  | 0.642641  | C  | 1.506825  | 2.972031  | -1.065720 |
| C                                                               | 0.507450  | 3.643543  | -0.741165 | O  | 1.359356  | 3.403435  | -2.202104 |
| C                                                               | 1.247655  | 4.864148  | 1.222354  | H  | -1.962479 | 0.207627  | 0.048017  |
| C                                                               | 0.812344  | 4.748474  | -1.535965 | Rh | 1.908989  | -2.713263 | -0.139533 |
| H                                                               | 0.120841  | 2.735668  | -1.192102 | Rh | 0.893756  | -0.510611 | 0.092599  |
| C                                                               | 1.549845  | 5.964322  | 0.425674  | O  | 3.285891  | -2.151932 | 1.285276  |
| H                                                               | 1.403217  | 4.883959  | 2.296111  | O  | 2.321532  | -0.111388 | 1.536892  |
| C                                                               | 1.331677  | 5.907948  | -0.955473 | O  | 2.166241  | 0.128207  | -1.404086 |
| H                                                               | 0.642837  | 4.705645  | -2.608504 | O  | -0.310828 | -1.329831 | 1.579595  |
| H                                                               | 1.951436  | 6.867578  | 0.876814  | O  | -0.484515 | -1.110748 | -1.343631 |
| H                                                               | 1.565081  | 6.768656  | -1.576931 | O  | 0.472085  | -3.158404 | -1.556341 |
| <b>I-TS-II(x)_conf1</b>                                         |           |           |           | O  | 3.112849  | -1.922458 | -1.618924 |
| <b>1 imaginary frequency, value = -316.9622 cm<sup>-1</sup></b> |           |           |           | O  | 0.649287  | -3.374926 | 1.357258  |
| C                                                               | -1.633935 | 1.103526  | 0.593746  | C  | -0.157978 | -2.557679 | 1.892431  |
| C                                                               | -0.231102 | 1.389464  | 0.167217  | C  | 3.192468  | -1.002764 | 1.812965  |
| C                                                               | 0.326233  | 2.448915  | -0.312775 | C  | 2.987837  | -0.698959 | -1.924409 |
| C                                                               | -1.372883 | 3.674161  | -1.181425 | C  | -0.394618 | -2.282114 | -1.845951 |
| C                                                               | -2.558406 | 2.766291  | -0.989084 | C  | -1.423930 | -2.636858 | -2.899452 |
| H                                                               | -1.012051 | 3.820422  | -2.194921 | C  | -1.002012 | -3.075701 | 3.038907  |
| H                                                               | -3.471545 | 3.352324  | -1.141468 | C  | 4.213956  | -0.636080 | 2.868877  |
| H                                                               | -2.543096 | 1.961499  | -1.739378 | C  | 3.895018  | -0.146797 | -3.002966 |
| H                                                               | -1.635049 | 0.855248  | 1.657304  | H  | 4.525693  | 0.639426  | -2.574648 |
| N                                                               | -2.564824 | 2.228150  | 0.372905  | H  | 3.290895  | 0.311808  | -3.792092 |
| S                                                               | -4.055491 | 2.142734  | 1.174540  | H  | 4.520397  | -0.937515 | -3.419898 |
| O                                                               | -3.741486 | 1.791269  | 2.559469  | H  | 4.833360  | 0.187742  | 2.498484  |
| O                                                               | -4.764718 | 3.376001  | 0.821303  | H  | 4.845764  | -1.493597 | 3.104895  |
| C                                                               | -4.957487 | 0.771485  | 0.449988  | H  | 3.703157  | -0.285428 | 3.771116  |
| C                                                               | -5.833893 | 1.007754  | -0.612656 | H  | -0.434830 | -2.968433 | 3.971138  |
| C                                                               | -4.754812 | -0.523812 | 0.934908  | H  | -1.923974 | -2.497939 | 3.133315  |
| C                                                               | -6.500939 | -0.067612 | -1.196162 | H  | -1.222761 | -4.135910 | 2.896825  |
| H                                                               | -6.005580 | 2.021858  | -0.957418 | H  | -2.427144 | -2.393995 | -2.536317 |
| C                                                               | -5.429123 | -1.586700 | 0.336440  | H  | -1.360511 | -3.695721 | -3.154748 |
|                                                                 |           |           |           | H  | -1.243166 | -2.035384 | -3.797276 |

|   |          |          |           |
|---|----------|----------|-----------|
| C | 2.818921 | 3.048831 | -0.366848 |
| C | 2.947651 | 2.865414 | 1.016215  |
| C | 3.945504 | 3.405546 | -1.129574 |
| C | 4.188433 | 3.046603 | 1.629936  |
| H | 2.085836 | 2.579573 | 1.606834  |
| C | 5.182779 | 3.567241 | -0.516956 |
| H | 3.821770 | 3.558405 | -2.196511 |
| C | 5.305000 | 3.391925 | 0.867332  |
| H | 4.279910 | 2.917210 | 2.704552  |
| H | 6.051536 | 3.839014 | -1.110240 |
| H | 6.270032 | 3.529973 | 1.347961  |

# I-TS-II(x)\_conf2

1 imaginary frequency, value = -327.6742 cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.816019 | -0.144351 | -0.972933 |
| C | -0.656838 | 0.765527  | -0.724025 |
| C | -0.477773 | 2.020710  | -0.966976 |
| C | -2.013306 | 2.529832  | -2.585669 |
| C | -2.641433 | 1.195623  | -2.871947 |
| H | -1.381131 | 2.961089  | -3.355882 |
| H | -3.564278 | 1.346512  | -3.444316 |
| H | -1.966425 | 0.586099  | -3.491339 |
| H | -2.130735 | -0.572412 | -0.017527 |
| N | -2.973973 | 0.517326  | -1.611722 |
| S | -4.388495 | -0.443919 | -1.650574 |
| O | -5.322862 | 0.269411  | -2.529995 |
| O | -4.051702 | -1.851197 | -1.900311 |
| C | -4.961656 | -0.308076 | 0.039357  |
| C | -4.784030 | -1.379298 | 0.914298  |
| C | -5.614738 | 0.858031  | 0.449404  |
| C | -5.251955 | -1.268103 | 2.224392  |
| H | -4.301731 | -2.286018 | 0.565568  |
| C | -6.075341 | 0.949362  | 1.759059  |
| H | -5.775670 | 1.667177  | -0.255506 |
| C | -5.896302 | -0.106564 | 2.668624  |
| H | -5.119201 | -2.101942 | 2.908877  |
| H | -6.590894 | 1.850719  | 2.081354  |
| C | -6.377645 | 0.018182  | 4.094426  |
| H | -7.337015 | 0.544004  | 4.148425  |
| H | -6.499240 | -0.962683 | 4.564238  |
| H | -5.661261 | 0.587246  | 4.701562  |
| C | -2.202119 | 3.201164  | -1.413472 |
| H | -1.811289 | 4.204499  | -1.283687 |
| H | -2.887038 | 2.824251  | -0.662774 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.558888  | 3.079094  | -1.174030 |
| O  | 0.731673  | 3.542085  | -2.294114 |
| H  | -1.455891 | -0.982207 | -1.584647 |
| Rh | 2.897671  | -1.997735 | 0.386280  |
| Rh | 1.073317  | -0.457866 | -0.094737 |
| O  | 3.050347  | -1.127030 | 2.247858  |
| O  | 1.331699  | 0.295392  | 1.820797  |
| O  | 2.493847  | 0.842023  | -0.843978 |
| O  | -0.208949 | -1.893452 | 0.696250  |
| O  | 0.939271  | -1.361742 | -1.956866 |
| O  | 2.641983  | -2.792531 | -1.502849 |
| O  | 4.195379  | -0.585220 | -0.375309 |
| O  | 1.499081  | -3.326823 | 1.121138  |
| C  | 0.276022  | -2.998429 | 1.114363  |
| C  | 2.248900  | -0.196014 | 2.560187  |
| C  | 3.725205  | 0.505166  | -0.819166 |
| C  | 1.738863  | -2.314061 | -2.251209 |
| C  | 1.589511  | -2.906218 | -3.636858 |
| C  | -0.722287 | -4.011738 | 1.635650  |
| C  | 2.392975  | 0.410268  | 3.940966  |
| C  | 4.702683  | 1.515911  | -1.380080 |
| H  | 4.593971  | 2.463822  | -0.843435 |
| H  | 4.465825  | 1.706351  | -2.432097 |
| H  | 5.726472  | 1.149805  | -1.290749 |
| H  | 2.736698  | 1.445841  | 3.843950  |
| H  | 3.110069  | -0.157571 | 4.535608  |
| H  | 1.419850  | 0.429478  | 4.441268  |
| H  | -1.403404 | -3.531814 | 2.344767  |
| H  | -1.323423 | -4.387657 | 0.799992  |
| H  | -0.206915 | -4.846330 | 2.113334  |
| H  | 0.537828  | -3.135024 | -3.832971 |
| H  | 2.197121  | -3.807010 | -3.735155 |
| H  | 1.911172  | -2.168389 | -4.380406 |
| C  | 1.274544  | 3.622200  | 0.012847  |
| C  | 0.903368  | 3.306904  | 1.326444  |
| C  | 2.305511  | 4.551191  | -0.215437 |
| C  | 1.551491  | 3.921615  | 2.399132  |
| H  | 0.122989  | 2.578311  | 1.507647  |
| C  | 2.958092  | 5.149923  | 0.856261  |
| H  | 2.568379  | 4.791961  | -1.240113 |
| C  | 2.578208  | 4.838179  | 2.167718  |
| H  | 1.252369  | 3.682564  | 3.415730  |
| H  | 3.755472  | 5.865567  | 0.675698  |
| H  | 3.081566  | 5.313714  | 3.005478  |

## II(x)\_conf1

### 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 1.712582  | -0.265210 | -0.752069 |
| C  | 0.456753  | 0.536521  | -0.837320 |
| C  | 0.421773  | 1.689055  | -1.698744 |
| C  | 1.734943  | 2.120047  | -2.422483 |
| C  | 3.024867  | 1.497220  | -1.930940 |
| H  | 1.784807  | 3.189483  | -2.616922 |
| H  | 3.797569  | 1.586938  | -2.698271 |
| H  | 3.370577  | 2.025993  | -1.025723 |
| H  | 1.472291  | -1.323989 | -0.877110 |
| N  | 2.796279  | 0.074730  | -1.685746 |
| S  | 4.145872  | -0.948244 | -1.681227 |
| O  | 3.611246  | -2.308899 | -1.620477 |
| O  | 5.001207  | -0.488046 | -2.776908 |
| C  | 5.010562  | -0.630832 | -0.141870 |
| C  | 6.002578  | 0.353021  | -0.098492 |
| C  | 4.661482  | -1.345549 | 1.007987  |
| C  | 6.638885  | 0.624353  | 1.111299  |
| H  | 6.285498  | 0.876854  | -1.005427 |
| C  | 5.308609  | -1.058398 | 2.208809  |
| H  | 3.911817  | -2.127731 | 0.953343  |
| C  | 6.303570  | -0.072431 | 2.281582  |
| H  | 7.414666  | 1.385314  | 1.145756  |
| H  | 5.040873  | -1.615069 | 3.103449  |
| C  | 7.021684  | 0.206895  | 3.580394  |
| H  | 7.897035  | -0.446524 | 3.692159  |
| H  | 7.379173  | 1.240647  | 3.626919  |
| H  | 6.372157  | 0.030504  | 4.443985  |
| C  | 0.766893  | 1.334380  | -3.195325 |
| H  | 0.085293  | 1.845790  | -3.866869 |
| H  | 0.983120  | 0.294331  | -3.410027 |
| C  | -0.579173 | 2.837621  | -1.575592 |
| O  | -1.114769 | 3.289084  | -2.577988 |
| Rh | -1.147916 | -0.374451 | -0.026139 |
| Rh | -3.135503 | -1.654763 | 0.648913  |
| O  | -0.024460 | -1.635309 | 1.186173  |
| O  | -1.868748 | -2.804402 | 1.818406  |
| O  | -3.367268 | -0.323159 | 2.208173  |
| O  | -2.795227 | -2.919241 | -0.952226 |
| O  | -4.250278 | -0.407434 | -0.575141 |
| O  | -2.408753 | 0.779023  | -1.170159 |
| O  | -1.495193 | 0.819701  | 1.623197  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -0.957495 | -1.744746 | -1.580606 |
| C | -1.803248 | -2.699911 | -1.701464 |
| C | -0.628272 | -2.565332 | 1.828078  |
| C | -2.511597 | 0.593864  | 2.366029  |
| C | -3.662462 | 0.520112  | -1.200875 |
| C | -4.508289 | 1.417576  | -2.079578 |
| C | -1.579774 | -3.630444 | -2.874809 |
| C | 0.254949  | -3.466946 | 2.666820  |
| C | -2.674267 | 1.507361  | 3.562680  |
| H | -3.691007 | 1.439454  | 3.953566  |
| H | -2.433209 | 2.536517  | 3.286066  |
| H | -1.973051 | 1.196554  | 4.346201  |
| H | -0.353507 | -4.131577 | 3.281847  |
| H | 0.911470  | -2.862368 | 3.299951  |
| H | 0.891131  | -4.065858 | 2.005410  |
| H | -0.522796 | -3.902768 | -2.942152 |
| H | -2.198291 | -4.523633 | -2.773688 |
| H | -1.847865 | -3.110579 | -3.801699 |
| H | -5.287874 | 1.888242  | -1.471859 |
| H | -5.009839 | 0.809081  | -2.839228 |
| H | -3.893633 | 2.180280  | -2.560022 |
| H | 2.024890  | -0.156739 | 0.306584  |
| C | -0.740161 | 3.524793  | -0.258647 |
| C | 0.123192  | 3.313997  | 0.824546  |
| C | -1.749133 | 4.497069  | -0.149805 |
| C | -0.012813 | 4.064916  | 1.992429  |
| H | 0.908679  | 2.568335  | 0.763595  |
| C | -1.897956 | 5.231931  | 1.021315  |
| H | -2.399340 | 4.662732  | -1.002089 |
| C | -1.024041 | 5.021317  | 2.094529  |
| H | 0.667456  | 3.898098  | 2.822822  |
| H | -2.686201 | 5.975757  | 1.098647  |
| H | -1.130866 | 5.604828  | 3.005352  |

## 1v\_conf1

### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.654806  | 1.641531  | -0.080967 |
| H | 1.745103  | 1.645140  | -0.207450 |
| H | 0.401094  | 2.481268  | 0.567860  |
| N | 0.357074  | 0.405141  | 0.668282  |
| S | -1.024634 | 0.328385  | 1.639014  |
| O | -1.253661 | 1.695662  | 2.109112  |
| O | -0.798794 | -0.790127 | 2.558736  |
| C | -2.417374 | -0.135152 | 0.602420  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | -2.708408 | -1.487651 | 0.406919  | H  | -4.077224 | -1.543349 | -1.481503 |
| C                            | -3.199349 | 0.856615  | 0.004694  | C  | -7.292583 | -0.020631 | 0.055691  |
| C                            | -3.781447 | -1.842994 | -0.409460 | H  | -6.061068 | 0.458832  | 1.766564  |
| H                            | -2.120190 | -2.247896 | 0.909702  | C  | -7.354395 | -0.602232 | -1.218163 |
| C                            | -4.270801 | 0.482633  | -0.802382 | H  | -6.207310 | -1.603680 | -2.746082 |
| H                            | -2.974885 | 1.901729  | 0.183160  | H  | -8.194820 | 0.393719  | 0.498615  |
| C                            | -4.578202 | -0.868294 | -1.025526 | C  | -8.659681 | -0.680927 | -1.973488 |
| H                            | -4.009909 | -2.895158 | -0.560302 | H  | -8.508161 | -0.551644 | -3.050502 |
| H                            | -4.883062 | 1.253478  | -1.264218 | H  | -9.138363 | -1.658402 | -1.828409 |
| C                            | -5.760808 | -1.258394 | -1.880018 | H  | -9.366394 | 0.082892  | -1.634217 |
| H                            | -5.663906 | -2.281470 | -2.256783 | C  | -1.912722 | 0.937875  | -0.720657 |
| H                            | -6.694579 | -1.207441 | -1.304574 | H  | -1.689881 | -0.109252 | -0.948034 |
| H                            | -5.873381 | -0.587603 | -2.738650 | H  | -2.540913 | 1.343967  | -1.530933 |
| C                            | 0.870578  | -0.873123 | 0.154013  | C  | -0.641903 | 1.666672  | -0.708951 |
| H                            | 0.629879  | -1.642650 | 0.894157  | C  | 0.396767  | 2.307619  | -0.722489 |
| H                            | 0.384599  | -1.164668 | -0.791765 | C  | -2.322994 | 3.420833  | 1.036098  |
| C                            | 2.318420  | -0.848049 | -0.048941 | H  | -1.471339 | 3.260388  | 1.693673  |
| C                            | 3.512602  | -0.833505 | -0.244616 | C  | -2.487626 | 4.591214  | 0.418843  |
| C                            | -0.017027 | 1.781588  | -1.424690 | H  | -3.325949 | 4.776061  | -0.250758 |
| H                            | 0.091704  | 0.947100  | -2.118010 | H  | -1.784070 | 5.405866  | 0.561902  |
| C                            | -0.677366 | 2.873220  | -1.812949 | C  | 1.332020  | 3.419983  | -0.602556 |
| H                            | -0.799146 | 3.730586  | -1.153652 | O  | 1.280098  | 4.225860  | 0.302353  |
| H                            | -1.112553 | 2.957027  | -2.805206 | Rh | 1.489701  | 0.061946  | -0.238987 |
| C                            | 4.937657  | -0.897564 | -0.487644 | Rh | 2.823185  | -1.832633 | 0.388004  |
| O                            | 5.525631  | -1.895096 | -0.849871 | O  | 2.938828  | 1.259226  | 0.629635  |
| O                            | 5.520181  | 0.297272  | -0.261512 | O  | 4.191012  | -0.537222 | 1.214550  |
| C                            | 6.942729  | 0.328054  | -0.474225 | O  | 1.796949  | -1.901483 | 2.167332  |
| H                            | 7.180688  | 0.076527  | -1.511177 | O  | 3.778988  | -1.682665 | -1.431718 |
| H                            | 7.245751  | 1.349907  | -0.245952 | O  | 1.400016  | -3.061057 | -0.439027 |
| H                            | 7.444482  | -0.381185 | 0.189177  | O  | 0.160189  | -1.280193 | -1.083716 |
| <b>I(v)-Yne_conf1</b>        |           |           |           | O  | 0.546101  | -0.106046 | 1.580284  |
| <b>0 imaginary frequency</b> |           |           |           | O  | 2.516178  | 0.104143  | -2.033023 |
| C                            | -3.287189 | 2.271559  | 0.915243  | C  | 3.424122  | -0.764028 | -2.236891 |
| H                            | -3.771736 | 2.106447  | 1.882472  | C  | 3.958508  | 0.710055  | 1.160758  |
| H                            | -4.068679 | 2.510066  | 0.175317  | C  | 0.879782  | -1.044599 | 2.375262  |
| N                            | -2.608380 | 1.002941  | 0.574140  | C  | 0.377734  | -2.533738 | -0.973398 |
| S                            | -3.381632 | -0.413455 | 1.094198  | C  | -0.690139 | -3.454665 | -1.514080 |
| O                            | -3.696293 | -0.208856 | 2.509706  | C  | 4.172830  | -0.682542 | -3.549915 |
| O                            | -2.552836 | -1.535956 | 0.646897  | C  | 4.999521  | 1.634926  | 1.752622  |
| C                            | -4.939533 | -0.508818 | 0.203617  | C  | 0.113527  | -1.130703 | 3.674408  |
| C                            | -4.974751 | -1.100439 | -1.063057 | H  | 0.454706  | -1.981923 | 4.265461  |
| C                            | -6.096574 | 0.029498  | 0.771083  | H  | -0.955643 | -1.222645 | 3.459153  |
| C                            | -6.178259 | -1.140037 | -1.762996 | H  | 0.255088  | -0.204260 | 4.240845  |
|                              |           |           |           | H  | 5.713885  | 1.914207  | 0.968820  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 5.547254  | 1.127507  | 2.549315  |
| H | 4.527499  | 2.545386  | 2.128439  |
| H | 3.628734  | -0.063290 | -4.265008 |
| H | 5.158706  | -0.238107 | -3.370488 |
| H | 4.330368  | -1.686571 | -3.952485 |
| H | -0.346161 | -4.489920 | -1.503721 |
| H | -0.958444 | -3.156105 | -2.532281 |
| H | -1.580274 | -3.350909 | -0.884558 |
| O | 2.207766  | 3.454028  | -1.616966 |
| C | 3.172888  | 4.516747  | -1.548263 |
| H | 3.781651  | 4.413923  | -0.646224 |
| H | 3.786435  | 4.406486  | -2.442139 |
| H | 2.674930  | 5.489919  | -1.537980 |

#### I(v)-Ene\_conf2

##### 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.813105 | 0.275173  | 0.612576  |
| H | 2.065732 | -0.786480 | 0.671864  |
| H | 1.533816 | 0.488337  | -0.423120 |
| N | 2.991595 | 1.107003  | 0.955113  |
| S | 4.282130 | 0.347858  | 1.739753  |
| O | 3.683753 | -0.508177 | 2.763148  |
| O | 5.240320 | 1.409559  | 2.058452  |
| C | 5.050251 | -0.728812 | 0.523730  |
| C | 5.991402 | -0.204591 | -0.369116 |
| C | 4.680059 | -2.073929 | 0.459262  |
| C | 6.544045 | -1.034480 | -1.341121 |
| H | 6.303224 | 0.831227  | -0.283834 |
| C | 5.245818 | -2.890141 | -0.520481 |
| H | 3.977898 | -2.475568 | 1.181875  |
| C | 6.179452 | -2.386904 | -1.435998 |
| H | 7.278234 | -0.628565 | -2.033012 |
| H | 4.960642 | -3.938053 | -0.569143 |
| C | 6.805762 | -3.279918 | -2.480659 |
| H | 6.866838 | -2.776913 | -3.452195 |
| H | 7.828679 | -3.559756 | -2.196956 |
| H | 6.235804 | -4.204826 | -2.611798 |
| C | 3.328108 | 2.206567  | 0.039021  |
| H | 4.215549 | 2.707447  | 0.436843  |
| H | 3.577622 | 1.831470  | -0.968814 |
| C | 2.239088 | 3.175368  | -0.082007 |
| C | 1.337985 | 3.972978  | -0.212259 |
| C | 0.650955 | 0.582653  | 1.524184  |
| H | 0.284128 | 1.606007  | 1.501398  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.135615  | -0.298976 | 2.412606  |
| H  | 0.534279  | -1.305419 | 2.506782  |
| H  | -0.622881 | -0.002392 | 3.128618  |
| C  | 0.218478  | 4.882861  | -0.311355 |
| O  | -0.896057 | 4.648142  | 0.110817  |
| Rh | -1.437976 | -0.512360 | 0.501290  |
| Rh | -3.306620 | -1.080170 | -0.914756 |
| O  | -0.579096 | -2.327126 | -0.008138 |
| O  | -2.368530 | -2.882690 | -1.290744 |
| O  | -4.244188 | -1.910475 | 0.710115  |
| O  | -2.335621 | -0.231816 | -2.515509 |
| O  | -4.116126 | 0.762812  | -0.469225 |
| O  | -2.394589 | 1.254344  | 0.923240  |
| O  | -2.480971 | -1.425529 | 2.048662  |
| O  | -0.585170 | 0.341569  | -1.197982 |
| C  | -1.201862 | 0.297136  | -2.313533 |
| C  | -1.234419 | -3.113941 | -0.769377 |
| C  | -3.641374 | -1.903883 | 1.826945  |
| C  | -3.491417 | 1.527592  | 0.331696  |
| C  | -4.081555 | 2.887458  | 0.624722  |
| C  | -0.495697 | 0.918495  | -3.499218 |
| C  | -0.608779 | -4.463667 | -1.049453 |
| C  | -4.362296 | -2.501138 | 3.015464  |
| H  | -5.253925 | -3.039862 | 2.691186  |
| H  | -4.653919 | -1.696318 | 3.699547  |
| H  | -3.690259 | -3.169870 | 3.560784  |
| H  | -1.003366 | -4.880899 | -1.977831 |
| H  | -0.856634 | -5.146154 | -0.227876 |
| H  | 0.479167  | -4.375796 | -1.098226 |
| H  | -0.079176 | 1.889393  | -3.216800 |
| H  | 0.337231  | 0.272930  | -3.800920 |
| H  | -1.183676 | 1.029065  | -4.338812 |
| H  | -4.965060 | 3.064152  | 0.009285  |
| H  | -3.320861 | 3.652457  | 0.441086  |
| H  | -4.354634 | 2.942326  | 1.684230  |
| O  | 0.574119  | 6.024191  | -0.933017 |
| C  | -0.477559 | 6.996671  | -1.069365 |
| H  | -0.850914 | 7.296338  | -0.086695 |
| H  | -0.021712 | 7.843143  | -1.582819 |
| H  | -1.303997 | 6.587785  | -1.656675 |

#### I-TS-II(v)\_conf1

##### 1 imaginary frequency, value = -293.3057 cm<sup>-1</sup>

|   |           |          |          |
|---|-----------|----------|----------|
| C | -1.644223 | 0.851793 | 0.612549 |
|---|-----------|----------|----------|

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.358790 | 1.496065  | 0.223799  |
| C  | -0.058103 | 2.687219  | -0.149567 |
| C  | -1.989657 | 3.644090  | -0.789302 |
| C  | -2.944629 | 2.477718  | -0.729238 |
| H  | -1.693317 | 3.998345  | -1.772366 |
| H  | -3.966579 | 2.864610  | -0.802255 |
| H  | -2.775447 | 1.806593  | -1.584572 |
| H  | -1.551396 | 0.475976  | 1.633991  |
| N  | -2.800471 | 1.765959  | 0.543500  |
| S  | -4.217251 | 1.249468  | 1.317527  |
| O  | -3.795146 | 0.753201  | 2.627248  |
| O  | -5.173373 | 2.349910  | 1.166864  |
| C  | -4.841645 | -0.144176 | 0.376037  |
| C  | -5.793668 | 0.071577  | -0.624066 |
| C  | -4.360170 | -1.429568 | 0.639751  |
| C  | -6.253160 | -1.011287 | -1.370678 |
| H  | -6.188093 | 1.068655  | -0.787854 |
| C  | -4.829908 | -2.499946 | -0.119981 |
| H  | -3.651570 | -1.589599 | 1.445370  |
| C  | -5.775917 | -2.309709 | -1.138032 |
| H  | -7.003975 | -0.846924 | -2.139674 |
| H  | -4.465724 | -3.502147 | 0.091848  |
| C  | -6.262305 | -3.471478 | -1.971120 |
| H  | -6.186763 | -4.416650 | -1.424215 |
| H  | -7.305022 | -3.336271 | -2.276815 |
| H  | -5.665537 | -3.574575 | -2.887143 |
| C  | -1.567001 | 4.309150  | 0.318284  |
| H  | -0.947252 | 5.193774  | 0.226348  |
| H  | -1.898573 | 4.012852  | 1.307510  |
| C  | 0.965117  | 3.552152  | -0.770059 |
| O  | 0.746061  | 4.335907  | -1.674851 |
| H  | -1.780599 | -0.018714 | -0.047124 |
| Rh | 2.824550  | -1.874374 | -0.028001 |
| Rh | 1.238237  | -0.035740 | 0.106101  |
| O  | 4.086321  | -0.783071 | 1.181004  |
| O  | 2.570555  | 0.895359  | 1.379202  |
| O  | 2.164558  | 0.768876  | -1.569410 |
| O  | 0.409680  | -0.999241 | 1.747550  |
| O  | 0.000375  | -1.147122 | -1.147730 |
| O  | 1.471480  | -2.873498 | -1.229829 |
| O  | 3.624003  | -0.966155 | -1.701438 |
| O  | 1.930876  | -2.681224 | 1.650326  |
| C  | 0.940109  | -2.082645 | 2.166820  |
| C  | 3.681830  | 0.330785  | 1.637657  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.128125  | 0.128789  | -2.106352 |
| C | 0.378824  | -2.306578 | -1.526969 |
| C | -0.572644 | -3.055083 | -2.438160 |
| C | 0.342942  | -2.685802 | 3.420821  |
| C | 4.600198  | 1.045516  | 2.607323  |
| C | 3.758000  | 0.744406  | -3.339849 |
| H | 3.132450  | 1.545120  | -3.738639 |
| H | 3.913721  | -0.027554 | -4.098479 |
| H | 4.742384  | 1.148824  | -3.077420 |
| H | 4.350764  | 2.106742  | 2.663931  |
| H | 5.642021  | 0.907664  | 2.307330  |
| H | 4.477727  | 0.603772  | 3.603207  |
| H | 0.841823  | -2.249830 | 4.294509  |
| H | -0.722126 | -2.453541 | 3.490300  |
| H | 0.505452  | -3.765460 | 3.436389  |
| H | -1.597639 | -2.961357 | -2.068098 |
| H | -0.286838 | -4.105821 | -2.509265 |
| H | -0.538372 | -2.606769 | -3.437801 |
| O | 2.153447  | 3.379897  | -0.186624 |
| C | 3.252696  | 4.059107  | -0.814919 |
| H | 4.124408  | 3.809435  | -0.210655 |
| H | 3.379003  | 3.700882  | -1.839491 |
| H | 3.082135  | 5.138652  | -0.825296 |

# I-TS-II(v)\_conf2

1 imaginary frequency, value = -302.9974 cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.681514 | 0.452093  | -0.796388 |
| C | -0.622576 | 1.170536  | -0.033715 |
| C | -0.552389 | 2.356332  | 0.456110  |
| C | -2.123369 | 3.557170  | -0.640788 |
| C | -2.593223 | 2.571398  | -1.677334 |
| H | -1.519681 | 4.392641  | -0.984003 |
| H | -3.511544 | 2.948154  | -2.141175 |
| H | -1.839898 | 2.471060  | -2.472631 |
| H | -1.964992 | -0.439456 | -0.228495 |
| N | -2.884277 | 1.275935  | -1.046845 |
| S | -4.194642 | 0.406877  | -1.719500 |
| O | -5.167638 | 1.423205  | -2.138248 |
| O | -3.710229 | -0.602882 | -2.669186 |
| C | -4.832694 | -0.449219 | -0.283757 |
| C | -4.605797 | -1.816762 | -0.139879 |
| C | -5.582881 | 0.261519  | 0.658902  |
| C | -5.125330 | -2.475290 | 0.976537  |
| H | -4.044423 | -2.353020 | -0.897342 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -6.092417 | -0.411915 | 1.763404  |
| H  | -5.775934 | 1.319380  | 0.513254  |
| C  | -5.868977 | -1.788243 | 1.943201  |
| H  | -4.953353 | -3.542231 | 1.092173  |
| H  | -6.680475 | 0.134605  | 2.496786  |
| C  | -6.422949 | -2.499933 | 3.154223  |
| H  | -5.944399 | -2.142863 | 4.074877  |
| H  | -7.499610 | -2.322794 | 3.261516  |
| H  | -6.262877 | -3.580411 | 3.092829  |
| C  | -2.468603 | 3.478754  | 0.672544  |
| H  | -2.174176 | 4.257298  | 1.366863  |
| H  | -3.118688 | 2.688829  | 1.031561  |
| C  | 0.345709  | 3.389960  | 1.009050  |
| O  | 0.380312  | 4.545843  | 0.631181  |
| H  | -1.237119 | 0.098932  | -1.736430 |
| Rh | 3.181355  | -1.487333 | -0.183157 |
| Rh | 1.231327  | -0.041823 | 0.001874  |
| O  | 3.404383  | -1.326977 | 1.859009  |
| O  | 1.534409  | -0.051053 | 2.046790  |
| O  | 2.513236  | 1.571001  | -0.246082 |
| O  | 0.091811  | -1.766550 | 0.205863  |
| O  | 1.066067  | -0.188975 | -2.066132 |
| O  | 2.856311  | -1.574517 | -2.219585 |
| O  | 4.321335  | 0.212570  | -0.447253 |
| O  | 1.922719  | -3.102559 | 0.081231  |
| C  | 0.677539  | -2.901118 | 0.198908  |
| C  | 2.531949  | -0.684435 | 2.521340  |
| C  | 3.755630  | 1.347249  | -0.428285 |
| C  | 1.894470  | -0.914534 | -2.713886 |
| C  | 1.703406  | -0.968395 | -4.214981 |
| C  | -0.214334 | -4.120295 | 0.310770  |
| C  | 2.675944  | -0.695908 | 4.029579  |
| C  | 4.649815  | 2.555206  | -0.623277 |
| H  | 4.057424  | 3.456515  | -0.790843 |
| H  | 5.321617  | 2.382527  | -1.468729 |
| H  | 5.273781  | 2.688656  | 0.267871  |
| H  | 2.130916  | 0.138063  | 4.475958  |
| H  | 3.732653  | -0.660351 | 4.306008  |
| H  | 2.260003  | -1.633120 | 4.417796  |
| H  | -1.075104 | -3.905383 | 0.948596  |
| H  | -0.585724 | -4.380510 | -0.687697 |
| H  | 0.350618  | -4.969164 | 0.700684  |
| H  | 0.657491  | -1.187468 | -4.449553 |
| H  | 2.356230  | -1.722350 | -4.657325 |

|   |          |          |           |
|---|----------|----------|-----------|
| H | 1.938544 | 0.012312 | -4.643467 |
| O | 1.086408 | 2.892428 | 2.002608  |
| C | 2.111339 | 3.764867 | 2.505029  |
| H | 2.598462 | 3.203000 | 3.301557  |
| H | 2.823411 | 4.001435 | 1.710768  |
| H | 1.674883 | 4.689687 | 2.890887  |

# I-TS-II(v)\_conf3

1 imaginary frequency, value = -318.6977 cm<sup>-1</sup>

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.453905 | -0.628083 | -0.364651 |
| C  | -0.614065 | 0.590584  | -0.199707 |
| C  | -0.868533 | 1.845646  | -0.330727 |
| C  | -2.706742 | 1.984597  | -1.555468 |
| C  | -2.955246 | 0.543466  | -1.927561 |
| H  | -2.346880 | 2.650366  | -2.334836 |
| H  | -3.958724 | 0.455691  | -2.358894 |
| H  | -2.252421 | 0.223296  | -2.709613 |
| H  | -1.451588 | -1.197491 | 0.566001  |
| N  | -2.850040 | -0.314021 | -0.741477 |
| S  | -3.947736 | -1.615908 | -0.657767 |
| O  | -4.283678 | -2.079091 | -2.010789 |
| O  | -3.400480 | -2.533653 | 0.344195  |
| C  | -5.410982 | -0.831838 | 0.018293  |
| C  | -5.420464 | -0.444599 | 1.363102  |
| C  | -6.535015 | -0.656203 | -0.786451 |
| C  | -6.566170 | 0.141072  | 1.890329  |
| H  | -4.548752 | -0.618354 | 1.986003  |
| C  | -7.676775 | -0.066834 | -0.238725 |
| H  | -6.517317 | -0.993310 | -1.817343 |
| C  | -7.710569 | 0.343511  | 1.098952  |
| H  | -6.580157 | 0.438264  | 2.936215  |
| H  | -8.557117 | 0.067199  | -0.862055 |
| C  | -8.941398 | 0.991659  | 1.686814  |
| H  | -9.799427 | 0.908704  | 1.013078  |
| H  | -9.215122 | 0.531524  | 2.643170  |
| H  | -8.771841 | 2.058852  | 1.879809  |
| C  | -3.010617 | 2.492145  | -0.329479 |
| H  | -2.901067 | 3.551726  | -0.129750 |
| H  | -3.438162 | 1.864173  | 0.444148  |
| C  | -0.267387 | 3.190547  | -0.433908 |
| O  | -0.561562 | 4.014387  | -1.280130 |
| H  | -0.964469 | -1.258611 | -1.120559 |
| Rh | 3.747974  | -0.925115 | 0.232508  |
| Rh | 1.502950  | -0.003107 | 0.061170  |

|                              |          |           |           |    |           |           |           |
|------------------------------|----------|-----------|-----------|----|-----------|-----------|-----------|
| O                            | 3.960895 | 0.112952  | 2.001556  | H  | 1.399783  | -0.184356 | -1.355989 |
| O                            | 1.857919 | 0.960505  | 1.854748  | N  | 2.765086  | 1.351542  | -0.963577 |
| O                            | 2.328473 | 1.573037  | -1.016387 | S  | 4.094722  | 0.586476  | -1.684091 |
| O                            | 0.855760 | -1.655576 | 1.130963  | O  | 3.529452  | -0.399951 | -2.605283 |
| O                            | 1.318640 | -1.067307 | -1.717010 | O  | 4.980992  | 1.662572  | -2.132046 |
| O                            | 3.414605 | -1.919956 | -1.545040 | C  | 4.933318  | -0.306117 | -0.373781 |
| O                            | 4.420682 | 0.708578  | -0.834073 | C  | 5.939501  | 0.329404  | 0.359199  |
| O                            | 2.948854 | -2.518289 | 1.274252  | C  | 4.551392  | -1.617810 | -0.076579 |
| C                            | 1.702297 | -2.537931 | 1.500094  | C  | 6.557526  | -0.357406 | 1.402468  |
| C                            | 2.984497 | 0.804162  | 2.427837  | H  | 6.246427  | 1.336307  | 0.096818  |
| C                            | 3.584599 | 1.573169  | -1.236361 | C  | 5.180605  | -2.287287 | 0.971586  |
| C                            | 2.294735 | -1.786087 | -2.121309 | H  | 3.789592  | -2.108614 | -0.672741 |
| C                            | 2.072477 | -2.549587 | -3.410066 | C  | 6.189593  | -1.671652 | 1.726529  |
| C                            | 1.149507 | -3.700376 | 2.296667  | H  | 7.344241  | 0.133023  | 1.970472  |
| C                            | 3.168955 | 1.492114  | 3.765286  | H  | 4.887233  | -3.308281 | 1.202740  |
| C                            | 4.140237 | 2.729765  | -2.043575 | C  | 6.887326  | -2.419240 | 2.837696  |
| H                            | 3.336180 | 3.296892  | -2.516206 | H  | 7.749514  | -2.979041 | 2.451665  |
| H                            | 4.830547 | 2.350539  | -2.802218 | H  | 7.260611  | -1.736812 | 3.608046  |
| H                            | 4.712119 | 3.390201  | -1.381703 | H  | 6.218283  | -3.141935 | 3.316076  |
| H                            | 2.440897 | 2.295928  | 3.889643  | C  | 0.806581  | 3.381601  | -1.153956 |
| H                            | 4.188192 | 1.877654  | 3.850100  | H  | 0.159460  | 4.245076  | -1.266951 |
| H                            | 3.022376 | 0.758006  | 4.566138  | H  | 1.016448  | 2.801328  | -2.045017 |
| H                            | 0.834840 | -3.342000 | 3.283306  | C  | -0.564828 | 3.277399  | 1.026595  |
| H                            | 0.265139 | -4.107431 | 1.797972  | O  | -1.013047 | 4.385308  | 0.808030  |
| H                            | 1.907792 | -4.475277 | 2.418897  | Rh | -1.180390 | -0.065286 | 0.029468  |
| H                            | 1.258493 | -3.269168 | -3.270275 | Rh | -3.173615 | -1.480905 | -0.251170 |
| H                            | 2.980919 | -3.076930 | -3.704543 | O  | -0.059911 | -1.807366 | 0.140203  |
| H                            | 1.766607 | -1.857759 | -4.201133 | O  | -1.901420 | -3.111806 | -0.129056 |
| O                            | 0.614390 | 3.391467  | 0.548492  | O  | -3.370409 | -1.493809 | 1.802592  |
| C                            | 1.382632 | 4.601584  | 0.450022  | O  | -2.865916 | -1.402405 | -2.293469 |
| H                            | 2.037804 | 4.594252  | 1.320584  | O  | -4.287365 | 0.264988  | -0.356337 |
| H                            | 1.968552 | 4.598475  | -0.472080 | O  | -2.442530 | 1.565407  | -0.110306 |
| H                            | 0.726681 | 5.475906  | 0.462573  | O  | -1.519106 | -0.202503 | 2.070153  |
| <b>II(v)_conf1</b>           |          |           |           | O  | -1.002437 | -0.131601 | -2.039982 |
| <b>0 imaginary frequency</b> |          |           |           | C  | -1.866132 | -0.772531 | -2.737595 |
| C                            | 1.667813 | 0.475871  | -0.526033 | C  | -0.661614 | -2.933495 | 0.032193  |
| C                            | 0.434870 | 1.135776  | -0.017452 | C  | -2.515717 | -0.875620 | 2.501385  |
| C                            | 0.426951 | 2.567508  | 0.136079  | C  | -3.698481 | 1.380146  | -0.281203 |
| C                            | 1.763495 | 3.354006  | -0.043951 | C  | -4.542228 | 2.629770  | -0.426421 |
| C                            | 3.027831 | 2.523620  | -0.129077 | C  | -1.649354 | -0.743884 | -4.235687 |
| H                            | 1.828914 | 4.236777  | 0.587970  | C  | 0.224085  | -4.161618 | 0.087864  |
| H                            | 3.821760 | 3.104814  | -0.604317 | C  | -2.703994 | -0.907417 | 4.005407  |
| H                            | 3.357009 | 2.245307  | 0.886556  | H  | -3.111669 | -1.874469 | 4.309061  |
|                              |          |           |           | H  | -3.427545 | -0.134524 | 4.291094  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H                            | -1.760252 | -0.711173 | 4.518205  | H  | 5.292200  | -4.452707 | -1.478095 |
| H                            | -0.382978 | -5.065113 | 0.161562  | H  | 5.436516  | -3.470664 | -2.947580 |
| H                            | 0.905867  | -4.092703 | 0.940659  | C  | 1.241187  | 2.792562  | -1.742301 |
| H                            | 0.832481  | -4.209006 | -0.822561 | H  | 0.785058  | 3.207251  | -2.635189 |
| H                            | -0.616509 | -1.020547 | -4.467389 | H  | 1.900509  | 1.942574  | -1.873634 |
| H                            | -2.343975 | -1.422091 | -4.733440 | C  | -1.118077 | 3.374492  | -0.890004 |
| H                            | -1.806925 | 0.275607  | -4.604785 | O  | -1.341943 | 3.994737  | -1.910653 |
| H                            | -5.466165 | 2.523136  | 0.148471  | Rh | -1.117287 | -0.001725 | 0.179479  |
| H                            | -4.821190 | 2.747634  | -1.479865 | Rh | -2.624091 | -1.925429 | -0.101123 |
| H                            | -3.986291 | 3.512841  | -0.106061 | O  | -0.324538 | -0.960403 | 1.833509  |
| H                            | 1.972147  | -0.196750 | 0.301057  | O  | -1.717961 | -2.738609 | 1.578066  |
| O                            | -0.778620 | 2.580312  | 2.147606  | O  | -3.970750 | -0.956579 | 1.122556  |
| C                            | -1.753461 | 3.124357  | 3.047909  | O  | -1.188884 | -2.799659 | -1.310190 |
| H                            | -2.732098 | 3.153450  | 2.561973  | O  | -3.416950 | -0.956696 | -1.755175 |
| H                            | -1.770778 | 2.444876  | 3.899269  | O  | -2.013356 | 0.810240  | -1.499126 |
| H                            | -1.472208 | 4.133947  | 3.358599  | O  | -2.568856 | 0.806972  | 1.414710  |
| <b>II(v)_conf2</b>           |           |           |           | O  | 0.224646  | -1.046886 | -1.023024 |
| <b>0 imaginary frequency</b> |           |           |           | C  | -0.097895 | -2.193404 | -1.495381 |
| C                            | 1.543348  | 1.106861  | 0.844384  | C  | -0.804777 | -2.098639 | 2.173308  |
| C                            | 0.255308  | 1.468974  | 0.190717  | C  | -3.655850 | 0.165796  | 1.613885  |
| C                            | 0.188547  | 2.682880  | -0.582252 | C  | -2.945790 | 0.165319  | -2.095440 |
| C                            | 1.411050  | 3.653141  | -0.566819 | C  | -3.512511 | 0.814443  | -3.341362 |
| C                            | 2.485967  | 3.367701  | 0.459829  | C  | 0.941063  | -2.856560 | -2.376346 |
| H                            | 1.127699  | 4.698692  | -0.663564 | C  | -0.229882 | -2.708948 | 3.434810  |
| H                            | 3.420792  | 3.857529  | 0.178715  | C  | -4.677616 | 0.841086  | 2.506784  |
| H                            | 2.175941  | 3.761385  | 1.441214  | H  | -5.248786 | 0.089209  | 3.055993  |
| H                            | 1.757120  | 0.055267  | 0.627157  | H  | -5.378911 | 1.406901  | 1.881759  |
| N                            | 2.721347  | 1.918524  | 0.493691  | H  | -4.189667 | 1.532490  | 3.196838  |
| S                            | 4.167603  | 1.430401  | 1.263905  | H  | -0.383823 | -3.789652 | 3.436801  |
| O                            | 5.142334  | 2.487337  | 0.975802  | H  | -0.747004 | -2.281359 | 4.301953  |
| O                            | 3.889488  | 1.017636  | 2.645704  | H  | 0.832137  | -2.469358 | 3.527673  |
| C                            | 4.602318  | -0.034093 | 0.331473  | H  | 1.931378  | -2.767584 | -1.920786 |
| C                            | 4.401834  | -1.293886 | 0.893995  | H  | 0.687021  | -3.905397 | -2.538160 |
| C                            | 5.164066  | 0.107897  | -0.941335 | H  | 0.972882  | -2.342100 | -3.343697 |
| C                            | 4.758485  | -2.427356 | 0.160707  | H  | -4.599240 | 0.696434  | -3.360231 |
| H                            | 3.985293  | -1.379052 | 1.891890  | H  | -3.109320 | 0.301693  | -4.222391 |
| C                            | 5.514019  | -1.032671 | -1.655927 | H  | -3.236036 | 1.869357  | -3.388656 |
| H                            | 5.333280  | 1.097169  | -1.353593 | H  | 1.325578  | 1.139467  | 1.929458  |
| C                            | 5.318385  | -2.316798 | -1.118546 | O  | -1.940646 | 3.324394  | 0.162878  |
| H                            | 4.606324  | -3.411885 | 0.595441  | C  | -3.238775 | 3.904326  | -0.027569 |
| H                            | 5.953224  | -0.928524 | -2.645076 | H  | -3.778974 | 3.358835  | -0.805786 |
| C                            | 5.734403  | -3.543135 | -1.895625 | H  | -3.744656 | 3.801204  | 0.931691  |
| H                            | 6.825005  | -3.666995 | -1.877045 | H  | -3.154127 | 4.955839  | -0.313806 |

**1y\_conf1****0 imaginary frequency**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.676906  | 1.476478  | 0.397481  |
| H | 2.744392  | 1.533857  | 0.149835  |
| H | 1.543199  | 1.929373  | 1.381252  |
| N | 1.395300  | 0.035047  | 0.532438  |
| S | 0.112395  | -0.469732 | 1.502178  |
| O | -0.003976 | 0.531801  | 2.564731  |
| O | 0.357609  | -1.886211 | 1.789208  |
| C | -1.397912 | -0.403819 | 0.527695  |
| C | -1.770115 | -1.509951 | -0.240067 |
| C | -2.188191 | 0.748234  | 0.547468  |
| C | -2.934260 | -1.449042 | -1.005373 |
| H | -1.170234 | -2.413428 | -0.215251 |
| C | -3.350843 | 0.788802  | -0.218006 |
| H | -1.897527 | 1.590236  | 1.164776  |
| C | -3.741591 | -0.303506 | -1.007469 |
| H | -3.225632 | -2.310296 | -1.601602 |
| H | -3.969126 | 1.683222  | -0.199266 |
| C | -5.019810 | -0.254975 | -1.810830 |
| H | -5.018534 | -1.000074 | -2.612637 |
| H | -5.891723 | -0.457865 | -1.175001 |
| H | -5.172180 | 0.731558  | -2.262239 |
| C | 1.799008  | -0.868231 | -0.563168 |
| H | 1.596664  | -1.887920 | -0.222987 |
| H | 1.192508  | -0.697009 | -1.467687 |
| C | 3.219616  | -0.736080 | -0.893305 |
| C | 4.386502  | -0.635090 | -1.193812 |
| C | 0.872326  | 2.214360  | -0.644086 |
| H | 0.858027  | 1.784860  | -1.646017 |
| C | 0.234931  | 3.362947  | -0.413552 |
| H | 0.232916  | 3.825773  | 0.571597  |
| H | -0.301516 | 3.888833  | -1.198964 |
| C | 5.801151  | -0.528353 | -1.542097 |
| H | 6.186557  | -1.483528 | -1.918719 |
| H | 5.969164  | 0.228373  | -2.317887 |
| H | 6.402245  | -0.250949 | -0.667896 |

**I(y)-Yne\_conf1****0 imaginary frequency**

|   |           |          |          |
|---|-----------|----------|----------|
| C | -2.394241 | 2.083202 | 0.333931 |
| H | -1.417454 | 2.513785 | 0.084926 |
| H | -2.515889 | 2.173659 | 1.414185 |
| N | -2.281280 | 0.648916 | 0.018885 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| S  | -3.115784 | -0.475807 | 0.935356  |
| O  | -3.198758 | 0.077115  | 2.292183  |
| O  | -2.494485 | -1.778402 | 0.672780  |
| C  | -4.794014 | -0.573004 | 0.298176  |
| C  | -5.078569 | -1.436221 | -0.763204 |
| C  | -5.793192 | 0.230073  | 0.851795  |
| C  | -6.373604 | -1.480064 | -1.277146 |
| H  | -4.301679 | -2.079339 | -1.163048 |
| C  | -7.083023 | 0.168808  | 0.328848  |
| H  | -5.560157 | 0.882099  | 1.685795  |
| C  | -7.394585 | -0.681614 | -0.742000 |
| H  | -6.596649 | -2.152293 | -2.102164 |
| H  | -7.862533 | 0.791252  | 0.761585  |
| C  | -8.802986 | -0.759991 | -1.282022 |
| H  | -8.812581 | -1.048613 | -2.338148 |
| H  | -9.393211 | -1.506726 | -0.734362 |
| H  | -9.323125 | 0.198851  | -1.185557 |
| C  | -1.781539 | 0.223840  | -1.298294 |
| H  | -1.505047 | -0.830163 | -1.220581 |
| H  | -2.558269 | 0.323163  | -2.074776 |
| C  | -0.606462 | 0.985494  | -1.742995 |
| C  | 0.266221  | 1.649819  | -2.276392 |
| C  | -3.492417 | 2.817921  | -0.394357 |
| H  | -3.522709 | 2.697942  | -1.477815 |
| C  | -4.376601 | 3.618781  | 0.201591  |
| H  | -4.373303 | 3.768958  | 1.279712  |
| H  | -5.130395 | 4.162094  | -0.362005 |
| Rh | 1.603729  | 0.265993  | -0.513909 |
| Rh | 3.244819  | -0.793105 | 0.887301  |
| O  | 2.689045  | 2.025598  | -0.309900 |
| O  | 4.234157  | 1.010809  | 1.003332  |
| O  | 2.116690  | -0.279315 | 2.523958  |
| O  | 4.296658  | -1.273069 | -0.819995 |
| O  | 2.177147  | -2.543103 | 0.736162  |
| O  | 0.651580  | -1.559439 | -0.618242 |
| O  | 0.583990  | 0.749533  | 1.210226  |
| O  | 2.756768  | -0.273746 | -2.151452 |
| C  | 3.832312  | -0.928310 | -1.949837 |
| C  | 3.749642  | 2.015663  | 0.399275  |
| C  | 1.037903  | 0.367631  | 2.338955  |
| C  | 1.109536  | -2.547462 | 0.048049  |
| C  | 0.293034  | -3.817046 | 0.008022  |
| C  | 4.608149  | -1.357699 | -3.176478 |
| C  | 4.480233  | 3.333495  | 0.543469  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.216686  | 0.731862  | 3.554182  |
| H | 0.612322  | 0.239069  | 4.443654  |
| H | -0.827464 | 0.448649  | 3.389683  |
| H | 0.248516  | 1.818066  | 3.697542  |
| H | 5.460297  | 3.179962  | 0.997562  |
| H | 3.889492  | 4.003521  | 1.178308  |
| H | 4.585742  | 3.812297  | -0.434310 |
| H | 4.548526  | -0.590559 | -3.952387 |
| H | 5.648558  | -1.561736 | -2.917073 |
| H | 4.160470  | -2.275660 | -3.575314 |
| H | 0.770944  | -4.601036 | 0.597159  |
| H | 0.178264  | -4.147543 | -1.029691 |
| H | -0.705609 | -3.598500 | 0.399800  |
| C | 1.216252  | 2.490206  | -3.004268 |
| H | 1.773982  | 3.122209  | -2.307116 |
| H | 1.938672  | 1.862229  | -3.535817 |
| H | 0.692385  | 3.124723  | -3.728484 |

#### I(y)-Ene\_conf2

##### 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.469394 | -1.457681 | -0.285973 |
| H | 0.730266 | -2.047469 | 0.266058  |
| H | 1.391554 | -1.731510 | -1.338894 |
| N | 2.788213 | -1.885195 | 0.207070  |
| S | 4.123260 | -1.883421 | -0.814485 |
| O | 3.598633 | -2.105557 | -2.164746 |
| O | 5.095981 | -2.791614 | -0.198379 |
| C | 4.867086 | -0.247852 | -0.806532 |
| C | 5.769132 | 0.097296  | 0.203650  |
| C | 4.551083 | 0.656015  | -1.821437 |
| C | 6.346984 | 1.364150  | 0.194342  |
| H | 6.023850 | -0.621985 | 0.973796  |
| C | 5.141171 | 1.919791  | -1.815880 |
| H | 3.870097 | 0.361040  | -2.611908 |
| C | 6.045358 | 2.293862  | -0.813010 |
| H | 7.054222 | 1.632608  | 0.975683  |
| H | 4.901594 | 2.623057  | -2.609645 |
| C | 6.710004 | 3.650110  | -0.832536 |
| H | 6.797731 | 4.068790  | 0.176144  |
| H | 7.725837 | 3.584148  | -1.244240 |
| H | 6.152014 | 4.361677  | -1.449259 |
| C | 2.984760 | -2.098552 | 1.647774  |
| H | 2.097710 | -2.637042 | 2.005749  |
| H | 3.834894 | -2.776892 | 1.763811  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 3.189271  | -0.886943 | 2.458493  |
| C  | 3.369949  | 0.096268  | 3.140395  |
| C  | 1.171676  | 0.012903  | -0.086090 |
| H  | 1.311768  | 0.397910  | 0.920909  |
| C  | 0.830793  | 0.863573  | -1.083598 |
| H  | 0.746683  | 0.525852  | -2.113460 |
| H  | 0.716778  | 1.928268  | -0.906632 |
| Rh | -1.398707 | 0.227268  | -0.197381 |
| Rh | -3.767641 | -0.012713 | 0.184627  |
| O  | -1.528314 | -1.347553 | -1.525867 |
| O  | -3.757726 | -1.566230 | -1.169281 |
| O  | -3.358973 | -1.339113 | 1.699965  |
| O  | -4.115915 | 1.317393  | -1.338615 |
| O  | -3.639792 | 1.557572  | 1.515300  |
| O  | -1.411770 | 1.791722  | 1.150705  |
| O  | -1.130021 | -1.124548 | 1.364504  |
| O  | -1.894426 | 1.559265  | -1.712673 |
| C  | -3.120793 | 1.808573  | -1.954006 |
| C  | -2.664510 | -1.894137 | -1.725230 |
| C  | -2.148725 | -1.605046 | 1.964351  |
| C  | -2.514013 | 2.112819  | 1.707263  |
| C  | -2.461235 | 3.244240  | 2.710851  |
| C  | -3.403042 | 2.766300  | -3.090715 |
| C  | -2.704383 | -3.019068 | -2.735525 |
| C  | -1.872778 | -2.581326 | 3.086882  |
| H  | -2.804403 | -2.891510 | 3.562032  |
| H  | -1.212791 | -2.115178 | 3.825322  |
| H  | -1.353295 | -3.459147 | 2.687956  |
| H  | -3.635687 | -3.580452 | -2.645535 |
| H  | -1.843564 | -3.678561 | -2.596963 |
| H  | -2.638293 | -2.595479 | -3.744285 |
| H  | -3.135201 | 2.287243  | -4.039065 |
| H  | -4.459343 | 3.038578  | -3.108805 |
| H  | -2.781683 | 3.660430  | -2.986460 |
| H  | -3.450524 | 3.688199  | 2.835793  |
| H  | -1.737978 | 3.998791  | 2.392407  |
| H  | -2.131795 | 2.846791  | 3.678120  |
| C  | 3.602648  | 1.294395  | 3.943242  |
| H  | 4.245100  | 2.004393  | 3.408144  |
| H  | 2.663283  | 1.807636  | 4.181140  |
| H  | 4.096746  | 1.047084  | 4.890705  |

#### I(y)-Ene\_conf3

##### 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 1.411916  | -0.209515 | 0.069857  |
| H  | 1.046863  | 0.518336  | 0.800104  |
| H  | 1.451753  | -1.184829 | 0.553757  |
| N  | 2.798712  | 0.206583  | -0.256086 |
| S  | 3.716704  | -0.953358 | -1.113984 |
| O  | 3.862480  | -0.544129 | -2.518705 |
| O  | 3.133701  | -2.255248 | -0.767330 |
| C  | 5.338210  | -0.860913 | -0.356453 |
| C  | 5.506899  | -1.295305 | 0.960866  |
| C  | 6.422286  | -0.423714 | -1.113868 |
| C  | 6.779632  | -1.276021 | 1.521554  |
| H  | 4.654285  | -1.645465 | 1.533158  |
| C  | 7.693255  | -0.415268 | -0.536471 |
| H  | 6.266468  | -0.099819 | -2.136796 |
| C  | 7.892531  | -0.839679 | 0.783216  |
| H  | 6.916104  | -1.610266 | 2.547291  |
| H  | 8.543478  | -0.079351 | -1.125051 |
| C  | 9.272988  | -0.856464 | 1.396439  |
| H  | 9.263364  | -0.455732 | 2.416467  |
| H  | 9.664469  | -1.880384 | 1.456398  |
| H  | 9.982027  | -0.267407 | 0.806405  |
| C  | 2.936917  | 1.605522  | -0.737422 |
| H  | 2.887990  | 1.647498  | -1.833765 |
| H  | 2.058674  | 2.139855  | -0.357404 |
| C  | 4.152638  | 2.273358  | -0.267279 |
| C  | 5.145037  | 2.859563  | 0.096973  |
| C  | 0.491004  | -0.249838 | -1.128083 |
| H  | 0.405182  | 0.666506  | -1.709130 |
| C  | -0.116377 | -1.373101 | -1.581190 |
| H  | 0.008169  | -2.324466 | -1.072580 |
| H  | -0.667194 | -1.381283 | -2.515888 |
| Rh | -1.892174 | -0.233221 | -0.285603 |
| Rh | -4.000754 | 0.378319  | 0.715676  |
| O  | -1.398526 | -1.150644 | 1.498270  |
| O  | -3.385530 | -0.579076 | 2.433148  |
| O  | -3.143927 | 2.123384  | 1.384242  |
| O  | -4.803159 | -1.380219 | 0.025649  |
| O  | -4.490778 | 1.299204  | -1.064064 |
| O  | -2.508721 | 0.724756  | -2.006327 |
| O  | -1.154314 | 1.574753  | 0.449634  |
| O  | -2.829333 | -1.975266 | -0.915725 |
| C  | -4.058003 | -2.166634 | -0.635659 |
| C  | -2.244255 | -1.134687 | 2.453506  |
| C  | -1.925832 | 2.344708  | 1.113879  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.659040 | 1.277833  | -2.022033 |
| C | -4.054808 | 1.966837  | -3.309717 |
| C | -4.681282 | -3.438964 | -1.165794 |
| C | -1.851068 | -1.871739 | 3.714992  |
| C | -1.322102 | 3.641683  | 1.607558  |
| H | -2.026297 | 4.170875  | 2.251039  |
| H | -1.066336 | 4.272551  | 0.749233  |
| H | -0.395909 | 3.435754  | 2.152824  |
| H | -2.475809 | -1.556418 | 4.552317  |
| H | -0.794657 | -1.701039 | 3.937621  |
| H | -1.988375 | -2.947521 | 3.555099  |
| H | -3.983772 | -4.273268 | -1.055727 |
| H | -5.617399 | -3.650387 | -0.646248 |
| H | -4.888197 | -3.315831 | -2.235199 |
| H | -5.044222 | 2.416447  | -3.215882 |
| H | -4.052402 | 1.239671  | -4.128260 |
| H | -3.316173 | 2.736912  | -3.554468 |
| C | 6.361903  | 3.535310  | 0.538332  |
| H | 7.223081  | 2.858405  | 0.482118  |
| H | 6.582105  | 4.407796  | -0.088885 |
| H | 6.276408  | 3.883133  | 1.574963  |

# I-TS-II(y)\_conf1

1 imaginary frequency, value = -409.6562 cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.611187 | 1.041572  | 0.333202  |
| C | -0.383220 | 1.643557  | -0.255228 |
| C | -0.153093 | 2.770065  | -0.849359 |
| C | -2.082119 | 3.535721  | -1.432974 |
| C | -3.029878 | 2.387578  | -1.185899 |
| H | -1.889406 | 3.790818  | -2.472614 |
| H | -4.057090 | 2.758982  | -1.265601 |
| H | -2.887129 | 1.608978  | -1.951019 |
| H | -1.444919 | 0.884812  | 1.401706  |
| N | -2.825737 | 1.868770  | 0.164484  |
| S | -4.193562 | 1.383137  | 1.037852  |
| O | -3.734199 | 1.173927  | 2.410652  |
| O | -5.243251 | 2.350740  | 0.702803  |
| C | -4.690329 | -0.210597 | 0.379772  |
| C | -5.629882 | -0.268293 | -0.653830 |
| C | -4.123983 | -1.378992 | 0.896218  |
| C | -5.990025 | -1.507932 | -1.177435 |
| H | -6.092750 | 0.643668  | -1.015769 |
| C | -4.495832 | -2.610441 | 0.357671  |
| H | -3.425477 | -1.323799 | 1.724195  |

|    |           |           |           |                              |           |           |           |
|----|-----------|-----------|-----------|------------------------------|-----------|-----------|-----------|
| C  | -5.425743 | -2.695902 | -0.688332 | H                            | 1.396100  | 4.261120  | -0.890720 |
| H  | -6.730495 | -1.555131 | -1.972259 |                              |           |           |           |
| H  | -4.065388 | -3.520933 | 0.767065  | <b>II(y)_conf1</b>           |           |           |           |
| C  | -5.805269 | -4.031119 | -1.283075 | <b>0 imaginary frequency</b> |           |           |           |
| H  | -5.224484 | -4.235173 | -2.192412 | C                            | -1.537526 | 1.051917  | 0.327049  |
| H  | -5.615845 | -4.850882 | -0.583121 | C                            | -0.325443 | 1.501432  | -0.405677 |
| H  | -6.863920 | -4.058751 | -1.562390 | C                            | -0.361000 | 2.693161  | -1.206777 |
| C  | -1.603941 | 4.324104  | -0.428471 | C                            | -1.775710 | 3.262335  | -1.532245 |
| H  | -1.017987 | 5.211417  | -0.640869 | C                            | -2.982742 | 2.438522  | -1.129192 |
| H  | -1.881171 | 4.135506  | 0.602187  | H                            | -1.835781 | 3.706318  | -2.523656 |
| C  | 0.912352  | 3.532068  | -1.549654 | H                            | -3.869788 | 3.074458  | -1.077324 |
| H  | 1.660702  | 2.806765  | -1.883115 | H                            | -3.160824 | 1.646369  | -1.876480 |
| H  | -1.739740 | 0.049846  | -0.126531 | H                            | -1.275860 | 0.947724  | 1.387769  |
| Rh | 3.101413  | -1.341970 | 0.235617  | N                            | -2.740773 | 1.890240  | 0.205765  |
| Rh | 1.305393  | 0.285743  | -0.081046 | S                            | -4.083060 | 1.414390  | 1.120008  |
| O  | 4.292827  | 0.224438  | 0.873581  | O                            | -3.563731 | 1.111923  | 2.454439  |
| O  | 2.623875  | 1.738853  | 0.584164  | O                            | -5.108067 | 2.434761  | 0.889517  |
| O  | 2.019141  | 0.553611  | -2.016216 | C                            | -4.669712 | -0.123350 | 0.404696  |
| O  | 0.738228  | -0.107017 | 1.874446  | C                            | -5.588915 | -0.089861 | -0.647519 |
| O  | 0.118650  | -1.295284 | -0.728594 | C                            | -4.181291 | -1.340822 | 0.888301  |
| O  | 1.788885  | -2.801644 | -0.418610 | C                            | -6.008529 | -1.287988 | -1.223197 |
| O  | 3.666190  | -0.981213 | -1.720894 | H                            | -5.985739 | 0.859849  | -0.990480 |
| O  | 2.418153  | -1.605384 | 2.168442  | C                            | -4.614378 | -2.528431 | 0.300915  |
| C  | 1.412897  | -0.944610 | 2.563924  | H                            | -3.492088 | -1.352078 | 1.725800  |
| C  | 3.806339  | 1.393362  | 0.919252  | C                            | -5.529527 | -2.522902 | -0.762540 |
| C  | 3.026802  | -0.130620 | -2.404932 | H                            | -6.726157 | -1.263925 | -2.039527 |
| C  | 0.614445  | -2.471997 | -0.755643 | H                            | -4.242289 | -3.476616 | 0.681607  |
| C  | -0.293329 | -3.569591 | -1.274320 | C                            | -6.012942 | -3.817843 | -1.370856 |
| C  | 0.978351  | -1.133579 | 4.002688  | H                            | -6.850677 | -4.232737 | -0.794955 |
| C  | 4.700166  | 2.495520  | 1.451381  | H                            | -6.362333 | -3.672923 | -2.398023 |
| C  | 3.494614  | 0.120819  | -3.824573 | H                            | -5.221577 | -4.574700 | -1.382861 |
| H  | 2.651693  | 0.024174  | -4.515785 | C                            | -0.993703 | 3.954466  | -0.498667 |
| H  | 4.285599  | -0.579596 | -4.096465 | H                            | -0.462554 | 4.868485  | -0.745495 |
| H  | 3.872124  | 1.146159  | -3.907219 | H                            | -1.298570 | 3.856047  | 0.536776  |
| H  | 4.523836  | 3.425658  | 0.905138  | C                            | 0.755306  | 3.001956  | -2.193776 |
| H  | 5.749251  | 2.202491  | 1.381003  | H                            | 0.851786  | 2.200725  | -2.929664 |
| H  | 4.455277  | 2.674250  | 2.505015  | H                            | -1.711093 | 0.019130  | -0.030995 |
| H  | 1.448190  | -0.358235 | 4.619442  | Rh                           | 3.104703  | -1.286253 | 0.353182  |
| H  | -0.104856 | -1.023945 | 4.093780  | Rh                           | 1.245769  | 0.261802  | -0.121198 |
| H  | 1.299939  | -2.109836 | 4.370780  | O                            | 4.346451  | 0.365699  | 0.456821  |
| H  | -1.329857 | -3.373566 | -0.988377 | O                            | 2.625421  | 1.800572  | 0.075970  |
| H  | 0.033439  | -4.541202 | -0.898668 | O                            | 1.731689  | 0.043170  | -2.129754 |
| H  | -0.241766 | -3.585354 | -2.369534 | O                            | 0.912730  | 0.319852  | 1.920734  |
| H  | 0.530208  | 4.058013  | -2.431057 | O                            | 0.026954  | -1.411428 | -0.261352 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 1.731336  | -2.832744 | 0.217118  |
| O | 3.421888  | -1.410635 | -1.686115 |
| O | 2.658375  | -1.063089 | 2.364495  |
| C | 1.681721  | -0.340324 | 2.706829  |
| C | 3.851734  | 1.519284  | 0.316231  |
| C | 2.693025  | -0.732969 | -2.464659 |
| C | 0.529579  | -2.574059 | -0.067388 |
| C | -0.415323 | -3.747631 | -0.229262 |
| C | 1.373153  | -0.212124 | 4.183791  |
| C | 4.783068  | 2.707231  | 0.449440  |
| C | 2.967506  | -0.832814 | -3.951915 |
| H | 3.213402  | 0.158699  | -4.346515 |
| H | 2.067155  | -1.178092 | -4.470489 |
| H | 3.792643  | -1.520586 | -4.142167 |
| H | 4.707856  | 3.340533  | -0.440204 |
| H | 5.812324  | 2.371277  | 0.583001  |
| H | 4.479239  | 3.312875  | 1.310069  |
| H | 1.550934  | 0.820573  | 4.503117  |
| H | 0.316337  | -0.431665 | 4.363711  |
| H | 2.003061  | -0.887797 | 4.764166  |
| H | -1.454909 | -3.426195 | -0.139581 |
| H | -0.183029 | -4.516839 | 0.511362  |
| H | -0.267917 | -4.185186 | -1.223680 |
| H | 0.545064  | 3.940537  | -2.719417 |
| H | 1.710035  | 3.094341  | -1.672124 |

#### 1z\_conf1

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.886301 | -2.340115 | 1.192281  |
| H | -1.565731 | -3.391336 | 1.193200  |
| H | -2.942947 | -2.325084 | 1.468895  |
| N | -1.782439 | -1.908182 | -0.212762 |
| S | -2.707557 | -0.617552 | -0.768328 |
| O | -3.919395 | -0.614816 | 0.054962  |
| O | -2.755926 | -0.760961 | -2.227279 |
| C | -1.835706 | 0.918427  | -0.434406 |
| C | -0.928847 | 1.413592  | -1.373203 |
| C | -2.087353 | 1.612039  | 0.751480  |
| C | -0.264700 | 2.611791  | -1.111910 |
| H | -0.763124 | 0.879910  | -2.302472 |
| C | -1.415704 | 2.807594  | 0.995503  |
| H | -2.807353 | 1.222164  | 1.461316  |
| C | -0.496595 | 3.327307  | 0.071659  |
| H | 0.434662  | 3.003450  | -1.846631 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.613624 | 3.350543  | 1.916682  |
| C | 0.195497  | 4.644618  | 0.331814  |
| H | 1.101647  | 4.749087  | -0.273368 |
| H | -0.462090 | 5.488900  | 0.085987  |
| H | 0.474687  | 4.749551  | 1.385979  |
| C | -0.684572 | -2.412296 | -1.046139 |
| H | -0.666474 | -3.504232 | -0.926261 |
| H | -0.954668 | -2.220343 | -2.089041 |
| C | 0.650409  | -1.867577 | -0.755033 |
| C | 1.761643  | -1.433306 | -0.534837 |
| C | -1.069939 | -1.557285 | 2.192335  |
| H | -0.015891 | -1.423540 | 1.956302  |
| C | -1.574155 | -1.069427 | 3.326505  |
| H | -2.625969 | -1.187226 | 3.581018  |
| H | -0.955717 | -0.540062 | 4.046540  |
| C | 3.063102  | -0.902640 | -0.272210 |
| C | 3.242287  | 0.481410  | -0.080228 |
| C | 4.183604  | -1.752882 | -0.202254 |
| C | 4.511247  | 0.995654  | 0.175855  |
| H | 2.379253  | 1.138048  | -0.134871 |
| C | 5.449200  | -1.229149 | 0.051278  |
| H | 4.048756  | -2.820079 | -0.349581 |
| C | 5.617676  | 0.144722  | 0.241833  |
| H | 4.638094  | 2.064834  | 0.323486  |
| H | 6.306267  | -1.895218 | 0.101451  |
| H | 6.605996  | 0.550112  | 0.440539  |

#### I(z)-Yne\_conf1

##### 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 2.508689 | 1.441627  | -1.622394 |
| H | 1.496737 | 1.853840  | -1.713915 |
| H | 2.713534 | 0.892263  | -2.542366 |
| N | 2.434250 | 0.460419  | -0.526531 |
| S | 3.403577 | -0.904871 | -0.565245 |
| O | 3.598453 | -1.228447 | -1.982993 |
| O | 2.815967 | -1.869258 | 0.369840  |
| C | 5.011712 | -0.465226 | 0.108386  |
| C | 5.215676 | -0.527667 | 1.489579  |
| C | 6.037338 | -0.056794 | -0.746211 |
| C | 6.455487 | -0.165053 | 2.012445  |
| H | 4.421253 | -0.878373 | 2.139848  |
| C | 7.272412 | 0.296398  | -0.205898 |
| H | 5.869189 | -0.030180 | -1.816719 |
| C | 7.502213 | 0.250410  | 1.176666  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 6.615887  | -0.215298 | 3.086737  |
| H  | 8.073565  | 0.609992  | -0.870747 |
| C  | 8.854253  | 0.604733  | 1.749113  |
| H  | 8.766303  | 1.020158  | 2.758470  |
| H  | 9.496918  | -0.283138 | 1.817498  |
| H  | 9.375848  | 1.336203  | 1.123248  |
| C  | 1.825824  | 0.842633  | 0.755088  |
| H  | 1.661832  | -0.071080 | 1.330750  |
| H  | 2.489218  | 1.506784  | 1.333917  |
| C  | 0.535211  | 1.533100  | 0.592628  |
| C  | -0.389826 | 2.333141  | 0.568527  |
| C  | 3.510758  | 2.551463  | -1.422660 |
| H  | 3.454903  | 3.093130  | -0.477910 |
| C  | 4.410996  | 2.916499  | -2.336262 |
| H  | 4.492461  | 2.403554  | -3.292900 |
| H  | 5.094103  | 3.745114  | -2.169602 |
| Rh | -1.417264 | -0.092799 | 0.147863  |
| Rh | -2.790315 | -2.025093 | -0.236371 |
| O  | -2.687712 | 0.960590  | -1.097015 |
| O  | -4.007480 | -0.856043 | -1.415961 |
| O  | -1.624266 | -2.473472 | -1.868410 |
| O  | -3.892017 | -1.497559 | 1.424534  |
| O  | -1.516487 | -3.123986 | 0.943696  |
| O  | -0.261287 | -1.289332 | 1.375240  |
| O  | -0.332187 | -0.643769 | -1.517562 |
| O  | -2.610246 | 0.339618  | 1.784671  |
| C  | -3.571153 | -0.449694 | 2.065964  |
| C  | -3.693308 | 0.361343  | -1.599807 |
| C  | -0.652935 | -1.702938 | -2.151474 |
| C  | -0.529372 | -2.532798 | 1.481237  |
| C  | 0.422879  | -3.357713 | 2.313729  |
| C  | -4.395705 | -0.099959 | 3.286476  |
| C  | -4.576353 | 1.170064  | -2.525248 |
| C  | 0.197659  | -2.053427 | -3.351004 |
| H  | -0.063163 | -3.043690 | -3.727684 |
| H  | 1.256069  | -2.012973 | -3.076509 |
| H  | 0.030135  | -1.310514 | -4.139343 |
| H  | -5.604356 | 0.803821  | -2.481729 |
| H  | -4.215115 | 1.051186  | -3.553746 |
| H  | -4.531672 | 2.229326  | -2.263825 |
| H  | -4.745690 | 0.934095  | 3.209912  |
| H  | -5.245343 | -0.777364 | 3.383076  |
| H  | -3.767070 | -0.170595 | 4.180827  |
| H  | 0.083151  | -4.392665 | 2.373957  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.498186  | -2.929911 | 3.318904  |
| H | 1.414860  | -3.308162 | 1.853987  |
| C | -1.400828 | 3.345495  | 0.559860  |
| C | -1.623085 | 4.114934  | -0.597408 |
| C | -2.160564 | 3.600108  | 1.717129  |
| C | -2.582986 | 5.123642  | -0.591457 |
| H | -1.042919 | 3.910576  | -1.491434 |
| C | -3.117411 | 4.612073  | 1.712494  |
| H | -2.001333 | 2.989220  | 2.598554  |
| C | -3.330905 | 5.375917  | 0.561865  |
| H | -2.747576 | 5.714563  | -1.488275 |
| H | -3.699738 | 4.804713  | 2.609387  |
| H | -4.078038 | 6.164964  | 0.563633  |

# I(z)-Ene\_conf2

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.711836 | -0.926774 | -1.929385 |
| H | -0.307970 | -0.723671 | -2.928347 |
| H | -0.077219 | -1.688244 | -1.473115 |
| N | -2.045085 | -1.519460 | -2.088937 |
| S | -2.495516 | -2.870705 | -1.194302 |
| O | -1.254825 | -3.589520 | -0.886913 |
| O | -3.588590 | -3.504202 | -1.938141 |
| C | -3.183614 | -2.309790 | 0.368263  |
| C | -4.565319 | -2.326170 | 0.551042  |
| C | -2.328196 | -1.876677 | 1.387492  |
| C | -5.095010 | -1.901783 | 1.771527  |
| H | -5.209539 | -2.681770 | -0.245266 |
| C | -2.876064 | -1.449701 | 2.593746  |
| H | -1.252824 | -1.874711 | 1.239171  |
| C | -4.264501 | -1.457177 | 2.808054  |
| H | -6.171693 | -1.926256 | 1.921010  |
| H | -2.214061 | -1.111997 | 3.387819  |
| C | -4.837278 | -1.012603 | 4.133221  |
| H | -5.930712 | -0.979049 | 4.106842  |
| H | -4.544483 | -1.696543 | 4.939886  |
| H | -4.474339 | -0.015624 | 4.410070  |
| C | -3.062397 | -0.815440 | -2.880380 |
| H | -2.551121 | -0.420527 | -3.768369 |
| H | -3.776070 | -1.564554 | -3.236810 |
| C | -3.772916 | 0.271588  | -2.192850 |
| C | -4.400150 | 1.157029  | -1.650812 |
| C | -0.680543 | 0.333115  | -1.091583 |
| H | -1.175664 | 0.278677  | -0.125104 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.136949 | 1.507167  | -1.490308 |
| H  | 0.308578  | 1.622057  | -2.475178 |
| H  | -0.208978 | 2.401065  | -0.879298 |
| Rh | 1.773633  | 0.501827  | -0.251735 |
| Rh | 3.919786  | 0.017994  | 0.732757  |
| O  | 2.613032  | 2.268722  | -0.953109 |
| O  | 4.613905  | 1.810081  | 0.008288  |
| O  | 3.262046  | 0.959637  | 2.444335  |
| O  | 4.450686  | -0.898205 | -1.034097 |
| O  | 3.170775  | -1.772081 | 1.411878  |
| O  | 1.132322  | -1.307058 | 0.547297  |
| O  | 1.253887  | 1.449735  | 1.507448  |
| O  | 2.423549  | -0.469728 | -1.955566 |
| C  | 3.603666  | -0.956509 | -1.976956 |
| C  | 3.828517  | 2.535008  | -0.676494 |
| C  | 2.103189  | 1.478464  | 2.458944  |
| C  | 1.959153  | -2.056166 | 1.171154  |
| C  | 1.428433  | -3.377630 | 1.677955  |
| C  | 4.013134  | -1.673911 | -3.244062 |
| C  | 4.383116  | 3.825105  | -1.239920 |
| C  | 1.700872  | 2.228208  | 3.710288  |
| H  | 2.158946  | 1.768584  | 4.588902  |
| H  | 0.613931  | 2.254718  | 3.810073  |
| H  | 2.066868  | 3.259220  | 3.637168  |
| H  | 5.318529  | 4.087755  | -0.743222 |
| H  | 3.650808  | 4.629089  | -1.127919 |
| H  | 4.572754  | 3.694290  | -2.311541 |
| H  | 3.826721  | -1.031579 | -4.110070 |
| H  | 5.066610  | -1.953939 | -3.202477 |
| H  | 3.399361  | -2.573445 | -3.362983 |
| H  | 2.249771  | -4.081966 | 1.823143  |
| H  | 0.688104  | -3.778230 | 0.981057  |
| H  | 0.936775  | -3.217529 | 2.645318  |
| C  | -5.139345 | 2.196471  | -1.005867 |
| C  | -5.695372 | 1.990410  | 0.271963  |
| C  | -5.329634 | 3.439326  | -1.640682 |
| C  | -6.420393 | 3.004274  | 0.893841  |
| H  | -5.550292 | 1.032713  | 0.762567  |
| C  | -6.058771 | 4.446155  | -1.012421 |
| H  | -4.903142 | 3.601186  | -2.625928 |
| C  | -6.605921 | 4.233358  | 0.255484  |
| H  | -6.844597 | 2.834211  | 1.879874  |
| H  | -6.200264 | 5.399811  | -1.513747 |
| H  | -7.174303 | 5.020699  | 0.742979  |

# I-TS-II(z)\_conf1

1 imaginary frequency, value = -435.8378 cm<sup>-1</sup>

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 1.671704  | 0.779909  | -0.627803 |
| C  | 0.319370  | 1.297037  | -0.269759 |
| C  | -0.107155 | 2.507857  | -0.037627 |
| C  | 1.611528  | 3.704495  | 0.325103  |
| C  | 2.754795  | 2.728160  | 0.447537  |
| H  | 1.303498  | 4.224905  | 1.228259  |
| H  | 3.697038  | 3.286141  | 0.425882  |
| H  | 2.697418  | 2.190288  | 1.406363  |
| H  | 1.607055  | 0.287700  | -1.601413 |
| N  | 2.724356  | 1.814453  | -0.691458 |
| S  | 4.196178  | 1.372942  | -1.398354 |
| O  | 3.849174  | 0.688849  | -2.643792 |
| O  | 5.025208  | 2.582274  | -1.374918 |
| C  | 4.959885  | 0.170595  | -0.307865 |
| C  | 5.841635  | 0.604385  | 0.686268  |
| C  | 4.649580  | -1.184766 | -0.447047 |
| C  | 6.406781  | -0.331645 | 1.549349  |
| H  | 6.097046  | 1.656052  | 0.761494  |
| C  | 5.224170  | -2.106281 | 0.427539  |
| H  | 3.985626  | -1.511264 | -1.240256 |
| C  | 6.108884  | -1.698029 | 1.435921  |
| H  | 7.097844  | 0.003001  | 2.319260  |
| H  | 4.988259  | -3.161777 | 0.317454  |
| C  | 6.756084  | -2.706343 | 2.355089  |
| H  | 6.157930  | -3.619501 | 2.434549  |
| H  | 7.747761  | -2.995430 | 1.982619  |
| H  | 6.894399  | -2.299606 | 3.362501  |
| C  | 1.086545  | 4.057494  | -0.887438 |
| H  | 0.349877  | 4.847499  | -0.968619 |
| H  | 1.477732  | 3.629070  | -1.802811 |
| H  | 1.922229  | 0.003420  | 0.111890  |
| Rh | -2.598240 | -2.251755 | -0.019979 |
| Rh | -1.092848 | -0.324112 | -0.110512 |
| O  | -3.932082 | -1.161685 | -1.158874 |
| O  | -2.537301 | 0.629231  | -1.248432 |
| O  | -1.982798 | 0.329026  | 1.641467  |
| O  | -0.300962 | -1.154359 | -1.844744 |
| O  | 0.248097  | -1.437875 | 1.023236  |
| O  | -1.157226 | -3.220137 | 1.112399  |
| O  | -3.410996 | -1.437475 | 1.698179  |
| O  | -1.696927 | -2.943184 | -1.748399 |

|                                                                 |           |           |           |    |           |           |           |
|-----------------------------------------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                                                               | -0.774331 | -2.258259 | -2.280495 | S  | -3.993373 | -1.510619 | -0.839895 |
| C                                                               | -3.623176 | 0.013695  | -1.515235 | O  | -4.262888 | -1.776575 | -2.260163 |
| C                                                               | -2.931421 | -0.355818 | 2.151200  | O  | -3.486771 | -2.564320 | 0.041769  |
| C                                                               | -0.074988 | -2.621404 | 1.379723  | C  | -5.489168 | -0.827587 | -0.126141 |
| C                                                               | 0.933929  | -3.361396 | 2.236279  | C  | -5.567464 | -0.654103 | 1.259758  |
| C                                                               | -0.188464 | -2.772916 | -3.579649 | C  | -6.570697 | -0.519953 | -0.950123 |
| C                                                               | -4.636342 | 0.781767  | -2.340618 | C  | -6.740104 | -0.151325 | 1.813247  |
| C                                                               | -3.521702 | 0.181894  | 3.439804  | H  | -4.725882 | -0.924054 | 1.889722  |
| H                                                               | -2.799731 | 0.042218  | 4.252709  | C  | -7.739351 | -0.014853 | -0.376283 |
| H                                                               | -4.444301 | -0.345877 | 3.686831  | H  | -6.497801 | -0.689388 | -2.019204 |
| H                                                               | -3.709442 | 1.254940  | 3.343016  | C  | -7.843846 | 0.176268  | 1.006691  |
| H                                                               | -4.928018 | 1.690440  | -1.803389 | H  | -6.806613 | -0.016995 | 2.890243  |
| H                                                               | -5.517387 | 0.168108  | -2.534040 | H  | -8.584808 | 0.226515  | -1.015516 |
| H                                                               | -4.181890 | 1.089896  | -3.287902 | C  | -9.119276 | 0.693499  | 1.628195  |
| H                                                               | -0.724954 | -2.311379 | -4.417243 | H  | -9.772068 | 1.154915  | 0.880958  |
| H                                                               | 0.865232  | -2.496332 | -3.662245 | H  | -9.682906 | -0.121019 | 2.101535  |
| H                                                               | -0.310160 | -3.855841 | -3.647552 | H  | -8.912410 | 1.436638  | 2.406375  |
| H                                                               | 1.951421  | -3.061304 | 1.973901  | C  | -2.709055 | 2.422222  | 0.247654  |
| H                                                               | 0.808428  | -4.440062 | 2.122196  | H  | -2.520131 | 3.413883  | 0.640168  |
| H                                                               | 0.764292  | -3.103739 | 3.288565  | H  | -3.077622 | 1.666214  | 0.930337  |
| C                                                               | -1.289600 | 3.235926  | 0.425809  | H  | -1.108606 | -1.196526 | -1.312460 |
| C                                                               | -2.241215 | 3.709595  | -0.493647 | Rh | 3.655593  | -1.258642 | 0.345133  |
| C                                                               | -1.491327 | 3.467850  | 1.796467  | Rh | 1.462037  | -0.226913 | 0.004160  |
| C                                                               | -3.368651 | 4.398373  | -0.049779 | O  | 3.987372  | 0.134646  | 1.833921  |
| H                                                               | -2.096290 | 3.513129  | -1.550615 | O  | 1.940804  | 1.077721  | 1.541033  |
| C                                                               | -2.616542 | 4.163111  | 2.237509  | O  | 2.369483  | 1.023636  | -1.376922 |
| H                                                               | -0.771214 | 3.082201  | 2.511273  | O  | 0.726441  | -1.573531 | 1.401093  |
| C                                                               | -3.556416 | 4.630624  | 1.315567  | O  | 1.159982  | -1.627225 | -1.502032 |
| H                                                               | -4.100558 | 4.755879  | -0.768960 | O  | 3.189100  | -2.588342 | -1.167073 |
| H                                                               | -2.761713 | 4.336717  | 3.300341  | O  | 4.405615  | 0.070214  | -1.047464 |
| H                                                               | -4.432651 | 5.173490  | 1.659748  | O  | 2.764002  | -2.523750 | 1.716870  |
| <b>I-TS-II(z)_conf2</b>                                         |           |           |           | C  | 1.521990  | -2.418194 | 1.936459  |
| <b>1 imaginary frequency, value = -453.8217 cm<sup>-1</sup></b> |           |           |           | C  | 3.080789  | 0.976559  | 2.105763  |
| C                                                               | -1.490142 | -0.614740 | -0.460945 | C  | 3.621221  | 0.901662  | -1.593478 |
| C                                                               | -0.545549 | 0.518515  | -0.255744 | C  | 2.070095  | -2.489497 | -1.750197 |
| C                                                               | -0.730776 | 1.810152  | -0.220257 | C  | 1.761152  | -3.481485 | -2.852835 |
| C                                                               | -2.627717 | 2.165915  | -1.094000 | C  | 0.898286  | -3.380502 | 2.926558  |
| C                                                               | -3.053399 | 0.846772  | -1.685804 | C  | 3.358588  | 1.964260  | 3.221848  |
| H                                                               | -2.379433 | 2.963355  | -1.789618 | C  | 4.211556  | 1.844899  | -2.623088 |
| H                                                               | -4.106754 | 0.921074  | -1.982515 | H  | 3.850775  | 1.564596  | -3.619296 |
| H                                                               | -2.482431 | 0.624192  | -2.598751 | H  | 5.301411  | 1.794207  | -2.608411 |
| H                                                               | -1.447135 | -1.273584 | 0.408833  | H  | 3.875361  | 2.866627  | -2.423660 |
| N                                                               | -2.903088 | -0.205472 | -0.676200 | H  | 3.148377  | 2.980629  | 2.875281  |
|                                                                 |           |           |           | H  | 4.394926  | 1.885387  | 3.553821  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H                            | 2.689800  | 1.756508  | 4.064614  | C  | -9.044281 | 0.445865  | 1.877773  |
| H                            | 0.412222  | -2.817514 | 3.729972  | H  | -9.641348 | -0.447139 | 2.104436  |
| H                            | 0.123394  | -3.969044 | 2.424176  | H  | -8.814510 | 0.931219  | 2.832726  |
| H                            | 1.656062  | -4.045251 | 3.343812  | H  | -9.674860 | 1.123332  | 1.293831  |
| H                            | 0.862999  | -4.051099 | -2.591978 | C  | -2.041526 | 2.223994  | 0.910923  |
| H                            | 2.600676  | -4.162001 | -3.002116 | H  | -1.910572 | 3.104241  | 1.531454  |
| H                            | 1.548253  | -2.942816 | -3.782010 | H  | -2.453888 | 1.353787  | 1.408425  |
| C                            | 0.015944  | 3.069677  | -0.196135 | H  | -1.118317 | -0.750748 | -1.612465 |
| C                            | 0.231609  | 3.755035  | 1.011791  | Rh | 3.515079  | -1.408630 | 0.317498  |
| C                            | 0.531586  | 3.608273  | -1.386728 | Rh | 1.370061  | -0.238108 | 0.001266  |
| C                            | 0.943348  | 4.952872  | 1.026879  | O  | 3.715251  | -0.393816 | 2.107587  |
| H                            | -0.148336 | 3.330252  | 1.935436  | O  | 1.740093  | 0.695416  | 1.819607  |
| C                            | 1.240773  | 4.808978  | -1.369695 | O  | 2.439719  | 1.210835  | -1.009815 |
| H                            | 0.388641  | 3.068480  | -2.317009 | O  | 0.496319  | -1.823250 | 1.027122  |
| C                            | 1.446028  | 5.484173  | -0.164335 | O  | 1.176134  | -1.293306 | -1.767170 |
| H                            | 1.106959  | 5.472319  | 1.967211  | O  | 3.168546  | -2.348170 | -1.496514 |
| H                            | 1.634841  | 5.216071  | -2.296903 | O  | 4.425806  | 0.162349  | -0.665339 |
| H                            | 1.996858  | 6.420872  | -0.152081 | O  | 2.469751  | -2.913950 | 1.282857  |
| <b>II(z)_conf1</b>           |           |           |           | C  | 1.220682  | -2.802796 | 1.425653  |
| <b>0 imaginary frequency</b> |           |           |           | C  | 2.814707  | 0.420361  | 2.457829  |
| C                            | -1.471851 | -0.394490 | -0.624064 | C  | 3.708687  | 1.100604  | -1.118342 |
| C                            | -0.448357 | 0.610330  | -0.234690 | C  | 2.098627  | -2.109975 | -2.122791 |
| C                            | -0.827448 | 1.996106  | -0.068381 | C  | 1.852744  | -2.851120 | -3.420204 |
| C                            | -2.264077 | 2.385799  | -0.533590 | C  | 0.483965  | -3.914810 | 2.142775  |
| C                            | -3.072325 | 1.357019  | -1.295589 | C  | 3.017397  | 1.172050  | 3.758605  |
| H                            | -2.320704 | 3.397013  | -0.928171 | C  | 4.401964  | 2.204365  | -1.890059 |
| H                            | -4.135349 | 1.617533  | -1.244973 | H  | 3.992156  | 3.175520  | -1.601425 |
| H                            | -2.780009 | 1.343972  | -2.356752 | H  | 4.211446  | 2.065754  | -2.960712 |
| H                            | -1.386685 | -1.267589 | 0.031414  | H  | 5.478537  | 2.170750  | -1.714163 |
| N                            | -2.878758 | 0.051852  | -0.657973 | H  | 3.218716  | 2.226223  | 3.536440  |
| S                            | -3.988981 | -1.152989 | -1.136851 | H  | 3.859326  | 0.754203  | 4.312617  |
| O                            | -4.271720 | -1.046462 | -2.575204 | H  | 2.106856  | 1.128012  | 4.363472  |
| O                            | -3.484220 | -2.402678 | -0.561890 | H  | 0.066220  | -3.528620 | 3.079030  |
| C                            | -5.464702 | -0.653117 | -0.252933 | H  | -0.352774 | -4.261472 | 1.528490  |
| C                            | -5.525688 | -0.832314 | 1.132720  | H  | 1.161220  | -4.742299 | 2.358981  |
| C                            | -6.546361 | -0.126473 | -0.957962 | H  | 0.965517  | -3.484780 | -3.314714 |
| C                            | -6.682308 | -0.463429 | 1.811558  | H  | 2.715874  | -3.467456 | -3.675659 |
| H                            | -4.682536 | -1.263012 | 1.662960  | H  | 1.650488  | -2.135450 | -4.223208 |
| C                            | -7.698446 | 0.238438  | -0.259077 | C  | 0.189474  | 3.114539  | -0.102006 |
| H                            | -6.484633 | -0.017479 | -2.035558 | C  | 0.817097  | 3.574624  | 1.061100  |
| C                            | -7.785802 | 0.076784  | 1.129195  | C  | 0.476240  | 3.744681  | -1.319169 |
| H                            | -6.734983 | -0.600106 | 2.888953  | C  | 1.713553  | 4.643018  | 1.007342  |
| H                            | -8.543598 | 0.650883  | -0.804334 | H  | 0.617508  | 3.079075  | 2.005189  |
|                              |           |           |           | C  | 1.368808  | 4.815536  | -1.375936 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | -0.001940 | 3.392430 | -2.229938 |
| C | 1.989662  | 5.269343 | -0.210102 |
| H | 2.192445  | 4.991087 | 1.918983  |
| H | 1.576260  | 5.295786 | -2.328616 |
| H | 2.679829  | 6.108066 | -0.249004 |

# 1u\_conf1

## 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.864644 | -0.884100 | 1.170557  |
| H | -0.400877 | -0.725663 | 2.149289  |
| H | -0.291456 | -1.664441 | 0.643084  |
| N | -0.779773 | 0.406539  | 0.460653  |
| S | 0.566993  | 1.373077  | 0.838123  |
| O | 0.664151  | 1.376811  | 2.298751  |
| O | 0.411206  | 2.606059  | 0.063026  |
| C | 2.015943  | 0.518080  | 0.206601  |
| C | 2.441956  | 0.753567  | -1.104070 |
| C | 2.692645  | -0.392231 | 1.022440  |
| C | 3.544092  | 0.058630  | -1.597506 |
| H | 1.931405  | 1.489836  | -1.715613 |
| C | 3.793721  | -1.077893 | 0.511513  |
| H | 2.373755  | -0.540194 | 2.048653  |
| C | 4.236104  | -0.866936 | -0.802075 |
| H | 3.878616  | 0.244720  | -2.615245 |
| H | 4.322845  | -1.783507 | 1.147309  |
| C | 5.449587  | -1.588878 | -1.337686 |
| H | 5.344552  | -1.812665 | -2.404619 |
| H | 6.353231  | -0.975875 | -1.222024 |
| H | 5.623693  | -2.530349 | -0.807033 |
| C | -1.191697 | 0.404046  | -0.959134 |
| H | -0.798205 | 1.316146  | -1.416189 |
| H | -0.744182 | -0.455576 | -1.484887 |
| C | -2.645987 | 0.388404  | -1.124103 |
| C | -3.844854 | 0.395566  | -1.283671 |
| C | -2.283284 | -1.342970 | 1.387498  |
| H | -2.960609 | -0.598342 | 1.800015  |
| C | -2.699463 | -2.590059 | 1.163986  |
| H | -2.041089 | -3.350073 | 0.747335  |
| H | -3.712714 | -2.901440 | 1.403891  |
| C | -5.298754 | 0.250526  | -1.411205 |
| H | -5.808776 | 1.170319  | -1.104522 |
| H | -5.556627 | 0.077706  | -2.469260 |
| O | -5.820667 | -0.780477 | -0.576505 |
| H | -5.236752 | -1.549268 | -0.675764 |

# I(u)-Ene\_conf1

## 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.812607 | 0.931452  | -0.336748 |
| H  | -2.052283 | 0.090057  | 0.315310  |
| H  | -1.289432 | 1.680780  | 0.265107  |
| N  | -3.079805 | 1.480062  | -0.874846 |
| S  | -4.388161 | 1.407019  | 0.226652  |
| O  | -5.464108 | 2.199486  | -0.380822 |
| O  | -3.952368 | 1.673162  | 1.603369  |
| C  | -4.814819 | -0.332313 | 0.123496  |
| C  | -4.722052 | -1.126703 | 1.264343  |
| C  | -5.288844 | -0.857282 | -1.083007 |
| C  | -5.097884 | -2.469966 | 1.189020  |
| H  | -4.368465 | -0.691470 | 2.192875  |
| C  | -5.657324 | -2.196748 | -1.139631 |
| H  | -5.368581 | -0.222218 | -1.959118 |
| C  | -5.566013 | -3.025329 | -0.007563 |
| H  | -5.031605 | -3.092097 | 2.078046  |
| H  | -6.027569 | -2.608963 | -2.075344 |
| C  | -5.959787 | -4.480817 | -0.092793 |
| H  | -5.993159 | -4.946410 | 0.896812  |
| H  | -6.945864 | -4.599846 | -0.556555 |
| H  | -5.246259 | -5.048174 | -0.704199 |
| C  | -2.962796 | 2.747734  | -1.638837 |
| H  | -2.599510 | 2.484684  | -2.639536 |
| H  | -3.970806 | 3.153364  | -1.754187 |
| C  | -2.049121 | 3.723244  | -1.031349 |
| C  | -1.200071 | 4.423986  | -0.527526 |
| C  | -0.948238 | 0.436803  | -1.471825 |
| H  | -1.189775 | -0.548751 | -1.864722 |
| C  | 0.008302  | 1.173859  | -2.088034 |
| H  | 0.220124  | 2.194711  | -1.785897 |
| H  | 0.520376  | 0.804722  | -2.970439 |
| C  | -0.091687 | 5.142154  | 0.116182  |
| Rh | 1.357785  | -0.085549 | -0.461169 |
| Rh | 3.188908  | -1.089397 | 0.740044  |
| O  | 1.354499  | 1.432859  | 0.973258  |
| O  | 3.023191  | 0.417664  | 2.125296  |
| O  | 1.835145  | -2.198090 | 1.817539  |
| O  | 4.495548  | 0.041678  | -0.364368 |
| O  | 3.243595  | -2.557567 | -0.706816 |
| O  | 1.485590  | -1.637432 | -1.806354 |
| O  | 0.098243  | -1.226636 | 0.735626  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| O                            | 2.791787  | 0.971393  | -1.533586 | H  | 7.936592  | 0.302510  | -0.941758 |
| C                            | 4.026403  | 0.816682  | -1.252525 | C  | 8.780248  | -0.024008 | 1.636815  |
| C                            | 2.161108  | 1.333653  | 1.968045  | H  | 8.752980  | 0.193644  | 2.709333  |
| C                            | 0.597827  | -2.017442 | 1.602829  | H  | 9.391724  | -0.925959 | 1.501243  |
| C                            | 2.389217  | -2.525667 | -1.643814 | H  | 9.300815  | 0.798594  | 1.134964  |
| C                            | 2.416337  | -3.656745 | -2.647481 | C  | 1.821684  | 0.864507  | 0.908880  |
| C                            | 5.008793  | 1.644730  | -2.050619 | H  | 1.563584  | -0.079890 | 1.394356  |
| C                            | 2.059464  | 2.387684  | 3.045043  | H  | 2.585690  | 1.372595  | 1.520208  |
| C                            | -0.376754 | -2.781520 | 2.471249  | C  | 0.625202  | 1.718083  | 0.888800  |
| H                            | 0.043230  | -3.752088 | 2.744429  | C  | -0.253693 | 2.557322  | 0.997407  |
| H                            | -1.333700 | -2.903722 | 1.959702  | C  | 3.564278  | 2.622810  | -1.160260 |
| H                            | -0.546628 | -2.213132 | 3.393438  | H  | 3.585767  | 3.067438  | -0.164810 |
| H                            | 2.839283  | 2.237218  | 3.792543  | C  | 4.463565  | 3.004379  | -2.067970 |
| H                            | 1.073870  | 2.321867  | 3.518700  | H  | 4.470008  | 2.589021  | -3.074106 |
| H                            | 2.131382  | 3.387155  | 2.607712  | H  | 5.220510  | 3.751954  | -1.846243 |
| H                            | 4.847900  | 2.706112  | -1.833123 | C  | -1.257221 | 3.617100  | 1.237139  |
| H                            | 6.034059  | 1.370951  | -1.797802 | Rh | -1.564209 | 0.393958  | 0.215310  |
| H                            | 4.832025  | 1.497787  | -3.120439 | Rh | -3.163905 | -1.285822 | -0.412268 |
| H                            | 3.413850  | -4.097915 | -2.692735 | O  | -2.692950 | 1.752170  | -0.870499 |
| H                            | 2.106763  | -3.300524 | -3.632588 | O  | -4.216083 | 0.168105  | -1.424368 |
| H                            | 1.709040  | -4.431118 | -2.327527 | O  | -2.052163 | -1.652016 | -2.093667 |
| H                            | 0.615855  | 5.483141  | -0.658406 | O  | -4.208609 | -0.858023 | 1.320226  |
| H                            | -0.457099 | 6.038404  | 0.629798  | O  | -2.036246 | -2.667044 | 0.604115  |
| O                            | 0.560141  | 4.358210  | 1.106049  | O  | -0.563780 | -1.075187 | 1.255361  |
| H                            | 0.714192  | 3.458773  | 0.761997  | O  | -0.543506 | -0.065524 | -1.506101 |
| <b>I(u)-Yne_conf2</b>        |           |           |           | O  | -2.739530 | 0.762444  | 1.899516  |
| <b>0 imaginary frequency</b> |           |           |           | C  | -3.796228 | 0.060083  | 2.085223  |
| C                            | 2.461073  | 1.629850  | -1.430812 | C  | -3.758066 | 1.350932  | -1.448102 |
| H                            | 1.488864  | 2.136725  | -1.443977 | C  | -0.985567 | -0.982686 | -2.274890 |
| H                            | 2.589265  | 1.161689  | -2.407655 | C  | -0.982688 | -2.280015 | 1.199242  |
| N                            | 2.325810  | 0.551567  | -0.435757 | C  | -0.138710 | -3.318336 | 1.897526  |
| S                            | 3.172915  | -0.880013 | -0.635686 | C  | -4.602734 | 0.367473  | 3.326203  |
| O                            | 3.301029  | -1.079570 | -2.083620 | C  | -4.530306 | 2.386375  | -2.235482 |
| O                            | 2.522892  | -1.875529 | 0.223227  | C  | -0.165857 | -1.279416 | -3.508523 |
| C                            | 4.828027  | -0.643688 | 0.024028  | H  | -0.547850 | -2.166502 | -4.015956 |
| C                            | 5.061842  | -0.863774 | 1.384098  | H  | 0.882734  | -1.418111 | -3.227823 |
| C                            | 5.860307  | -0.224843 | -0.818459 | H  | -0.217077 | -0.421749 | -4.188999 |
| C                            | 6.338672  | -0.647335 | 1.899969  | H  | -5.464542 | 1.965662  | -2.609799 |
| H                            | 4.260901  | -1.222104 | 2.022103  | H  | -3.918997 | 2.729679  | -3.077084 |
| C                            | 7.131141  | -0.019532 | -0.286137 | H  | -4.735345 | 3.255251  | -1.602484 |
| H                            | 5.668099  | -0.075544 | -1.874727 | H  | -4.950757 | 1.405500  | 3.289805  |
| C                            | 7.391589  | -0.223346 | 1.077203  | H  | -5.458267 | -0.304720 | 3.402301  |
| H                            | 6.521789  | -0.819791 | 2.957736  | H  | -3.966523 | 0.265829  | 4.211253  |
|                              |           |           |           | H  | -0.590235 | -4.306953 | 1.803688  |

|   |           |           |          |
|---|-----------|-----------|----------|
| H | -0.033382 | -3.054890 | 2.955196 |
| H | 0.860346  | -3.309832 | 1.450384 |
| H | -0.737650 | 4.578044  | 1.327675 |
| H | -1.920600 | 3.674338  | 0.362923 |
| O | -1.970778 | 3.421776  | 2.441743 |
| H | -2.362169 | 2.526270  | 2.397790 |

#### I(u)-Yne\_conf3

##### 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.610785  | -1.883727 | 2.002656  |
| H  | 3.313366  | -2.717324 | 2.097274  |
| H  | 1.609163  | -2.330311 | 1.917477  |
| N  | 2.921573  | -1.162457 | 0.763408  |
| S  | 4.148064  | -1.742372 | -0.256346 |
| O  | 3.584183  | -2.059421 | -1.572062 |
| O  | 4.887999  | -2.743027 | 0.519671  |
| C  | 5.198318  | -0.303221 | -0.466017 |
| C  | 6.010810  | 0.114271  | 0.593732  |
| C  | 5.212397  | 0.368003  | -1.687301 |
| C  | 6.830788  | 1.224045  | 0.421579  |
| H  | 6.001715  | -0.428407 | 1.533366  |
| C  | 6.042252  | 1.481211  | -1.840919 |
| H  | 4.592758  | 0.012719  | -2.503705 |
| C  | 6.860301  | 1.925844  | -0.796123 |
| H  | 7.464702  | 1.550863  | 1.242529  |
| H  | 6.055892  | 2.006830  | -2.792375 |
| C  | 7.771424  | 3.117822  | -0.969247 |
| H  | 7.657826  | 3.830837  | -0.144186 |
| H  | 8.824756  | 2.809836  | -0.985114 |
| H  | 7.566684  | 3.647401  | -1.904617 |
| C  | 1.817111  | -0.432651 | 0.125938  |
| H  | 1.379977  | 0.221931  | 0.883870  |
| H  | 2.214898  | 0.209456  | -0.665257 |
| C  | 0.765093  | -1.309277 | -0.430329 |
| C  | 0.030846  | -2.162147 | -0.903839 |
| C  | 2.682670  | -1.023829 | 3.241538  |
| H  | 2.307002  | -1.514103 | 4.140628  |
| C  | 3.165563  | 0.216802  | 3.318651  |
| H  | 3.554660  | 0.729250  | 2.443060  |
| H  | 3.198780  | 0.752210  | 4.263349  |
| C  | -0.754659 | -3.234554 | -1.548516 |
| Rh | -1.554093 | -0.219708 | -0.162656 |
| Rh | -3.402948 | 1.240667  | 0.340404  |
| O  | -2.669589 | -1.765991 | 0.640108  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -4.392311 | -0.377725 | 1.138545  |
| O | -2.539199 | 1.603680  | 2.171326  |
| O | -4.194050 | 0.819613  | -1.515026 |
| O | -2.322662 | 2.790523  | -0.480047 |
| O | -0.567328 | 1.426543  | -0.930671 |
| O | -0.816385 | 0.205906  | 1.711930  |
| O | -2.459259 | -0.543711 | -2.014222 |
| C | -3.569759 | 0.034296  | -2.285780 |
| C | -3.828272 | -1.515026 | 1.112899  |
| C | -1.458306 | 1.009540  | 2.468584  |
| C | -1.157243 | 2.557970  | -0.926879 |
| C | -0.380110 | 3.726593  | -1.491765 |
| C | -4.160071 | -0.243150 | -3.649067 |
| C | -4.595782 | -2.690198 | 1.676467  |
| C | -0.890292 | 1.248172  | 3.848918  |
| H | -1.062649 | 2.284149  | 4.150418  |
| H | 0.174293  | 1.007434  | 3.871633  |
| H | -1.413255 | 0.599672  | 4.561893  |
| H | -5.493688 | -2.349195 | 2.193712  |
| H | -3.956412 | -3.258424 | 2.358183  |
| H | -4.880930 | -3.359763 | 0.857254  |
| H | -4.195054 | -1.322269 | -3.827932 |
| H | -5.160392 | 0.184580  | -3.727183 |
| H | -3.513778 | 0.196166  | -4.417065 |
| H | -1.037797 | 4.582737  | -1.649397 |
| H | 0.100822  | 3.435940  | -2.429752 |
| H | 0.410180  | 4.006817  | -0.785882 |
| H | -0.114909 | -4.120712 | -1.630155 |
| H | -1.601864 | -3.490576 | -0.895266 |
| O | -1.172150 | -2.904879 | -2.857898 |
| H | -1.687113 | -2.078530 | -2.782068 |

#### I-TS-II(u)\_conf1

##### 1 imaginary frequency, value = -335.8495 cm<sup>-1</sup>

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -1.671728 | 0.881444 | 0.255971  |
| C | -0.422181 | 1.451949 | -0.314955 |
| C | -0.144486 | 2.572238 | -0.889618 |
| C | -2.037658 | 3.553652 | -1.317484 |
| C | -3.034047 | 2.430643 | -1.132344 |
| H | -1.858276 | 3.873356 | -2.342100 |
| H | -4.045070 | 2.849354 | -1.159579 |
| H | -2.942562 | 1.707626 | -1.957178 |
| H | -1.497212 | 0.645059 | 1.308373  |
| N | -2.830638 | 1.793172 | 0.167508  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| S  | -4.195879 | 1.366733  | 1.072188  |
| O  | -3.704771 | 1.065451  | 2.416826  |
| O  | -5.186747 | 2.416831  | 0.817759  |
| C  | -4.826528 | -0.160979 | 0.372405  |
| C  | -5.781670 | -0.112637 | -0.646482 |
| C  | -4.338548 | -1.385706 | 0.837104  |
| C  | -6.239818 | -1.303849 | -1.206304 |
| H  | -6.175241 | 0.843364  | -0.975416 |
| C  | -4.807490 | -2.566206 | 0.263449  |
| H  | -3.619943 | -1.409473 | 1.649217  |
| C  | -5.762209 | -2.546240 | -0.764010 |
| H  | -6.987027 | -1.268644 | -1.995315 |
| H  | -4.432195 | -3.519697 | 0.627073  |
| C  | -6.289986 | -3.832826 | -1.352859 |
| H  | -7.148024 | -4.203887 | -0.776822 |
| H  | -6.626206 | -3.693644 | -2.385360 |
| H  | -5.528722 | -4.619783 | -1.344312 |
| C  | -1.508814 | 4.251579  | -0.276902 |
| H  | -0.847912 | 5.097425  | -0.429261 |
| H  | -1.758073 | 3.988393  | 0.745050  |
| C  | 0.981937  | 3.357931  | -1.470947 |
| H  | 1.611991  | 2.624823  | -1.995120 |
| H  | -1.867407 | -0.068553 | -0.265673 |
| Rh | 3.099016  | -1.472601 | 0.283099  |
| Rh | 1.281793  | 0.114980  | -0.102383 |
| O  | 4.269262  | 0.127540  | 0.890430  |
| O  | 2.589258  | 1.612075  | 0.555062  |
| O  | 2.018097  | 0.345814  | -2.030895 |
| O  | 0.690845  | -0.237600 | 1.852125  |
| O  | 0.130047  | -1.483352 | -0.722882 |
| O  | 1.814895  | -2.959478 | -0.352646 |
| O  | 3.685535  | -1.152313 | -1.672817 |
| O  | 2.391283  | -1.697922 | 2.211081  |
| C  | 1.368587  | -1.044944 | 2.574635  |
| C  | 3.786253  | 1.293099  | 0.892215  |
| C  | 3.041512  | -0.331811 | -2.389511 |
| C  | 0.640996  | -2.654639 | -0.714132 |
| C  | -0.244433 | -3.775501 | -1.218373 |
| C  | 0.915916  | -1.203569 | 4.010773  |
| C  | 4.675572  | 2.430247  | 1.348350  |
| C  | 3.522821  | -0.111253 | -3.808828 |
| H  | 3.886590  | 0.916961  | -3.913664 |
| H  | 2.689435  | -0.237648 | -4.506645 |
| H  | 4.326659  | -0.807277 | -4.052711 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 4.582460  | 3.278415  | 0.663204  |
| H | 5.714462  | 2.102510  | 1.406174  |
| H | 4.349469  | 2.767193  | 2.339109  |
| H | 1.394655  | -0.427845 | 4.620211  |
| H | -0.165836 | -1.074105 | 4.089217  |
| H | 1.218074  | -2.179111 | 4.397011  |
| H | -1.292161 | -3.567688 | -0.988419 |
| H | 0.065422  | -4.727166 | -0.782032 |
| H | -0.142504 | -3.845306 | -2.307886 |
| H | 0.617731  | 4.075536  | -2.211741 |
| O | 1.709913  | 4.087036  | -0.503864 |
| H | 2.084599  | 3.404387  | 0.090454  |

# I-TS-II(u)\_conf2

1 imaginary frequency, value = -338.9476 cm<sup>-1</sup>

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.628221 | 0.929982  | -0.798370 |
| C | -0.524339 | 1.446219  | 0.055942  |
| C | -0.423064 | 2.452651  | 0.856644  |
| C | -2.198203 | 3.693935  | 0.539401  |
| C | -2.750280 | 3.140621  | -0.751676 |
| H | -1.745678 | 4.682058  | 0.483608  |
| H | -3.737785 | 3.573837  | -0.941795 |
| H | -2.097645 | 3.424613  | -1.590724 |
| H | -1.806402 | -0.116290 | -0.530919 |
| N | -2.893007 | 1.684105  | -0.648159 |
| S | -4.221188 | 1.004185  | -1.477882 |
| O | -5.282823 | 2.016793  | -1.423605 |
| O | -3.790048 | 0.438641  | -2.762473 |
| C | -4.666065 | -0.356117 | -0.402892 |
| C | -4.353499 | -1.661315 | -0.778661 |
| C | -5.352226 | -0.091847 | 0.786760  |
| C | -4.722427 | -2.714564 | 0.061079  |
| H | -3.842711 | -1.844024 | -1.717896 |
| C | -5.711430 | -1.153670 | 1.609657  |
| H | -5.611933 | 0.928557  | 1.049212  |
| C | -5.401761 | -2.480205 | 1.262629  |
| H | -4.484470 | -3.734681 | -0.229220 |
| H | -6.247259 | -0.954291 | 2.534569  |
| C | -5.815244 | -3.620842 | 2.161667  |
| H | -6.906952 | -3.730738 | 2.181567  |
| H | -5.391389 | -4.571586 | 1.824985  |
| H | -5.490051 | -3.451441 | 3.194816  |
| C | -2.356871 | 3.080775  | 1.743150  |
| H | -2.004333 | 3.525247  | 2.666930  |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H                            | -2.880134 | 2.133881  | 1.812515  | C  | -2.918555 | 2.525616  | -0.990174 |
| C                            | 0.522770  | 3.144149  | 1.779772  | H  | -1.698057 | 3.897666  | -2.217744 |
| H                            | 1.513670  | 3.040571  | 1.315382  | H  | -3.805801 | 3.159768  | -0.921483 |
| H                            | -1.280523 | 0.934771  | -1.841170 | H  | -3.063107 | 1.803702  | -1.811731 |
| Rh                           | 3.193152  | -1.279009 | -0.210328 | H  | -1.328546 | 0.783960  | 1.437695  |
| Rh                           | 1.274906  | 0.224005  | -0.045137 | N  | -2.732611 | 1.861609  | 0.299111  |
| O                            | 3.449454  | -1.055551 | 1.834590  | S  | -4.101401 | 1.377879  | 1.165320  |
| O                            | 1.636764  | 0.293141  | 2.019038  | O  | -3.611383 | 0.993514  | 2.489847  |
| O                            | 2.598407  | 1.796881  | -0.320655 | O  | -5.092882 | 2.438198  | 0.971409  |
| O                            | 0.092440  | -1.462728 | 0.216606  | C  | -4.722948 | -0.104997 | 0.369566  |
| O                            | 1.067330  | 0.030713  | -2.087677 | C  | -5.629707 | 0.006616  | -0.688674 |
| O                            | 2.826592  | -1.397792 | -2.236238 | C  | -4.282471 | -1.357572 | 0.804745  |
| O                            | 4.370385  | 0.391583  | -0.523596 | C  | -6.087748 | -1.149719 | -1.316172 |
| O                            | 1.887586  | -2.849278 | 0.111170  | H  | -5.987703 | 0.984127  | -0.994214 |
| C                            | 0.650542  | -2.611195 | 0.242727  | C  | -4.753729 | -2.503722 | 0.165139  |
| C                            | 2.646464  | -0.341605 | 2.495156  | H  | -3.602098 | -1.428379 | 1.646509  |
| C                            | 3.837328  | 1.539428  | -0.507924 | C  | -5.660047 | -2.420246 | -0.901582 |
| C                            | 1.872215  | -0.726977 | -2.729995 | H  | -6.797174 | -1.065664 | -2.135826 |
| C                            | 1.664305  | -0.799573 | -4.227785 | H  | -4.421052 | -3.479962 | 0.509296  |
| C                            | -0.256170 | -3.804525 | 0.466711  | C  | -6.194776 | -3.667491 | -1.564099 |
| C                            | 2.863487  | -0.226846 | 3.989375  | H  | -7.151817 | -3.967881 | -1.117438 |
| C                            | 4.739000  | 2.735543  | -0.732077 | H  | -6.371574 | -3.509230 | -2.633172 |
| H                            | 4.670877  | 3.413763  | 0.124931  | H  | -5.504118 | -4.509345 | -1.452825 |
| H                            | 4.400839  | 3.288042  | -1.614864 | C  | -0.971339 | 3.972117  | -0.138033 |
| H                            | 5.772714  | 2.415212  | -0.869121 | H  | -0.388709 | 4.877393  | -0.273517 |
| H                            | 2.727456  | 0.809790  | 4.311859  | H  | -1.327291 | 3.784939  | 0.868279  |
| H                            | 3.860236  | -0.580177 | 4.257422  | C  | 0.903067  | 3.219147  | -1.754908 |
| H                            | 2.116726  | -0.838431 | 4.509178  | H  | 1.296852  | 2.357495  | -2.303662 |
| H                            | -0.028850 | -4.250315 | 1.441290  | H  | -1.731152 | 0.000576  | -0.076785 |
| H                            | -1.305784 | -3.506683 | 0.439563  | Rh | 2.996412  | -1.522266 | 0.283866  |
| H                            | -0.056922 | -4.564105 | -0.295045 | Rh | 1.220790  | 0.155497  | -0.067086 |
| H                            | 0.598949  | -0.891784 | -4.455898 | O  | 4.291506  | 0.040122  | 0.704453  |
| H                            | 2.219866  | -1.638757 | -4.649432 | O  | 2.667659  | 1.588458  | 0.381546  |
| H                            | 2.021473  | 0.131008  | -4.683760 | O  | 1.796497  | 0.178648  | -2.065018 |
| H                            | 0.294310  | 4.211762  | 1.846309  | O  | 0.786527  | -0.044795 | 1.946897  |
| O                            | 0.498168  | 2.627097  | 3.095464  | O  | -0.044492 | -1.424735 | -0.484921 |
| H                            | 0.797285  | 1.699552  | 2.996093  | O  | 1.588645  | -2.969046 | -0.166693 |
| <b>II(u)_conf1</b>           |           |           |           | O  | 3.445900  | -1.345783 | -1.726073 |
| <b>0 imaginary frequency</b> |           |           |           | O  | 2.424371  | -1.582871 | 2.274631  |
| C                            | -1.551793 | 0.990525  | 0.382981  | C  | 1.472995  | -0.852325 | 2.668951  |
| C                            | -0.306160 | 1.492998  | -0.254862 | C  | 3.873491  | 1.225567  | 0.651460  |
| C                            | -0.292500 | 2.765488  | -0.906880 | C  | 2.770490  | -0.560130 | -2.448319 |
| C                            | -1.695979 | 3.381345  | -1.260234 | C  | 0.408360  | -2.623403 | -0.448562 |
|                              |           |           |           | C  | -0.573676 | -3.716899 | -0.814725 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.101501  | -0.898944 | 4.135849  |
| C | 4.848353  | 2.347155  | 0.936883  |
| C | 3.138774  | -0.455129 | -3.913869 |
| H | 3.543613  | 0.542925  | -4.115254 |
| H | 2.244523  | -0.578038 | -4.532240 |
| H | 3.883851  | -1.208328 | -4.174094 |
| H | 4.820554  | 3.080006  | 0.123959  |
| H | 5.858470  | 1.952038  | 1.051864  |
| H | 4.549658  | 2.864253  | 1.855352  |
| H | 1.439236  | 0.024329  | 4.620262  |
| H | 0.014971  | -0.949942 | 4.248624  |
| H | 1.576752  | -1.752866 | 4.621034  |
| H | -1.598644 | -3.402260 | -0.606413 |
| H | -0.331755 | -4.633338 | -0.272021 |
| H | -0.487992 | -3.924156 | -1.888039 |
| H | 0.552335  | 3.957794  | -2.485151 |
| O | 1.905014  | 3.864380  | -0.994791 |
| H | 2.279859  | 3.180988  | -0.402429 |

#### 1aa\_conf1

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.748517  | 1.487023  | 0.789801  |
| H | 0.339016  | 1.665597  | 1.788547  |
| H | 0.087049  | 1.972159  | 0.053063  |
| N | 0.761229  | 0.022031  | 0.603961  |
| S | -0.517369 | -0.839863 | 1.310718  |
| O | -0.671713 | -0.294955 | 2.660664  |
| O | -0.235933 | -2.256396 | 1.066031  |
| C | -2.002159 | -0.421809 | 0.388397  |
| C | -2.390847 | -1.218534 | -0.691843 |
| C | -2.744044 | 0.708405  | 0.743320  |
| C | -3.522526 | -0.867362 | -1.425609 |
| H | -1.827576 | -2.113574 | -0.933547 |
| C | -3.872301 | 1.044392  | -0.002620 |
| H | -2.452848 | 1.298715  | 1.605633  |
| C | -4.279347 | 0.266483  | -1.096492 |
| H | -3.827817 | -1.489914 | -2.263128 |
| H | -4.451651 | 1.921544  | 0.275207  |
| C | -5.523739 | 0.619356  | -1.876106 |
| H | -5.455698 | 0.281280  | -2.915212 |
| H | -6.410117 | 0.143711  | -1.435773 |
| H | -5.702498 | 1.699562  | -1.879329 |
| C | 1.243550  | -0.468932 | -0.703008 |
| H | 0.777255  | -1.439351 | -0.893851 |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 0.923934 | 0.215969  | -1.503041 |
| C | 2.697036 | -0.642675 | -0.751450 |
| C | 3.888373 | -0.832891 | -0.827203 |
| C | 2.128855 | 2.079443  | 0.704677  |
| H | 2.871507 | 1.640908  | 1.368050  |
| C | 2.448096 | 3.099220  | -0.092095 |
| H | 1.722809 | 3.546793  | -0.769152 |
| H | 3.446279 | 3.527212  | -0.097351 |
| C | 5.330320 | -1.039657 | -0.897949 |
| H | 5.719760 | -1.357837 | 0.077624  |
| H | 5.572623 | -1.818437 | -1.632559 |
| F | 5.997749 | 0.125034  | -1.269874 |

#### 1aa\_conf2

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.777980 | -1.346499 | 1.441871  |
| H | 0.234379  | -1.184156 | 1.831361  |
| H | -1.026757 | -2.403397 | 1.616445  |
| N | -0.735993 | -1.045791 | -0.005086 |
| S | 0.678533  | -1.580633 | -0.791367 |
| O | 0.404386  | -1.485992 | -2.230411 |
| O | 1.153043  | -2.844078 | -0.209762 |
| C | 1.845642  | -0.301618 | -0.330262 |
| C | 3.025887  | -0.657137 | 0.319757  |
| C | 1.586418  | 1.027351  | -0.680274 |
| C | 3.955456  | 0.337924  | 0.629117  |
| H | 3.206092  | -1.695471 | 0.576423  |
| C | 2.523661  | 2.004219  | -0.363203 |
| H | 0.660558  | 1.287728  | -1.182794 |
| C | 3.722807  | 1.676744  | 0.293210  |
| H | 4.875686  | 0.066085  | 1.139876  |
| H | 2.324790  | 3.039953  | -0.627918 |
| C | 4.739217  | 2.748176  | 0.608828  |
| H | 5.486203  | 2.394422  | 1.325937  |
| H | 5.273015  | 3.062456  | -0.297534 |
| H | 4.261784  | 3.641465  | 1.027260  |
| C | -2.002932 | -1.233762 | -0.744671 |
| H | -1.758259 | -1.551946 | -1.762454 |
| H | -2.587023 | -2.040812 | -0.280202 |
| C | -2.804484 | -0.009295 | -0.811767 |
| C | -3.480240 | 0.988280  | -0.915525 |
| C | -1.742194 | -0.449378 | 2.168065  |
| H | -1.599055 | 0.619710  | 2.021929  |
| C | -2.709189 | -0.897409 | 2.968899  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -2.877932 | -1.961430 | 3.123207  |
| H | -3.366959 | -0.217856 | 3.503093  |
| C | -4.296334 | 2.193167  | -1.013198 |
| H | -3.685489 | 3.050073  | -1.325576 |
| H | -5.095229 | 2.056733  | -1.753526 |
| F | -4.889359 | 2.511454  | 0.206472  |

#### 1aa\_conf3

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.256634 | -0.251654 | 0.598484  |
| H | -3.324547 | -1.336132 | 0.721799  |
| H | -4.108451 | 0.034525  | -0.041077 |
| N | -1.984863 | 0.046935  | -0.078253 |
| S | -1.224662 | -1.230512 | -0.917691 |
| O | -1.175156 | -0.902537 | -2.348529 |
| O | -1.858029 | -2.469297 | -0.450454 |
| C | 0.455513  | -1.204914 | -0.295583 |
| C | 0.691693  | -1.431020 | 1.063533  |
| C | 1.509978  | -1.025933 | -1.187705 |
| C | 2.002535  | -1.459615 | 1.526995  |
| H | -0.138221 | -1.578732 | 1.746893  |
| C | 2.820125  | -1.063186 | -0.704970 |
| H | 1.301880  | -0.864053 | -2.239553 |
| C | 3.087366  | -1.274484 | 0.653183  |
| H | 2.190401  | -1.631479 | 2.584099  |
| H | 3.647032  | -0.931771 | -1.398626 |
| C | 4.503702  | -1.295005 | 1.177274  |
| H | 4.707818  | -0.413214 | 1.798216  |
| H | 4.684487  | -2.177044 | 1.802562  |
| H | 5.233449  | -1.303376 | 0.361940  |
| C | -1.942014 | 1.362749  | -0.755047 |
| H | -2.317015 | 1.283832  | -1.784620 |
| H | -2.630745 | 2.005357  | -0.196711 |
| C | -0.619226 | 1.987090  | -0.759454 |
| C | 0.464770  | 2.521402  | -0.782127 |
| C | -3.381113 | 0.425532  | 1.941367  |
| H | -4.370904 | 0.335223  | 2.390411  |
| C | -2.418071 | 1.083394  | 2.587027  |
| H | -1.422063 | 1.193562  | 2.167019  |
| H | -2.598356 | 1.530864  | 3.560217  |
| C | 1.789444  | 3.130844  | -0.799499 |
| H | 2.560143  | 2.351005  | -0.853079 |
| H | 1.901723  | 3.787055  | -1.672093 |
| F | 2.021009  | 3.890832  | 0.343824  |

#### 1aa\_conf4

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.149104  | -0.706208 | 0.542322  |
| H | 4.087546  | -0.334919 | 0.096991  |
| H | 3.077641  | -1.755339 | 0.241707  |
| N | 1.999787  | 0.007980  | -0.029453 |
| S | 1.116025  | -0.757978 | -1.278457 |
| O | 1.705834  | -2.089848 | -1.461355 |
| O | 1.015949  | 0.195077  | -2.388928 |
| C | -0.526276 | -0.992915 | -0.601025 |
| C | -1.501883 | -0.014927 | -0.792848 |
| C | -0.806329 | -2.158459 | 0.117034  |
| C | -2.766948 | -0.202334 | -0.237838 |
| H | -1.279446 | 0.882523  | -1.355533 |
| C | -2.079214 | -2.332352 | 0.654405  |
| H | -0.042244 | -2.918664 | 0.238075  |
| C | -3.077583 | -1.359645 | 0.488342  |
| H | -3.515121 | 0.574626  | -0.369087 |
| H | -2.302170 | -3.239386 | 1.211279  |
| C | -4.461069 | -1.571583 | 1.056272  |
| H | -4.989208 | -0.622041 | 1.189348  |
| H | -5.069826 | -2.193537 | 0.386541  |
| H | -4.424278 | -2.080970 | 2.025457  |
| C | 2.166978  | 1.470963  | -0.157545 |
| H | 2.919933  | 1.751316  | 0.586591  |
| H | 2.557772  | 1.736499  | -1.148314 |
| C | 0.942950  | 2.229304  | 0.109333  |
| C | -0.066172 | 2.858657  | 0.325722  |
| C | 3.229013  | -0.603424 | 2.045892  |
| H | 4.157099  | -0.992114 | 2.466957  |
| C | 2.292323  | -0.105456 | 2.852666  |
| H | 1.357148  | 0.286950  | 2.462965  |
| H | 2.431709  | -0.082772 | 3.929726  |
| C | -1.342936 | 3.537694  | 0.512487  |
| H | -1.755748 | 3.332274  | 1.507584  |
| H | -1.230647 | 4.623114  | 0.401259  |
| F | -2.280122 | 3.107390  | -0.433235 |

#### I(aa)-Yne\_conf1

##### 0 imaginary frequency

|   |          |          |           |
|---|----------|----------|-----------|
| C | 1.320632 | 2.277248 | -1.086850 |
| H | 0.750151 | 2.799834 | -0.311126 |
| H | 0.654962 | 2.144267 | -1.939613 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | 1.531814  | 0.901203  | -0.497492 |
| S  | 2.442144  | -0.114438 | -1.637668 |
| O  | 3.823271  | 0.371759  | -1.721585 |
| O  | 1.596086  | -0.178708 | -2.828590 |
| C  | 2.517149  | -1.724684 | -0.848354 |
| C  | 1.515832  | -2.664763 | -1.088671 |
| C  | 3.650779  | -2.049256 | -0.096266 |
| C  | 1.650181  | -3.942722 | -0.546747 |
| H  | 0.648359  | -2.389327 | -1.675665 |
| C  | 3.760152  | -3.328373 | 0.442812  |
| H  | 4.431820  | -1.311773 | 0.052011  |
| C  | 2.767250  | -4.295811 | 0.223173  |
| H  | 0.875133  | -4.682574 | -0.732645 |
| H  | 4.637445  | -3.584859 | 1.031685  |
| C  | 2.921761  | -5.694904 | 0.770708  |
| H  | 1.952774  | -6.190481 | 0.888063  |
| H  | 3.526167  | -6.314478 | 0.094936  |
| H  | 3.425144  | -5.692288 | 1.743420  |
| C  | 2.088309  | 0.889263  | 0.891726  |
| H  | 1.381882  | 1.481628  | 1.481006  |
| H  | 1.998775  | -0.137199 | 1.259338  |
| C  | 3.449408  | 1.383369  | 1.114110  |
| C  | 4.566088  | 1.763637  | 1.381969  |
| C  | 2.523283  | 3.091268  | -1.490141 |
| H  | 3.292298  | 3.258163  | -0.741634 |
| C  | 2.621648  | 3.659588  | -2.692333 |
| H  | 1.872373  | 3.498361  | -3.464750 |
| H  | 3.459898  | 4.299771  | -2.953094 |
| C  | 5.916232  | 2.249863  | 1.642926  |
| Rh | -0.899362 | 0.290574  | -0.066772 |
| Rh | -3.178196 | -0.095090 | 0.605560  |
| O  | -1.633426 | 1.692113  | -1.397982 |
| O  | -3.774709 | 1.331881  | -0.745610 |
| O  | -3.340285 | -1.514933 | -0.862978 |
| O  | -2.944769 | 1.358394  | 2.047670  |
| O  | -2.476771 | -1.521283 | 1.921826  |
| O  | -0.325639 | -1.129442 | 1.319957  |
| O  | -1.193240 | -1.171653 | -1.502176 |
| O  | -0.811507 | 1.753802  | 1.400191  |
| C  | -1.838452 | 1.969771  | 2.130558  |
| C  | -2.889387 | 1.902165  | -1.457125 |
| C  | -2.329459 | -1.741057 | -1.598028 |
| C  | -1.226381 | -1.725098 | 2.000369  |
| C  | -0.744474 | -2.750647 | 3.002767  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.709848 | 3.059282  | 3.171510  |
| C | -3.364131 | 2.902902  | -2.486601 |
| C | -2.474588 | -2.800904 | -2.667794 |
| H | -3.524043 | -2.918469 | -2.944515 |
| H | -2.112903 | -3.758684 | -2.274401 |
| H | -1.871903 | -2.541373 | -3.541136 |
| H | -4.377451 | 3.236208  | -2.256280 |
| H | -3.363396 | 2.424225  | -3.472756 |
| H | -2.679718 | 3.753980  | -2.529273 |
| H | -1.594305 | 4.026493  | 2.670127  |
| H | -2.593072 | 3.084281  | 3.811180  |
| H | -0.811987 | 2.892973  | 3.774510  |
| H | -1.569148 | -3.388480 | 3.325104  |
| H | -0.333979 | -2.232038 | 3.876995  |
| H | 0.057754  | -3.349395 | 2.563268  |
| H | 6.425115  | 1.610117  | 2.375416  |
| H | 6.503736  | 2.245637  | 0.715866  |
| F | 5.903024  | 3.549444  | 2.142837  |

# I(aa)-Ene\_conf2

## 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.754064 | 0.603119  | -0.230539 |
| H | 1.395343 | -0.109441 | 0.514913  |
| H | 1.976556 | 0.061205  | -1.162077 |
| N | 2.967256 | 1.231200  | 0.322983  |
| S | 3.849125 | 0.287358  | 1.431868  |
| O | 2.870830 | -0.255587 | 2.375956  |
| O | 4.971049 | 1.121239  | 1.868232  |
| C | 4.528509 | -1.095957 | 0.508796  |
| C | 5.795008 | -0.981221 | -0.070616 |
| C | 3.777659 | -2.265390 | 0.357656  |
| C | 6.301653 | -2.044163 | -0.816328 |
| H | 6.381951 | -0.082019 | 0.083660  |
| C | 4.301166 | -3.317310 | -0.391676 |
| H | 2.809426 | -2.353846 | 0.838409  |
| C | 5.566406 | -3.225437 | -0.990451 |
| H | 7.288846 | -1.957811 | -1.263611 |
| H | 3.720808 | -4.229699 | -0.506097 |
| C | 6.138357 | -4.384764 | -1.771131 |
| H | 6.840852 | -4.043952 | -2.538561 |
| H | 6.684630 | -5.070707 | -1.110180 |
| H | 5.350782 | -4.965498 | -2.262422 |
| C | 3.771780 | 2.046394  | -0.608983 |
| H | 4.767595 | 2.161991  | -0.171903 |

|                   |           |           |           |                                                           |           |           |           |
|-------------------|-----------|-----------|-----------|-----------------------------------------------------------|-----------|-----------|-----------|
| H                 | 3.886969  | 1.523601  | -1.572671 | 1 imaginary frequency, value = -346.9468 cm <sup>-1</sup> |           |           |           |
| C                 | 3.215629  | 3.381227  | -0.836083 | C                                                         | -1.632556 | 0.927363  | 0.378808  |
| C                 | 2.805698  | 4.497415  | -1.054239 | C                                                         | -0.384632 | 1.528562  | -0.162360 |
| C                 | 0.653239  | 1.609430  | -0.458518 | C                                                         | -0.122006 | 2.670088  | -0.702260 |
| H                 | 0.455391  | 2.279764  | 0.374171  | C                                                         | -2.080038 | 3.545812  | -1.265155 |
| C                 | -0.048255 | 1.729425  | -1.609844 | C                                                         | -3.032804 | 2.394428  | -1.051342 |
| H                 | 0.170954  | 1.112368  | -2.477516 | H                                                         | -1.899540 | 3.834690  | -2.298892 |
| H                 | -0.789853 | 2.510330  | -1.740529 | H                                                         | -4.057859 | 2.777210  | -1.099160 |
| C                 | 2.299476  | 5.844633  | -1.294358 | H                                                         | -2.911385 | 1.652024  | -1.855577 |
| Rh                | -1.568463 | 0.252444  | -0.312934 | H                                                         | -1.469696 | 0.694969  | 1.434395  |
| Rh                | -3.377324 | -1.127281 | 0.473223  | N                                                         | -2.818804 | 1.802377  | 0.268336  |
| O                 | -2.639190 | 0.474105  | -2.082614 | S                                                         | -4.191996 | 1.308262  | 1.134035  |
| O                 | -4.335695 | -0.822536 | -1.321690 | O                                                         | -3.719649 | 0.996449  | 2.482511  |
| O                 | -2.398874 | -2.755407 | -0.334134 | O                                                         | -5.211205 | 2.329901  | 0.876637  |
| O                 | -4.250429 | 0.576480  | 1.234970  | C                                                         | -4.751847 | -0.222359 | 0.383738  |
| O                 | -2.362767 | -1.400976 | 2.240502  | C                                                         | -5.694509 | -0.182065 | -0.647202 |
| O                 | -0.666363 | -0.091038 | 1.515253  | C                                                         | -4.223169 | -1.440165 | 0.821818  |
| O                 | -0.681260 | -1.461185 | -1.058498 | C                                                         | -6.098023 | -1.373589 | -1.247006 |
| O                 | -2.555062 | 1.881132  | 0.478570  | H                                                         | -6.121561 | 0.766763  | -0.954333 |
| C                 | -3.665480 | 1.692462  | 1.079336  | C                                                         | -4.638573 | -2.621074 | 0.208865  |
| C                 | -3.773391 | -0.095567 | -2.197398 | H                                                         | -3.514953 | -1.459902 | 1.643132  |
| C                 | -1.286693 | -2.575939 | -0.917870 | C                                                         | -5.578694 | -2.608652 | -0.832403 |
| C                 | -1.237172 | -0.831371 | 2.384255  | H                                                         | -6.835101 | -1.344583 | -2.045713 |
| C                 | -0.511212 | -1.013051 | 3.696647  | H                                                         | -4.232773 | -3.569423 | 0.552573  |
| C                 | -4.337317 | 2.921385  | 1.651128  | C                                                         | -6.047310 | -3.897113 | -1.465401 |
| C                 | -4.526283 | 0.144679  | -3.487942 | H                                                         | -6.894293 | -4.320696 | -0.909633 |
| C                 | -0.627625 | -3.790478 | -1.535505 | H                                                         | -6.379757 | -3.739988 | -2.496525 |
| H                 | -0.907008 | -4.692509 | -0.987223 | H                                                         | -5.254132 | -4.651852 | -1.473097 |
| H                 | 0.457782  | -3.668939 | -1.553102 | C                                                         | -1.549816 | 4.277053  | -0.247996 |
| H                 | -0.976785 | -3.895378 | -2.569601 | H                                                         | -0.927383 | 5.143943  | -0.433821 |
| H                 | -5.276318 | -0.633153 | -3.642090 | H                                                         | -1.793719 | 4.044945  | 0.782671  |
| H                 | -3.831203 | 0.181867  | -4.330293 | C                                                         | 0.935764  | 3.431990  | -1.394015 |
| H                 | -5.034199 | 1.114438  | -3.427537 | H                                                         | 1.787015  | 2.756274  | -1.509583 |
| H                 | -4.562316 | 3.623853  | 0.841716  | H                                                         | -1.786483 | -0.028415 | -0.145384 |
| H                 | -5.257244 | 2.649354  | 2.170370  | Rh                                                        | 3.066940  | -1.508589 | 0.189129  |
| H                 | -3.652638 | 3.424796  | 2.341032  | Rh                                                        | 1.289979  | 0.143650  | -0.042499 |
| H                 | -0.741489 | -1.992707 | 4.121579  | O                                                         | 4.297256  | 0.028965  | 0.821771  |
| H                 | -0.859454 | -0.247221 | 4.400184  | O                                                         | 2.637450  | 1.564370  | 0.614191  |
| H                 | 0.564242  | -0.886372 | 3.555234  | O                                                         | 1.958911  | 0.465699  | -1.983282 |
| H                 | 2.425371  | 6.120703  | -2.349344 | O                                                         | 0.757560  | -0.291225 | 1.910577  |
| H                 | 1.229922  | 5.898587  | -1.052607 | O                                                         | 0.068602  | -1.408262 | -0.701258 |
| F                 | 2.966167  | 6.787888  | -0.519783 | O                                                         | 1.723705  | -2.942227 | -0.455789 |
|                   |           |           |           | O                                                         | 3.578115  | -1.112680 | -1.776222 |
| I-TS-II(aa)_conf1 |           |           |           | O                                                         | 2.437798  | -1.801194 | 2.134431  |

I-TS-II(aa)\_conf1

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | 1.443538  | -1.146322 | 2.567252  | H  | -3.623475 | -1.480052 | 1.619956  |
| C                            | 3.827217  | 1.202602  | 0.906747  | C  | -5.669902 | -2.397771 | -0.964897 |
| C                            | 2.941220  | -0.228762 | -2.419063 | H  | -6.798735 | -1.008065 | -2.167426 |
| C                            | 0.546956  | -2.590712 | -0.763008 | H  | -4.440117 | -3.497805 | 0.422711  |
| C                            | -0.383111 | -3.666019 | -1.287736 | C  | -6.200702 | -3.625099 | -1.666571 |
| C                            | 1.037989  | -1.366286 | 4.009406  | H  | -7.163482 | -3.934671 | -1.238930 |
| C                            | 4.746040  | 2.284307  | 1.434189  | H  | -6.365157 | -3.437316 | -2.732861 |
| C                            | 3.374194  | 0.050941  | -3.843919 | H  | -5.513376 | -4.471515 | -1.570775 |
| H                            | 3.724469  | 1.085940  | -3.922742 | C  | -0.956432 | 3.934827  | -0.118303 |
| H                            | 2.519080  | -0.058687 | -4.518444 | H  | -0.387270 | 4.845055  | -0.270782 |
| H                            | 4.174092  | -0.628575 | -4.141234 | H  | -1.296709 | 3.755954  | 0.894890  |
| H                            | 4.493310  | 3.249721  | 0.990021  | C  | 0.882589  | 3.139374  | -1.748566 |
| H                            | 5.788355  | 2.026659  | 1.235711  | H  | 1.484733  | 2.276003  | -2.023559 |
| H                            | 4.610379  | 2.364687  | 2.519305  | H  | -1.753930 | -0.044813 | -0.023810 |
| H                            | 1.492514  | -0.584046 | 4.628761  | Rh | 3.051880  | -1.475033 | 0.276603  |
| H                            | -0.046651 | -1.289320 | 4.116949  | Rh | 1.206711  | 0.118813  | -0.060031 |
| H                            | 1.392495  | -2.337493 | 4.359752  | O  | 4.305291  | 0.161638  | 0.496210  |
| H                            | -1.418420 | -3.439136 | -1.021924 | O  | 2.578166  | 1.616966  | 0.253557  |
| H                            | -0.089411 | -4.643176 | -0.898966 | O  | 1.696398  | 0.084822  | -2.083063 |
| H                            | -0.310840 | -3.694465 | -2.381552 | O  | 0.863412  | -0.012913 | 1.975232  |
| H                            | 0.610484  | 3.779782  | -2.381193 | O  | -0.033565 | -1.523100 | -0.349032 |
| F                            | 1.338959  | 4.558560  | -0.675229 | O  | 1.659393  | -2.990743 | 0.020266  |
| <b>II(aa)_conf1</b>          |           |           |           | O  | 3.367173  | -1.421048 | -1.766890 |
| <b>0 imaginary frequency</b> |           |           |           | O  | 2.614175  | -1.421774 | 2.299264  |
| C                            | -1.558611 | 0.947026  | 0.425499  | C  | 1.636850  | -0.732349 | 2.702898  |
| C                            | -0.314855 | 1.433824  | -0.226123 | C  | 3.809212  | 1.323434  | 0.443555  |
| C                            | -0.288354 | 2.717088  | -0.868410 | C  | 2.653510  | -0.668392 | -2.485215 |
| C                            | -1.694791 | 3.334766  | -1.225412 | C  | 0.458676  | -2.700782 | -0.241147 |
| C                            | -2.919192 | 2.487143  | -0.941153 | C  | -0.496344 | -3.852583 | -0.482143 |
| H                            | -1.700558 | 3.841196  | -2.188174 | C  | 1.338664  | -0.720256 | 4.187147  |
| H                            | -3.801325 | 3.128624  | -0.873343 | C  | 4.736120  | 2.503157  | 0.645536  |
| H                            | -3.073179 | 1.760755  | -1.757253 | C  | 2.945845  | -0.623403 | -3.971039 |
| H                            | -1.321744 | 0.745663  | 1.478822  | H  | 3.349703  | 0.361561  | -4.231140 |
| N                            | -2.731549 | 1.831437  | 0.351772  | H  | 2.020508  | -0.760618 | -4.538471 |
| S                            | -4.109131 | 1.340240  | 1.205422  | H  | 3.671094  | -1.392985 | -4.239265 |
| O                            | -3.625231 | 0.927248  | 2.523149  | H  | 4.343684  | 3.378708  | 0.124149  |
| O                            | -5.091047 | 2.412316  | 1.028285  | H  | 5.741899  | 2.256831  | 0.298272  |
| C                            | -4.735590 | -0.119963 | 0.373682  | H  | 4.790106  | 2.733916  | 1.716126  |
| C                            | -5.637236 | 0.022200  | -0.685446 | H  | 1.612430  | 0.256993  | 4.600600  |
| C                            | -4.300202 | -1.384772 | 0.777658  | H  | 0.267112  | -0.859532 | 4.356329  |
| C                            | -6.093898 | -1.115696 | -1.346558 | H  | 1.908914  | -1.499214 | 4.695513  |
| H                            | -5.992082 | 1.008332  | -0.965843 | H  | -1.533437 | -3.526002 | -0.382876 |
| C                            | -4.770304 | -2.512023 | 0.104543  | H  | -0.279822 | -4.666410 | 0.214405  |
|                              |           |           |           | H  | -0.342755 | -4.233461 | -1.498607 |

|   |          |          |           |
|---|----------|----------|-----------|
| H | 0.511606 | 3.633542 | -2.655580 |
| F | 1.699118 | 4.065506 | -1.096781 |

## II(aa)\_conf2

### 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.553763 | 0.869627  | 0.522679  |
| C  | -0.325374 | 1.425787  | -0.098291 |
| C  | -0.344545 | 2.737000  | -0.671992 |
| C  | -1.740549 | 3.376656  | -0.938653 |
| C  | -2.956885 | 2.505375  | -0.698377 |
| H  | -1.758553 | 3.980376  | -1.842000 |
| H  | -3.840028 | 3.131667  | -0.552077 |
| H  | -3.129081 | 1.851823  | -1.570462 |
| H  | -1.311752 | 0.576727  | 1.552364  |
| N  | -2.739855 | 1.737689  | 0.529344  |
| S  | -4.097439 | 1.157306  | 1.356669  |
| O  | -3.590171 | 0.637702  | 2.627418  |
| O  | -5.096113 | 2.226101  | 1.287234  |
| C  | -4.716764 | -0.234600 | 0.409687  |
| C  | -5.635063 | -0.014652 | -0.621626 |
| C  | -4.255597 | -1.522580 | 0.693639  |
| C  | -6.081261 | -1.096736 | -1.376689 |
| H  | -6.010008 | 0.986119  | -0.808363 |
| C  | -4.715256 | -2.593434 | -0.072632 |
| H  | -3.567250 | -1.681044 | 1.516815  |
| C  | -5.630445 | -2.400128 | -1.116990 |
| H  | -6.799043 | -0.928498 | -2.175883 |
| H  | -4.364805 | -3.597728 | 0.152369  |
| C  | -6.149010 | -3.568443 | -1.921095 |
| H  | -7.121525 | -3.905920 | -1.539113 |
| H  | -6.290407 | -3.299407 | -2.973351 |
| H  | -5.465520 | -4.422066 | -1.875973 |
| C  | -0.974202 | 3.886184  | 0.205071  |
| H  | -0.430599 | 4.817342  | 0.090676  |
| H  | -1.289328 | 3.627873  | 1.209121  |
| C  | 0.804162  | 3.178367  | -1.573457 |
| H  | 1.749404  | 3.156105  | -1.028684 |
| H  | -1.732160 | -0.081991 | -0.014904 |
| Rh | 3.100513  | -1.449591 | 0.188122  |
| Rh | 1.240657  | 0.149799  | -0.024689 |
| O  | 4.312231  | 0.149155  | 0.697859  |
| O  | 2.598299  | 1.628095  | 0.505538  |
| O  | 1.779422  | 0.348202  | -2.021397 |
| O  | 0.848322  | -0.209908 | 1.976583  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 0.038785  | -1.461998 | -0.529753 |
| O | 1.754342  | -2.935860 | -0.334799 |
| O | 3.501590  | -1.119281 | -1.815068 |
| O | 2.571869  | -1.674694 | 2.177274  |
| C | 1.588397  | -1.026799 | 2.632500  |
| C | 3.816301  | 1.308930  | 0.747355  |
| C | 2.777420  | -0.319053 | -2.470150 |
| C | 0.552554  | -2.635117 | -0.575224 |
| C | -0.377801 | -3.756929 | -0.989503 |
| C | 1.240549  | -1.196845 | 4.096086  |
| C | 4.731701  | 2.455184  | 1.125346  |
| C | 3.103184  | -0.107924 | -3.934725 |
| H | 3.367728  | 0.941398  | -4.104121 |
| H | 2.220639  | -0.326232 | -4.544501 |
| H | 3.932778  | -0.748774 | -4.236506 |
| H | 4.774292  | 3.177731  | 0.303351  |
| H | 5.734696  | 2.085542  | 1.342813  |
| H | 4.327491  | 2.976222  | 1.999096  |
| H | 1.511737  | -0.283607 | 4.637758  |
| H | 0.162442  | -1.339115 | 4.212864  |
| H | 1.784957  | -2.041892 | 4.520194  |
| H | -1.420530 | -3.478204 | -0.824082 |
| H | -0.129537 | -4.668041 | -0.439899 |
| H | -0.235117 | -3.959298 | -2.057535 |
| H | 0.874585  | 2.537613  | -2.454183 |
| F | 0.571635  | 4.489541  | -2.007470 |

## 1ab\_conf1

### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.148339  | -1.147733 | -3.194166 |
| H | -0.794601 | -1.049163 | -3.741233 |
| H | 0.945743  | -1.266549 | -3.948587 |
| N | 0.041814  | -2.348003 | -2.352912 |
| S | -1.036131 | -3.552608 | -2.856973 |
| O | -2.237780 | -2.859246 | -3.325950 |
| O | -1.069666 | -4.542031 | -1.780832 |
| C | -0.280265 | -4.347971 | -4.281969 |
| C | 0.506820  | -5.488462 | -4.099921 |
| C | -0.463420 | -3.806138 | -5.557966 |
| C | 1.125033  | -6.074172 | -5.204529 |
| H | 0.607510  | -5.920522 | -3.109905 |
| C | 0.161236  | -4.405225 | -6.649415 |
| H | -1.106972 | -2.943263 | -5.693138 |
| C | 0.965923  | -5.544075 | -6.492219 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.735566  | -6.962761 | -5.063643 |
| H | 0.015549  | -3.986571 | -7.642362 |
| C | 1.612873  | -6.202112 | -7.687885 |
| H | 2.508490  | -6.762779 | -7.401704 |
| H | 0.923418  | -6.909352 | -8.167700 |
| H | 1.899069  | -5.464437 | -8.445090 |
| C | 1.301729  | -2.822486 | -1.731508 |
| H | 1.699041  | -3.694749 | -2.271250 |
| H | 2.029881  | -2.016420 | -1.869408 |
| C | 1.192596  | -3.117755 | -0.303253 |
| C | 1.152695  | -3.347978 | 0.881967  |
| C | 0.386597  | 0.117503  | -2.405611 |
| H | 0.663570  | 0.972637  | -3.023116 |
| C | 0.268592  | 0.261775  | -1.086194 |
| H | -0.004440 | -0.566428 | -0.439208 |
| H | 0.445076  | 1.223189  | -0.612196 |
| C | 1.049113  | -3.670176 | 2.302297  |
| H | -0.014244 | -3.796597 | 2.572052  |
| H | 1.541695  | -4.638459 | 2.502985  |
| C | 1.545820  | -2.920873 | 4.466398  |
| H | 2.020432  | -2.087870 | 4.990923  |
| H | 0.497241  | -3.001771 | 4.796987  |
| H | 2.065114  | -3.855777 | 4.735136  |
| O | 1.640980  | -2.645611 | 3.085204  |

#### 1ab\_conf2

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.078367  | -1.454035 | -3.069707 |
| H | -0.803493 | -1.761452 | -3.639663 |
| H | 0.869532  | -1.297660 | -3.821931 |
| N | 0.451310  | -2.560869 | -2.183161 |
| S | -0.330433 | -4.059653 | -2.363080 |
| O | 0.693665  | -5.089021 | -2.161499 |
| O | -1.123050 | -3.995685 | -3.597672 |
| C | -1.490993 | -4.158515 | -0.999566 |
| C | -2.829514 | -3.829051 | -1.219496 |
| C | -1.046592 | -4.561094 | 0.261965  |
| C | -3.728180 | -3.896450 | -0.155628 |
| H | -3.159367 | -3.539149 | -2.211059 |
| C | -1.958716 | -4.614074 | 1.312850  |
| H | -0.008645 | -4.822843 | 0.427668  |
| C | -3.309774 | -4.287346 | 1.123782  |
| H | -4.772038 | -3.642670 | -0.323933 |
| H | -1.605305 | -4.911403 | 2.296754  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.294125 | -4.383218 | 2.265595  |
| H | -5.157435 | -3.728534 | 2.108073  |
| H | -4.675484 | -5.407628 | 2.371944  |
| H | -3.828997 | -4.110945 | 3.219219  |
| C | 1.839963  | -2.581399 | -1.680426 |
| H | 2.422471  | -3.354352 | -2.195235 |
| H | 2.270037  | -1.609749 | -1.945519 |
| C | 1.952149  | -2.770817 | -0.230287 |
| C | 2.056126  | -2.954438 | 0.959818  |
| C | -0.195373 | -0.155727 | -2.350758 |
| H | -0.327645 | 0.698258  | -3.016666 |
| C | -0.289444 | 0.011287  | -1.032105 |
| H | -0.161866 | -0.818024 | -0.342330 |
| H | -0.501045 | 0.986925  | -0.603499 |
| C | 2.164422  | -3.198610 | 2.395995  |
| H | 3.228089  | -3.286425 | 2.678870  |
| H | 1.756023  | -2.343087 | 2.961898  |
| C | 1.602471  | -4.705504 | 4.107391  |
| H | 1.047112  | -5.630962 | 4.277194  |
| H | 2.656557  | -4.864622 | 4.385856  |
| H | 1.188796  | -3.913506 | 4.752617  |
| O | 1.467368  | -4.389739 | 2.736084  |

#### 1ab\_conf3

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.044596 | -1.705323 | -2.418717 |
| H | -0.032572 | -1.463724 | -1.345344 |
| H | -1.088632 | -1.670466 | -2.746102 |
| N | 0.452823  | -3.070794 | -2.628288 |
| S | -0.667670 | -4.298487 | -2.937233 |
| O | 0.130889  | -5.495857 | -3.215260 |
| O | -1.607950 | -3.742404 | -3.912530 |
| C | -1.603141 | -4.617375 | -1.435860 |
| C | -2.794583 | -3.924727 | -1.204503 |
| C | -1.133156 | -5.555287 | -0.514696 |
| C | -3.507671 | -4.168278 | -0.032687 |
| H | -3.166850 | -3.226502 | -1.946365 |
| C | -1.861560 | -5.788908 | 0.650719  |
| H | -0.221155 | -6.104846 | -0.719098 |
| C | -3.055287 | -5.101247 | 0.912127  |
| H | -4.436493 | -3.631895 | 0.146433  |
| H | -1.501463 | -6.525773 | 1.364715  |
| C | -3.856534 | -5.381955 | 2.161380  |
| H | -4.284875 | -4.463596 | 2.577760  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.692763 | -6.060798 | 1.948048  |
| H | -3.242191 | -5.853020 | 2.935256  |
| C | 1.697116  | -3.426536 | -1.922985 |
| H | 1.996985  | -4.420480 | -2.264908 |
| H | 2.461702  | -2.722166 | -2.271057 |
| C | 1.619643  | -3.378533 | -0.456021 |
| C | 1.556379  | -3.313153 | 0.749976  |
| C | 0.740280  | -0.666257 | -3.187725 |
| H | 0.607902  | 0.353139  | -2.824862 |
| C | 1.524050  | -0.900996 | -4.239293 |
| H | 1.663633  | -1.905577 | -4.629309 |
| H | 2.039393  | -0.092647 | -4.749979 |
| C | 1.457943  | -3.285039 | 2.207020  |
| H | 0.485655  | -3.707506 | 2.518396  |
| H | 2.238146  | -3.933508 | 2.644458  |
| C | 1.515099  | -1.892851 | 4.091508  |
| H | 1.629456  | -0.842315 | 4.369316  |
| H | 0.543742  | -2.258344 | 4.463582  |
| H | 2.313240  | -2.480271 | 4.574374  |
| O | 1.595681  | -1.956905 | 2.683209  |

#### 1ab\_conf4

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.017915 | -1.272402 | -3.170106 |
| H | 0.778819  | -0.789161 | -2.586746 |
| H | -0.948893 | -0.758121 | -2.905303 |
| N | -0.109570 | -2.647858 | -2.669567 |
| S | -1.541957 | -3.513834 | -2.839871 |
| O | -1.306376 | -4.718269 | -3.644191 |
| O | -2.560211 | -2.529367 | -3.216269 |
| C | -1.884523 | -4.072065 | -1.166427 |
| C | -2.361320 | -3.155769 | -0.223291 |
| C | -1.699036 | -5.412392 | -0.829614 |
| C | -2.638678 | -3.592274 | 1.067766  |
| H | -2.523565 | -2.120366 | -0.504920 |
| C | -1.980505 | -5.832414 | 0.472259  |
| H | -1.351545 | -6.111616 | -1.582677 |
| C | -2.452513 | -4.935355 | 1.437544  |
| H | -3.011238 | -2.882262 | 1.802400  |
| H | -1.835451 | -6.876664 | 0.737370  |
| C | -2.780659 | -5.396799 | 2.837708  |
| H | -2.382788 | -4.706284 | 3.590078  |
| H | -3.866493 | -5.449120 | 2.990506  |
| H | -2.370701 | -6.391230 | 3.039004  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.104656 | -3.380861 | -2.287394 |
| H | 1.713623 | -2.691310 | -1.687194 |
| H | 0.807575 | -4.186596 | -1.605120 |
| C | 1.934044 | -3.933164 | -3.365231 |
| C | 2.672183 | -4.404520 | -4.197696 |
| C | 0.243872 | -1.074881 | -4.645499 |
| H | 0.439901 | -0.035304 | -4.913383 |
| C | 0.214015 | -2.006826 | -5.595232 |
| H | 0.016714 | -3.051297 | -5.374547 |
| H | 0.390766 | -1.748288 | -6.635658 |
| C | 3.509769 | -4.985245 | -5.243648 |
| H | 3.616244 | -6.072485 | -5.079684 |
| H | 3.011343 | -4.862244 | -6.221719 |
| C | 5.618423 | -4.895575 | -6.261638 |
| H | 6.572579 | -4.366683 | -6.197695 |
| H | 5.796470 | -5.974249 | -6.118358 |
| H | 5.193176 | -4.746976 | -7.267874 |
| O | 4.784249 | -4.362713 | -5.255231 |

#### I(ab)-Ene\_conf1

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.199189  | -1.147777 | -2.844551 |
| H | -0.829028 | -1.000435 | -3.186299 |
| H | 0.853752  | -1.130433 | -3.735287 |
| N | 0.258577  | -2.449602 | -2.173216 |
| S | -0.862603 | -3.625890 | -2.638483 |
| O | -2.111906 | -2.931072 | -2.954576 |
| O | -0.797420 | -4.685749 | -1.632207 |
| C | -0.236595 | -4.325573 | -4.173965 |
| C | 0.504170  | -5.509379 | -4.142927 |
| C | -0.479128 | -3.668871 | -5.384901 |
| C | 1.013582  | -6.027286 | -5.334150 |
| H | 0.653703  | -6.024637 | -3.200053 |
| C | 0.038005  | -4.200228 | -6.563694 |
| H | -1.084472 | -2.768597 | -5.403235 |
| C | 0.791630  | -5.384643 | -6.559245 |
| H | 1.587062  | -6.950698 | -5.310378 |
| H | -0.153983 | -3.692513 | -7.505939 |
| C | 1.317039  | -5.968206 | -7.849338 |
| H | 2.173933  | -6.625972 | -7.672821 |
| H | 0.544730  | -6.564023 | -8.353551 |
| H | 1.627338  | -5.183440 | -8.547593 |
| C | 1.581377  | -2.957632 | -1.748282 |
| H | 1.904059  | -3.793833 | -2.386652 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 2.295477  | -2.146701 | -1.926798 |
| C  | 1.626945  | -3.360416 | -0.339715 |
| C  | 1.660711  | -3.691486 | 0.821273  |
| C  | 0.562356  | 0.041381  | -1.989338 |
| H  | 0.583149  | 0.973024  | -2.554650 |
| C  | 0.924824  | 0.065260  | -0.685819 |
| H  | 0.962142  | -0.831691 | -0.076351 |
| H  | 1.270684  | 0.986025  | -0.228262 |
| C  | 1.677098  | -4.129046 | 2.215229  |
| Rh | -1.477085 | 0.603824  | -0.393985 |
| Rh | -3.650262 | 0.986968  | 0.566366  |
| O  | -1.638675 | -1.336571 | 0.236287  |
| O  | -3.641230 | -0.964562 | 1.227858  |
| O  | -2.739343 | 1.570617  | 2.313822  |
| O  | -4.501088 | 0.367045  | -1.197752 |
| O  | -3.529116 | 2.923476  | -0.145630 |
| O  | -1.437590 | 2.597876  | -0.966332 |
| O  | -0.687103 | 1.136623  | 1.453887  |
| O  | -2.462667 | 0.156989  | -2.159931 |
| C  | -3.736852 | 0.079497  | -2.168630 |
| C  | -2.650877 | -1.701768 | 0.919404  |
| C  | -1.473335 | 1.510164  | 2.384095  |
| C  | -2.472606 | 3.306332  | -0.737378 |
| C  | -2.447488 | 4.731168  | -1.249301 |
| C  | -4.371580 | -0.409315 | -3.449137 |
| C  | -2.641523 | -3.134266 | 1.395618  |
| C  | -0.824366 | 1.935465  | 3.683736  |
| H  | -1.577648 | 2.075948  | 4.460468  |
| H  | -0.285064 | 2.876300  | 3.526425  |
| H  | -0.093113 | 1.183710  | 3.994470  |
| H  | -3.538333 | -3.354224 | 1.977227  |
| H  | -1.740266 | -3.300962 | 1.995503  |
| H  | -2.576319 | -3.799989 | 0.528852  |
| H  | -4.065006 | -1.448090 | -3.608746 |
| H  | -5.458871 | -0.342250 | -3.389578 |
| H  | -4.004152 | 0.181937  | -4.294027 |
| H  | -3.130378 | 5.355796  | -0.670211 |
| H  | -2.774597 | 4.737522  | -2.295912 |
| H  | -1.431722 | 5.131522  | -1.209810 |
| H  | 1.422454  | -5.201895 | 2.271596  |
| H  | 2.693844  | -4.021533 | 2.633055  |
| O  | 0.753683  | -3.366041 | 2.978164  |
| C  | 0.744670  | -3.757663 | 4.336656  |
| H  | 0.008679  | -3.129031 | 4.842939  |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 0.456950 | -4.814709 | 4.455348 |
| H | 1.729617 | -3.610563 | 4.808708 |

# I(ab)-Yne\_conf2

## 0 imaginary frequency

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.801257  | -3.917949 | 0.959315  |
| H  | 1.312180  | -4.765877 | 0.493373  |
| H  | 0.010174  | -3.601340 | 0.264780  |
| N  | 1.768122  | -2.822751 | 1.116656  |
| S  | 3.355674  | -3.042233 | 0.556847  |
| O  | 3.620948  | -2.168253 | -0.591042 |
| O  | 3.551626  | -4.492609 | 0.460900  |
| C  | 4.331927  | -2.420339 | 1.926530  |
| C  | 4.445346  | -3.185627 | 3.092279  |
| C  | 4.991352  | -1.198566 | 1.802778  |
| C  | 5.220505  | -2.706504 | 4.142722  |
| H  | 3.939439  | -4.142807 | 3.165495  |
| C  | 5.763180  | -0.732891 | 2.869796  |
| H  | 4.908280  | -0.633513 | 0.880509  |
| C  | 5.890632  | -1.474130 | 4.050068  |
| H  | 5.314194  | -3.298807 | 5.049904  |
| H  | 6.278653  | 0.219700  | 2.777525  |
| C  | 6.742381  | -0.979622 | 5.195109  |
| H  | 6.197766  | -1.022980 | 6.145596  |
| H  | 7.642545  | -1.596607 | 5.311706  |
| H  | 7.066321  | 0.053509  | 5.037370  |
| C  | 1.228685  | -1.456941 | 1.077731  |
| H  | 0.380303  | -1.426454 | 1.765053  |
| H  | 1.978560  | -0.762144 | 1.470725  |
| C  | 0.806873  | -1.001018 | -0.263446 |
| C  | 0.633642  | -0.705393 | -1.433655 |
| C  | 0.180734  | -4.365334 | 2.260533  |
| H  | -0.612433 | -5.104193 | 2.137910  |
| C  | 0.519501  | -3.958228 | 3.484067  |
| H  | 1.310998  | -3.230318 | 3.640197  |
| H  | 0.023332  | -4.349449 | 4.367703  |
| C  | 0.589911  | -0.439674 | -2.874416 |
| Rh | -1.483320 | 0.138152  | -0.180634 |
| Rh | -3.603839 | 1.075723  | 0.467312  |
| O  | -2.016143 | -1.578290 | 0.851435  |
| O  | -4.011361 | -0.685568 | 1.454217  |
| O  | -2.701422 | 1.823932  | 2.157243  |
| O  | -4.418634 | 0.291498  | -1.253010 |
| O  | -3.092972 | 2.791783  | -0.545625 |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| O                            | -1.095520 | 1.910581  | -1.159931 | H  | -5.774638 | -0.036416 | -0.888204 |
| O                            | -0.702862 | 0.931077  | 1.565936  | C  | -4.803083 | 0.082072  | 2.861891  |
| O                            | -2.425903 | -0.592822 | -1.874668 | H  | -3.697019 | -1.734951 | 2.468281  |
| C                            | -3.670928 | -0.364446 | -2.040082 | C  | -5.625977 | 1.088139  | 2.337282  |
| C                            | -3.149328 | -1.616467 | 1.438280  | H  | -6.604010 | 1.800482  | 0.551622  |
| C                            | -1.464750 | 1.602902  | 2.337694  | H  | -4.540525 | 0.101237  | 3.916840  |
| C                            | -1.966771 | 2.839151  | -1.133494 | C  | -6.171697 | 2.183092  | 3.223195  |
| C                            | -1.640378 | 4.102695  | -1.898802 | H  | -6.294351 | 3.121611  | 2.672204  |
| C                            | -4.298447 | -0.928756 | -3.296079 | H  | -7.157217 | 1.910303  | 3.623567  |
| C                            | -3.495896 | -2.900127 | 2.159240  | H  | -5.514008 | 2.372403  | 4.077693  |
| C                            | -0.820581 | 2.209403  | 3.564956  | C  | -2.906199 | -1.021673 | -2.458942 |
| H                            | -1.581802 | 2.516269  | 4.284046  | H  | -2.174937 | -1.423048 | -3.173913 |
| H                            | -0.239576 | 3.088609  | 3.263424  | H  | -3.893790 | -1.296518 | -2.839664 |
| H                            | -0.129739 | 1.494814  | 4.020188  | C  | -2.759583 | 0.440567  | -2.408083 |
| H                            | -4.329084 | -2.739147 | 2.845275  | C  | -2.602550 | 1.639751  | -2.419105 |
| H                            | -2.619110 | -3.272779 | 2.695167  | C  | -1.105211 | -0.692539 | 0.424872  |
| H                            | -3.785128 | -3.657419 | 1.421072  | H  | -1.391216 | 0.312946  | 0.126471  |
| H                            | -4.124192 | -2.008411 | -3.340579 | C  | -0.627771 | -0.918600 | 1.672144  |
| H                            | -5.369237 | -0.721643 | -3.316466 | H  | -0.393739 | -1.923714 | 2.013758  |
| H                            | -3.819813 | -0.482832 | -4.174511 | H  | -0.547637 | -0.120571 | 2.402749  |
| H                            | -2.113125 | 4.964718  | -1.423066 | C  | -2.424559 | 3.088721  | -2.426687 |
| H                            | -2.039258 | 4.014127  | -2.916382 | Rh | 1.421920  | -0.238579 | 0.456564  |
| H                            | -0.559166 | 4.239748  | -1.963250 | Rh | 3.660545  | 0.415063  | -0.150104 |
| H                            | 0.884577  | -1.365395 | -3.400514 | O  | 1.913870  | -2.172937 | -0.068291 |
| H                            | -0.439317 | -0.201017 | -3.177824 | O  | 4.011373  | -1.548198 | -0.670330 |
| O                            | 1.479325  | 0.614781  | -3.194111 | O  | 2.996007  | 0.823455  | -2.050218 |
| C                            | 1.502616  | 0.872800  | -4.582109 | O  | 4.261454  | 0.010297  | 1.772788  |
| H                            | 0.510885  | 1.171454  | -4.959497 | O  | 3.175828  | 2.341138  | 0.409973  |
| H                            | 2.205853  | 1.693778  | -4.740197 | O  | 1.055456  | 1.733031  | 0.944733  |
| H                            | 1.842990  | -0.005494 | -5.154832 | O  | 0.908753  | 0.128390  | -1.519050 |
| <b>I(ab)-Ene_conf3</b>       |           |           |           | O  | 2.154810  | -0.565803 | 2.377712  |
| <b>0 imaginary frequency</b> |           |           |           | C  | 3.394745  | -0.386634 | 2.610470  |
| C                            | -1.369443 | -1.783950 | -0.588382 | C  | 3.087128  | -2.404961 | -0.514102 |
| H                            | -0.664897 | -1.678577 | -1.418943 | C  | 1.777108  | 0.602498  | -2.325338 |
| H                            | -1.221927 | -2.769519 | -0.142174 | C  | 1.998527  | 2.583028  | 0.818149  |
| N                            | -2.711997 | -1.730908 | -1.189602 | C  | 1.663957  | 4.016844  | 1.168217  |
| S                            | -4.045618 | -2.299995 | -0.341099 | C  | 3.870445  | -0.698815 | 4.012747  |
| O                            | -3.540306 | -3.349865 | 0.546652  | C  | 3.410005  | -3.842775 | -0.856918 |
| O                            | -5.081942 | -2.557733 | -1.346898 | C  | 1.291565  | 0.935487  | -3.716525 |
| C                            | -4.662405 | -0.975277 | 0.704352  | H  | 2.121643  | 1.269326  | -4.341163 |
| C                            | -5.489176 | 0.009655  | 0.157204  | H  | 0.528076  | 1.717965  | -3.646229 |
| C                            | -4.320018 | -0.948977 | 2.057026  | H  | 0.820992  | 0.053563  | -4.163007 |
| C                            | -5.959229 | 1.034124  | 0.975274  | H  | 4.225567  | -3.886573 | -1.581205 |
|                              |           |           |           | H  | 2.523015  | -4.350263 | -1.243085 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 3.726629  | -4.362238 | 0.055295  |
| H | 3.866323  | -1.785025 | 4.158405  |
| H | 4.881887  | -0.319873 | 4.167277  |
| H | 3.184325  | -0.264943 | 4.745454  |
| H | 2.575576  | 4.605523  | 1.283008  |
| H | 1.068347  | 4.050657  | 2.084401  |
| H | 1.059722  | 4.446830  | 0.361059  |
| H | -3.100905 | 3.544817  | -3.171011 |
| H | -2.705474 | 3.506803  | -1.444563 |
| O | -1.074764 | 3.415855  | -2.728917 |
| C | -0.866523 | 4.813795  | -2.775725 |
| H | 0.189285  | 4.970366  | -3.008184 |
| H | -1.481256 | 5.291752  | -3.555277 |
| H | -1.098019 | 5.291788  | -1.810128 |

#### I(ab)-Yne\_conf4

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.427354  | -3.691623 | 0.355577  |
| H | 2.328646  | -4.226073 | 0.035533  |
| H | 0.840859  | -3.498269 | -0.555195 |
| N | 1.829058  | -2.415740 | 0.952907  |
| S | 3.467471  | -2.013841 | 1.007907  |
| O | 4.157432  | -3.204542 | 1.509511  |
| O | 3.531612  | -0.725525 | 1.702786  |
| C | 4.032743  | -1.766531 | -0.679640 |
| C | 3.737356  | -0.574027 | -1.346373 |
| C | 4.759387  | -2.777783 | -1.311692 |
| C | 4.163814  | -0.408438 | -2.661341 |
| H | 3.184621  | 0.214455  | -0.848987 |
| C | 5.185244  | -2.590243 | -2.626593 |
| H | 5.000999  | -3.685517 | -0.769555 |
| C | 4.895489  | -1.408041 | -3.320797 |
| H | 3.914425  | 0.512761  | -3.179983 |
| H | 5.755521  | -3.374554 | -3.118492 |
| C | 5.382292  | -1.198603 | -4.735349 |
| H | 4.637568  | -0.670918 | -5.341394 |
| H | 6.298352  | -0.593305 | -4.750559 |
| H | 5.610400  | -2.149524 | -5.227360 |
| C | 0.813840  | -1.362488 | 1.036969  |
| H | -0.070937 | -1.797478 | 1.510371  |
| H | 1.181606  | -0.571574 | 1.692895  |
| C | 0.419861  | -0.778439 | -0.263635 |
| C | 0.246653  | -0.341884 | -1.389344 |
| C | 0.638759  | -4.579754 | 1.291772  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 0.111146  | -5.395549 | 0.796639  |
| C  | 0.573622  | -4.451308 | 2.616502  |
| H  | 1.104554  | -3.657572 | 3.134511  |
| H  | 0.003683  | -5.148802 | 3.223753  |
| C  | 0.159615  | 0.149258  | -2.766718 |
| Rh | -1.899908 | 0.293865  | -0.013057 |
| Rh | -4.029602 | 1.111501  | 0.741547  |
| O  | -2.345336 | -1.489486 | 0.937917  |
| O  | -4.351213 | -0.709572 | 1.648011  |
| O  | -3.106789 | 1.802823  | 2.442480  |
| O  | -4.861156 | 0.383490  | -0.998651 |
| O  | -3.610897 | 2.898012  | -0.189138 |
| O  | -1.606896 | 2.126497  | -0.918253 |
| O  | -1.095117 | 1.025405  | 1.743666  |
| O  | -2.853931 | -0.384059 | -1.722857 |
| C  | -4.111890 | -0.199947 | -1.839807 |
| C  | -3.456438 | -1.605518 | 1.554262  |
| C  | -1.857452 | 1.617457  | 2.577826  |
| C  | -2.507607 | 3.021972  | -0.806049 |
| C  | -2.235214 | 4.343815  | -1.489659 |
| C  | -4.757909 | -0.736724 | -3.098620 |
| C  | -3.739872 | -2.940320 | 2.206594  |
| C  | -1.200846 | 2.145640  | 3.833321  |
| H  | -1.942794 | 2.594143  | 4.495310  |
| H  | -0.446179 | 2.890985  | 3.561406  |
| H  | -0.683049 | 1.330068  | 4.347936  |
| H  | -4.271114 | -2.790637 | 3.149632  |
| H  | -2.811739 | -3.491891 | 2.368554  |
| H  | -4.388416 | -3.527568 | 1.545822  |
| H  | -4.632773 | -1.824044 | -3.135590 |
| H  | -5.819451 | -0.486868 | -3.121998 |
| H  | -4.256070 | -0.319183 | -3.977333 |
| H  | -2.961261 | 5.094601  | -1.174214 |
| H  | -2.305157 | 4.209113  | -2.575080 |
| H  | -1.218391 | 4.675827  | -1.262598 |
| H  | 0.355695  | -0.687021 | -3.460541 |
| H  | -0.860985 | 0.505496  | -2.961223 |
| O  | 1.107854  | 1.187224  | -2.967348 |
| C  | 0.969580  | 1.777247  | -4.244519 |
| H  | -0.029220 | 2.220959  | -4.379506 |
| H  | 1.721716  | 2.566796  | -4.313270 |
| H  | 1.139057  | 1.047578  | -5.053470 |

#### I-TS-II(ab)\_conf1

**1 imaginary frequency, value = -345.7849 cm<sup>-1</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.662967 | 0.993356  | 0.353353  |
| C  | -0.414013 | 1.586869  | -0.197689 |
| C  | -0.152143 | 2.717839  | -0.760187 |
| C  | -2.106865 | 3.552617  | -1.369024 |
| C  | -3.055245 | 2.399887  | -1.141850 |
| H  | -1.906253 | 3.814619  | -2.406065 |
| H  | -4.082484 | 2.771612  | -1.218471 |
| H  | -2.912424 | 1.634462  | -1.920437 |
| H  | -1.510015 | 0.802120  | 1.418424  |
| N  | -2.857737 | 1.850228  | 0.198173  |
| S  | -4.233986 | 1.381040  | 1.066805  |
| O  | -3.775250 | 1.124878  | 2.431863  |
| O  | -5.259109 | 2.383436  | 0.760355  |
| C  | -4.778770 | -0.182485 | 0.374067  |
| C  | -5.715707 | -0.189596 | -0.662568 |
| C  | -4.245933 | -1.378727 | 0.863623  |
| C  | -6.109532 | -1.406740 | -1.215938 |
| H  | -6.146205 | 0.743656  | -1.010000 |
| C  | -4.651293 | -2.585803 | 0.296740  |
| H  | -3.542633 | -1.361463 | 1.689223  |
| C  | -5.585777 | -2.620944 | -0.749242 |
| H  | -6.842499 | -1.414075 | -2.018901 |
| H  | -4.242478 | -3.517147 | 0.681132  |
| C  | -6.043509 | -3.937070 | -1.331457 |
| H  | -6.872001 | -4.357251 | -0.746017 |
| H  | -6.397744 | -3.819323 | -2.360523 |
| H  | -5.237274 | -4.678048 | -1.330267 |
| C  | -1.613840 | 4.320756  | -0.360276 |
| H  | -0.990579 | 5.184723  | -0.554689 |
| H  | -1.878583 | 4.109914  | 0.669844  |
| C  | 0.911962  | 3.463544  | -1.468135 |
| H  | 1.760526  | 2.769354  | -1.532106 |
| H  | -1.804703 | 0.018413  | -0.136919 |
| Rh | 2.993841  | -1.504822 | 0.210504  |
| Rh | 1.245497  | 0.178193  | -0.050172 |
| O  | 4.242277  | 0.015870  | 0.848429  |
| O  | 2.615351  | 1.582257  | 0.605207  |
| O  | 1.933015  | 0.464709  | -1.991176 |
| O  | 0.692964  | -0.229982 | 1.903642  |
| O  | 0.006334  | -1.362729 | -0.704077 |
| O  | 1.634598  | -2.921962 | -0.437781 |
| O  | 3.531017  | -1.131220 | -1.752485 |
| O  | 2.338880  | -1.773759 | 2.151555  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.355887  | -1.093940 | 2.571534  |
| C | 3.791590  | 1.198088  | 0.919199  |
| C | 2.904447  | -0.252034 | -2.412369 |
| C | 0.465536  | -2.553187 | -0.753852 |
| C | -0.480853 | -3.616396 | -1.274658 |
| C | 0.936355  | -1.293165 | 4.012987  |
| C | 4.727589  | 2.260011  | 1.459092  |
| C | 3.320073  | -0.034679 | -3.853570 |
| H | 3.348206  | 1.034492  | -4.081724 |
| H | 2.576560  | -0.495109 | -4.514466 |
| H | 4.293814  | -0.489308 | -4.042978 |
| H | 4.425829  | 3.251645  | 1.115884  |
| H | 5.755964  | 2.042558  | 1.161215  |
| H | 4.682506  | 2.246071  | 2.554505  |
| H | 1.413386  | -0.522945 | 4.630533  |
| H | -0.145655 | -1.180824 | 4.115256  |
| H | 1.258155  | -2.273310 | 4.370149  |
| H | -1.508699 | -3.388786 | -0.981188 |
| H | -0.183559 | -4.600995 | -0.908374 |
| H | -0.436015 | -3.625937 | -2.370258 |
| H | 0.604970  | 3.709519  | -2.499592 |
| O | 1.268159  | 4.651177  | -0.778693 |
| C | 2.379014  | 5.294894  | -1.372372 |
| H | 3.276130  | 4.658232  | -1.346208 |
| H | 2.177961  | 5.572806  | -2.420198 |
| H | 2.567403  | 6.202281  | -0.793758 |

**I-TS-II(ab)\_conf2**

**1 imaginary frequency, value = -343.0026 cm<sup>-1</sup>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.677924 | 0.997532  | 0.422788  |
| C | -0.437989 | 1.605212  | -0.138509 |
| C | -0.214188 | 2.733798  | -0.729766 |
| C | -2.161498 | 3.472887  | -1.386910 |
| C | -3.092342 | 2.314150  | -1.123679 |
| H | -1.944143 | 3.692657  | -2.430234 |
| H | -4.124625 | 2.666657  | -1.220038 |
| H | -2.931274 | 1.521992  | -1.871035 |
| H | -1.529540 | 0.833699  | 1.492809  |
| N | -2.891681 | 1.821264  | 0.238094  |
| S | -4.265246 | 1.339736  | 1.105293  |
| O | -3.806630 | 1.099043  | 2.473356  |
| O | -5.301377 | 2.327472  | 0.789250  |
| C | -4.788377 | -0.233357 | 0.418206  |
| C | -5.730379 | -0.255607 | -0.613740 |



|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H                            | 1.768691  | 3.166839  | -0.850722 | C  | -2.023985 | 3.403097  | -0.592265 |
| H                            | -1.735452 | -0.043144 | -0.003601 | C  | -3.199711 | 2.464910  | -0.410908 |
| Rh                           | 3.053616  | -1.453087 | 0.377562  | H  | -2.076379 | 4.075403  | -1.443857 |
| Rh                           | 1.223262  | 0.176131  | 0.103125  | H  | -4.107629 | 3.039735  | -0.213395 |
| O                            | 4.263802  | 0.123753  | 0.955948  | H  | -3.351894 | 1.870469  | -1.327920 |
| O                            | 2.577311  | 1.627508  | 0.712934  | H  | -1.452898 | 0.454130  | 1.682791  |
| O                            | 1.854945  | 0.384118  | -1.866509 | N  | -2.938924 | 1.618563  | 0.754250  |
| O                            | 0.742283  | -0.199502 | 2.082367  | S  | -4.258260 | 0.922132  | 1.547810  |
| O                            | 0.026204  | -1.417042 | -0.473136 | O  | -3.713950 | 0.323690  | 2.767741  |
| O                            | 1.711758  | -2.916232 | -0.217649 | O  | -5.300186 | 1.950957  | 1.576209  |
| O                            | 3.544203  | -1.112357 | -1.602895 | C  | -4.838118 | -0.414439 | 0.499526  |
| O                            | 2.433582  | -1.692112 | 2.339092  | C  | -5.784094 | -0.150504 | -0.495385 |
| C                            | 1.439970  | -1.036141 | 2.758809  | C  | -4.315659 | -1.700112 | 0.665164  |
| C                            | 3.777577  | 1.288116  | 1.005252  | C  | -6.195496 | -1.183868 | -1.334579 |
| C                            | 2.859650  | -0.294156 | -2.278659 | H  | -6.206218 | 0.844348  | -0.590920 |
| C                            | 0.526797  | -2.595849 | -0.510390 | C  | -4.740943 | -2.721466 | -0.183641 |
| C                            | -0.397236 | -3.698769 | -0.985689 | H  | -3.605818 | -1.897524 | 1.461282  |
| C                            | 1.022457  | -1.222451 | 4.202266  | C  | -5.681996 | -2.481947 | -1.195425 |
| C                            | 4.683699  | 2.412044  | 1.465608  | H  | -6.934145 | -0.980912 | -2.106196 |
| C                            | 3.252412  | -0.073111 | -3.725852 | H  | -4.341601 | -3.724062 | -0.050984 |
| H                            | 3.562443  | 0.968192  | -3.865758 | C  | -6.160527 | -3.600855 | -2.089667 |
| H                            | 2.388450  | -0.248431 | -4.374646 | H  | -7.059544 | -4.076331 | -1.675577 |
| H                            | 4.070611  | -0.738631 | -4.004623 | H  | -6.418474 | -3.233187 | -3.088315 |
| H                            | 4.657051  | 3.233141  | 0.742579  | H  | -5.400307 | -4.380970 | -2.198824 |
| H                            | 5.706168  | 2.051494  | 1.586874  | C  | -1.265662 | 3.854291  | 0.579797  |
| H                            | 4.318018  | 2.804292  | 2.420857  | H  | -0.761990 | 4.812979  | 0.532235  |
| H                            | 1.258958  | -0.312633 | 4.765348  | H  | -1.552770 | 3.500401  | 1.562988  |
| H                            | -0.059178 | -1.373245 | 4.264069  | C  | 0.527177  | 3.353233  | -1.276409 |
| H                            | 1.550658  | -2.068478 | 4.644515  | H  | 1.477292  | 3.296758  | -0.731149 |
| H                            | -1.442483 | -3.422773 | -0.831021 | H  | -1.853055 | -0.105203 | 0.071989  |
| H                            | -0.162372 | -4.631422 | -0.467572 | Rh | 3.021528  | -1.299205 | 0.247227  |
| H                            | -0.235265 | -3.858177 | -2.058349 | Rh | 1.104617  | 0.243102  | 0.102232  |
| H                            | 0.937601  | 2.583658  | -2.305673 | O  | 4.178607  | 0.316140  | 0.823615  |
| O                            | 0.619920  | 4.583580  | -1.850347 | O  | 2.409449  | 1.738030  | 0.711842  |
| C                            | 1.662190  | 5.075958  | -2.664954 | O  | 1.636459  | 0.542975  | -1.883103 |
| H                            | 2.627696  | 5.070362  | -2.135197 | O  | 0.729384  | -0.216895 | 2.087475  |
| H                            | 1.769807  | 4.483538  | -3.587381 | O  | -0.037234 | -1.385751 | -0.482607 |
| H                            | 1.406636  | 6.105245  | -2.929903 | O  | 1.726846  | -2.807684 | -0.337859 |
| <b>II(ab)_conf2</b>          |           |           |           | O  | 3.404168  | -0.879124 | -1.743485 |
| <b>0 imaginary frequency</b> |           |           |           | O  | 2.509106  | -1.620660 | 2.226169  |
| C                            | -1.713158 | 0.810660  | 0.678412  | C  | 1.500014  | -1.033274 | 2.707262  |
| C                            | -0.514525 | 1.464012  | 0.091558  | C  | 3.637091  | 1.451075  | 0.939887  |
| C                            | -0.595790 | 2.806928  | -0.396667 | C  | 2.652224  | -0.073827 | -2.360932 |
|                              |           |           |           | C  | 0.517835  | -2.536727 | -0.577803 |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | -0.368294 | -3.668307 | -1.057861 | H  | -4.450633 | 3.619615  | 3.060842  |
| C                            | 1.151137  | -1.290293 | 4.158053  | C  | -3.546529 | 1.762296  | 5.788762  |
| C                            | 4.504805  | 2.602184  | 1.406695  | H  | -3.199404 | -0.363850 | 5.748174  |
| C                            | 2.964952  | 0.207559  | -3.817089 | H  | -3.975698 | 3.855883  | 5.484277  |
| H                            | 3.176804  | 1.274175  | -3.947457 | C  | -3.291264 | 1.910697  | 7.269681  |
| H                            | 2.092834  | -0.031299 | -4.434288 | H  | -4.230697 | 2.064091  | 7.816406  |
| H                            | 3.824019  | -0.380443 | -4.143111 | H  | -2.808512 | 1.021123  | 7.685384  |
| H                            | 4.406846  | 3.447147  | 0.718102  | H  | -2.651354 | 2.775139  | 7.479965  |
| H                            | 5.548139  | 2.290301  | 1.472315  | C  | -1.283336 | 4.154716  | 0.121281  |
| H                            | 4.160857  | 2.939325  | 2.390628  | H  | -0.748565 | 5.080399  | -0.057819 |
| H                            | 1.284467  | -0.366745 | 4.731877  | H  | -1.589980 | 3.956483  | 1.141573  |
| H                            | 0.098623  | -1.577396 | 4.242873  | C  | 0.511700  | 3.331884  | -1.614742 |
| H                            | 1.790263  | -2.072412 | 4.570301  | H  | 1.459132  | 3.293257  | -1.063067 |
| H                            | -1.420981 | -3.440804 | -0.877487 | H  | -2.014062 | 0.192672  | 0.151437  |
| H                            | -0.083653 | -4.600127 | -0.563574 | Rh | 2.843194  | -1.104186 | 0.636909  |
| H                            | -0.220235 | -3.800245 | -2.136219 | Rh | 0.975338  | 0.458766  | 0.238490  |
| H                            | 0.618815  | 2.734242  | -2.178510 | O  | 4.025407  | 0.544696  | 1.049644  |
| O                            | 0.227490  | 4.696884  | -1.626356 | O  | 2.307263  | 1.989534  | 0.694361  |
| C                            | 1.222783  | 5.277130  | -2.441798 | O  | 1.577972  | 0.492902  | -1.748908 |
| H                            | 2.200405  | 5.297854  | -1.935077 | O  | 0.525611  | 0.263296  | 2.253957  |
| H                            | 1.336863  | 4.731965  | -3.392165 | O  | -0.191993 | -1.200148 | -0.164646 |
| H                            | 0.909295  | 6.302558  | -2.654334 | O  | 1.526443  | -2.639880 | 0.191818  |
| <b>II(ab)_conf3</b>          |           |           |           | O  | 3.304921  | -0.933721 | -1.369784 |
| <b>0 imaginary frequency</b> |           |           |           | O  | 2.247578  | -1.170294 | 2.623429  |
| C                            | -1.839617 | 1.169052  | 0.640766  | C  | 1.250492  | -0.491285 | 2.994022  |
| C                            | -0.606831 | 1.701281  | 0.005128  | C  | 3.519014  | 1.700008  | 0.992367  |
| C                            | -0.637889 | 2.957114  | -0.681639 | C  | 2.588942  | -0.204197 | -2.111223 |
| C                            | -2.043569 | 3.558134  | -0.984076 | C  | 0.328550  | -2.370141 | -0.100645 |
| C                            | -3.250273 | 2.691305  | -0.693857 | C  | -0.599664 | -3.520146 | -0.430123 |
| H                            | -2.064978 | 4.101773  | -1.924426 | C  | 0.880904  | -0.534468 | 4.462918  |
| H                            | -4.150837 | 3.304198  | -0.615516 | C  | 4.416356  | 2.880787  | 1.305123  |
| H                            | -3.398972 | 1.966670  | -1.510691 | C  | 2.933407  | -0.147677 | -3.585927 |
| H                            | -1.596627 | 0.920805  | 1.682911  | H  | 2.961175  | 0.891796  | -3.926028 |
| N                            | -3.036392 | 2.026974  | 0.600749  | H  | 2.152870  | -0.661271 | -4.158385 |
| S                            | -4.424319 | 1.328538  | 1.306057  | H  | 3.893792  | -0.631151 | -3.770972 |
| O                            | -5.536485 | 2.219427  | 0.959480  | H  | 4.454640  | 3.552664  | 0.441186  |
| O                            | -4.489382 | -0.107166 | 0.999772  | H  | 5.422600  | 2.540409  | 1.553396  |
| C                            | -4.062574 | 1.497672  | 3.051446  | H  | 3.997624  | 3.448414  | 2.142507  |
| C                            | -3.720998 | 0.370207  | 3.796724  | H  | 1.463132  | 0.226776  | 4.995838  |
| C                            | -4.161537 | 2.756808  | 3.651950  | H  | -0.179890 | -0.314723 | 4.602158  |
| C                            | -3.462363 | 0.512906  | 5.161706  | H  | 1.132973  | -1.510311 | 4.883741  |
| H                            | -3.671250 | -0.599723 | 3.313736  | H  | -1.543058 | -3.407343 | 0.111867  |
| C                            | -3.899857 | 2.879244  | 5.012334  | H  | -0.128621 | -4.472013 | -0.180264 |
|                              |           |           |           | H  | -0.831867 | -3.500518 | -1.500853 |

|                              |           |           |           |                              |           |           |           |
|------------------------------|-----------|-----------|-----------|------------------------------|-----------|-----------|-----------|
| H                            | 0.569157  | 2.603014  | -2.433834 | O                            | 4.060252  | 0.533526  | 1.017610  |
| O                            | 0.280878  | 4.635082  | -2.130357 | O                            | 2.352249  | 1.979624  | 0.621535  |
| C                            | 1.282989  | 5.041786  | -3.037511 | O                            | 1.626535  | 0.422574  | -1.785036 |
| H                            | 2.274964  | 5.069977  | -2.559932 | O                            | 0.551839  | 0.308234  | 2.216924  |
| H                            | 1.337197  | 4.370180  | -3.908929 | O                            | -0.162662 | -1.216253 | -0.164887 |
| H                            | 1.022092  | 6.047251  | -3.377932 | O                            | 1.542199  | -2.657905 | 0.245017  |
| <b>II(ab)_conf4</b>          |           |           |           | O                            | 3.335750  | -1.012805 | -1.360722 |
| <b>0 imaginary frequency</b> |           |           |           | O                            | 2.267257  | -1.119658 | 2.634943  |
| C                            | -1.800293 | 1.180472  | 0.568446  | C                            | 1.271428  | -0.426568 | 2.981701  |
| C                            | -0.561254 | 1.690581  | -0.073202 | C                            | 3.561360  | 1.690157  | 0.930022  |
| C                            | -0.581662 | 2.929626  | -0.790085 | C                            | 2.630947  | -0.295281 | -2.124301 |
| C                            | -1.982362 | 3.530880  | -1.114037 | C                            | 0.348390  | -2.387765 | -0.063364 |
| C                            | -3.195299 | 2.677735  | -0.810014 | C                            | -0.586269 | -3.539882 | -0.366174 |
| H                            | -1.995905 | 4.052085  | -2.067138 | C                            | 0.896278  | -0.424163 | 4.449788  |
| H                            | -4.092837 | 3.297263  | -0.751438 | C                            | 4.465066  | 2.872695  | 1.216709  |
| H                            | -3.343323 | 1.934684  | -1.610257 | C                            | 2.983838  | -0.278595 | -3.598026 |
| H                            | -1.564353 | 0.956517  | 1.617706  | H                            | 3.067299  | 0.753732  | -3.951311 |
| N                            | -2.992652 | 2.043103  | 0.501408  | H                            | 2.180020  | -0.757496 | -4.167995 |
| S                            | -4.389450 | 1.362937  | 1.208171  | H                            | 3.919597  | -0.811984 | -3.771316 |
| O                            | -5.493740 | 2.256023  | 0.842665  | H                            | 4.502308  | 3.528687  | 0.340661  |
| O                            | -4.462205 | -0.076384 | 0.920833  | H                            | 5.470828  | 2.532667  | 1.467397  |
| C                            | -4.036974 | 1.553068  | 2.953197  | H                            | 4.052350  | 3.457194  | 2.045508  |
| C                            | -3.704044 | 0.433710  | 3.714531  | H                            | 1.467060  | 0.361844  | 4.958621  |
| C                            | -4.134892 | 2.819917  | 3.537386  | H                            | -0.167515 | -0.211433 | 4.577027  |
| C                            | -3.453014 | 0.592478  | 5.079120  | H                            | 1.157049  | -1.382170 | 4.904742  |
| H                            | -3.654952 | -0.542410 | 3.244110  | H                            | -1.534676 | -3.401894 | 0.160958  |
| C                            | -3.880859 | 2.958349  | 4.897723  | H                            | -0.126254 | -4.487173 | -0.080829 |
| H                            | -4.417258 | 3.676301  | 2.933828  | H                            | -0.806045 | -3.552785 | -1.439647 |
| C                            | -3.536273 | 1.849919  | 5.690088  | H                            | 0.633548  | 2.525142  | -2.525334 |
| H                            | -3.196915 | -0.277902 | 5.677998  | O                            | 0.353050  | 4.565785  | -2.275582 |
| H                            | -3.955948 | 3.941066  | 5.356985  | C                            | 1.362999  | 4.945902  | -3.185552 |
| C                            | -3.289419 | 2.015649  | 7.170593  | H                            | 2.351802  | 4.981881  | -2.701945 |
| H                            | -4.231801 | 2.176997  | 7.709913  | H                            | 1.420325  | 4.252800  | -4.039763 |
| H                            | -2.810592 | 1.130321  | 7.599689  | H                            | 1.108646  | 5.943705  | -3.552446 |
| H                            | -2.649369 | 2.881543  | 7.374302  | <b>1ac_conf1</b>             |           |           |           |
| C                            | -1.224361 | 4.149593  | -0.019332 | <b>0 imaginary frequency</b> |           |           |           |
| H                            | -0.683649 | 5.067877  | -0.217713 | C                            | 2.128254  | 1.330365  | 0.245924  |
| H                            | -1.537028 | 3.977598  | 1.003865  | H                            | 3.159432  | 1.403078  | -0.122336 |
| C                            | 0.574949  | 3.275181  | -1.725675 | H                            | 2.136051  | 1.617766  | 1.298455  |
| H                            | 1.518943  | 3.246378  | -1.167514 | N                            | 1.800143  | -0.107293 | 0.186412  |
| H                            | -1.977136 | 0.193425  | 0.101970  | S                            | 0.632680  | -0.734782 | 1.232196  |
| Rh                           | 2.868275  | -1.118748 | 0.648780  | O                            | 0.704026  | 0.082991  | 2.444883  |
| Rh                           | 1.012830  | 0.445636  | 0.199604  | O                            | 0.851790  | -2.183862 | 1.252232  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.986716 | -0.474669 | 0.495356  |
| C | -1.503777 | -1.428899 | -0.384757 |
| C | -1.716334 | 0.674109  | 0.810082  |
| C | -2.753795 | -1.215973 | -0.964349 |
| H | -0.946299 | -2.336778 | -0.589469 |
| C | -2.966343 | 0.866864  | 0.226547  |
| H | -1.311070 | 1.394658  | 1.510857  |
| C | -3.504105 | -0.069146 | -0.669549 |
| H | -3.157262 | -1.958958 | -1.647962 |
| H | -3.537109 | 1.758602  | 0.474484  |
| C | -4.873702 | 0.137669  | -1.271877 |
| H | -4.981929 | -0.402214 | -2.218027 |
| H | -5.658916 | -0.225974 | -0.595829 |
| H | -5.073411 | 1.198160  | -1.459001 |
| C | 2.005283  | -0.826135 | -1.082620 |
| H | 1.800467  | -1.882970 | -0.888583 |
| H | 1.299236  | -0.489960 | -1.859341 |
| C | 3.375765  | -0.684240 | -1.579839 |
| C | 4.493359  | -0.566200 | -2.019726 |
| C | 1.235444  | 2.248239  | -0.551944 |
| H | 1.086836  | 1.996911  | -1.602362 |
| C | 0.674717  | 3.352038  | -0.056139 |
| H | 0.807490  | 3.640074  | 0.985050  |
| H | 0.070224  | 4.013930  | -0.670630 |
| H | 5.487556  | -0.475923 | -2.394881 |

#### 1ac\_conf2

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.359472  | 0.305796  | -1.185527 |
| H | 2.045489  | -0.314638 | -2.030323 |
| H | 3.457987  | 0.315899  | -1.195124 |
| N | 1.929258  | -0.401030 | 0.030827  |
| S | 0.743810  | -1.591370 | -0.051254 |
| O | 0.837185  | -2.332397 | 1.209796  |
| O | 0.911810  | -2.242911 | -1.353441 |
| C | -0.862854 | -0.787856 | -0.081820 |
| C | -1.458684 | -0.492538 | -1.309900 |
| C | -1.504938 | -0.473377 | 1.118408  |
| C | -2.701867 | 0.138738  | -1.329345 |
| H | -0.966768 | -0.781589 | -2.232434 |
| C | -2.748130 | 0.153287  | 1.078966  |
| H | -1.044231 | -0.733056 | 2.064735  |
| C | -3.362994 | 0.476006  | -0.140272 |
| H | -3.171457 | 0.360536  | -2.284527 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.254268 | 0.389295  | 2.012008  |
| C | -4.698861 | 1.180180  | -0.166854 |
| H | -5.211469 | 1.033041  | -1.122752 |
| H | -5.357105 | 0.820681  | 0.631485  |
| H | -4.576659 | 2.262067  | -0.023118 |
| C | 2.351998  | 0.107100  | 1.340236  |
| H | 2.337975  | -0.732619 | 2.040549  |
| H | 3.399910  | 0.415558  | 1.232589  |
| C | 1.567312  | 1.223563  | 1.891463  |
| C | 0.935351  | 2.122252  | 2.392605  |
| C | 1.834249  | 1.712427  | -1.325397 |
| H | 0.753749  | 1.829160  | -1.255116 |
| C | 2.610625  | 2.772576  | -1.549557 |
| H | 3.693615  | 2.683891  | -1.616987 |
| H | 2.197493  | 3.769052  | -1.678525 |
| H | 0.373943  | 2.925394  | 2.812934  |

#### I(ac)-Yne\_conf1

##### 0 imaginary frequency

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.451280 | 2.129639  | -0.410293 |
| H | -1.488618 | 2.494655  | -0.786683 |
| H | -2.570399 | 2.533490  | 0.596154  |
| N | -2.299284 | 0.668918  | -0.284374 |
| S | -3.095828 | -0.149551 | 0.943311  |
| O | -3.154848 | 0.773984  | 2.081228  |
| O | -2.457625 | -1.465484 | 1.049437  |
| C | -4.785633 | -0.443355 | 0.407021  |
| C | -5.073356 | -1.569313 | -0.369214 |
| C | -5.792544 | 0.458603  | 0.756137  |
| C | -6.379891 | -1.779275 | -0.806429 |
| H | -4.289863 | -2.281878 | -0.605014 |
| C | -7.094165 | 0.228896  | 0.315291  |
| H | -5.556439 | 1.317525  | 1.373865  |
| C | -7.409563 | -0.887632 | -0.472507 |
| H | -6.605248 | -2.655936 | -1.408880 |
| H | -7.879791 | 0.928399  | 0.590452  |
| C | -8.829338 | -1.142180 | -0.920324 |
| H | -8.859330 | -1.699818 | -1.862118 |
| H | -9.376740 | -1.733053 | -0.173924 |
| H | -9.379708 | -0.206025 | -1.060609 |
| C | -1.789926 | -0.116189 | -1.417292 |
| H | -1.507590 | -1.102133 | -1.037788 |
| H | -2.553497 | -0.249655 | -2.201328 |
| C | -0.607694 | 0.493862  | -2.034587 |

|                              |           |           |           |    |           |           |           |
|------------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C                            | 0.333274  | 0.999617  | -2.616028 | S  | -3.862821 | -1.560266 | -0.956905 |
| C                            | -3.573568 | 2.583698  | -1.310350 | O  | -5.127888 | -2.300981 | -0.957768 |
| H                            | -3.602838 | 2.148585  | -2.309853 | O  | -2.965319 | -1.564273 | -2.115975 |
| C                            | -4.480886 | 3.498655  | -0.967439 | C  | -4.254489 | 0.154198  | -0.593769 |
| H                            | -4.479404 | 3.961715  | 0.017633  | C  | -3.293484 | 1.146393  | -0.811938 |
| H                            | -5.252524 | 3.828386  | -1.657897 | C  | -5.515693 | 0.475241  | -0.090921 |
| Rh                           | 1.655017  | 0.146550  | -0.667919 | C  | -3.608279 | 2.469564  | -0.510512 |
| Rh                           | 3.304936  | -0.441384 | 0.972381  | H  | -2.315674 | 0.888031  | -1.206015 |
| O                            | 2.779756  | 1.839789  | -1.082146 | C  | -5.813009 | 1.806590  | 0.198018  |
| O                            | 4.322525  | 1.282416  | 0.483925  | H  | -6.251341 | -0.307070 | 0.058487  |
| O                            | 2.211287  | 0.597332  | 2.368541  | C  | -4.869351 | 2.822234  | -0.005113 |
| O                            | 4.315329  | -1.468188 | -0.501864 | H  | -2.862427 | 3.243462  | -0.675700 |
| O                            | 2.208085  | -2.124773 | 1.405645  | H  | -6.796479 | 2.059443  | 0.586648  |
| O                            | 0.663905  | -1.589600 | -0.162342 | C  | -5.208731 | 4.265343  | 0.283784  |
| O                            | 0.668555  | 1.183157  | 0.816078  | H  | -4.337549 | 4.815478  | 0.655365  |
| O                            | 2.756899  | -0.920706 | -2.056297 | H  | -5.553168 | 4.778009  | -0.624227 |
| C                            | 3.827966  | -1.496565 | -1.674432 | H  | -6.007367 | 4.348252  | 1.027945  |
| C                            | 3.851160  | 2.039349  | -0.419356 | C  | -3.676007 | -2.696065 | 1.506121  |
| C                            | 1.136868  | 1.169431  | 2.002169  | H  | -4.601201 | -3.162770 | 1.156186  |
| C                            | 1.127568  | -2.329115 | 0.769744  | H  | -3.052458 | -3.498966 | 1.920497  |
| C                            | 0.307571  | -3.543638 | 1.133768  | C  | -3.980311 | -1.715489 | 2.560379  |
| C                            | 4.568330  | -2.311211 | -2.712893 | C  | -4.261398 | -0.934847 | 3.437822  |
| C                            | 4.610467  | 3.312509  | -0.723965 | C  | -1.074490 | -0.860033 | 1.306557  |
| C                            | 0.335260  | 1.907299  | 3.049745  | H  | -1.561972 | 0.100807  | 1.160924  |
| H                            | 0.755909  | 1.739618  | 4.042371  | C  | -0.184492 | -1.002881 | 2.316511  |
| H                            | -0.706441 | 1.572973  | 3.013291  | H  | 0.277029  | -1.962730 | 2.534940  |
| H                            | 0.348041  | 2.979755  | 2.824824  | H  | 0.031277  | -0.190482 | 3.002432  |
| H                            | 5.637091  | 3.240477  | -0.360873 | Rh | 1.291377  | -0.166523 | 0.498835  |
| H                            | 4.115467  | 4.151063  | -0.220353 | Rh | 3.176213  | 0.551750  | -0.820773 |
| H                            | 4.596638  | 3.512779  | -1.798394 | O  | 0.157387  | 0.028840  | -1.231104 |
| H                            | 4.536966  | -1.806826 | -3.681929 | O  | 1.949531  | 0.639169  | -2.469362 |
| H                            | 5.600387  | -2.480214 | -2.400781 | O  | 2.688315  | 2.494565  | -0.327333 |
| H                            | 4.069949  | -3.281395 | -2.823774 | O  | 3.553907  | -1.429908 | -1.234566 |
| H                            | 0.773517  | -4.088778 | 1.955869  | O  | 4.352931  | 0.428441  | 0.857243  |
| H                            | 0.216398  | -4.197777 | 0.259908  | O  | 2.603469  | -0.285270 | 2.108159  |
| H                            | -0.699016 | -3.215837 | 1.410716  | O  | 0.936350  | 1.817971  | 0.947862  |
| H                            | 1.092735  | 1.485909  | -3.188234 | O  | 1.757219  | -2.108665 | -0.027711 |
| <b>I(ac)-Ene_conf2</b>       |           |           |           | C  | 2.772208  | -2.317111 | -0.773736 |
| <b>0 imaginary frequency</b> |           |           |           | C  | 0.720565  | 0.361316  | -2.329115 |
| C                            | -1.514493 | -1.978932 | 0.387697  | C  | 1.705183  | 2.705252  | 0.448243  |
| H                            | -1.179553 | -1.774113 | -0.630623 | C  | 3.826783  | 0.031101  | 1.941680  |
| H                            | -1.054607 | -2.924701 | 0.698814  | C  | 4.731954  | -0.104952 | 3.146332  |
| N                            | -2.968340 | -2.179546 | 0.329651  | C  | 3.045993  | -3.754973 | -1.155145 |
|                              |           |           |           | C  | -0.167228 | 0.451007  | -3.549306 |

|   |           |           |           |    |           |           |           |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 1.437272  | 4.141327  | 0.843333  | H  | 1.628635  | 0.510812  | 0.118098  |
| H | 1.699328  | 4.812923  | 0.022705  | C  | 0.773490  | 0.883865  | -1.772552 |
| H | 2.068537  | 4.394925  | 1.703230  | H  | 0.524217  | 0.513374  | -2.763685 |
| H | 0.392466  | 4.272810  | 1.131772  | H  | 0.630505  | 1.944816  | -1.596164 |
| H | 0.400028  | 0.184107  | -4.443907 | Rh | -1.187201 | 0.278752  | -0.367712 |
| H | -0.508509 | 1.487052  | -3.664869 | Rh | -3.381523 | 0.097333  | 0.608865  |
| H | -1.040910 | -0.194029 | -3.434120 | O  | -0.452112 | -0.575063 | 1.383377  |
| H | 2.311503  | -4.070838 | -1.904927 | O  | -2.528903 | -0.762235 | 2.268929  |
| H | 4.048324  | -3.854753 | -1.574511 | O  | -3.094262 | 1.967905  | 1.426023  |
| H | 2.929399  | -4.403608 | -0.282756 | O  | -3.544212 | -1.765366 | -0.258505 |
| H | 5.661867  | 0.443847  | 2.988504  | O  | -4.173574 | 0.952332  | -1.082151 |
| H | 4.966359  | -1.164988 | 3.297909  | O  | -2.118337 | 1.118553  | -2.023008 |
| H | 4.221395  | 0.254762  | 4.043458  | O  | -1.033006 | 2.149428  | 0.495210  |
| H | -4.500575 | -0.233781 | 4.204875  | O  | -1.471863 | -1.603947 | -1.165757 |

#### I(ac)-Ene\_conf3

##### 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.706239 | -1.371654 | -1.066166 |
| H | 0.866945 | -2.019618 | -0.791622 |
| H | 1.916744 | -1.555872 | -2.121882 |
| N | 2.857616 | -1.829060 | -0.279799 |
| S | 4.421242 | -1.485911 | -0.796572 |
| O | 4.379217 | -1.537902 | -2.259292 |
| O | 5.305364 | -2.343834 | -0.003161 |
| C | 4.798558 | 0.211561  | -0.339787 |
| C | 5.255803 | 0.495531  | 0.951263  |
| C | 4.627888 | 1.232856  | -1.275329 |
| C | 5.521382 | 1.815824  | 1.304613  |
| H | 5.424414 | -0.310168 | 1.658105  |
| C | 4.904214 | 2.549193  | -0.905363 |
| H | 4.298180 | 0.992782  | -2.279949 |
| C | 5.349504 | 2.863192  | 0.385496  |
| H | 5.878818 | 2.037345  | 2.307519  |
| H | 4.776542 | 3.344827  | -1.635121 |
| C | 5.669140 | 4.286902  | 0.775604  |
| H | 5.265986 | 4.530394  | 1.765087  |
| H | 6.754020 | 4.448660  | 0.820381  |
| H | 5.258510 | 5.001953  | 0.056184  |
| C | 2.627247 | -2.193040 | 1.126530  |
| H | 3.602125 | -2.338752 | 1.598429  |
| H | 2.103461 | -1.382817 | 1.652621  |
| C | 1.843005 | -3.427937 | 1.252433  |
| C | 1.188996 | -4.434598 | 1.385337  |
| C | 1.341824 | 0.083596  | -0.839845 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.628635  | 0.510812  | 0.118098  |
| C  | 0.773490  | 0.883865  | -1.772552 |
| H  | 0.524217  | 0.513374  | -2.763685 |
| H  | 0.630505  | 1.944816  | -1.596164 |
| Rh | -1.187201 | 0.278752  | -0.367712 |
| Rh | -3.381523 | 0.097333  | 0.608865  |
| O  | -0.452112 | -0.575063 | 1.383377  |
| O  | -2.528903 | -0.762235 | 2.268929  |
| O  | -3.094262 | 1.967905  | 1.426023  |
| O  | -3.544212 | -1.765366 | -0.258505 |
| O  | -4.173574 | 0.952332  | -1.082151 |
| O  | -2.118337 | 1.118553  | -2.023008 |
| O  | -1.033006 | 2.149428  | 0.495210  |
| O  | -1.471863 | -1.603947 | -1.165757 |
| C  | -2.570617 | -2.214208 | -0.936976 |
| C  | -1.270273 | -0.911297 | 2.304925  |
| C  | -2.010543 | 2.585445  | 1.190411  |
| C  | -3.384666 | 1.265422  | -2.026021 |
| C  | -3.994699 | 1.845214  | -3.283168 |
| C  | -2.705303 | -3.598317 | -1.531423 |
| C  | -0.672358 | -1.540535 | 3.542925  |
| C  | -1.870958 | 3.980861  | 1.758095  |
| H  | -2.514147 | 4.101247  | 2.631831  |
| H  | -2.181293 | 4.705749  | 0.996135  |
| H  | -0.828910 | 4.185029  | 2.014749  |
| H  | -1.458131 | -1.826501 | 4.243585  |
| H  | 0.006131  | -0.827416 | 4.023613  |
| H  | -0.085003 | -2.418422 | 3.254685  |
| H  | -1.929647 | -4.247963 | -1.112312 |
| H  | -3.691026 | -4.013728 | -1.317833 |
| H  | -2.543622 | -3.551624 | -2.612916 |
| H  | -5.023473 | 2.158885  | -3.099178 |
| H  | -3.988929 | 1.080031  | -4.067912 |
| H  | -3.394839 | 2.687792  | -3.637469 |
| H  | 0.639426  | -5.342850 | 1.487577  |

#### I-TS-II(ac)\_conf1

##### 1 imaginary frequency, value = -359.2053 cm<sup>-1</sup>

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -1.674361 | 1.030171 | 0.333150  |
| C | -0.432083 | 1.590816 | -0.251195 |
| C | -0.158518 | 2.640221 | -0.922428 |
| C | -2.075453 | 3.396374 | -1.719714 |
| C | -3.004481 | 2.253398 | -1.372890 |
| H | -1.832635 | 3.508483 | -2.774821 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -4.034751 | 2.587188  | -1.533333 |
| H  | -2.814256 | 1.402971  | -2.044703 |
| H  | -1.559426 | 0.965302  | 1.418045  |
| N  | -2.856255 | 1.867935  | 0.032736  |
| S  | -4.265566 | 1.514930  | 0.905415  |
| O  | -3.849811 | 1.417495  | 2.304435  |
| O  | -5.268514 | 2.482548  | 0.450867  |
| C  | -4.803337 | -0.115235 | 0.381774  |
| C  | -5.698108 | -0.238362 | -0.685177 |
| C  | -4.299935 | -1.248486 | 1.026294  |
| C  | -6.077531 | -1.509312 | -1.111512 |
| H  | -6.107195 | 0.650146  | -1.154452 |
| C  | -4.690030 | -2.511840 | 0.583966  |
| H  | -3.630861 | -1.139096 | 1.873038  |
| C  | -5.580647 | -2.664005 | -0.488356 |
| H  | -6.777155 | -1.606687 | -1.938149 |
| H  | -4.302289 | -3.394144 | 1.087078  |
| C  | -6.024181 | -4.035543 | -0.938646 |
| H  | -5.280644 | -4.799429 | -0.690053 |
| H  | -6.964603 | -4.322874 | -0.450067 |
| H  | -6.197641 | -4.066259 | -2.019474 |
| C  | -1.659865 | 4.326452  | -0.822251 |
| H  | -1.061508 | 5.177577  | -1.131700 |
| H  | -1.959601 | 4.270664  | 0.218284  |
| H  | -1.794715 | 0.006271  | -0.052193 |
| Rh | 3.234400  | -1.173854 | 0.187440  |
| Rh | 1.356385  | 0.350679  | -0.090630 |
| O  | 4.387389  | 0.464604  | 0.686102  |
| O  | 2.637221  | 1.890029  | 0.432778  |
| O  | 1.925832  | 0.571843  | -2.073253 |
| O  | 0.920724  | 0.023504  | 1.908949  |
| O  | 0.205434  | -1.305930 | -0.592764 |
| O  | 1.960748  | -2.720113 | -0.326937 |
| O  | 3.661788  | -0.869540 | -1.812223 |
| O  | 2.687814  | -1.379257 | 2.169306  |
| C  | 1.676929  | -0.743732 | 2.594745  |
| C  | 3.854320  | 1.614805  | 0.700267  |
| C  | 2.934968  | -0.087023 | -2.494299 |
| C  | 0.751984  | -2.459940 | -0.598714 |
| C  | -0.132757 | -3.622052 | -1.003209 |
| C  | 1.337779  | -0.876034 | 4.064946  |
| C  | 4.746687  | 2.790317  | 1.042701  |
| C  | 3.272028  | 0.063646  | -3.964024 |
| H  | 2.632699  | -0.610066 | -4.546827 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 4.314717  | -0.204713 | -4.143819 |
| H | 3.075374  | 1.085607  | -4.297402 |
| H | 5.027288  | 3.308311  | 0.118034  |
| H | 5.654119  | 2.447003  | 1.542495  |
| H | 4.207017  | 3.501406  | 1.673543  |
| H | 1.702407  | 0.011793  | 4.594738  |
| H | 0.254240  | -0.921488 | 4.201582  |
| H | 1.815996  | -1.760621 | 4.489135  |
| H | -1.168742 | -3.433527 | -0.711704 |
| H | 0.231787  | -4.548403 | -0.554516 |
| H | -0.099648 | -3.731622 | -2.093745 |
| H | 0.598079  | 3.175387  | -1.461887 |

#### I-TS-II(ac)\_conf2

1 imaginary frequency, value = -359.1063 cm<sup>-1</sup>

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.675421 | -1.026490 | 0.331846  |
| C | 0.433018 | -1.585743 | -0.253541 |
| C | 0.159150 | -2.633860 | -0.926627 |
| C | 2.075324 | -3.389651 | -1.725104 |
| C | 3.004894 | -2.247707 | -1.376194 |
| H | 1.832238 | -3.499602 | -2.780376 |
| H | 4.034991 | -2.581740 | -1.537200 |
| H | 2.815130 | -1.395991 | -2.046482 |
| H | 1.560540 | -0.963525 | 1.416869  |
| N | 2.856704 | -1.864572 | 0.030058  |
| S | 4.265978 | -1.516252 | 0.904455  |
| O | 3.849134 | -1.419775 | 2.303226  |
| O | 5.266948 | -2.485691 | 0.449448  |
| C | 4.808384 | 0.113254  | 0.383602  |
| C | 5.704716 | 0.235531  | -0.682146 |
| C | 4.307117 | 1.246899  | 1.029068  |
| C | 6.087848 | 1.506068  | -1.106340 |
| H | 6.112097 | -0.653392 | -1.152111 |
| C | 4.700963 | 2.509848  | 0.588898  |
| H | 3.636812 | 1.138072  | 1.874915  |
| C | 5.593205 | 2.661187  | -0.482171 |
| H | 6.788688 | 1.602769  | -1.932026 |
| H | 4.314916 | 3.392463  | 1.092759  |
| C | 6.040822 | 4.032155  | -0.930139 |
| H | 5.300242 | 4.798049  | -0.678947 |
| H | 6.982902 | 4.315209  | -0.442259 |
| H | 6.212943 | 4.064563  | -2.011141 |
| C | 1.660006 | -4.321533 | -0.829416 |
| H | 1.061208 | -5.171816 | -1.140325 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.960006  | -4.267800 | 0.211153  |
| H  | 1.796468  | -0.001982 | -0.051664 |
| Rh | -3.239707 | 1.170639  | 0.185774  |
| Rh | -1.357295 | -0.348407 | -0.092480 |
| O  | -3.658711 | 0.874913  | -1.816735 |
| O  | -1.917407 | -0.559894 | -2.078594 |
| O  | -0.207681 | 1.313171  | -0.580552 |
| O  | -2.637799 | -1.893087 | 0.416332  |
| O  | -0.930873 | -0.030713 | 1.910770  |
| O  | -2.701530 | 1.367628  | 2.170978  |
| O  | -1.967449 | 2.722150  | -0.316182 |
| O  | -4.391647 | -0.472481 | 0.671051  |
| C  | -3.855760 | -1.621170 | 0.684200  |
| C  | -2.927214 | 0.097762  | -2.499957 |
| C  | -0.756949 | 2.465896  | -0.584055 |
| C  | -1.690689 | 0.732439  | 2.597097  |
| C  | -1.355356 | 0.860282  | 4.068611  |
| C  | -4.735382 | -2.799315 | 1.049994  |
| C  | -3.258924 | -0.047279 | -3.971444 |
| C  | 0.126525  | 3.631870  | -0.980103 |
| H  | 1.162820  | 3.442329  | -0.690481 |
| H  | -0.238874 | 4.554415  | -0.524269 |
| H  | 0.092537  | 3.749875  | -2.069733 |
| H  | -2.615939 | 0.626929  | -4.549620 |
| H  | -4.300438 | 0.223483  | -4.154293 |
| H  | -3.062930 | -1.068564 | -4.307334 |
| H  | -4.775765 | -3.500350 | 0.209528  |
| H  | -4.298593 | -3.332289 | 1.900560  |
| H  | -5.743249 | -2.463352 | 1.297901  |
| H  | -1.700805 | -0.039199 | 4.591452  |
| H  | -1.851241 | 1.731841  | 4.499290  |
| H  | -0.272883 | 0.927018  | 4.205771  |
| H  | -0.597881 | -3.168221 | -1.466250 |

# II(ac)\_conf1

## 0 imaginary frequency

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.583722 | -1.047293 | 0.349843  |
| C | 0.331353 | -1.444665 | -0.335980 |
| C | 0.313759 | -2.559780 | -1.226031 |
| C | 1.678576 | -3.049394 | -1.792409 |
| C | 2.904411 | -2.264090 | -1.359624 |
| H | 1.647999 | -3.315900 | -2.846472 |
| H | 3.796483 | -2.888681 | -1.447180 |
| H | 3.027334 | -1.380060 | -2.007661 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.402410  | -1.045165 | 1.432219  |
| N  | 2.753300  | -1.890533 | 0.050287  |
| S  | 4.159054  | -1.579990 | 0.941869  |
| O  | 3.714507  | -1.425977 | 2.327650  |
| O  | 5.127042  | -2.601233 | 0.535862  |
| C  | 4.772891  | 0.011212  | 0.385519  |
| C  | 5.672240  | 0.070001  | -0.683573 |
| C  | 4.320743  | 1.179875  | 1.004249  |
| C  | 6.108998  | 1.312605  | -1.136910 |
| H  | 6.039585  | -0.846477 | -1.133212 |
| C  | 4.768587  | 2.414362  | 0.535002  |
| H  | 3.648069  | 1.118651  | 1.853071  |
| C  | 5.665143  | 2.502218  | -0.539208 |
| H  | 6.812399  | 1.360126  | -1.964693 |
| H  | 4.422254  | 3.324328  | 1.018641  |
| C  | 6.170942  | 3.841221  | -1.020655 |
| H  | 7.151338  | 4.070124  | -0.582520 |
| H  | 6.291472  | 3.856311  | -2.109189 |
| H  | 5.490357  | 4.651536  | -0.741313 |
| C  | 0.993062  | -3.912091 | -0.822490 |
| H  | 0.442772  | -4.778620 | -1.174860 |
| H  | 1.390029  | -3.983492 | 0.183601  |
| H  | 1.744554  | 0.012034  | 0.071570  |
| Rh | -3.237125 | 1.149014  | 0.207445  |
| Rh | -1.263281 | -0.291361 | -0.087509 |
| O  | -4.335313 | -0.578821 | 0.511724  |
| O  | -2.513858 | -1.909813 | 0.228562  |
| O  | -1.735068 | -0.372746 | -2.103839 |
| O  | -0.936874 | -0.107338 | 1.945421  |
| O  | -0.155902 | 1.435843  | -0.376154 |
| O  | -1.977400 | 2.768773  | -0.118139 |
| O  | -3.549877 | 0.969354  | -1.833994 |
| O  | -2.771532 | 1.204028  | 2.228823  |
| C  | -1.755097 | 0.584135  | 2.650256  |
| C  | -3.756439 | -1.700592 | 0.459452  |
| C  | -2.761306 | 0.268411  | -2.527180 |
| C  | -0.748834 | 2.571571  | -0.327621 |
| C  | 0.121314  | 3.786117  | -0.581881 |
| C  | -1.463054 | 0.628105  | 4.135958  |
| C  | -4.595068 | -2.940003 | 0.697308  |
| C  | -3.025776 | 0.174249  | -4.016420 |

## [Rh<sub>2</sub>(OAc)<sub>4</sub>]-alkynal complex

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.713313 | 0.292110 | 0.269740 |
|---|----------|----------|----------|

|    |           |           |           |                                                         |           |           |           |
|----|-----------|-----------|-----------|---------------------------------------------------------|-----------|-----------|-----------|
| C  | 1.749440  | 1.364550  | 0.005953  | H                                                       | 3.894464  | 2.648666  | 0.999179  |
| C  | 1.023925  | 2.328532  | -0.193808 | C                                                       | 5.502217  | -1.457544 | 1.089729  |
| C  | 4.547147  | 1.776094  | 1.088782  | H                                                       | 4.561325  | -1.931253 | 1.379305  |
| H  | 5.563547  | 2.077457  | 0.834965  | H                                                       | 6.226516  | -2.219445 | 0.792410  |
| H  | 4.512369  | 1.417760  | 2.130259  | H                                                       | 5.907997  | -0.858050 | 1.907416  |
| H  | 2.540210  | -0.510266 | -0.452198 |                                                         |           |           |           |
| N  | 4.097140  | 0.763484  | 0.128974  | <b>[Rh<sub>2</sub>(OAc)<sub>4</sub>]-alkyne complex</b> |           |           |           |
| S  | 5.224553  | -0.400155 | -0.354070 | C                                                       | 2.726817  | 0.373073  | 0.052103  |
| O  | 4.569750  | -1.223481 | -1.372076 | C                                                       | 1.760457  | 1.425664  | -0.294647 |
| O  | 6.474716  | 0.309800  | -0.617094 | C                                                       | 1.070635  | 2.385359  | -0.594174 |
| C  | 0.323532  | 3.581795  | -0.444164 | C                                                       | 4.409809  | 1.840419  | 1.156914  |
| H  | -0.718150 | 3.480325  | -0.785463 | H                                                       | 5.430162  | 2.203961  | 1.035398  |
| O  | 0.868062  | 4.657424  | -0.291056 | H                                                       | 4.289414  | 1.392859  | 2.157104  |
| H  | 2.501540  | -0.106124 | 1.275756  | H                                                       | 2.670480  | -0.416204 | -0.700353 |
| Rh | -2.529239 | -1.092110 | 0.047831  | N                                                       | 4.103856  | 0.899100  | 0.076908  |
| Rh | -0.610340 | 0.349420  | -0.009076 | S                                                       | 5.320997  | -0.189238 | -0.351283 |
| O  | -3.200832 | -0.182480 | -1.667514 | O                                                       | 4.835930  | -0.938012 | -1.511382 |
| O  | -1.406219 | 1.200955  | -1.714788 | O                                                       | 6.570364  | 0.571061  | -0.389613 |
| O  | -1.679907 | 1.693360  | 1.139257  | C                                                       | 0.329770  | 3.582882  | -0.984241 |
| O  | 0.330732  | -1.089182 | -1.153372 | H                                                       | -0.346472 | 3.894157  | -0.182112 |
| O  | 0.052618  | -0.596858 | 1.712468  | H                                                       | 2.441077  | -0.059537 | 1.022686  |
| O  | -1.773513 | -1.938701 | 1.765841  | Rh                                                      | -2.517329 | -0.993139 | 0.213455  |
| O  | -3.491634 | 0.331517  | 1.179865  | Rh                                                      | -0.592612 | 0.416797  | -0.094372 |
| O  | -1.481098 | -2.445853 | -1.094037 | O                                                       | -3.253181 | -0.287046 | -1.572346 |
| C  | -0.296866 | -2.160300 | -1.451535 | O                                                       | -1.442345 | 1.045032  | -1.870579 |
| C  | -2.506883 | 0.749459  | -2.178879 | O                                                       | -1.623221 | 1.900372  | 0.920501  |
| C  | -2.874700 | 1.399976  | 1.479812  | O                                                       | 0.299528  | -1.162377 | -1.086590 |
| C  | -0.672192 | -1.513094 | 2.228522  | O                                                       | 0.120414  | -0.314477 | 1.713483  |
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| C  | 0.427700  | -3.153493 | -2.330192 | O                                                       | -3.430676 | 0.560812  | 1.206695  |
| C  | -3.004840 | 1.364067  | -3.466817 | O                                                       | -1.520309 | -2.482206 | -0.798342 |
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| H  | -2.493148 | 0.883241  | -4.308843 | C                                                       | -3.128956 | 1.051832  | -3.540576 |
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| H  | -0.729381 | -3.034860 | 3.750354  | H                                                       | -3.237820 | 2.140855  | -3.510267 |
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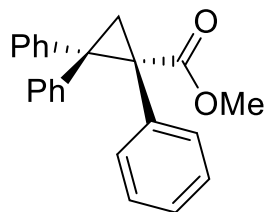
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| H                                                        | 0.091804  | -3.196079 | -3.096231 | C                                                       | 0.924771  | 3.424297  | -1.972933 |
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| H                                                        | -0.054473 | -4.321305 | -1.732284 | C                                                       | -3.198231 | -3.193805 | 0.905543  |
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| H                                                        | -0.541678 | -2.539523 | 4.012345  | C                                                       | 6.350858  | -0.340052 | -0.231032 |
| H                                                        | -0.210277 | -0.843009 | 4.436084  | H                                                       | 5.654157  | -0.091594 | -1.034937 |
| H                                                        | 3.721968  | 2.686236  | 1.074857  | H                                                       | 7.285816  | 0.209210  | -0.364637 |
| C                                                        | 5.454556  | -1.362819 | 1.022563  | H                                                       | 6.551012  | -1.413318 | -0.201549 |
| H                                                        | 4.503909  | -1.886537 | 1.146850  | F                                                       | 0.789046  | -3.630435 | -2.743093 |
| H                                                        | 6.240772  | -2.074441 | 0.760099  | F                                                       | 2.336762  | -2.108739 | -2.947954 |
| H                                                        | 5.727781  | -0.825994 | 1.933641  | F                                                       | 0.692515  | -2.187354 | -4.372262 |
| H                                                        | 1.025650  | 4.401298  | -1.202523 | F                                                       | -2.429697 | -4.283148 | 0.745120  |
| H                                                        | -0.269602 | 3.382203  | -1.877643 | F                                                       | -3.437217 | -3.025123 | 2.214556  |
| <b>[Rh<sub>2</sub>(TFA)<sub>4</sub>]-alkynal complex</b> |           |           |           | F                                                       | -4.357971 | -3.386780 | 0.275934  |
| C                                                        | 3.043849  | -0.232730 | 0.806967  | F                                                       | -3.441593 | 1.935166  | 3.205981  |
| C                                                        | 1.844792  | -0.307927 | 1.657663  | F                                                       | -2.659875 | 3.702883  | 2.195173  |
| C                                                        | 0.937271  | -0.418787 | 2.473685  | F                                                       | -4.545410 | 2.823096  | 1.552224  |
| C                                                        | 4.314200  | -2.132152 | 1.810637  | F                                                       | 0.947007  | 4.365768  | -1.018195 |
| H                                                        | 5.193400  | -2.319300 | 2.427411  | F                                                       | 2.188256  | 3.060096  | -2.247763 |
| H                                                        | 4.369910  | -2.728517 | 0.886716  | F                                                       | 0.375020  | 3.936508  | -3.074758 |
| H                                                        | 3.195447  | 0.809846  | 0.511497  | <b>[Rh<sub>2</sub>(TFA)<sub>4</sub>]-alkyne complex</b> |           |           |           |
| N                                                        | 4.220386  | -0.694851 | 1.543334  | C                                                       | 2.977606  | -0.462904 | -1.113599 |
| S                                                        | 5.652579  | 0.183292  | 1.354343  | C                                                       | 1.753524  | -0.106064 | -1.860213 |
| O                                                        | 5.258443  | 1.585861  | 1.218846  | C                                                       | 0.890644  | 0.207433  | -2.668482 |
| O                                                        | 6.562838  | -0.276195 | 2.400332  | C                                                       | 3.943885  | 1.820287  | -0.826480 |
| C                                                        | 0.044857  | -0.585063 | 3.623829  | H                                                       | 4.780690  | 2.429062  | -1.169125 |
| H                                                        | -0.943740 | -0.108146 | 3.537495  | H                                                       | 3.914621  | 1.796274  | 0.272286  |
| O                                                        | 0.401932  | -1.201838 | 4.604370  | H                                                       | 3.293673  | -1.460659 | -1.430215 |
| H                                                        | 2.864033  | -0.825542 | -0.102662 | N                                                       | 4.059105  | 0.482211  | -1.413238 |
| Rh                                                       | -1.988510 | 0.265426  | -1.409768 | S                                                       | 5.599178  | -0.151244 | -1.672942 |
| Rh                                                       | -0.306899 | -0.033521 | 0.315034  | O                                                       | 5.415398  | -1.409177 | -2.398853 |
| O                                                        | -3.037847 | 1.451336  | -0.093748 | O                                                       | 6.416072  | 0.938736  | -2.204143 |
| O                                                        | -1.443529 | 1.208676  | 1.507508  | C                                                       | -0.039092 | 0.567364  | -3.737383 |
| O                                                        | -1.401029 | -1.649478 | 0.983607  | H                                                       | -0.550176 | 1.508221  | -3.511650 |
| O                                                        | 0.667184  | 1.605082  | -0.478125 | H                                                       | 2.761822  | -0.495867 | -0.037979 |
| O                                                        | 0.696936  | -1.261525 | -1.013641 | Rh                                                      | -1.943764 | -0.073358 | 1.376521  |
| O                                                        | -0.854239 | -0.938599 | -2.642619 | Rh                                                      | -0.298505 | -0.015527 | -0.413948 |
| O                                                        | -2.949565 | -1.396137 | -0.661116 | O                                                       | -3.148417 | -1.201582 | 0.141875  |
| O                                                        | -0.936210 | 1.912793  | -2.060273 | O                                                       | -1.613092 | -1.140982 | -1.535768 |
| C                                                        | 0.135723  | 2.195696  | -1.463303 | O                                                       | -1.212665 | 1.714661  | -1.072248 |
| C                                                        | -2.536182 | 1.648571  | 1.043314  | O                                                       | 0.499619  | -1.745319 | 0.396225  |
| C                                                        | -2.452892 | -1.957442 | 0.350601  | O                                                       | 0.901184  | 1.103779  | 0.848310  |
| C                                                        | 0.207381  | -1.419436 | -2.169967 |                                                         |           |           |           |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | -0.645138 | 1.056069  | 2.516906  | H | 6.302876  | 0.338583  | 0.572118  |
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| C | -2.215000 | 2.142813  | -0.429928 | F | -1.979177 | 4.475740  | -0.657307 |
| C | 0.458462  | 1.374774  | 2.002177  | F | 1.261430  | 3.533681  | 2.502860  |
| C | 1.396375  | 2.247713  | 2.868129  | F | 2.678148  | 1.885476  | 2.680825  |
| C | 0.632157  | -3.504812 | 1.973195  | F | 1.107958  | 2.133997  | 4.165275  |
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- (31) NBO analysis was performed with NBO6.0 at Peking University Shenzhen Graduate School

## 12. The NMR spectra



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7.22  
7.16  
7.13  
7.11  
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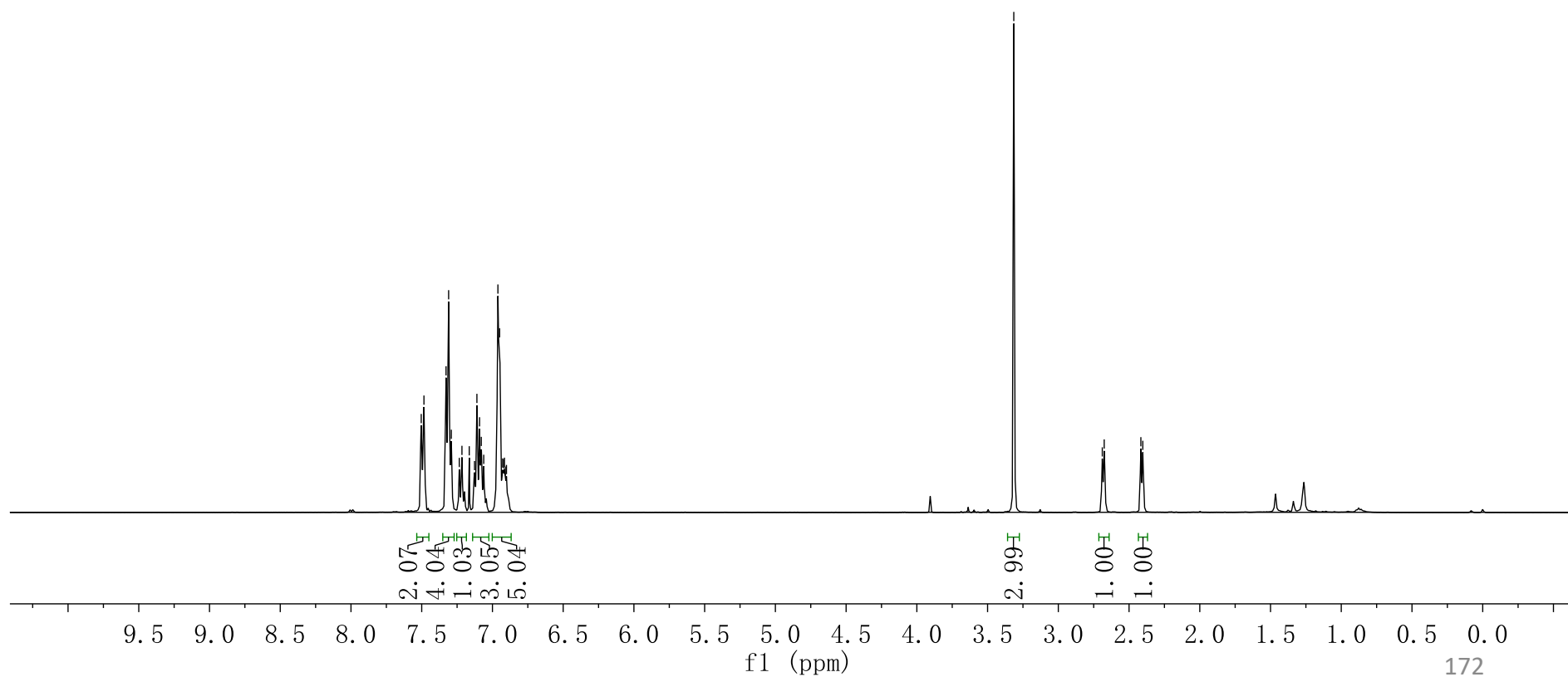
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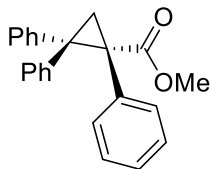
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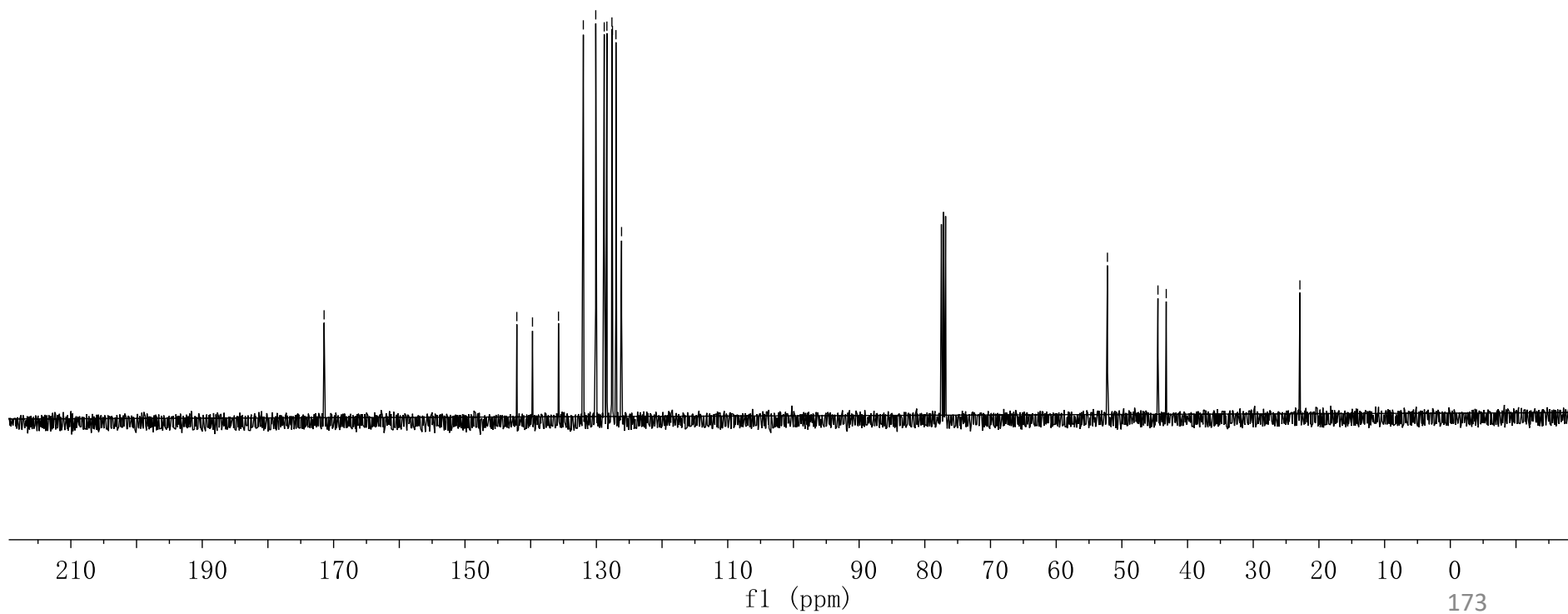


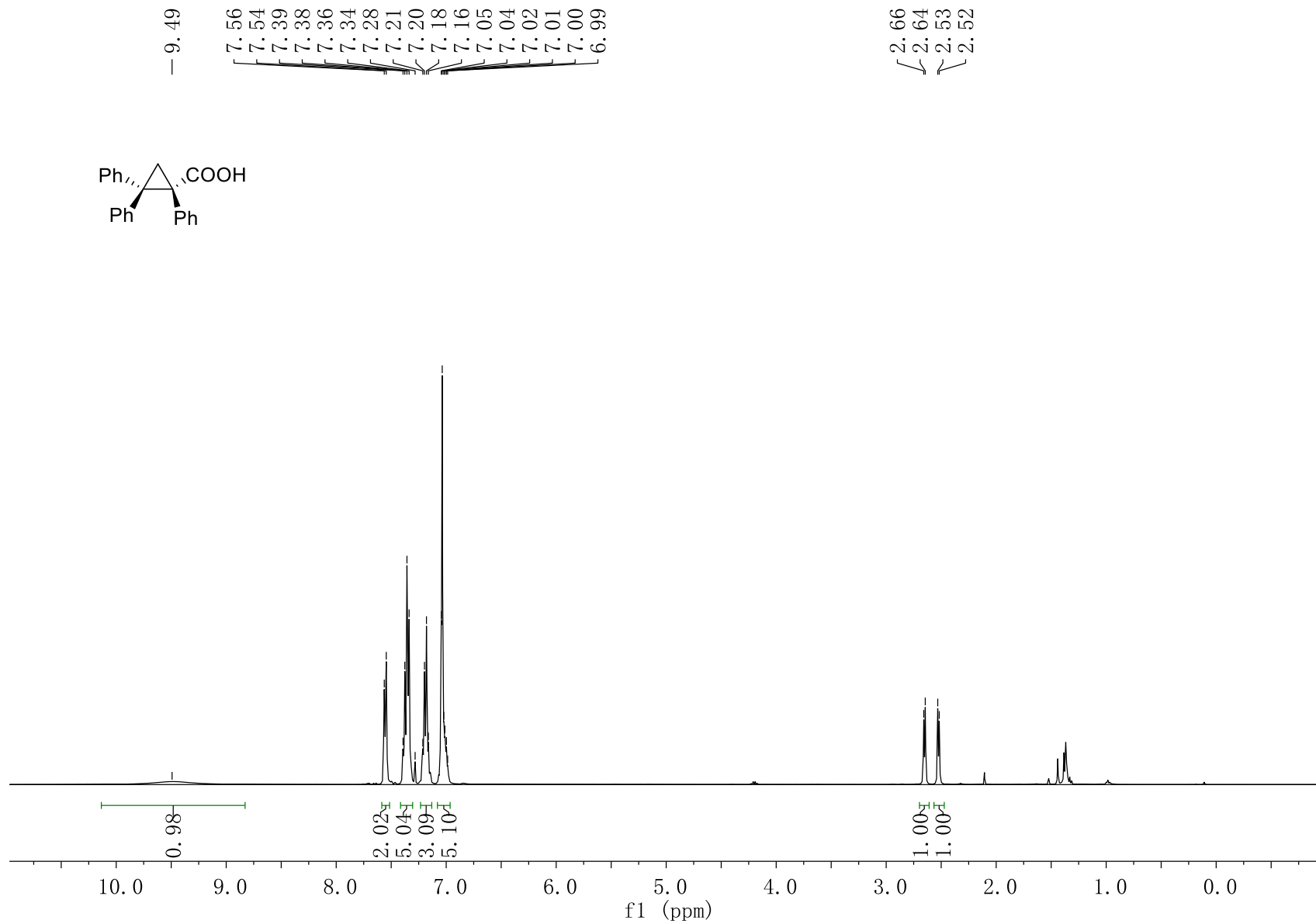
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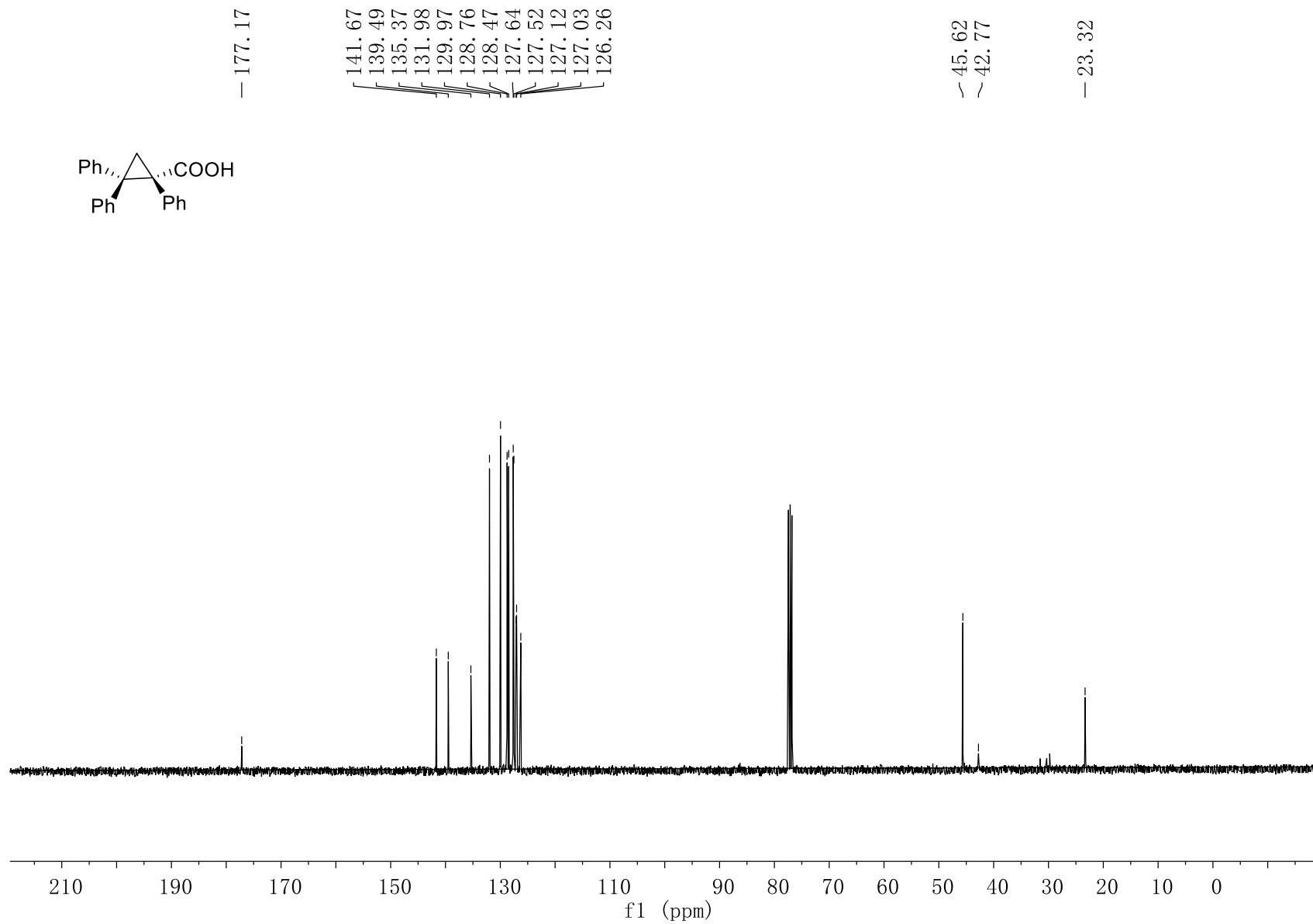
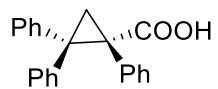
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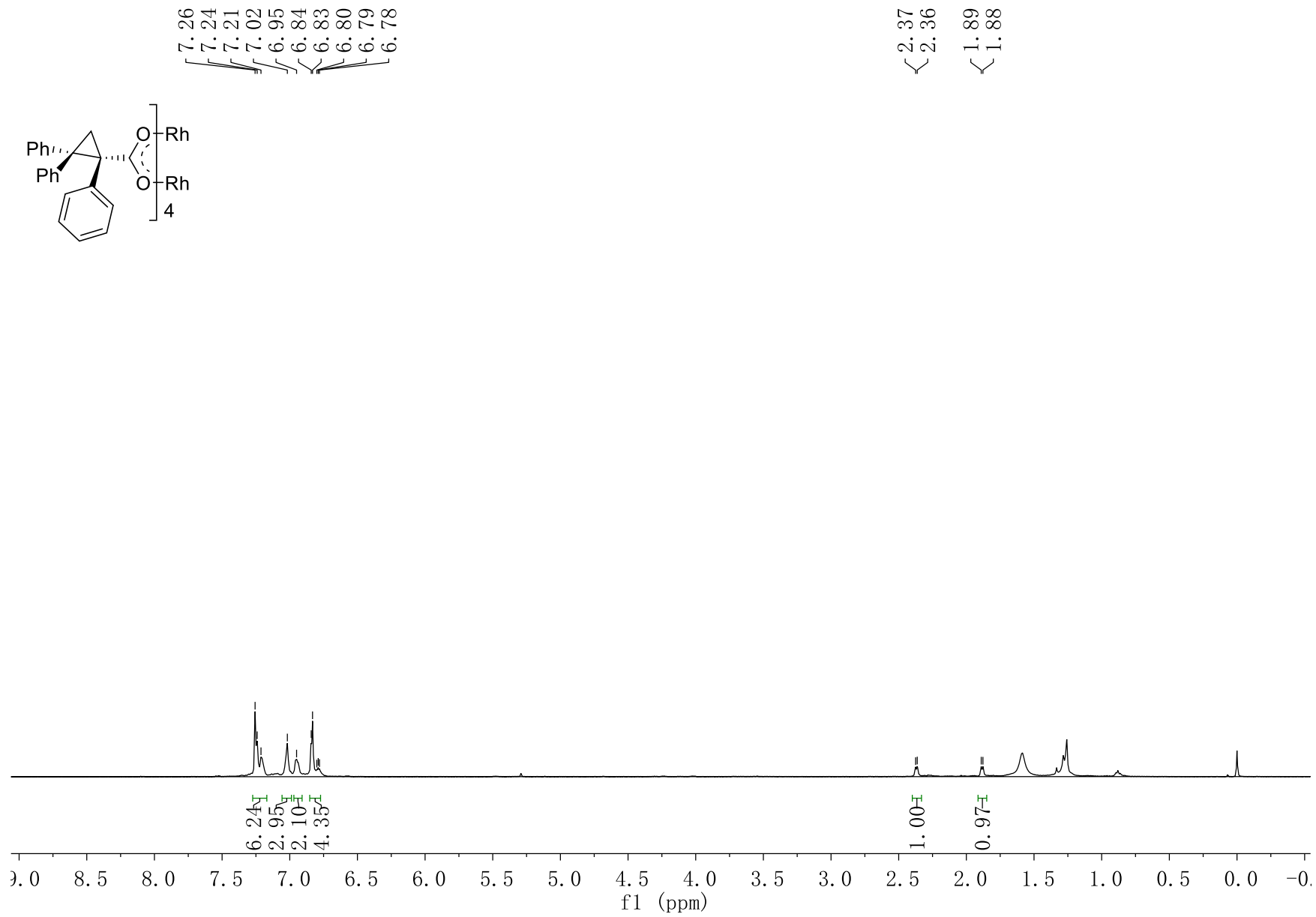
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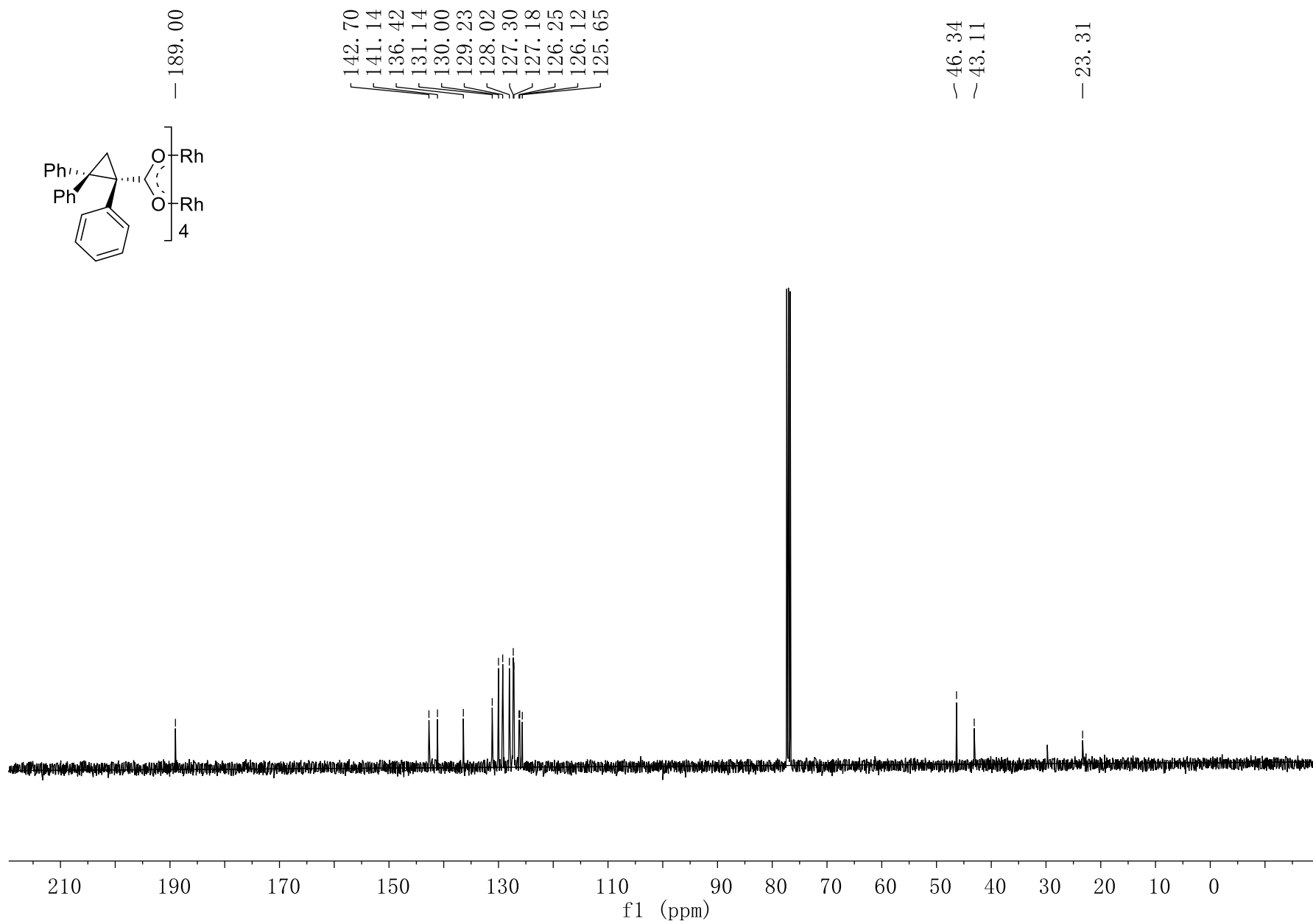
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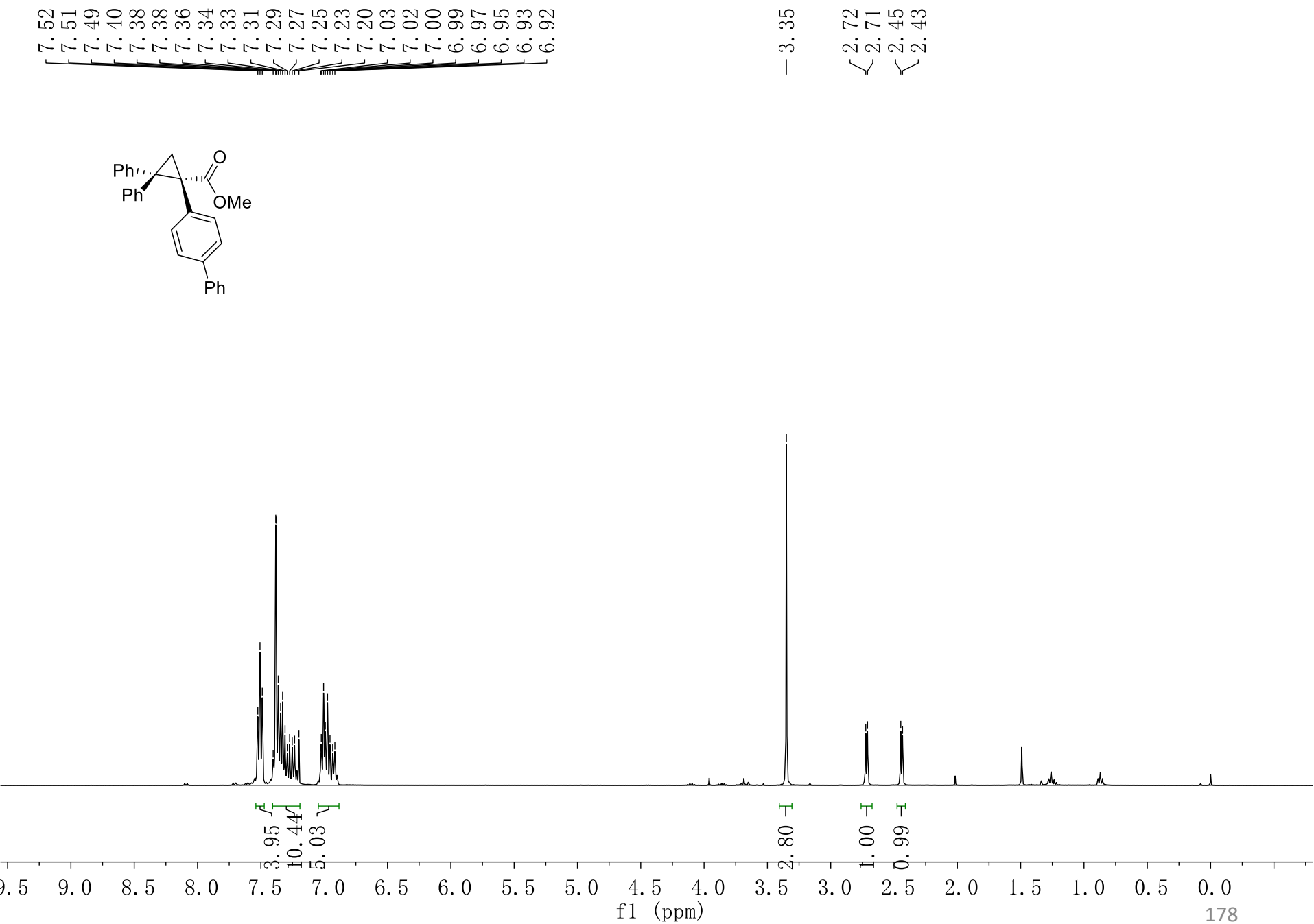


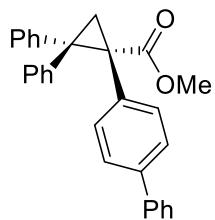








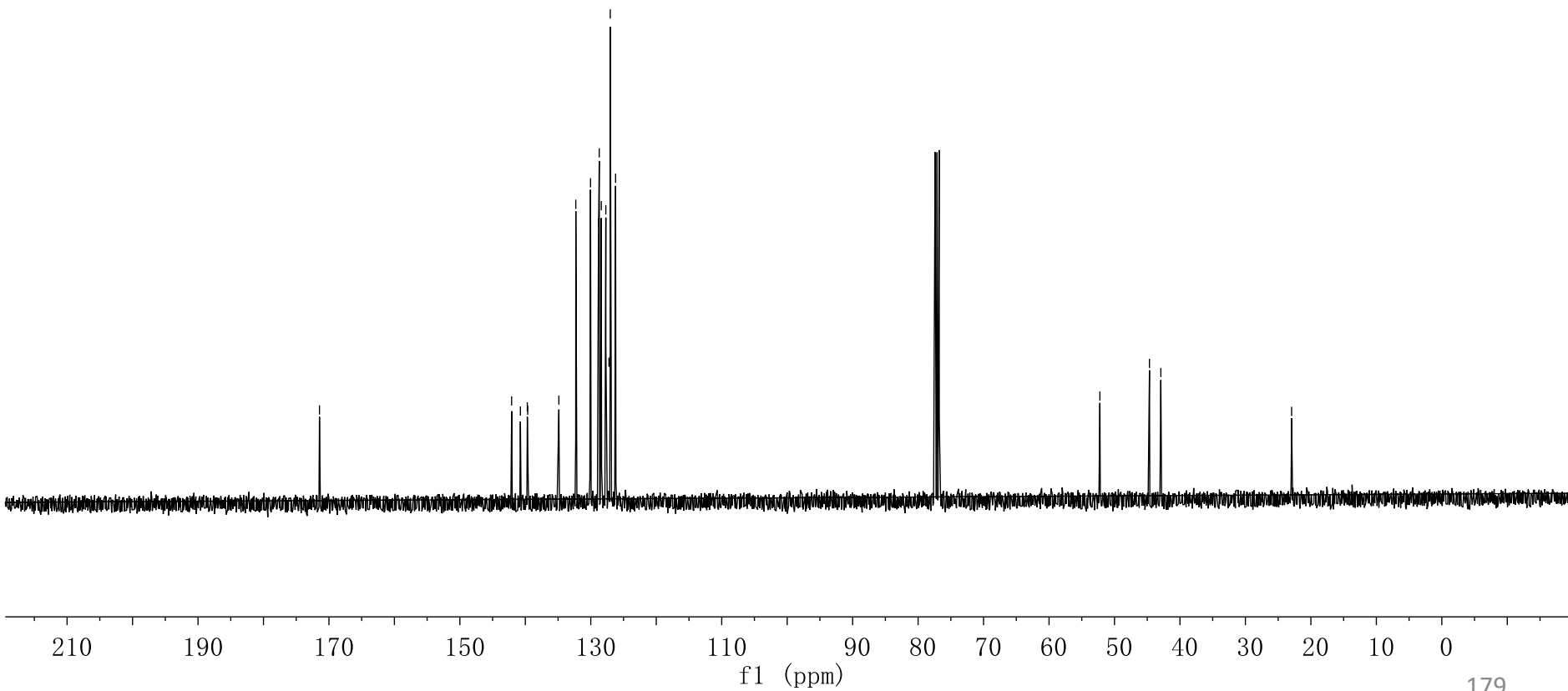


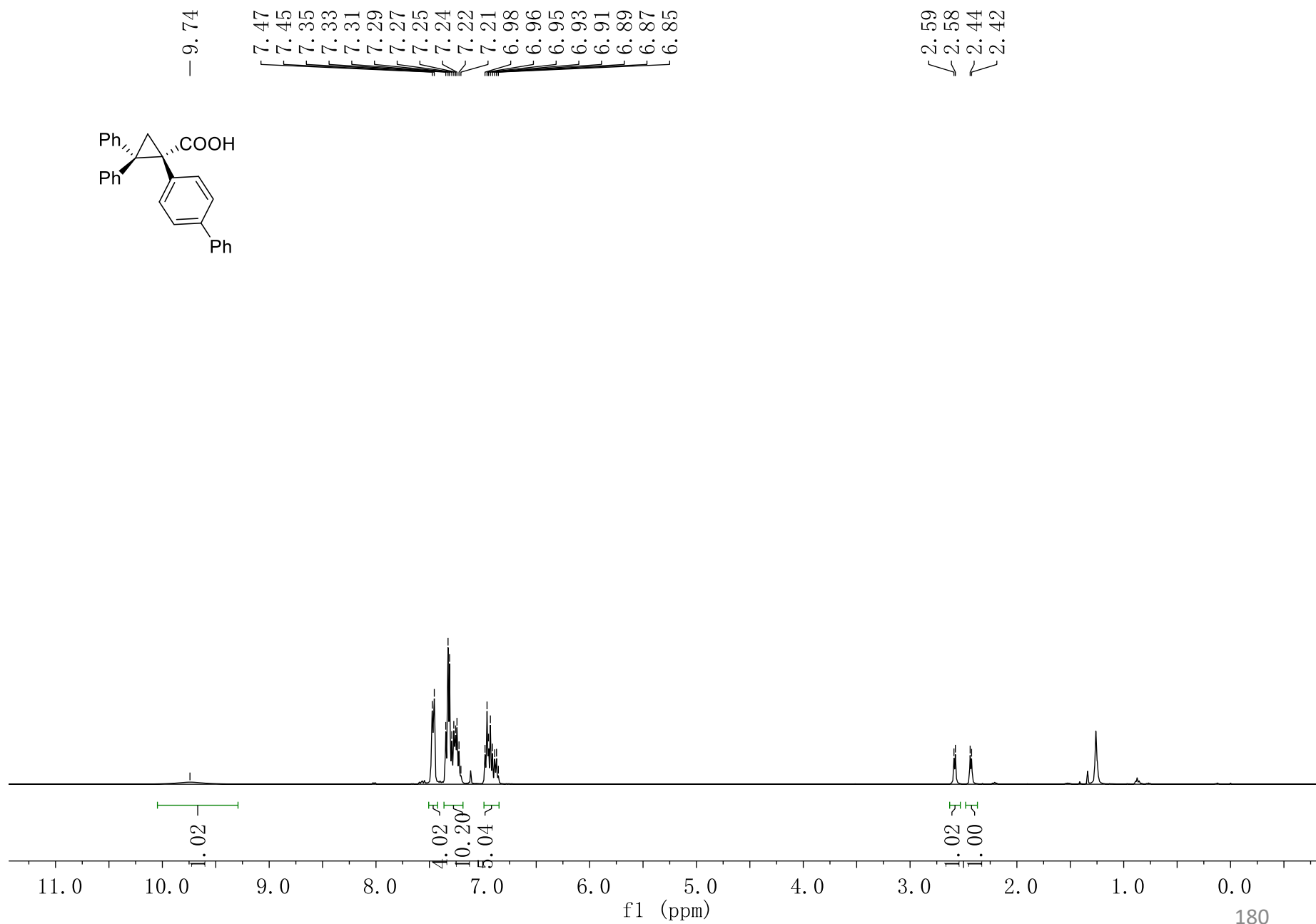


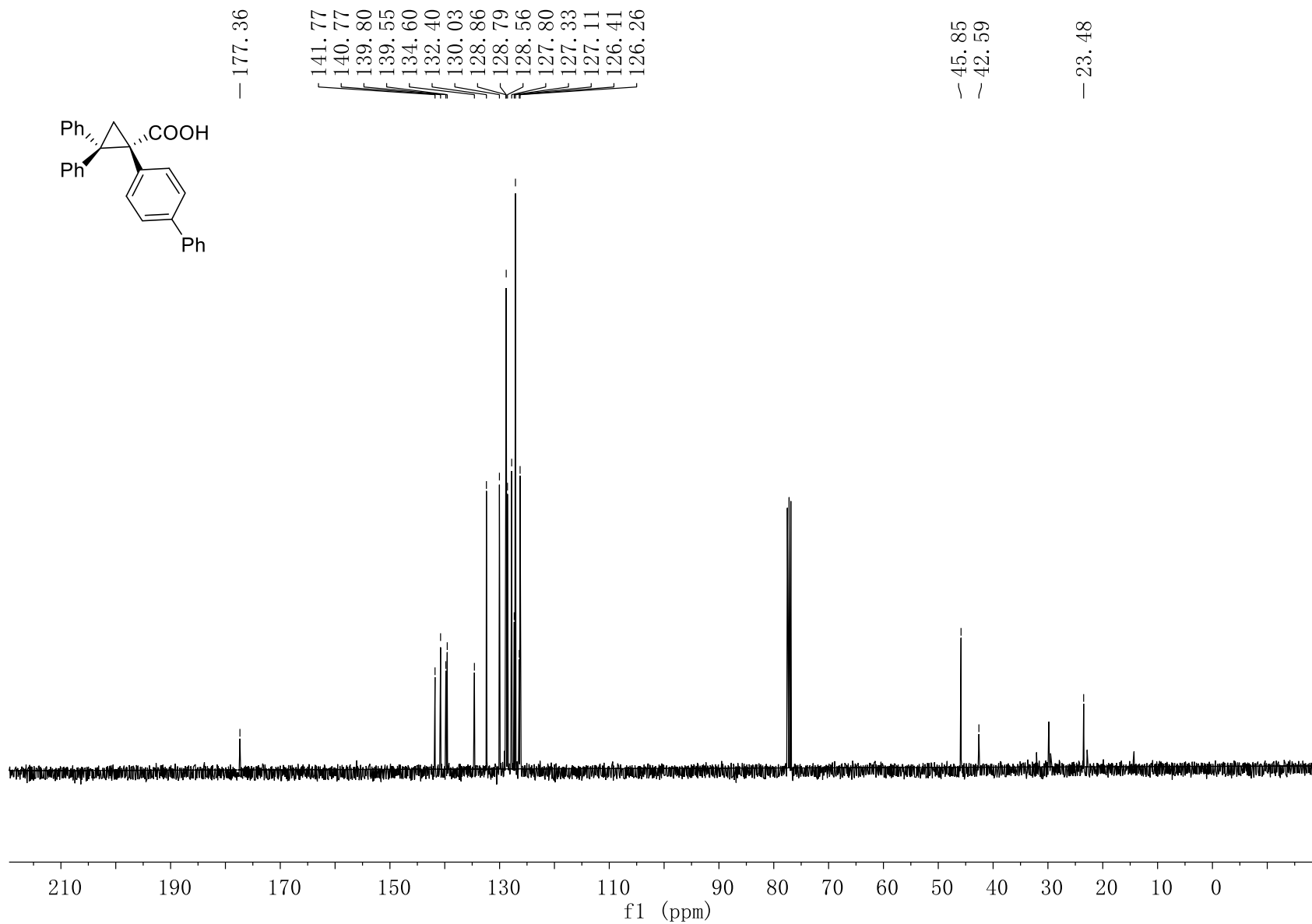
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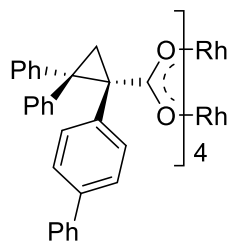
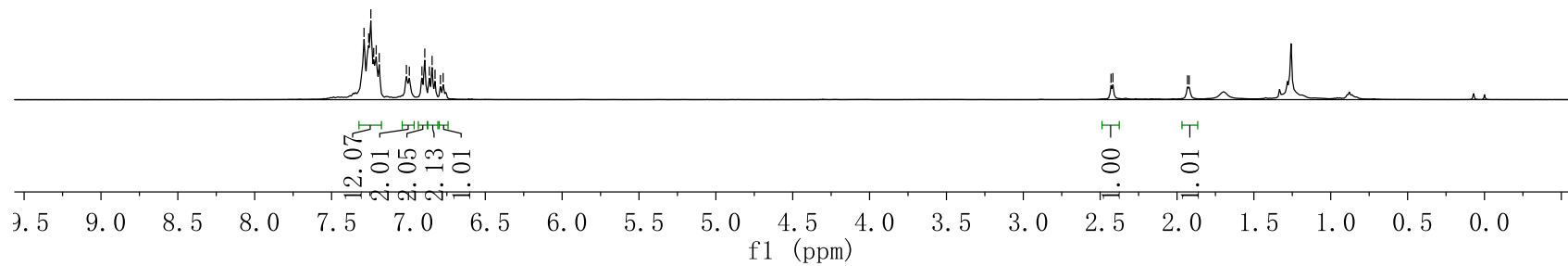
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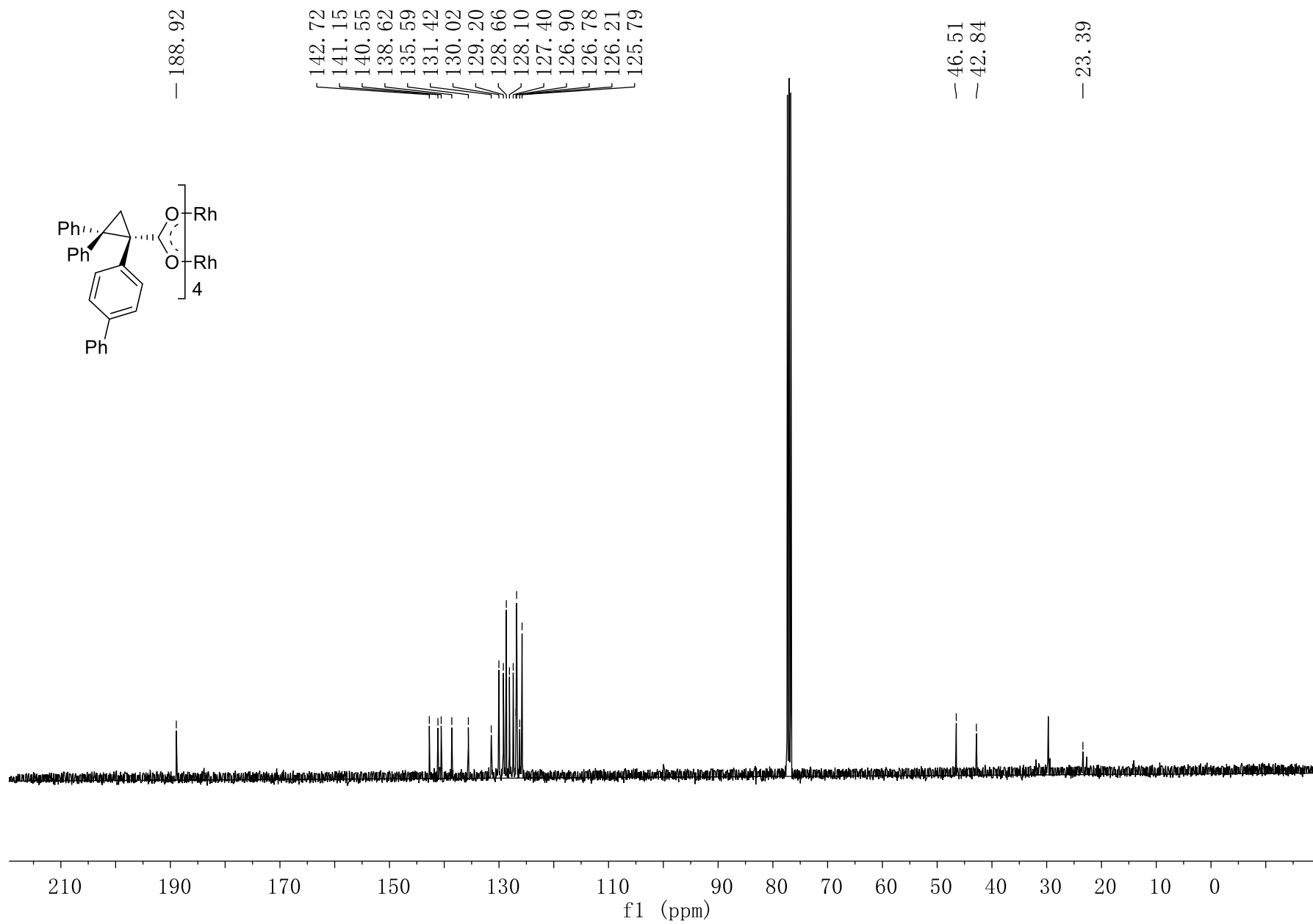
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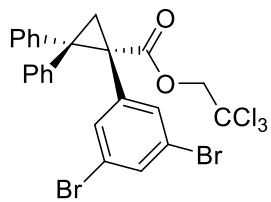








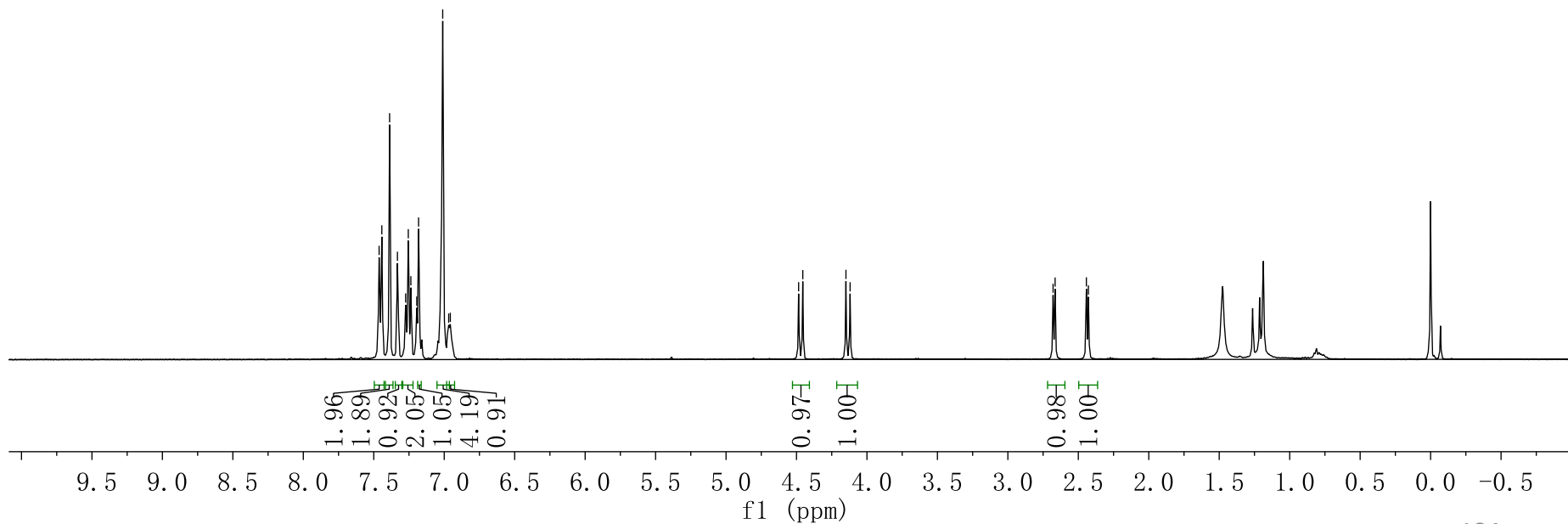


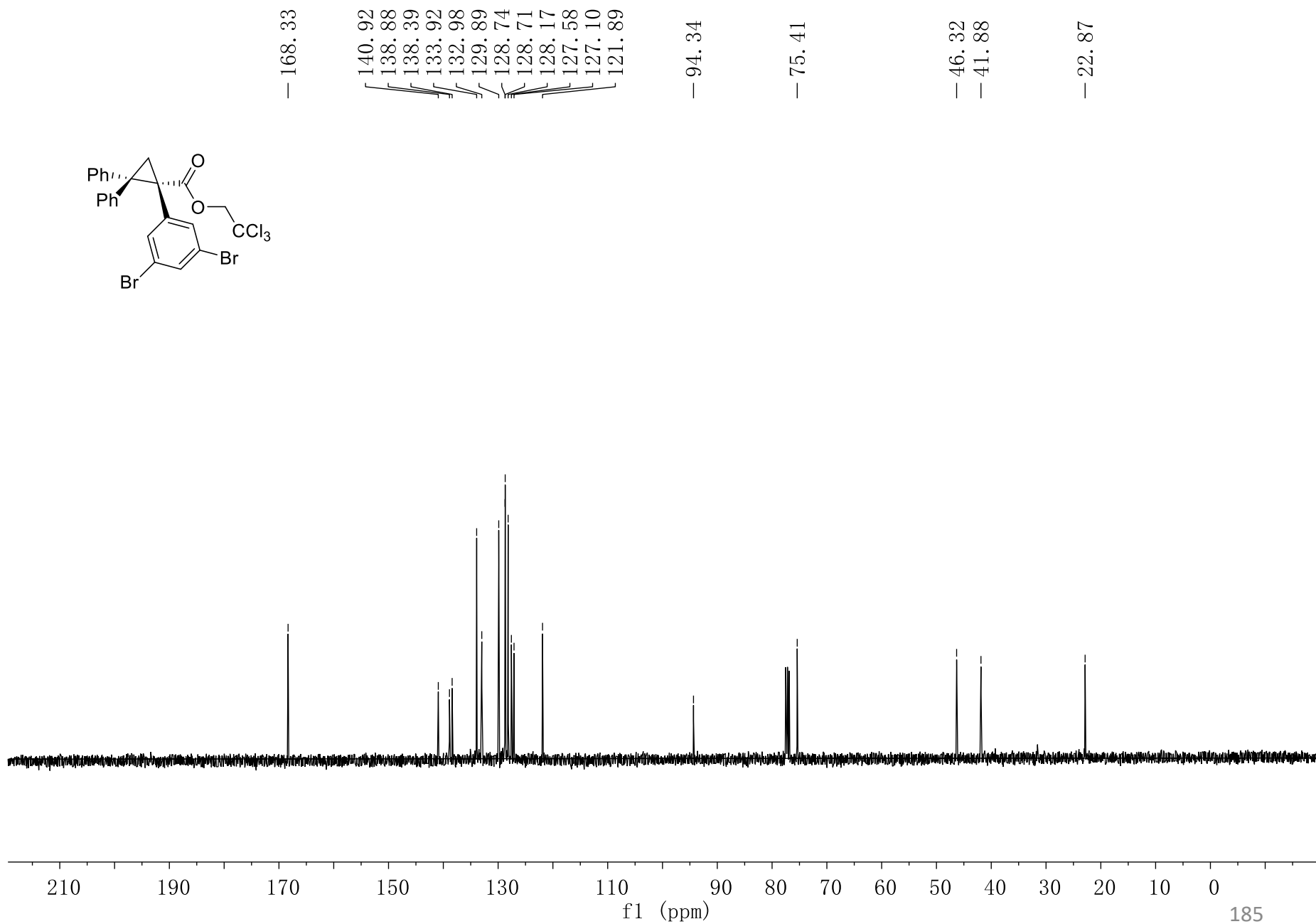
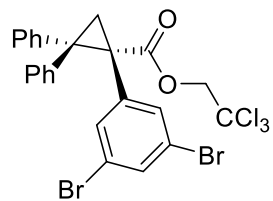


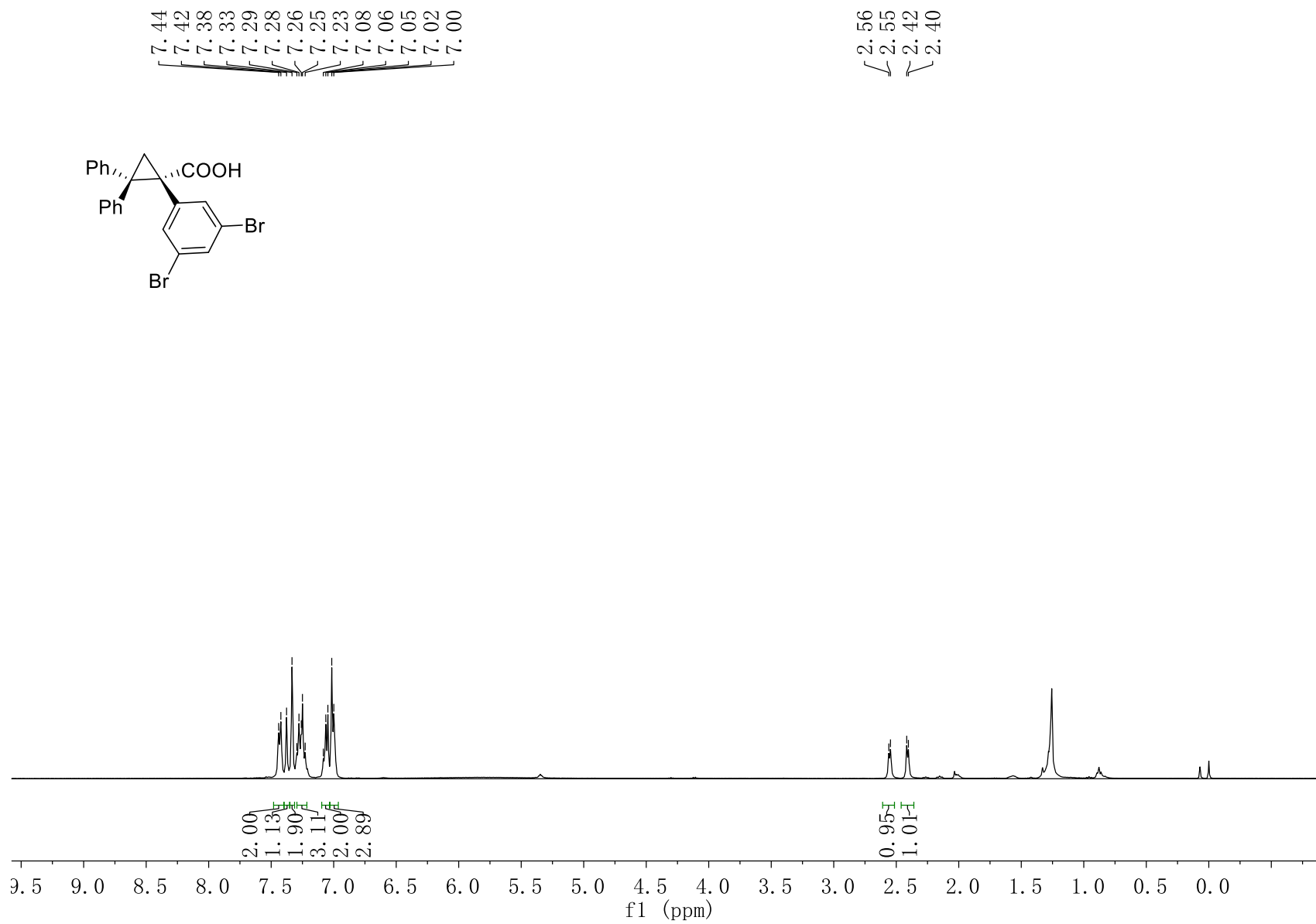
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6.96

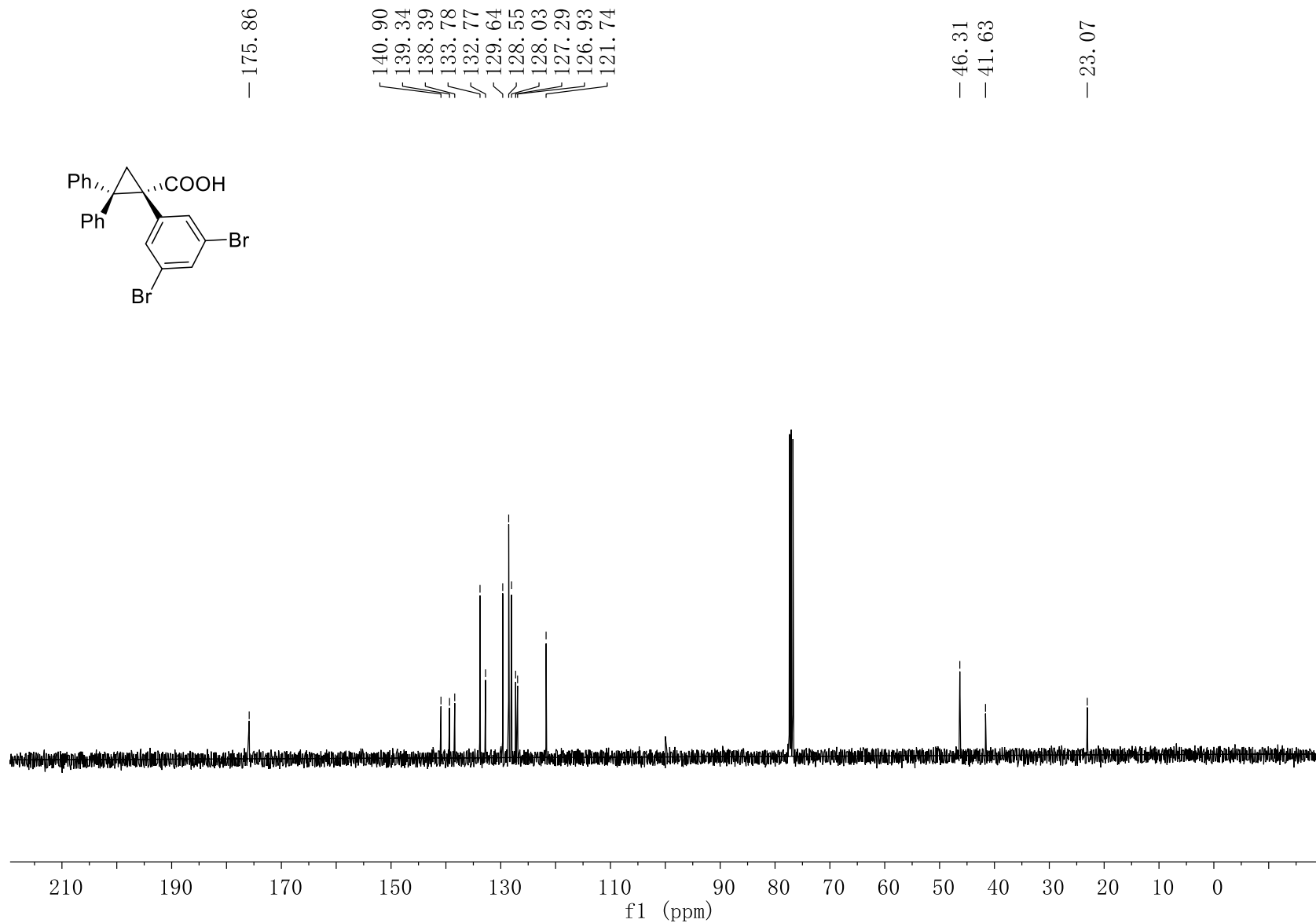
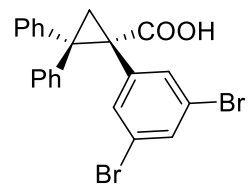
4.48  
4.46  
4.15  
4.12

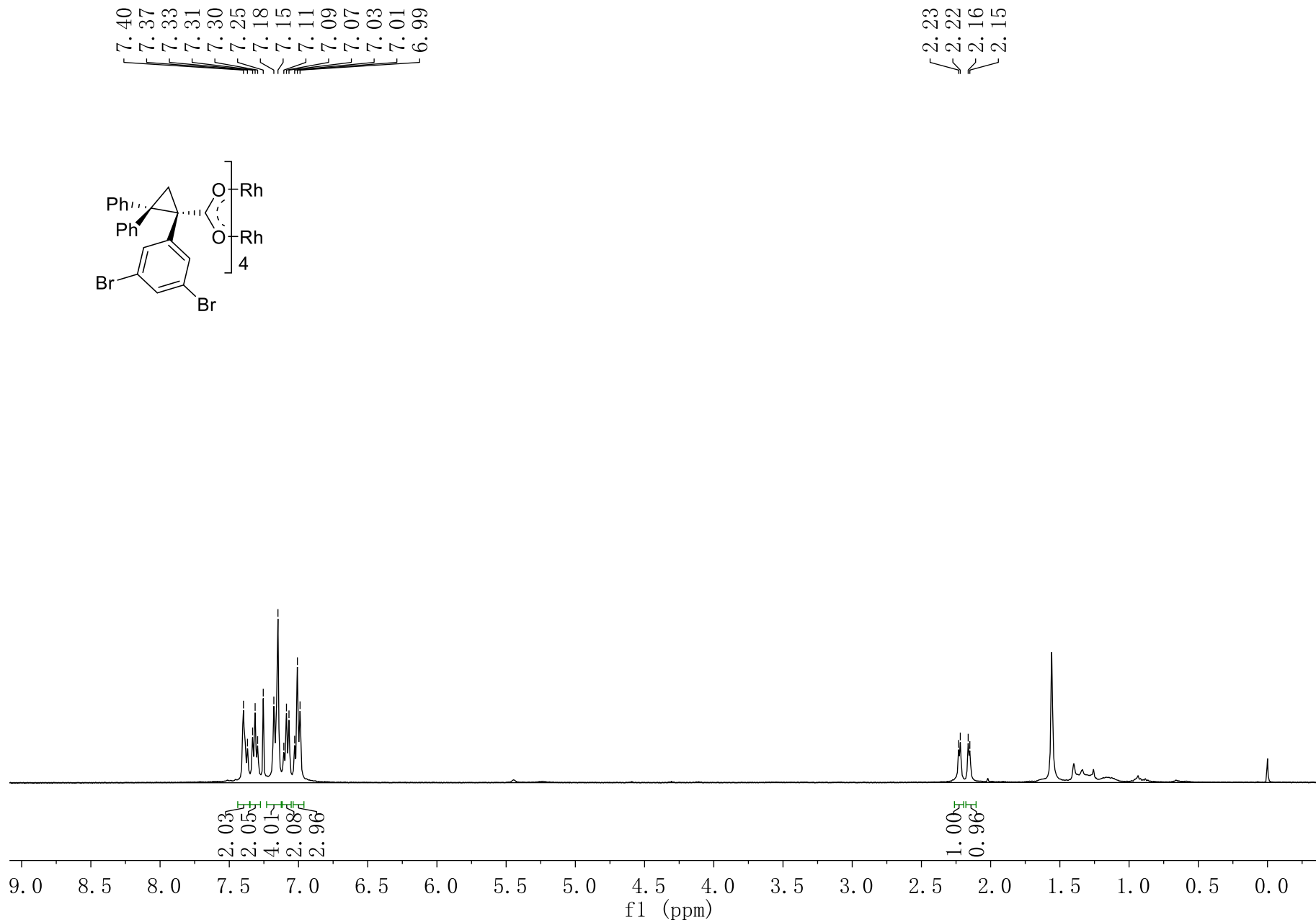
2.68  
2.66  
2.44  
2.43

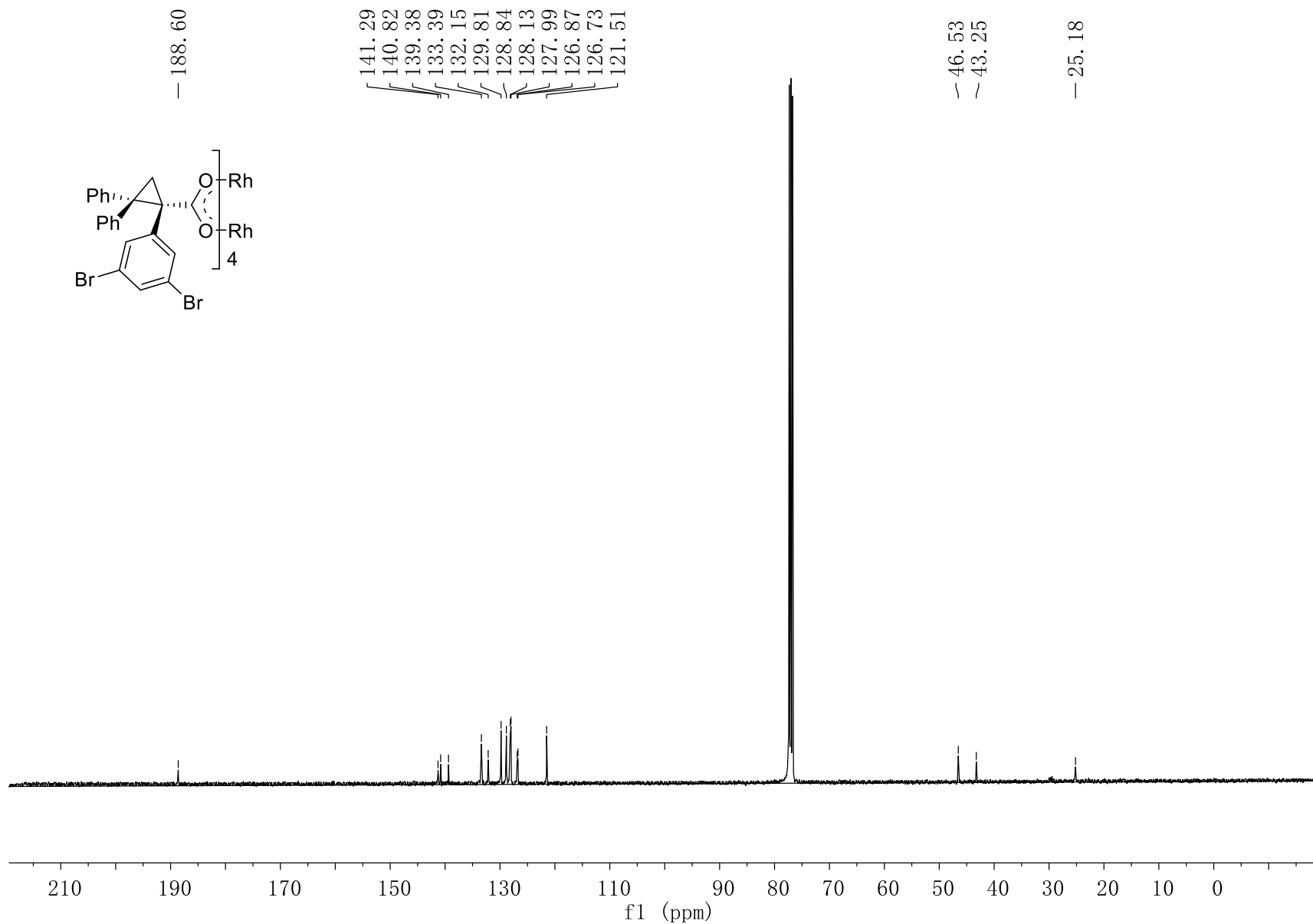


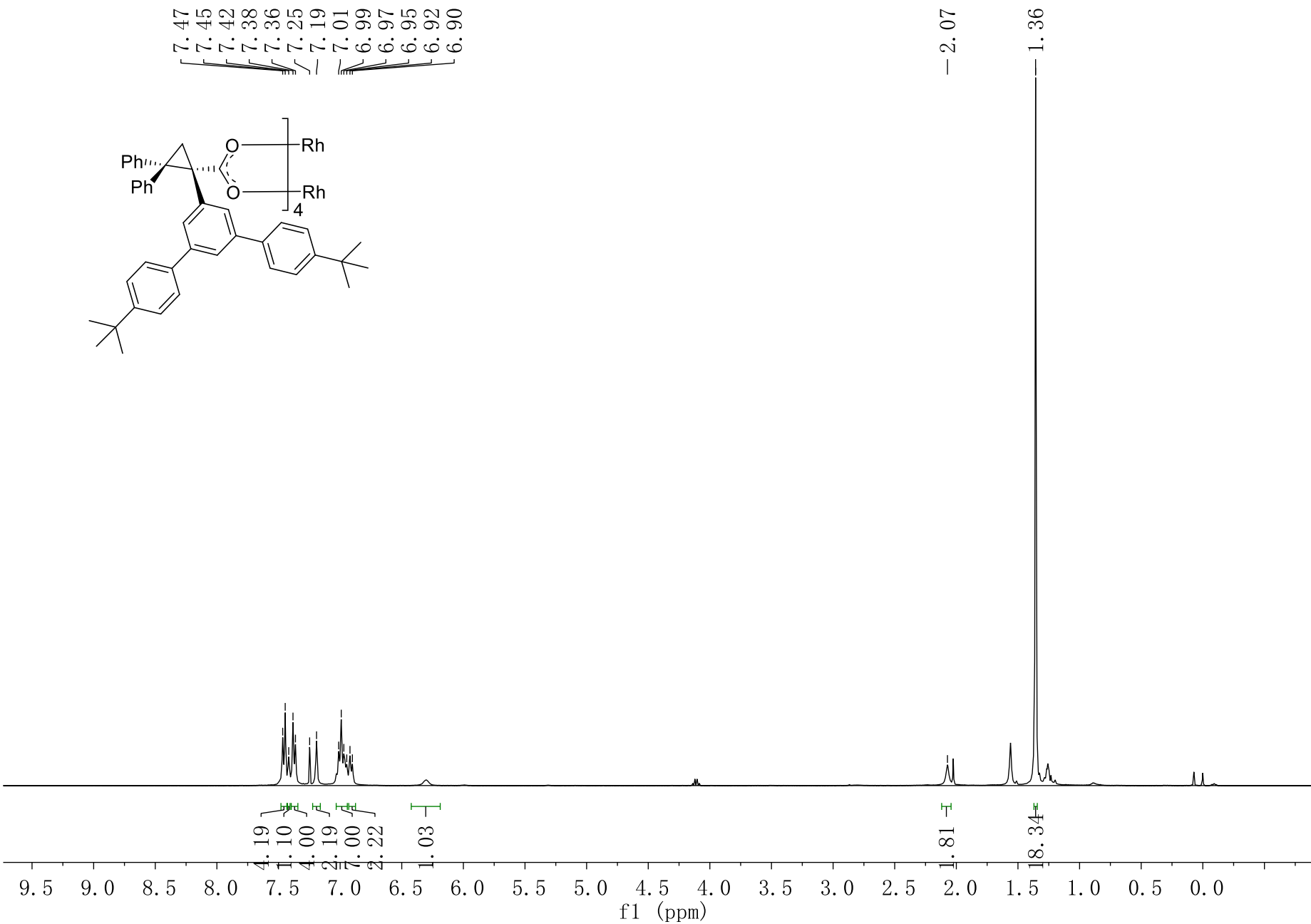


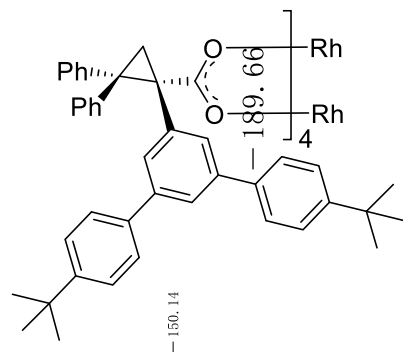






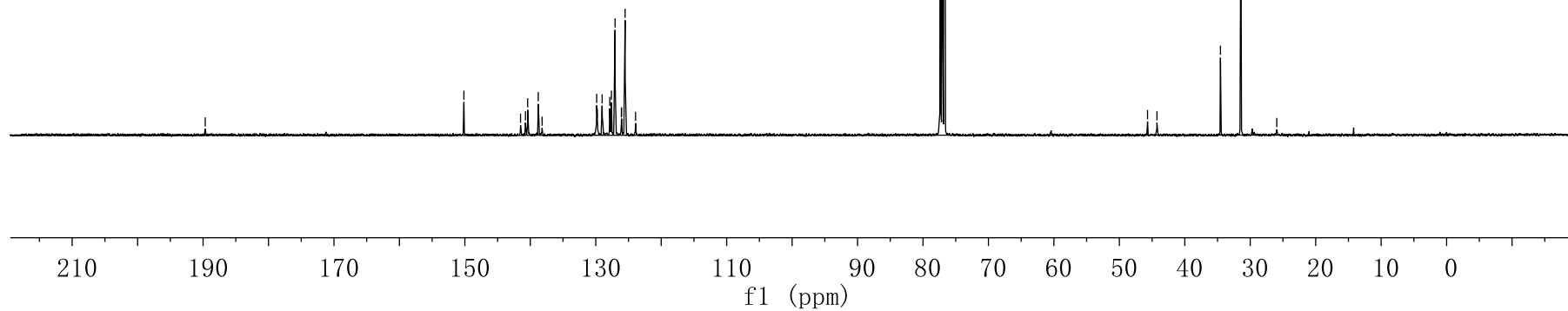
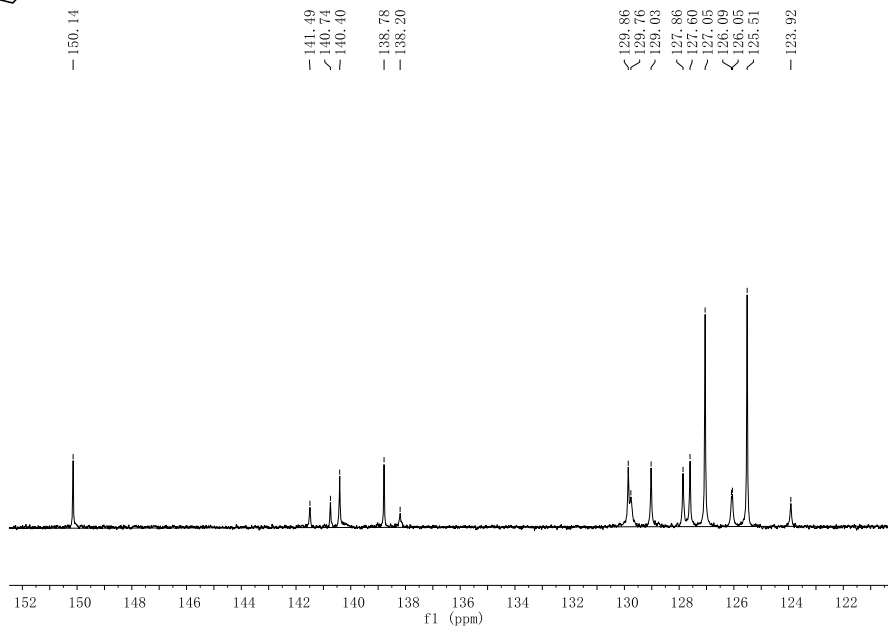


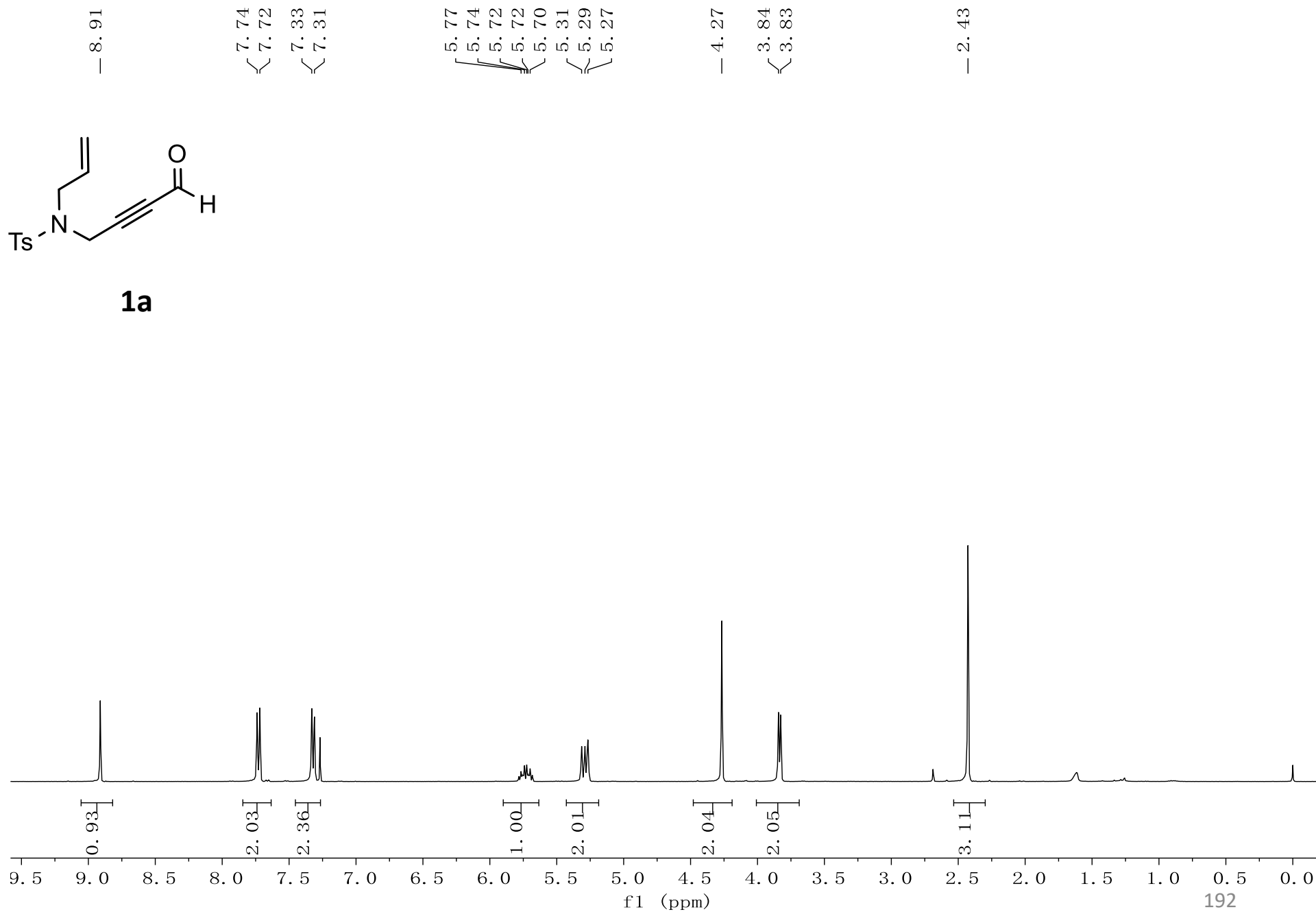
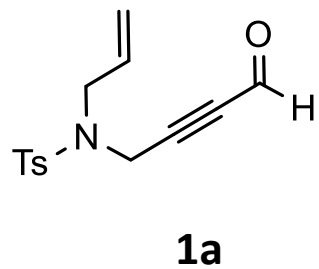


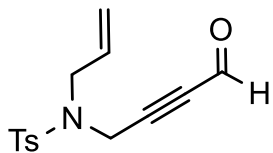


- 150.14  
 140.74  
 140.40  
 138.78  
 129.76  
 129.03  
 127.86  
 127.60  
 127.05  
 126.09  
 126.05  
 125.51  
 123.92

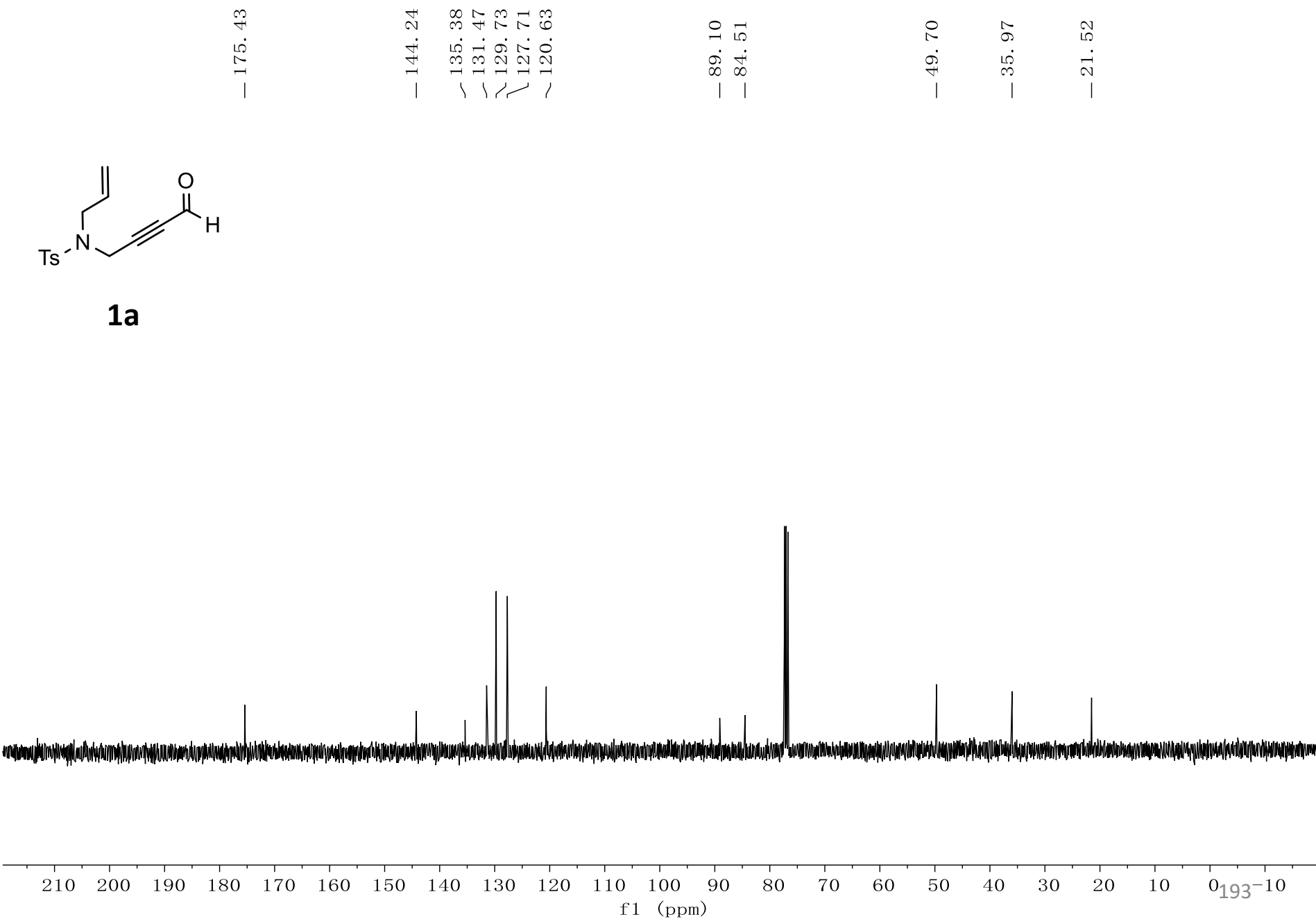
45.69  
 44.25  
 34.55  
 31.43  
 25.94

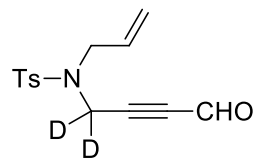




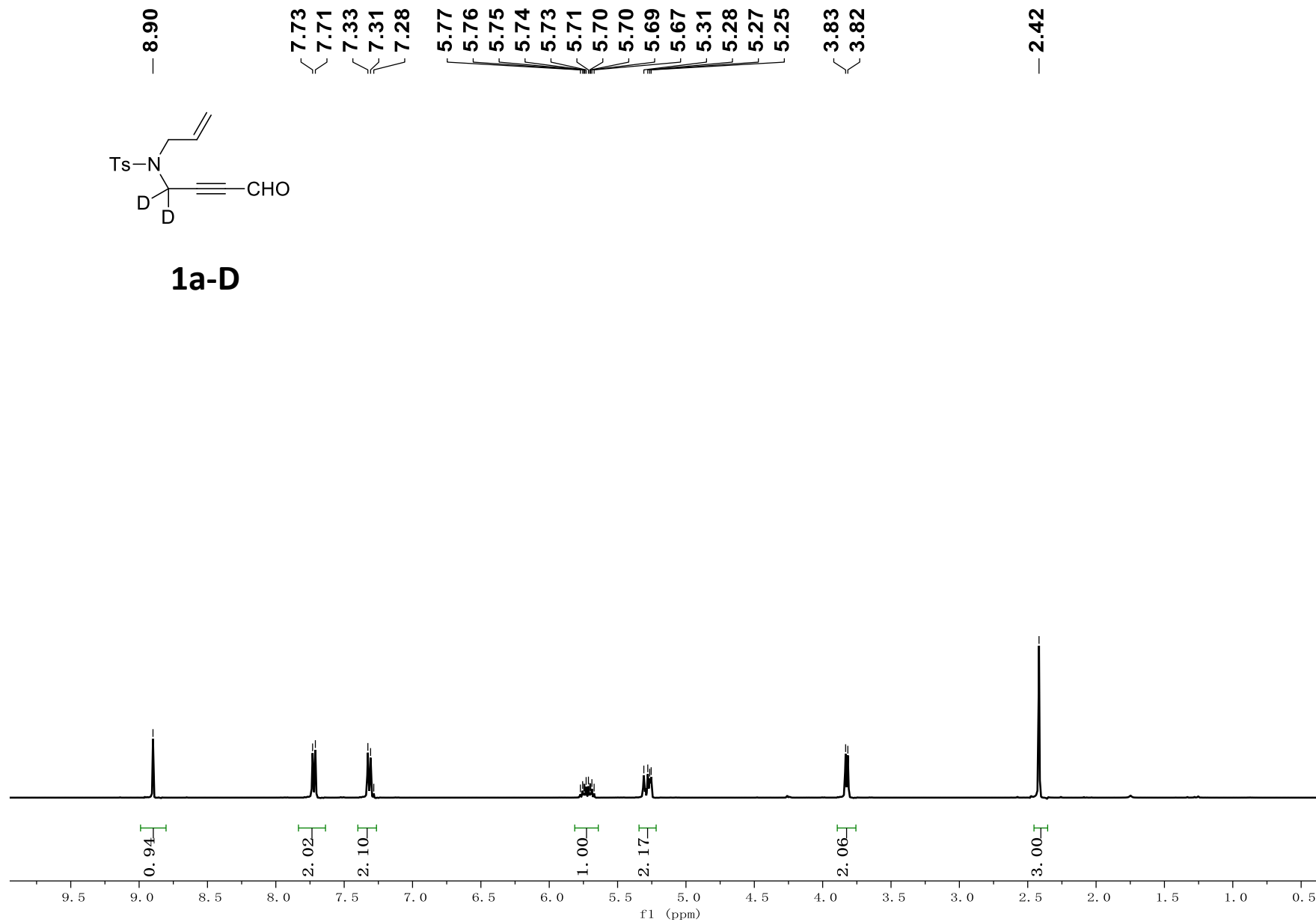


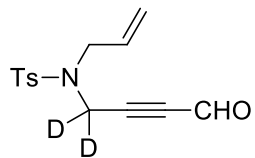
**1a**





**1a-D**





**1a-D**

— 175.55

— 144.27

— 135.32

— 131.47

— 129.76

— 127.70

— 120.63

— 89.01

— 84.52

— 49.65

— 35.82

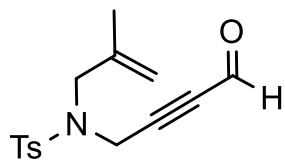
— 35.60

— 35.38

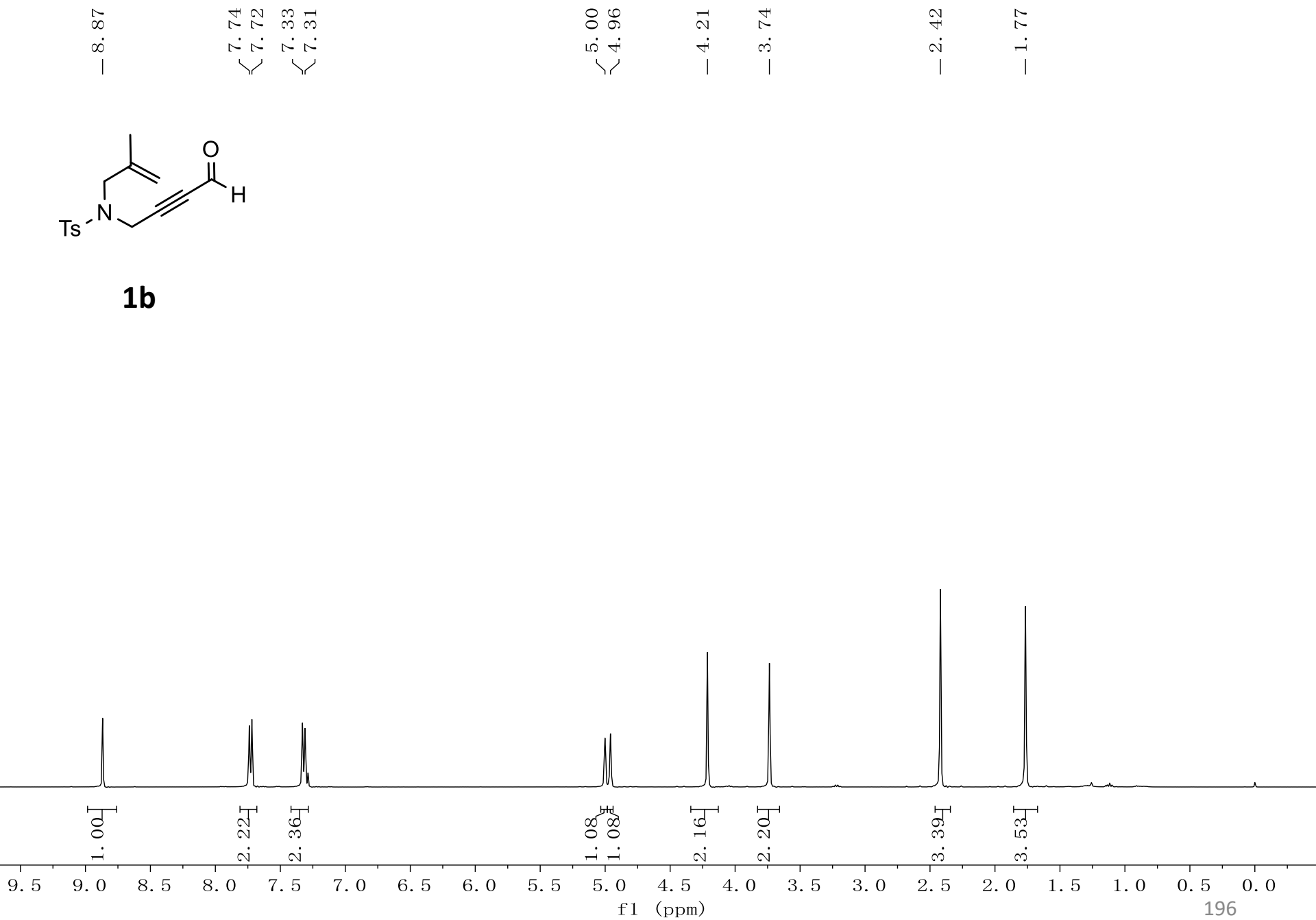
— 21.52

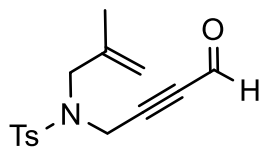
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

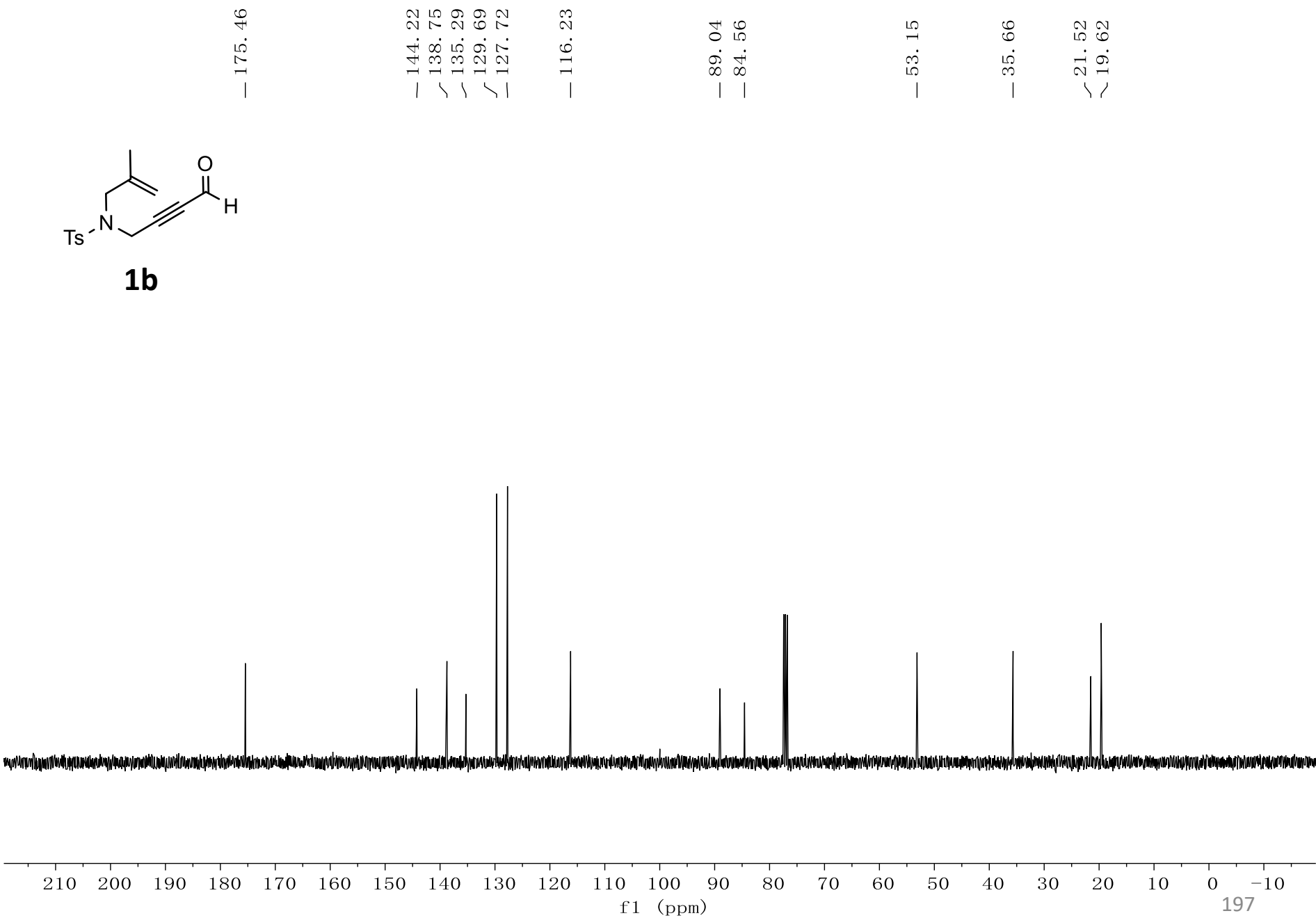


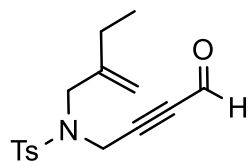
**1b**



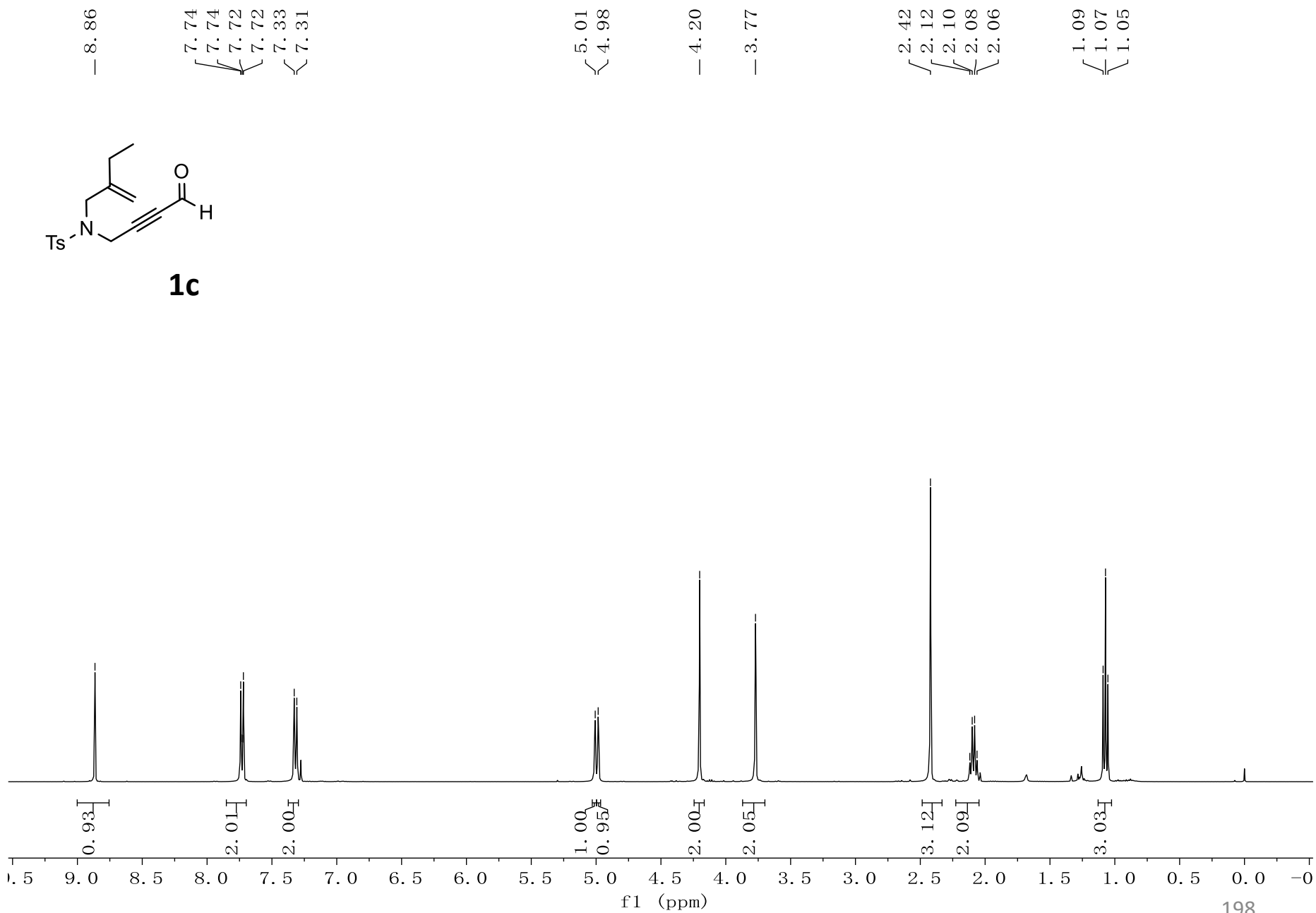


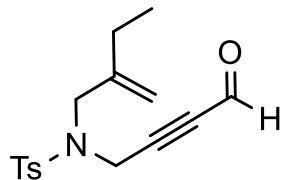
**1b**



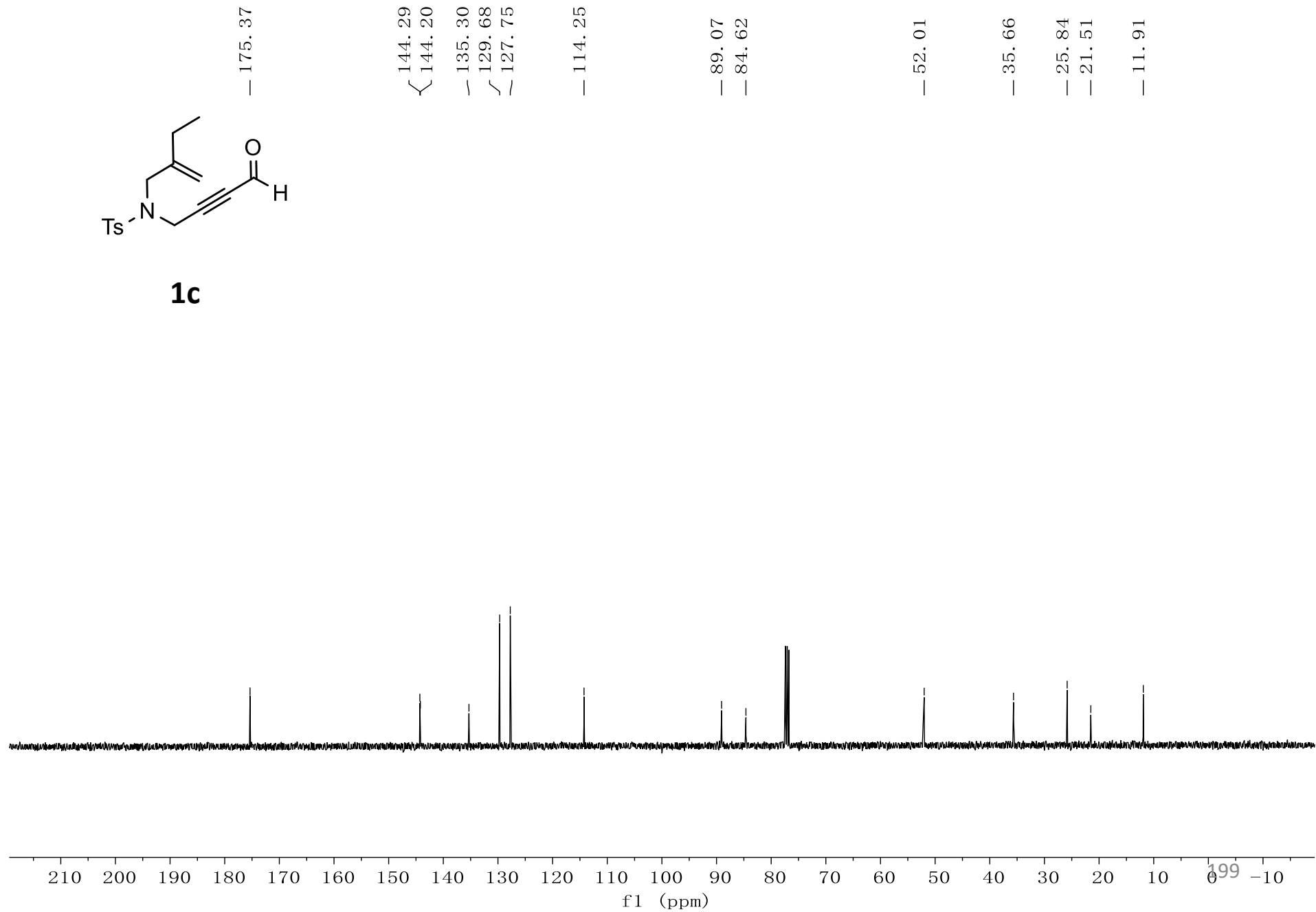


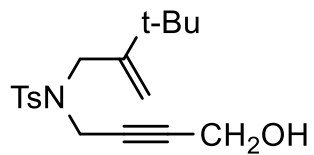
**1c**





**1c**





**1d**

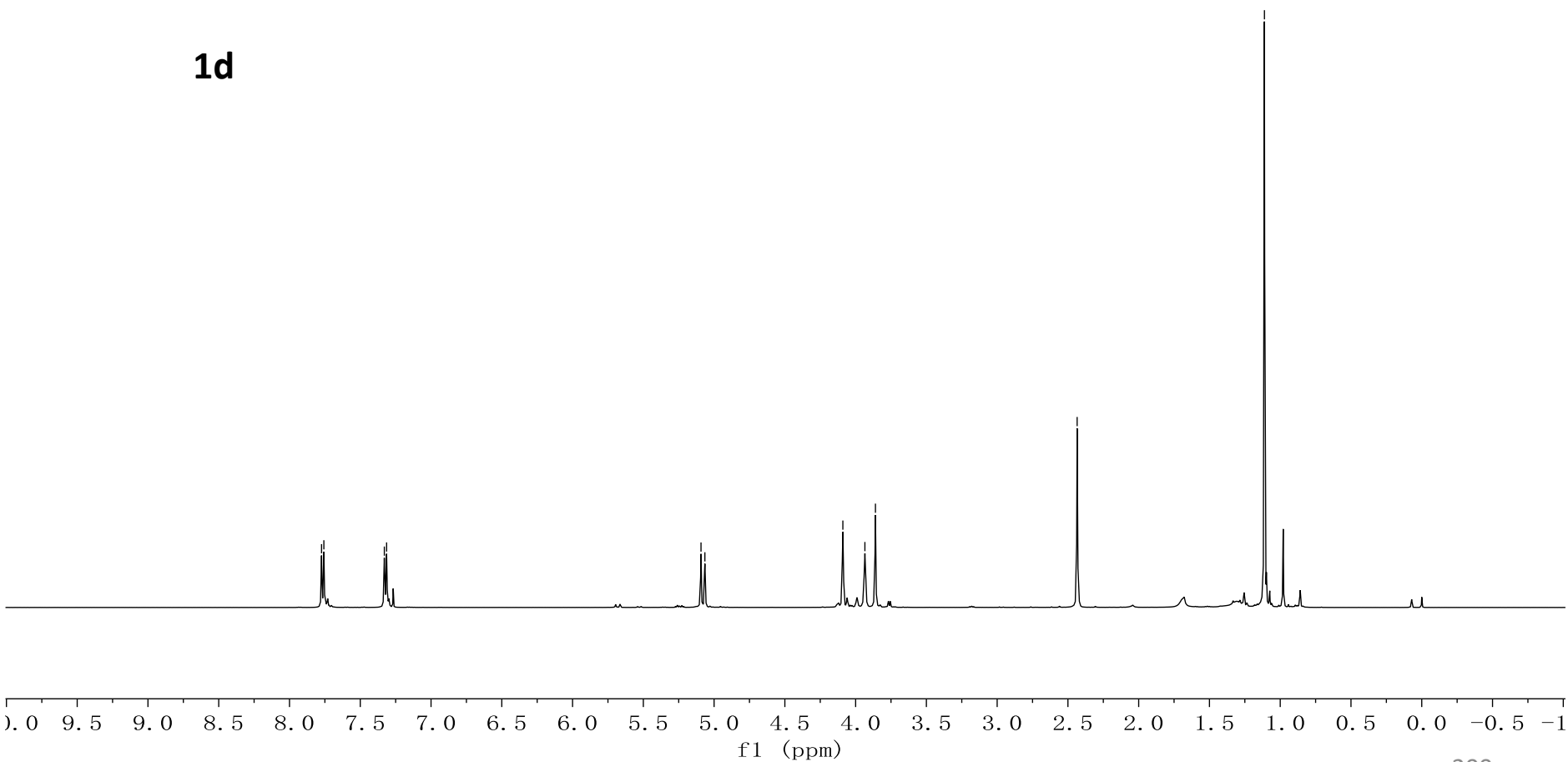
7.77  
7.76  
7.33  
7.31

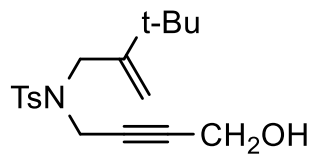
5.09  
5.07

4.09  
3.93  
3.86

2.43

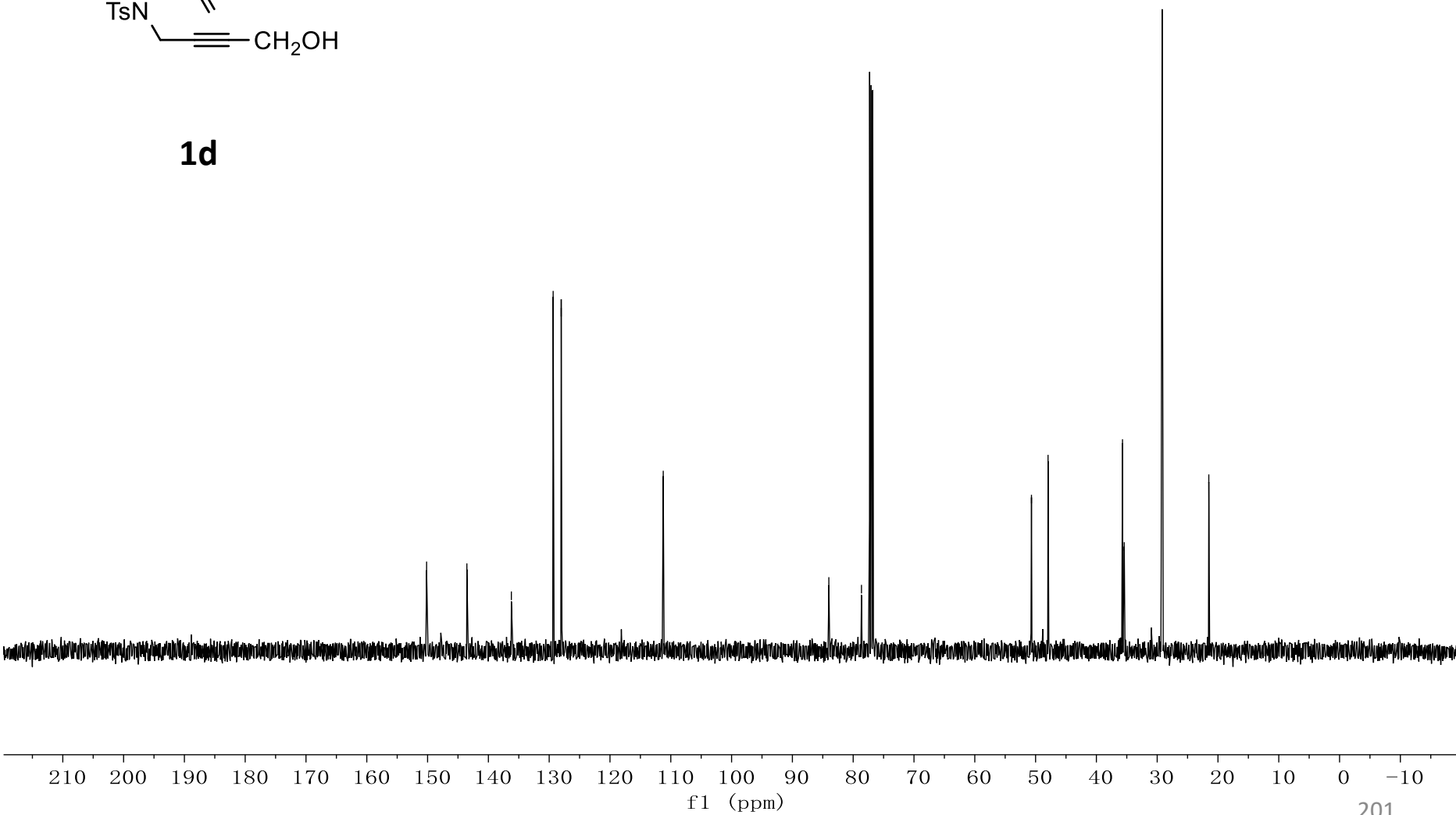
1.11

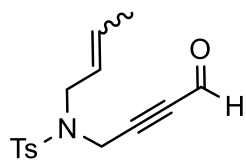




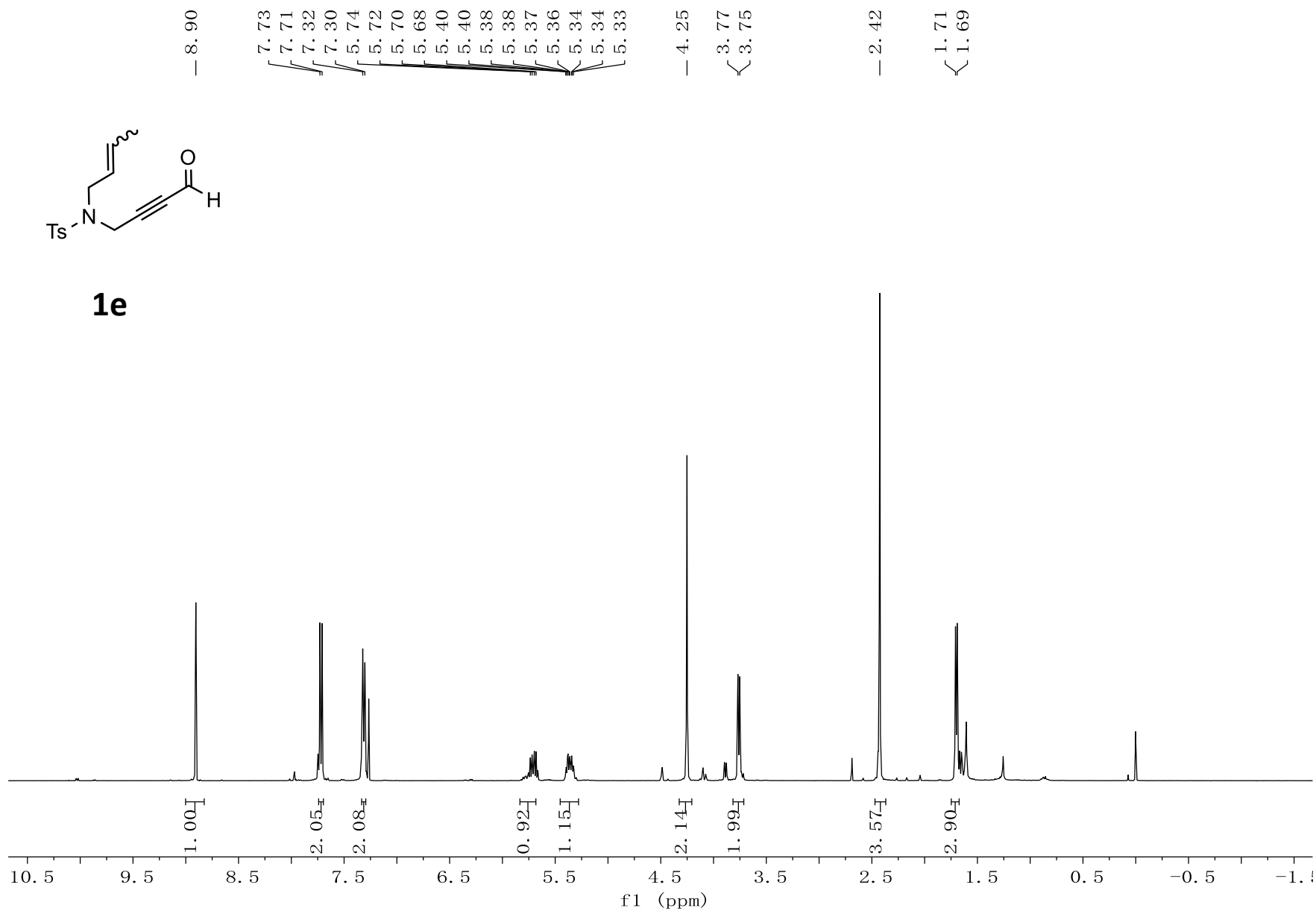
**1d**

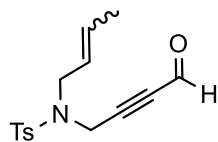
$\sim 150.16$   
 $\sim 143.54$   
 $\sim 136.22$   
 $\sim 129.35$   
 $\sim 128.02$   
  
 $-111.24$   
  
 $-84.00$   
 $-78.64$   
  
 $\sim 50.68$   
 $\sim 47.95$   
  
 $\sim 35.70$   
 $\sim 35.42$   
 $\sim 29.19$   
 $\sim 21.51$



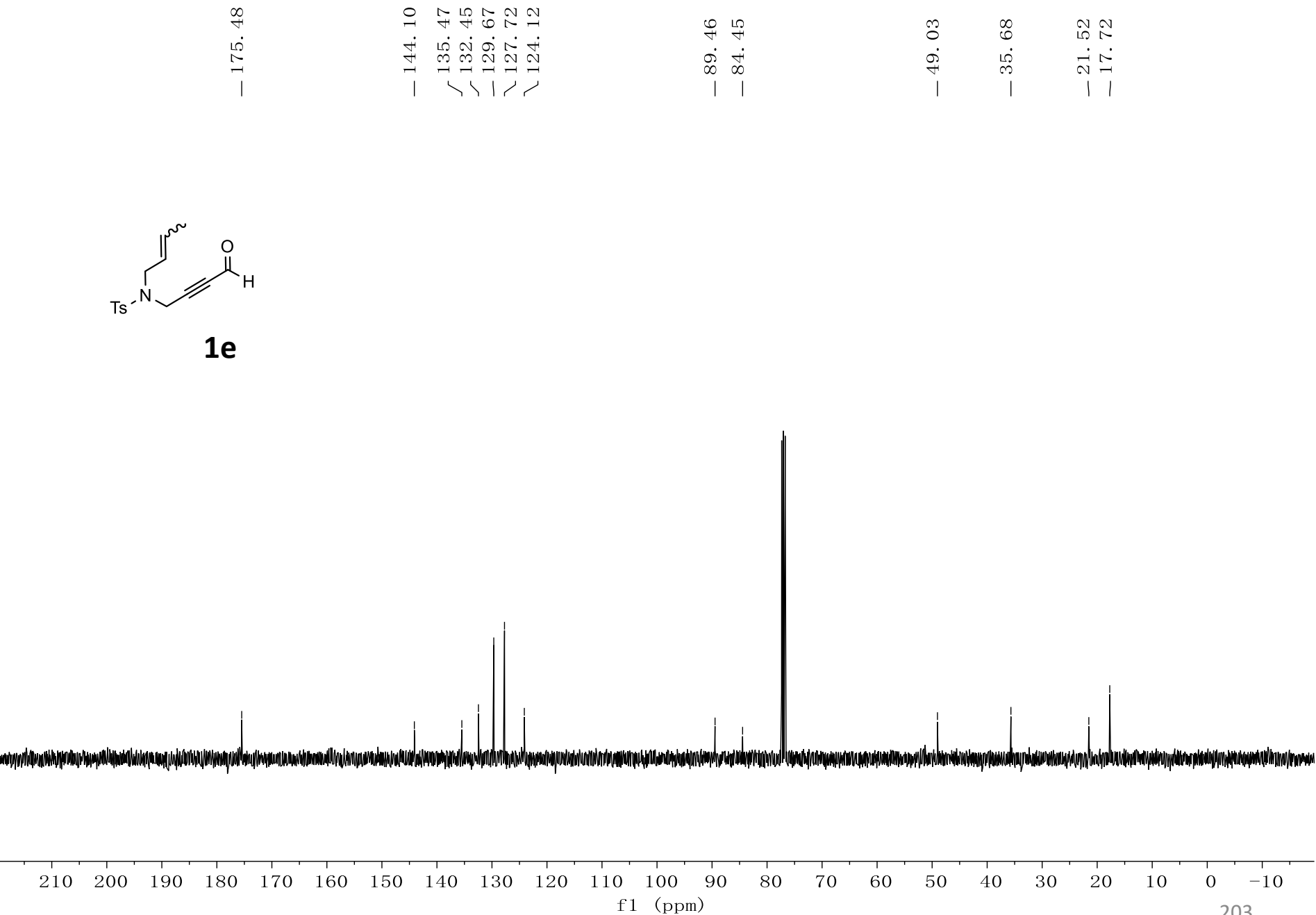


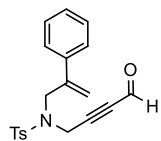
**1e**



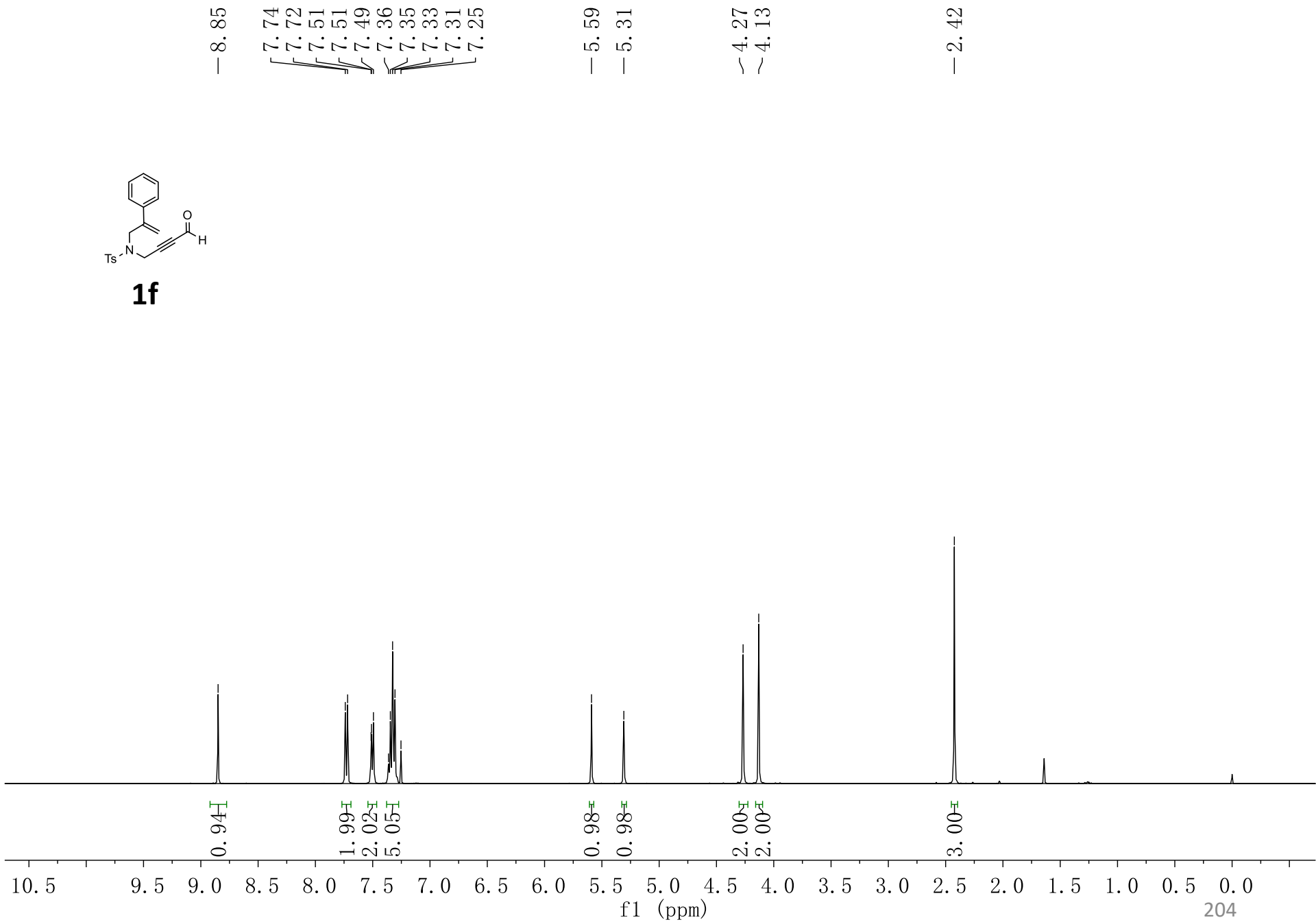


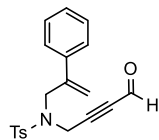
**1e**





**1f**





**1f**

— 175.36

144.39

141.09

137.20

134.93

129.76

128.59

128.43

127.93

126.39

— 117.78

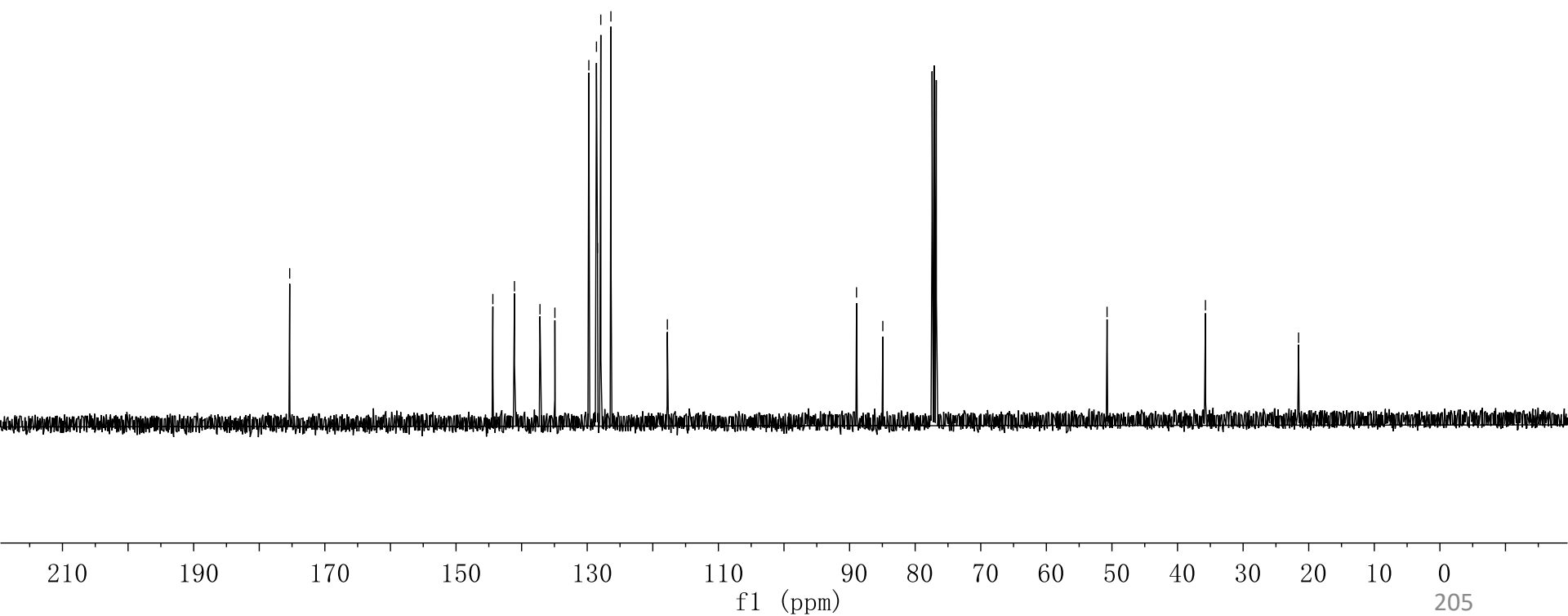
— 88.94

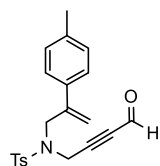
— 84.93

— 50.74

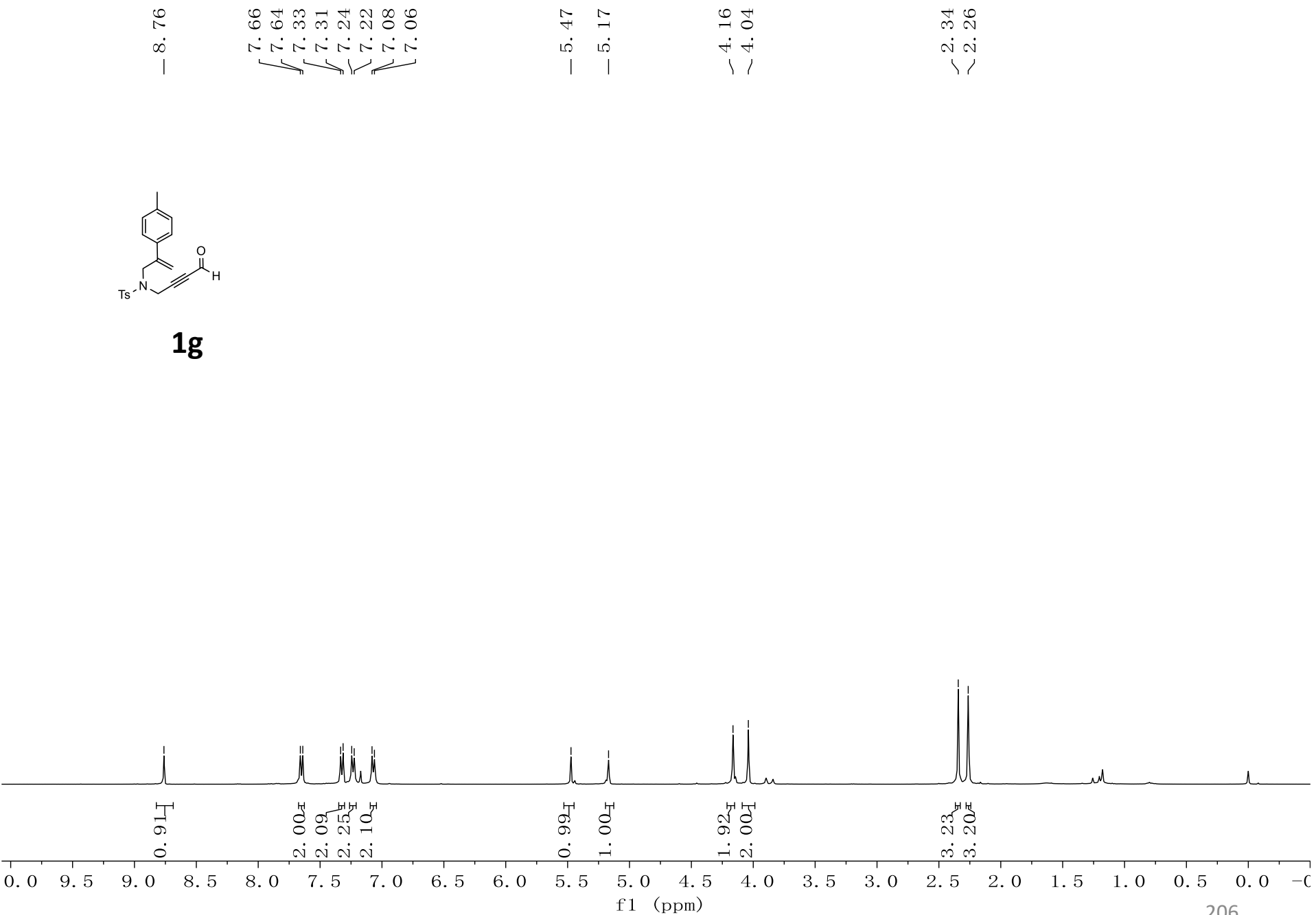
— 35.74

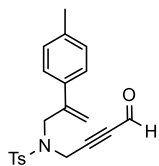
— 21.54





**1g**





**1g**

— 175.38

144.34

140.82

138.32

134.90

134.22

129.72

129.27

127.92

126.26

— 116.96

— 89.01

— 84.91

— 50.77

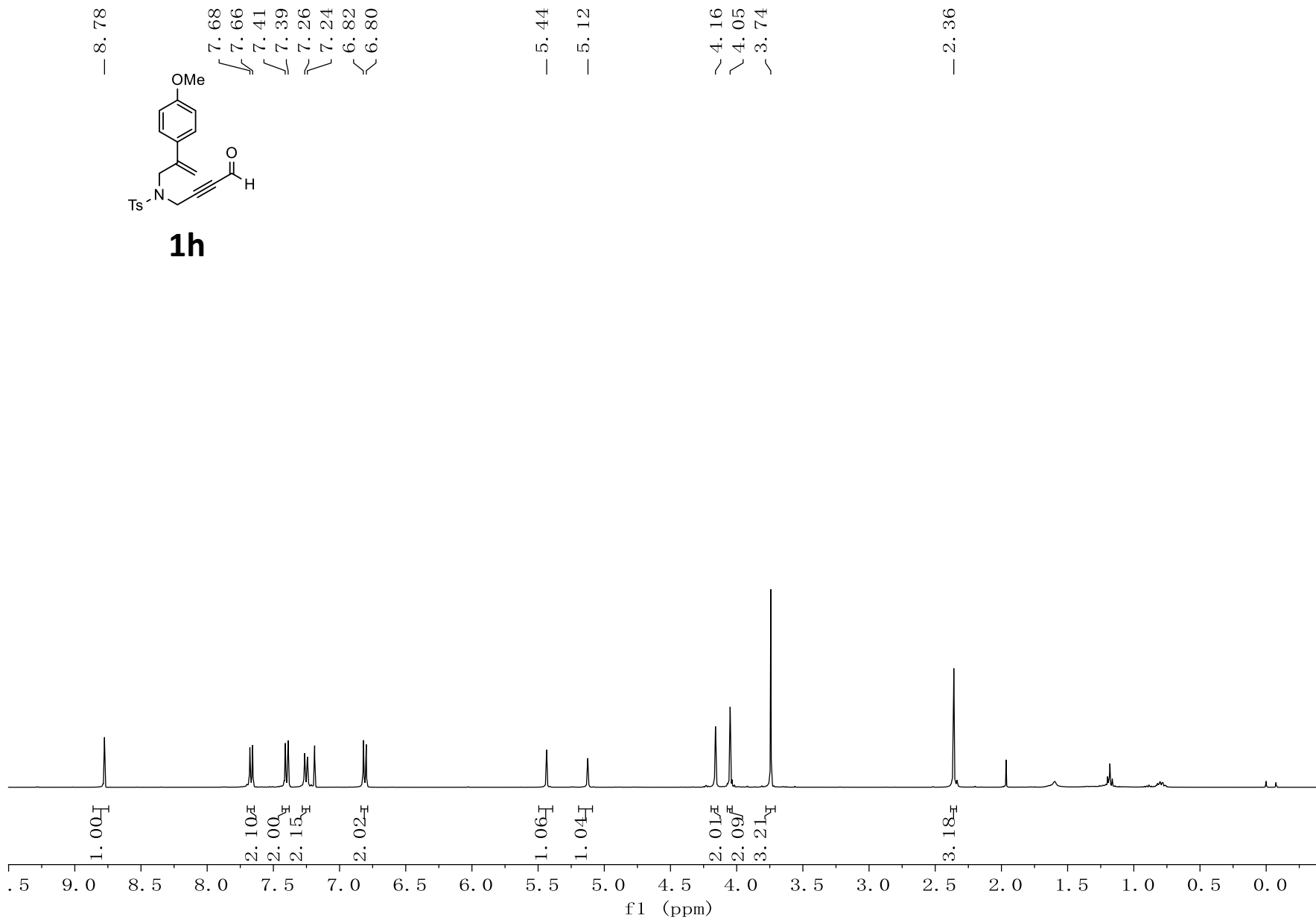
— 35.68

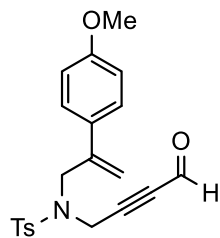
21.55

21.17

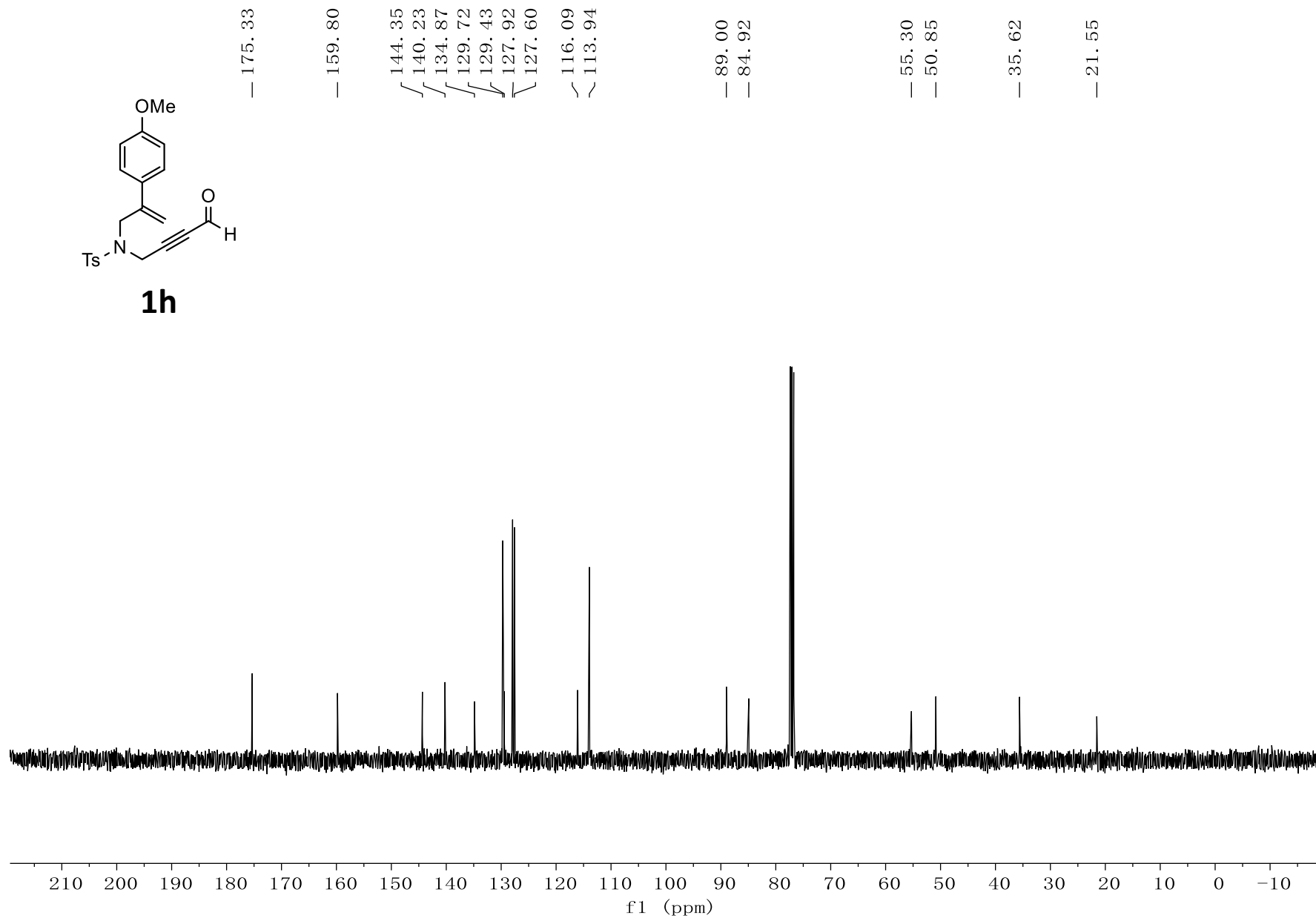
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

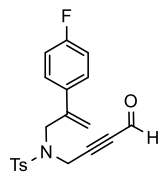
f1 (ppm)



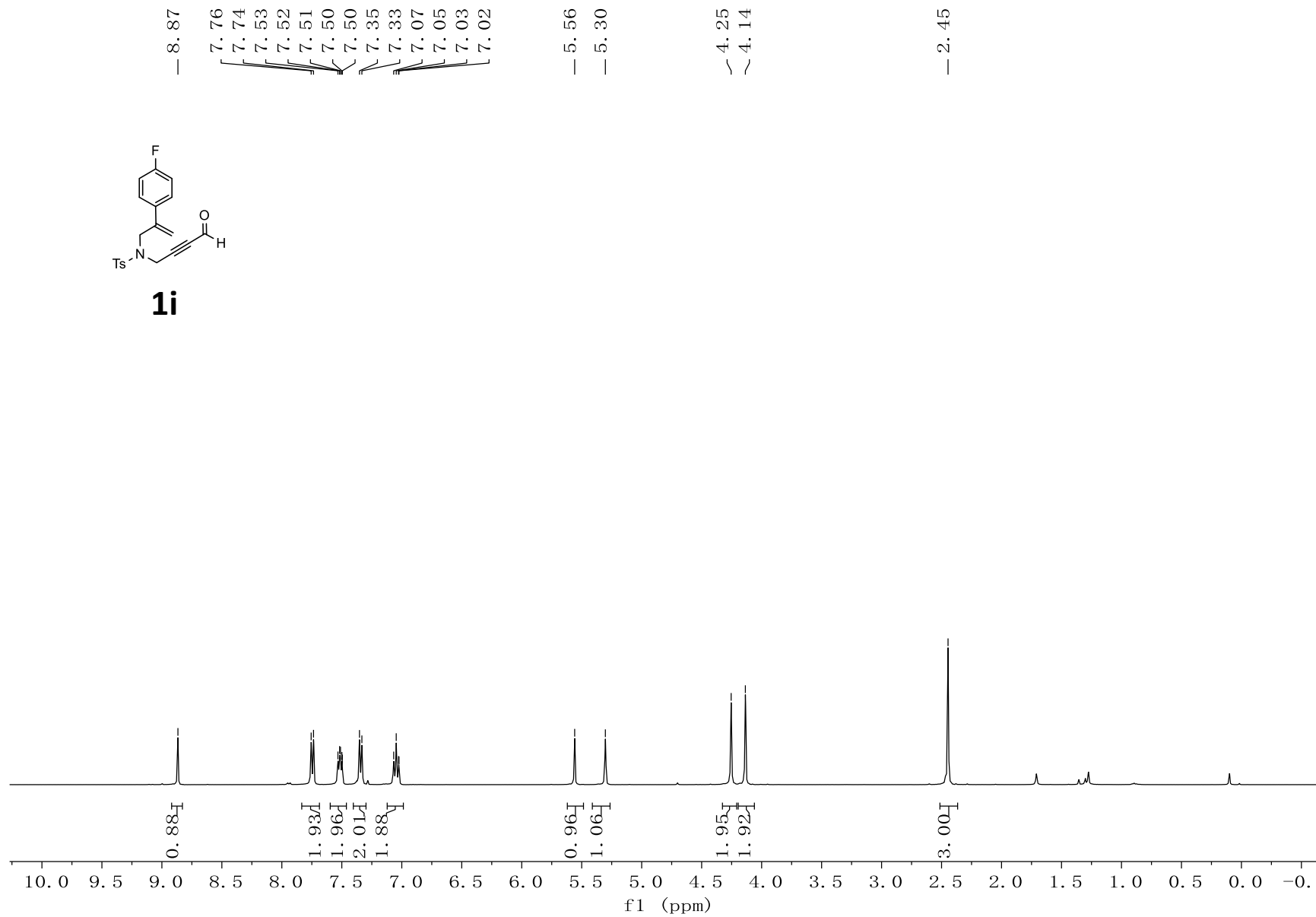


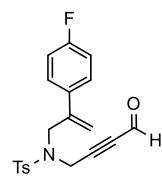
**1h**



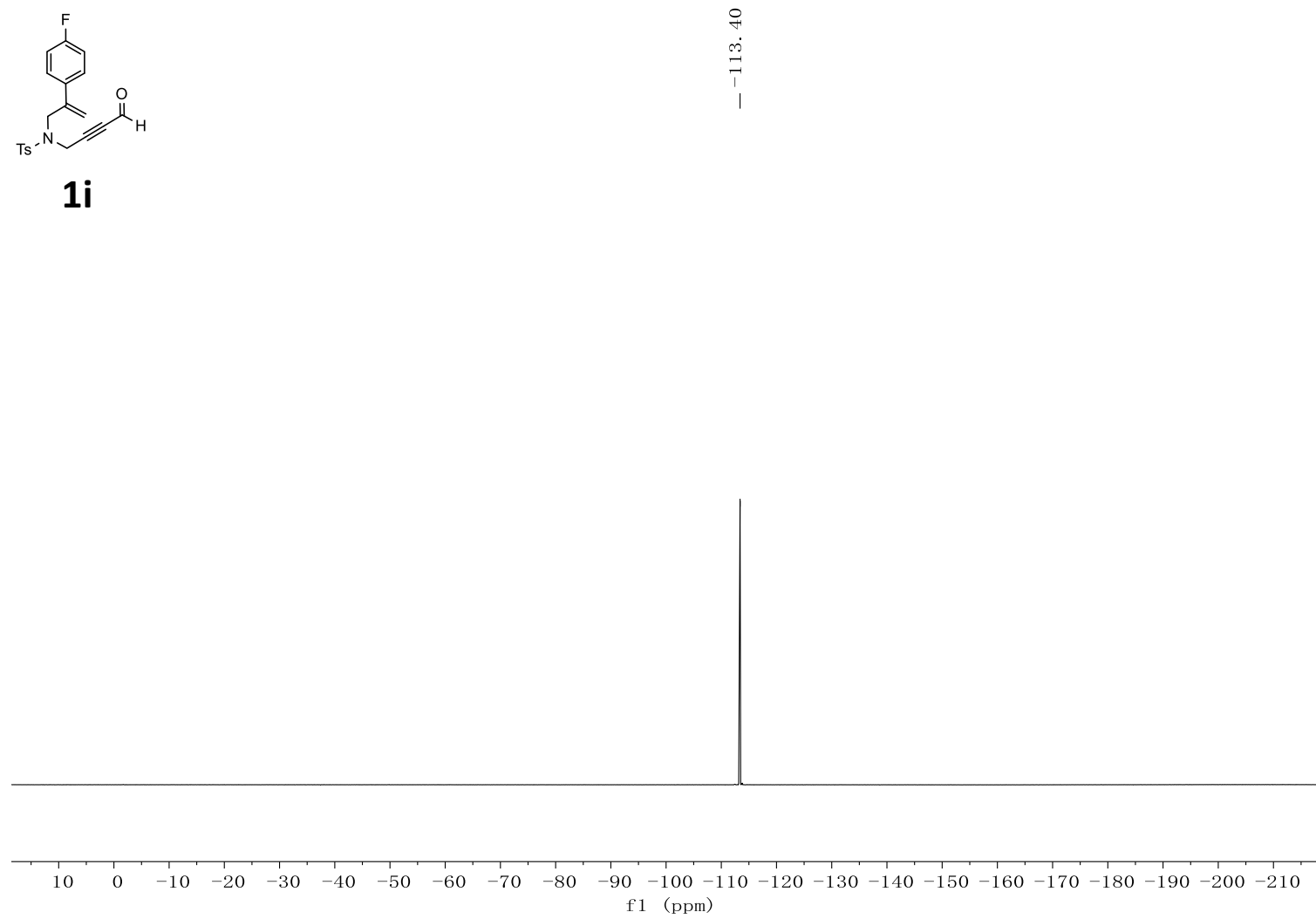


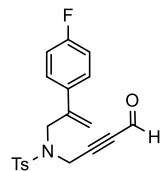
**1i**



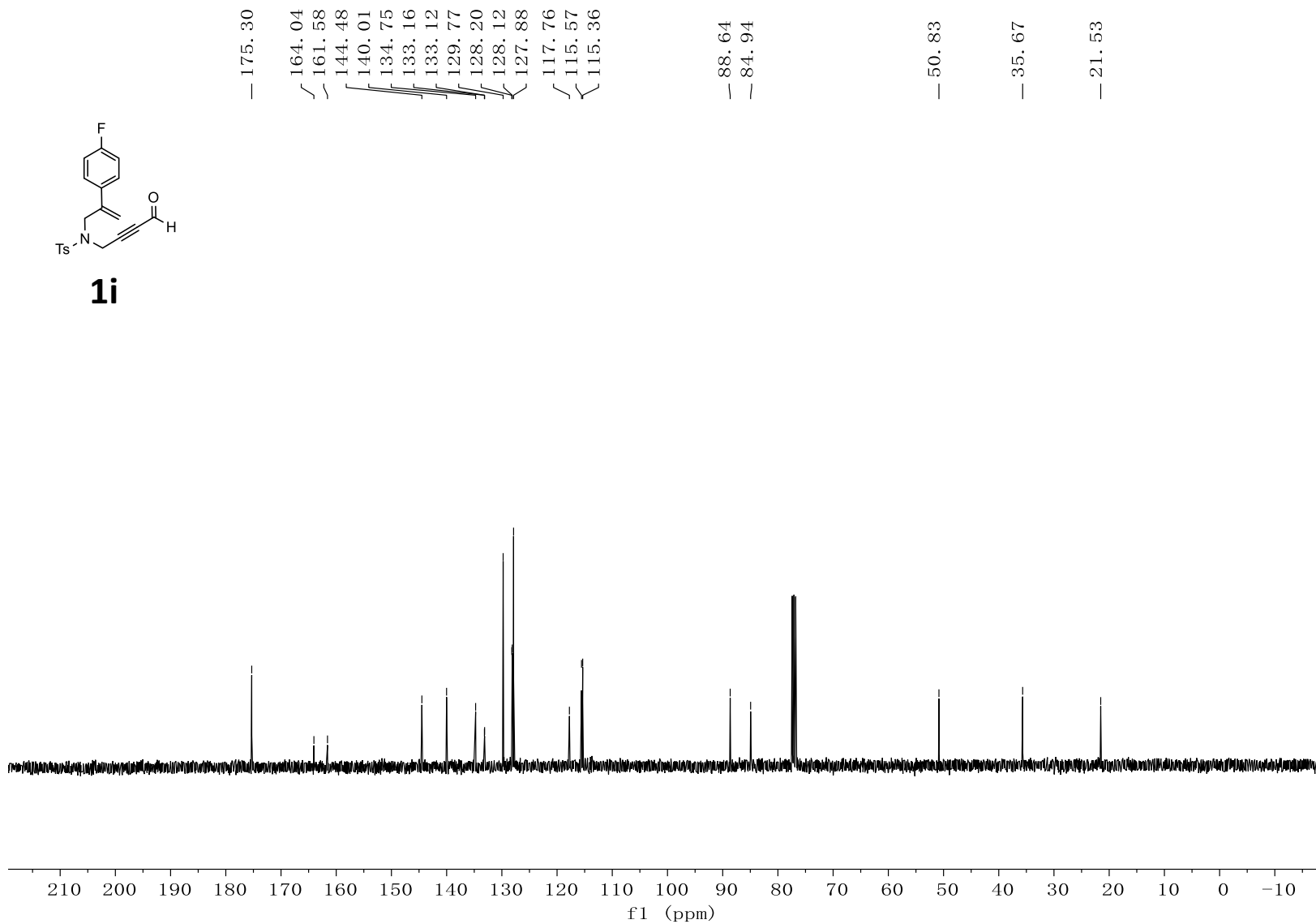


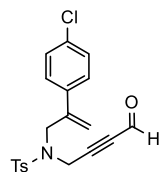
**1i**



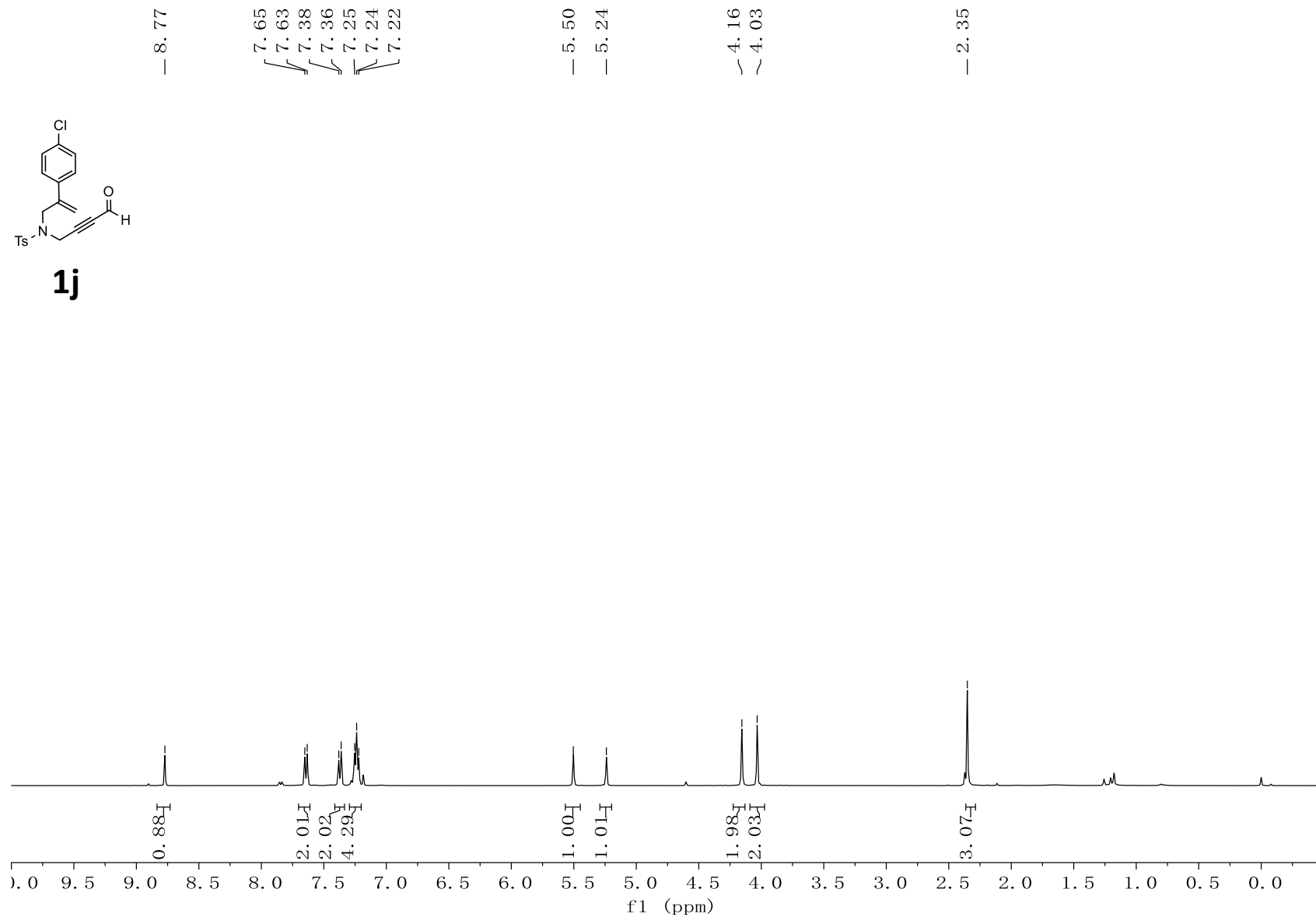


**1i**

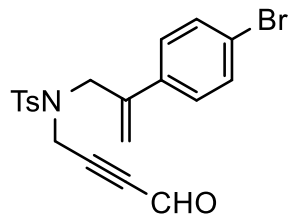




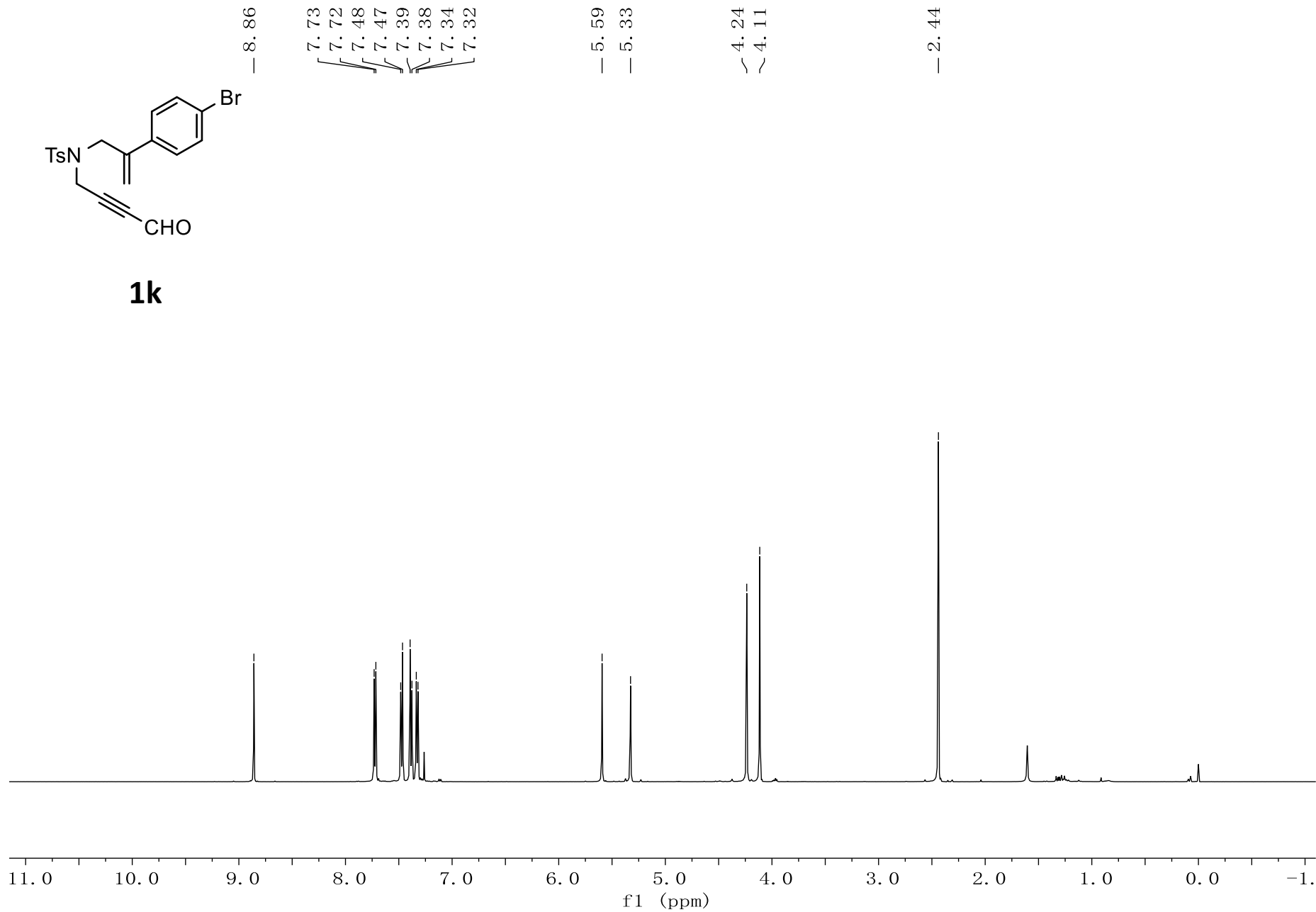
**1j**

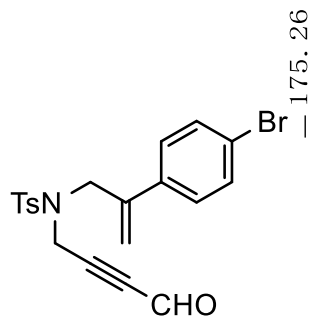




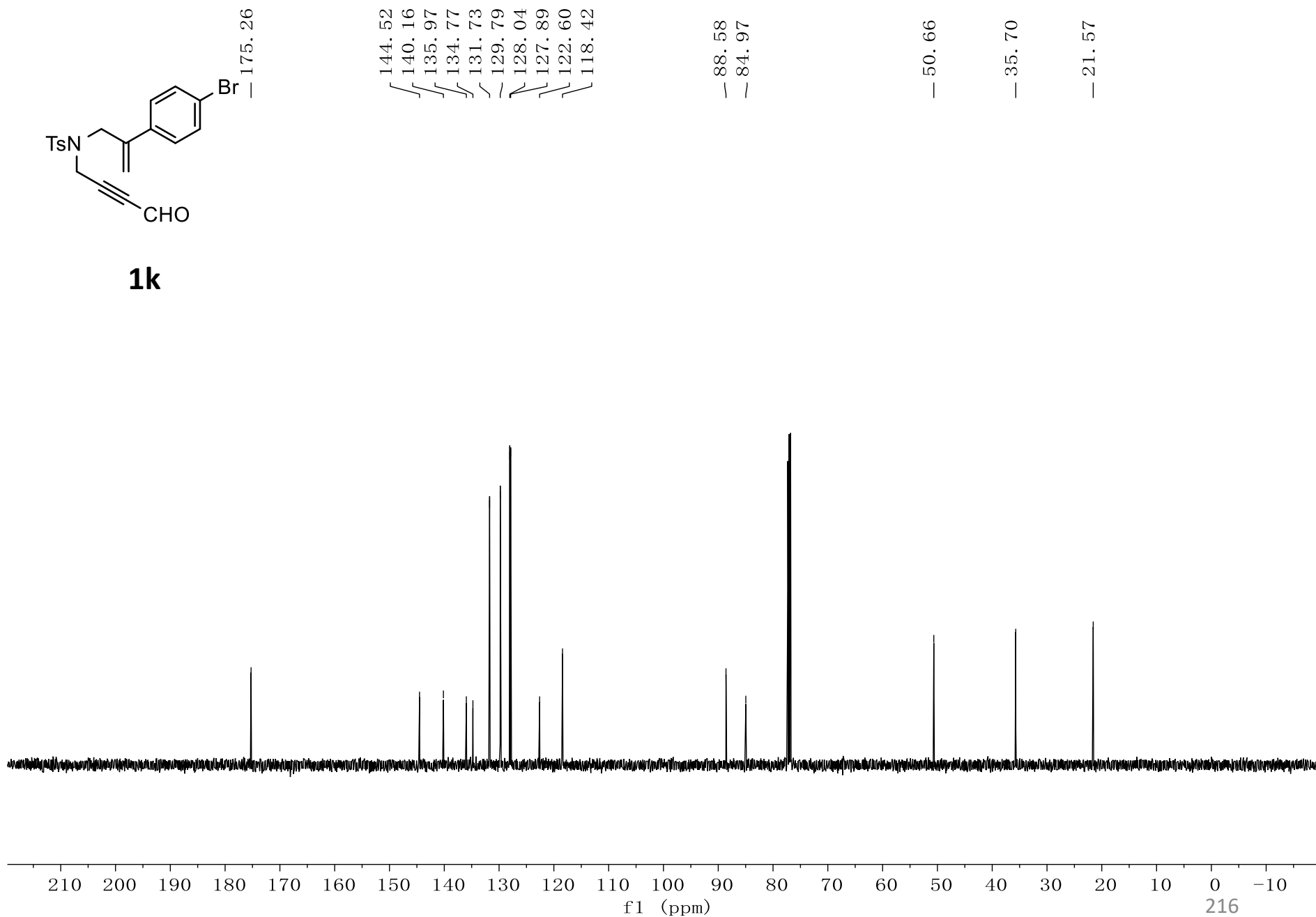


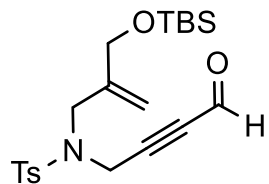
**1k**





**1k**





**1l**

8.87

7.74

7.72

7.33

7.31

5.33

5.11

4.25

4.12

3.82

2.42

0.91

0.08

0.95

2.00

2.01

1.00

1.00

1.98

2.10

1.98

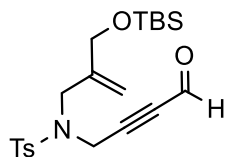
3.08

9.14

6.13

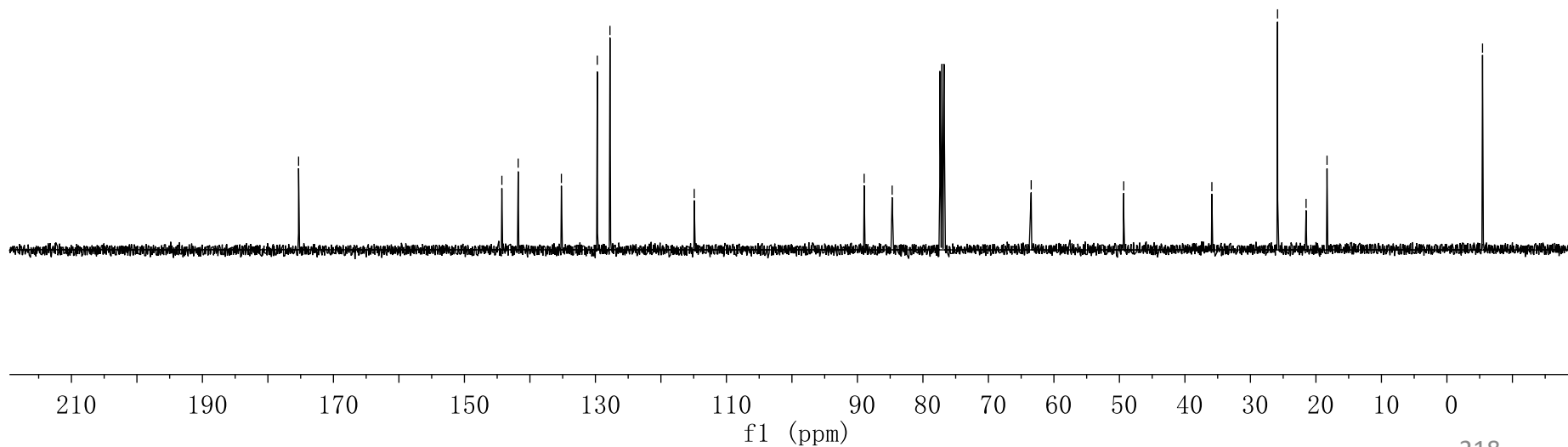
f1 (ppm)

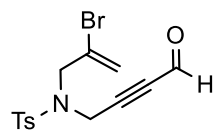
217



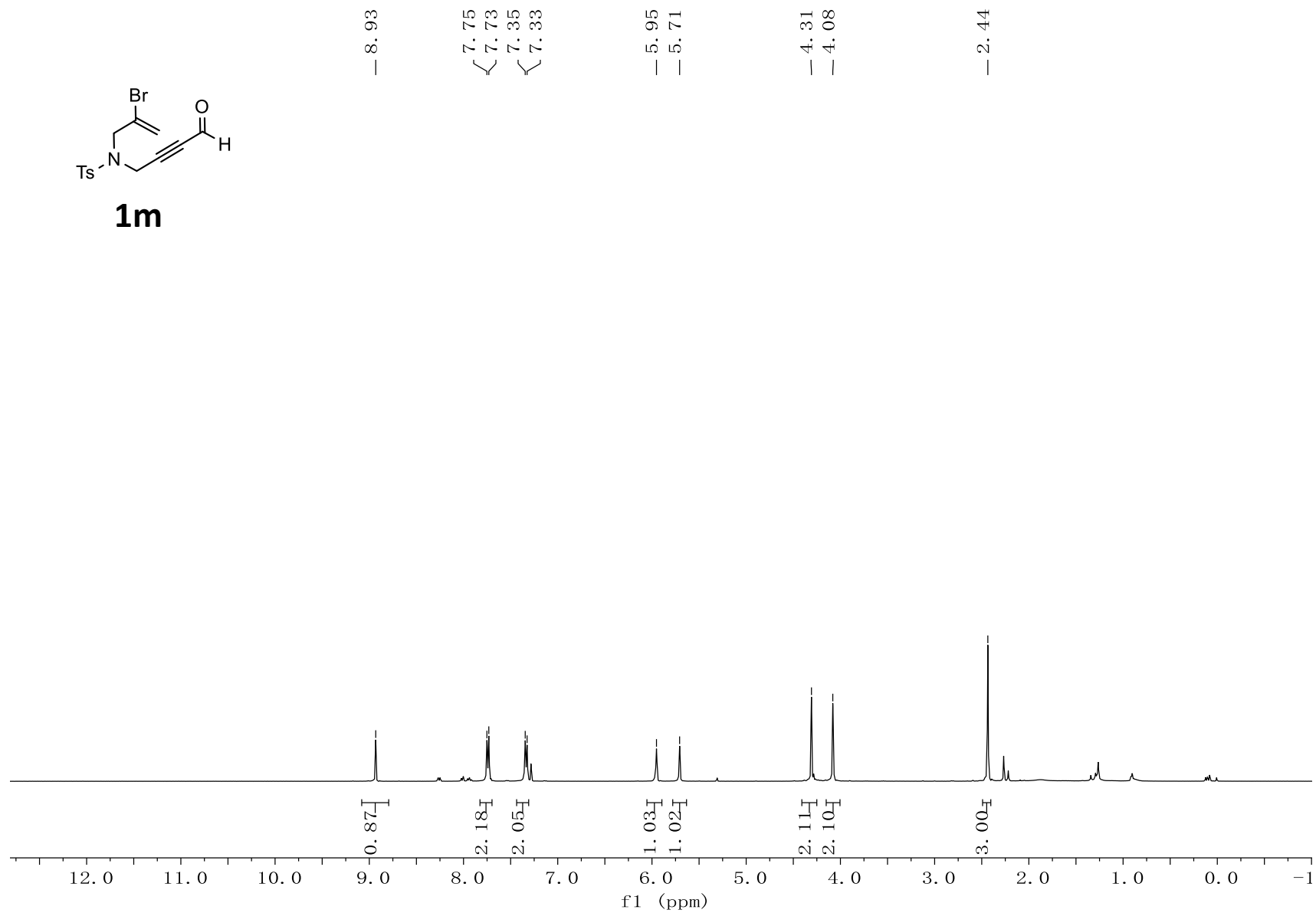
**1l**

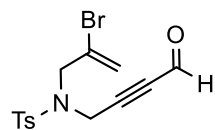
— 175.32  
 — 144.28  
 ~ 141.79  
 ~ 135.19  
 ~ 129.71  
 — 127.78  
 — 114.91  
 — 88.97  
 — 84.70  
 — 63.47  
 — 49.34  
 — 35.89  
 ~ 25.86  
 ~ 21.50  
 ~ 18.31  
 — -5.44





**1m**





**1m**

— 175.32

— 144.56

✓ 135.30

✓ 129.83

✓ 127.71

✓ 126.45

✓ 121.14

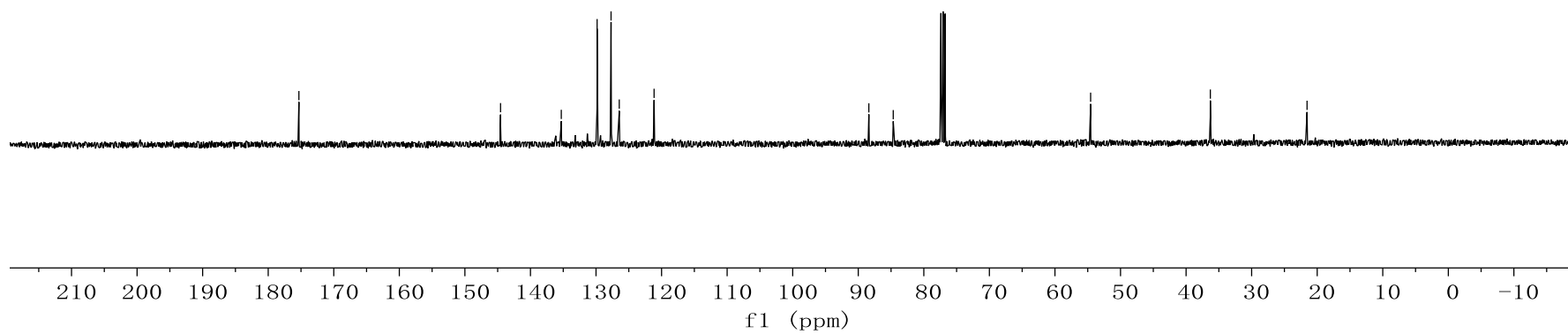
— 88.39

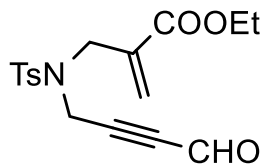
— 84.66

— 54.56

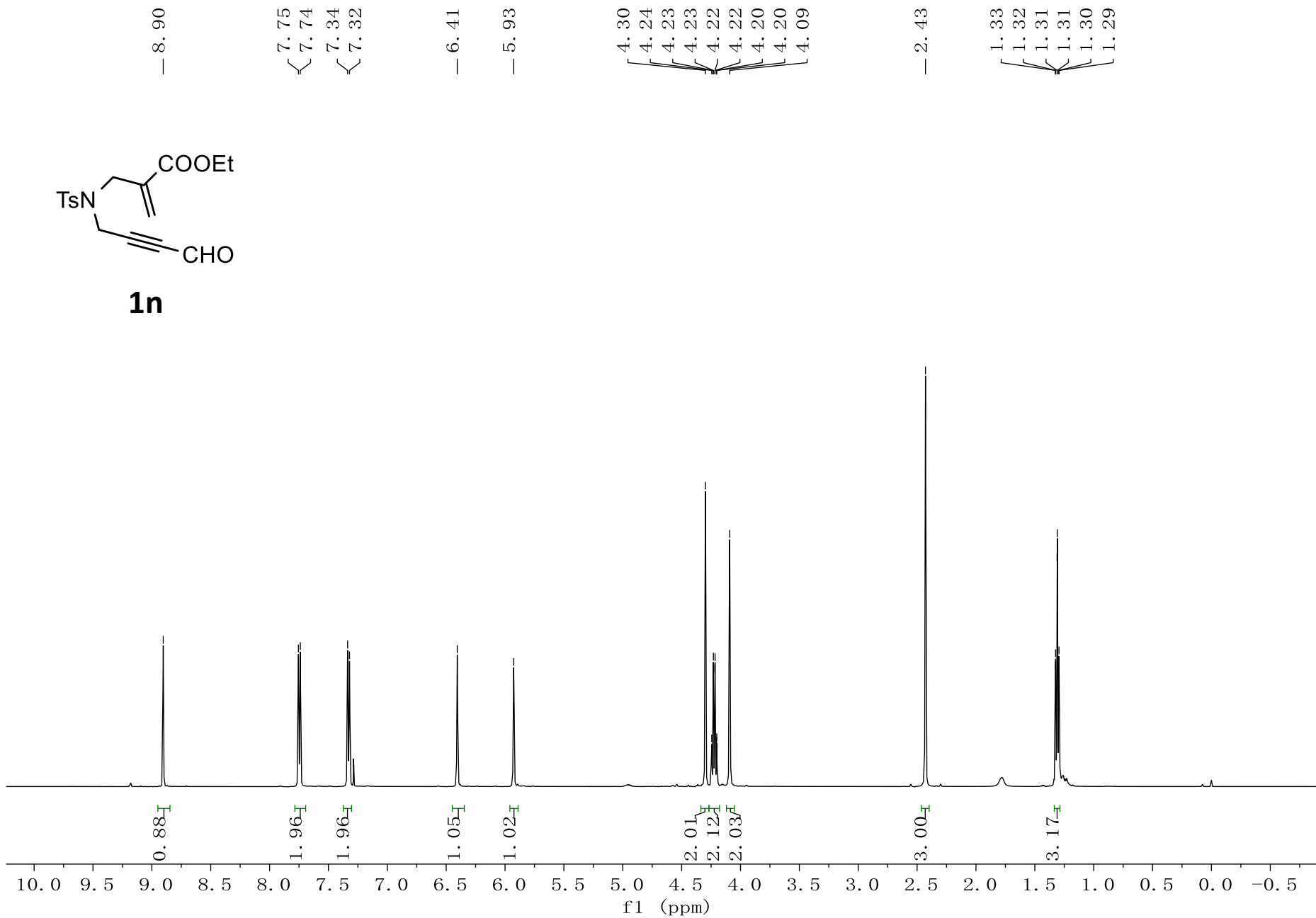
— 36.30

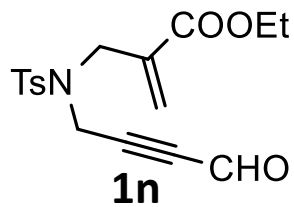
— 21.55



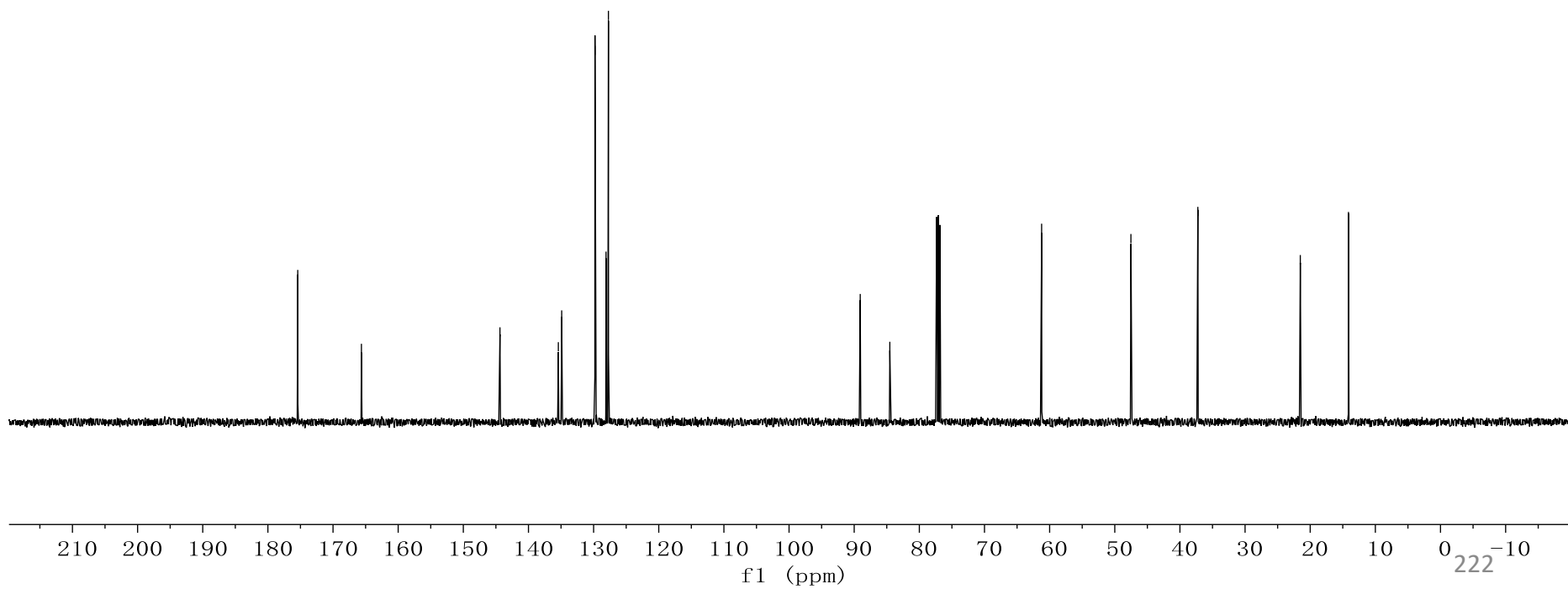


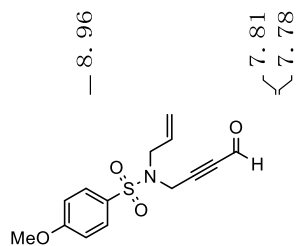
**1n**



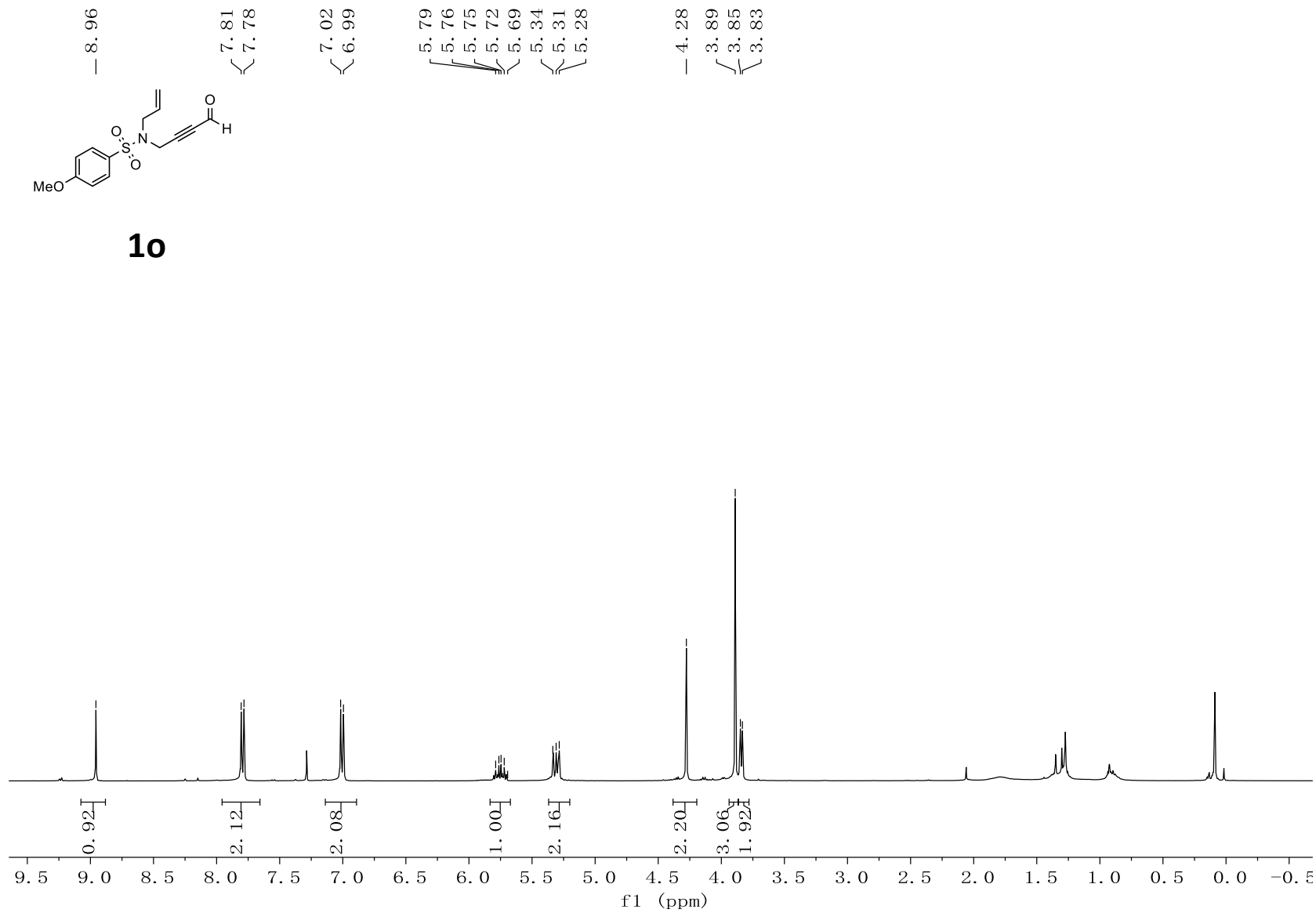


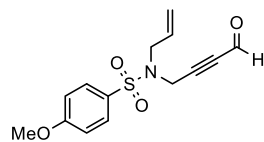
— 175.42  
 — 165.64  
 — 144.38  
 135.41  
 134.90  
 129.79  
 128.10  
 127.73  
 — 89.07  
 — 84.53  
 — 61.23  
 — 47.52  
 — 37.25  
 — 21.52  
 — 14.12





**1o**





**1o**

— 175.52

— 163.45

131.53

129.87

129.80

— 120.61

— 114.31

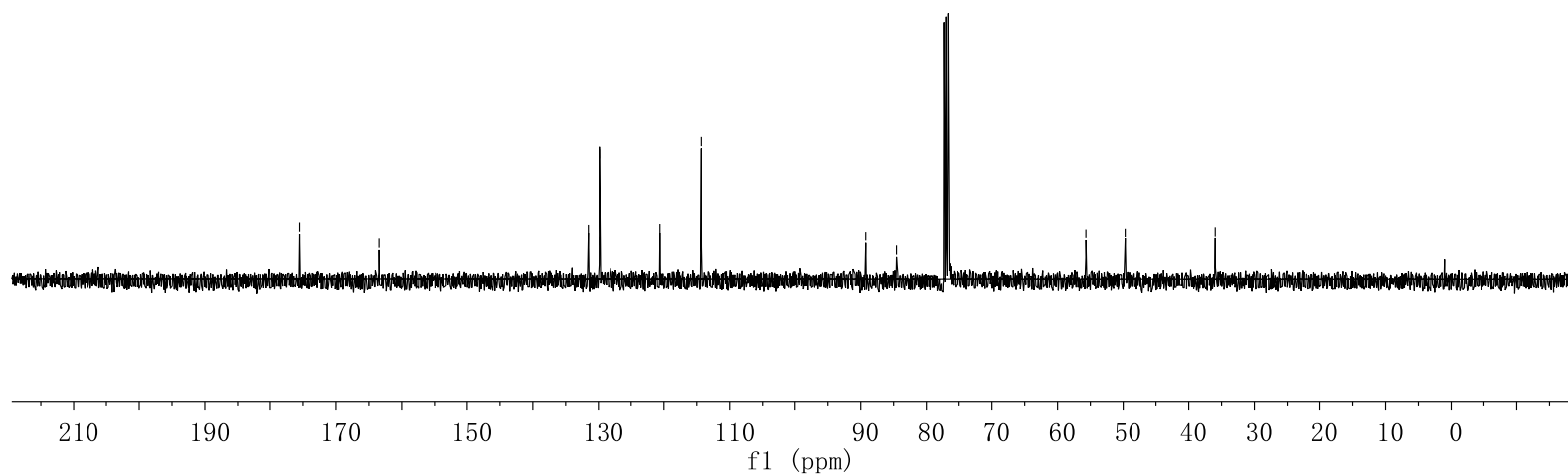
— 89.24

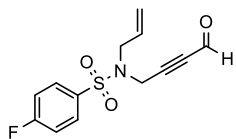
— 84.57

— 55.68

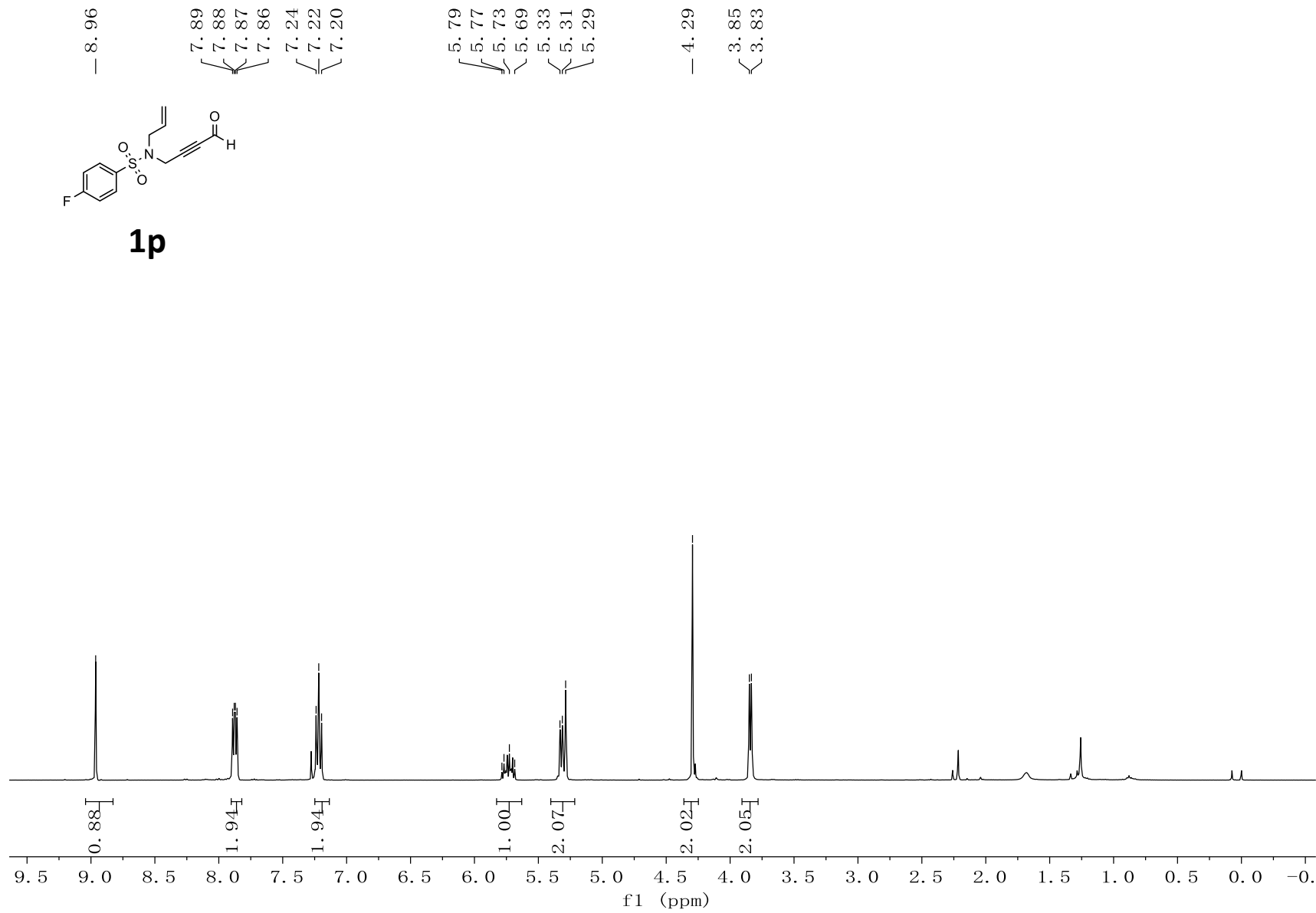
— 49.69

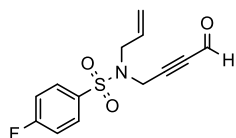
— 35.96





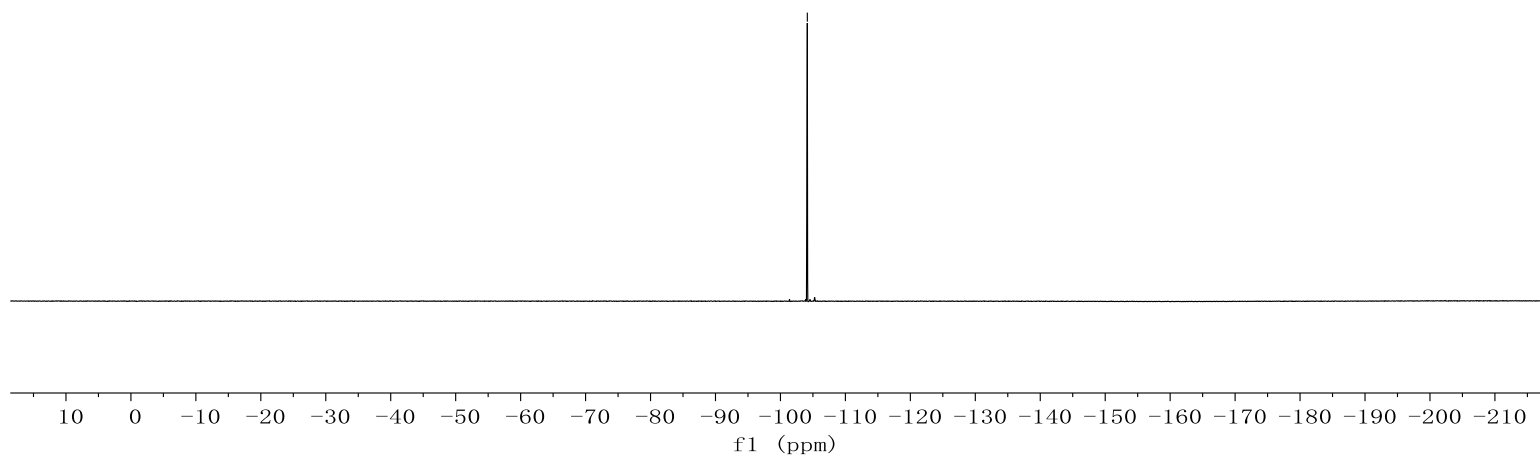
**1p**

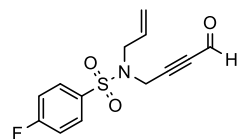




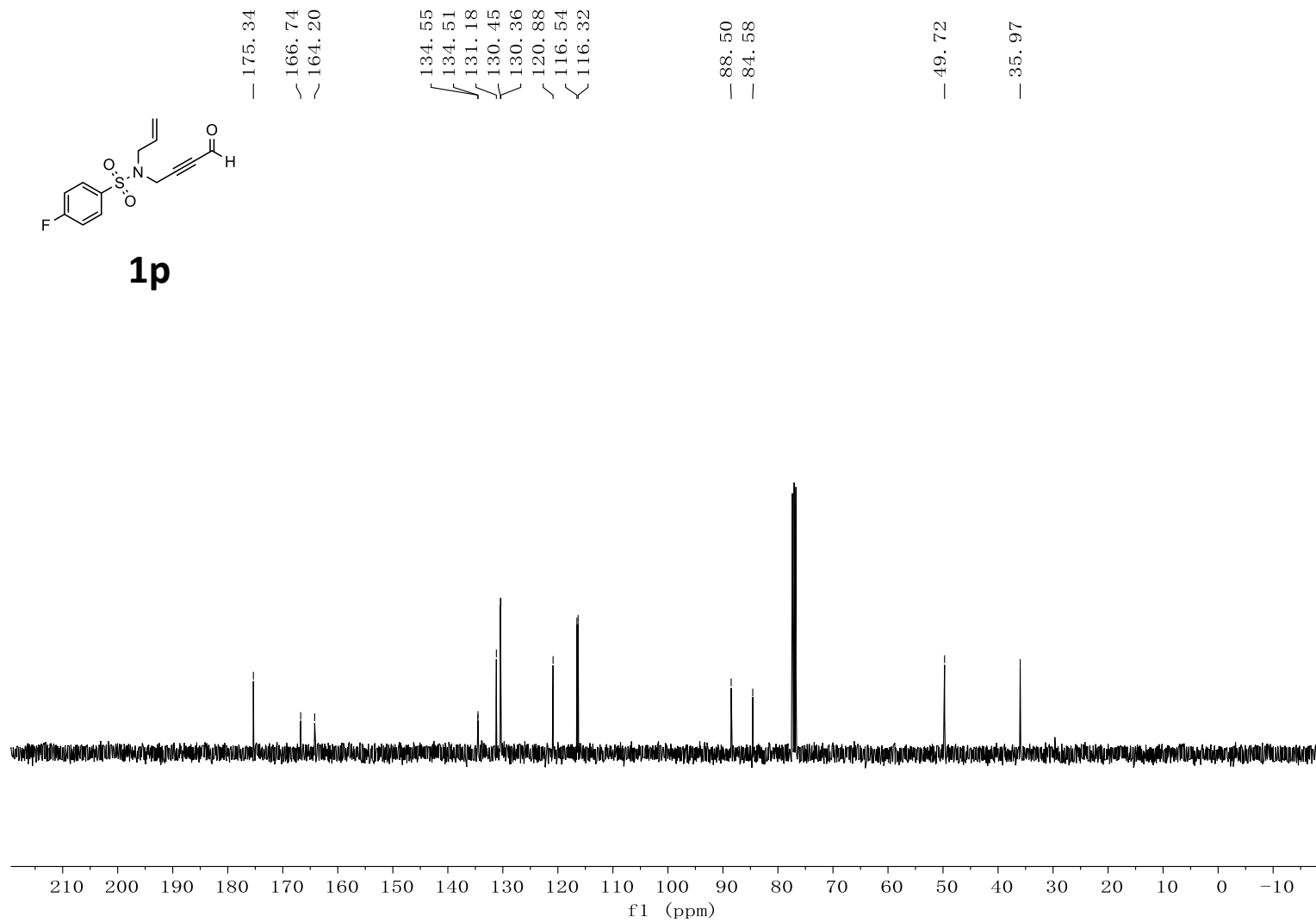
**1p**

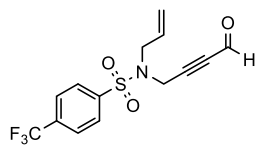
— -104.14



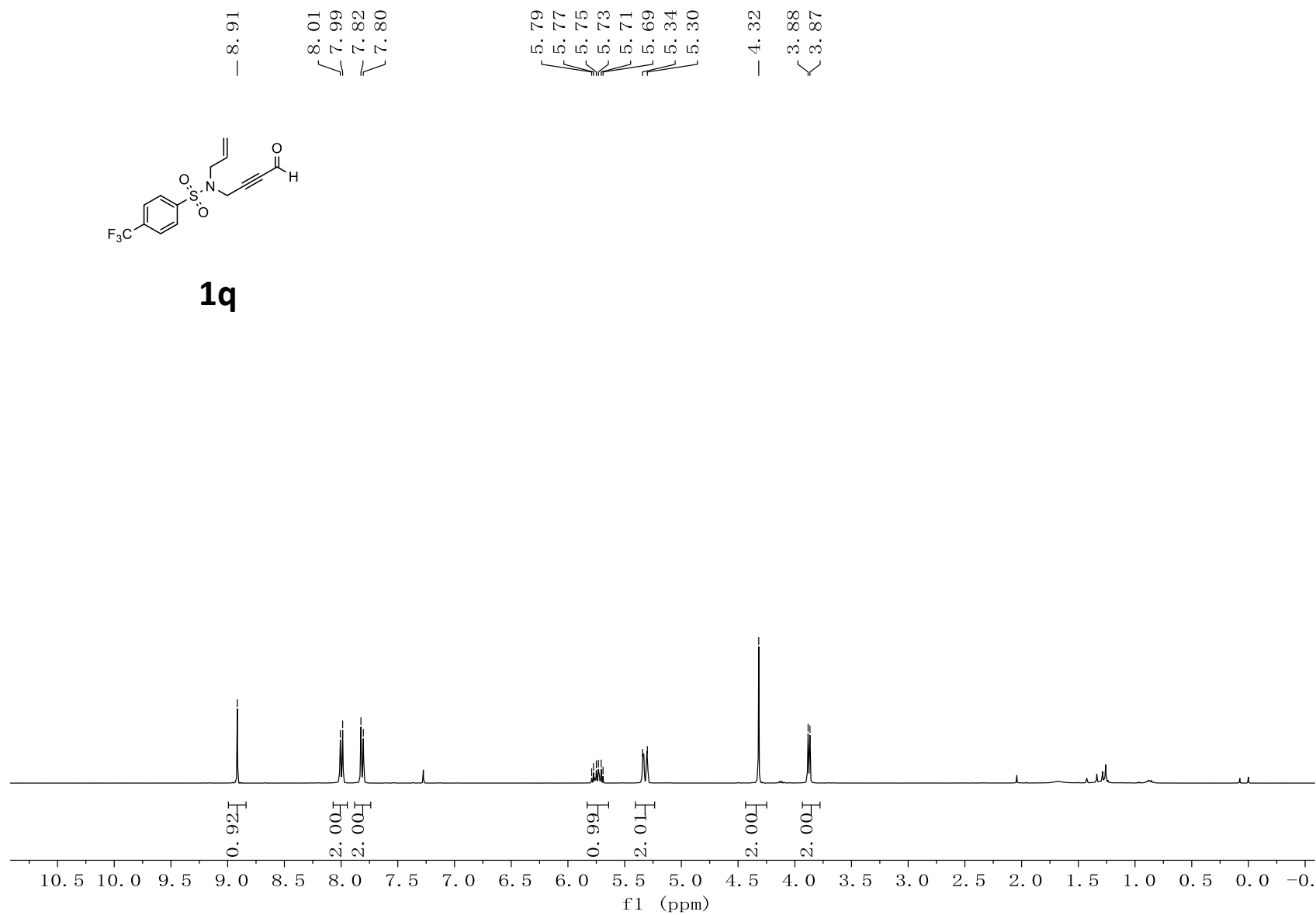


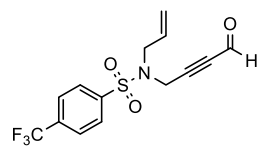
**1p**





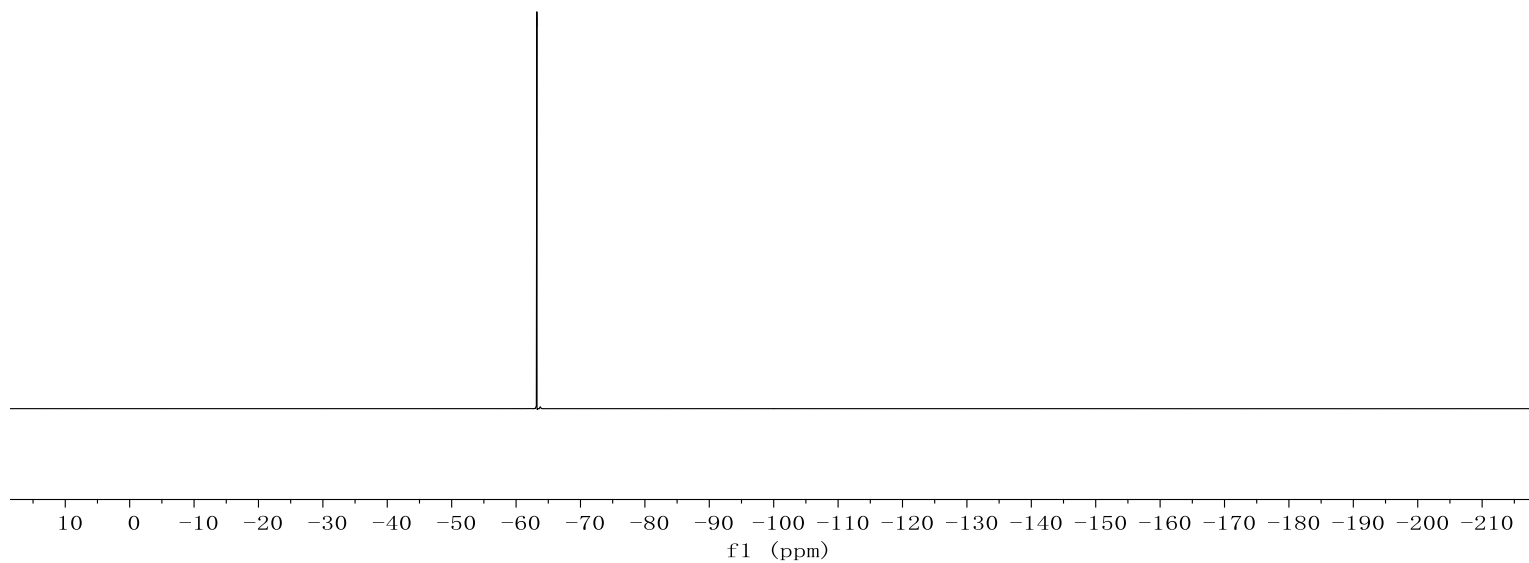
**1q**

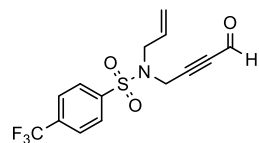




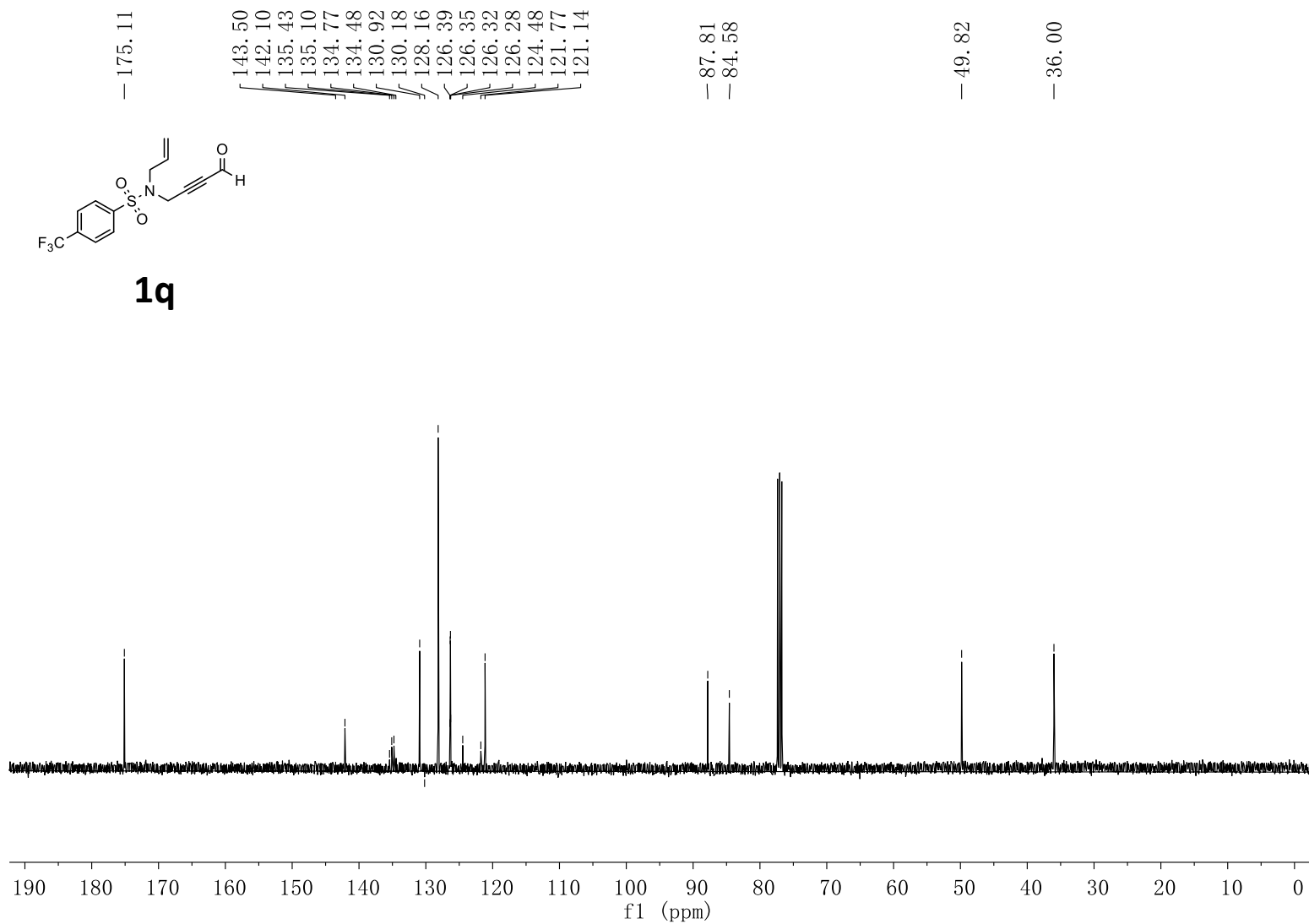
**1q**

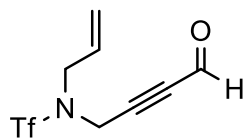
— -63.22



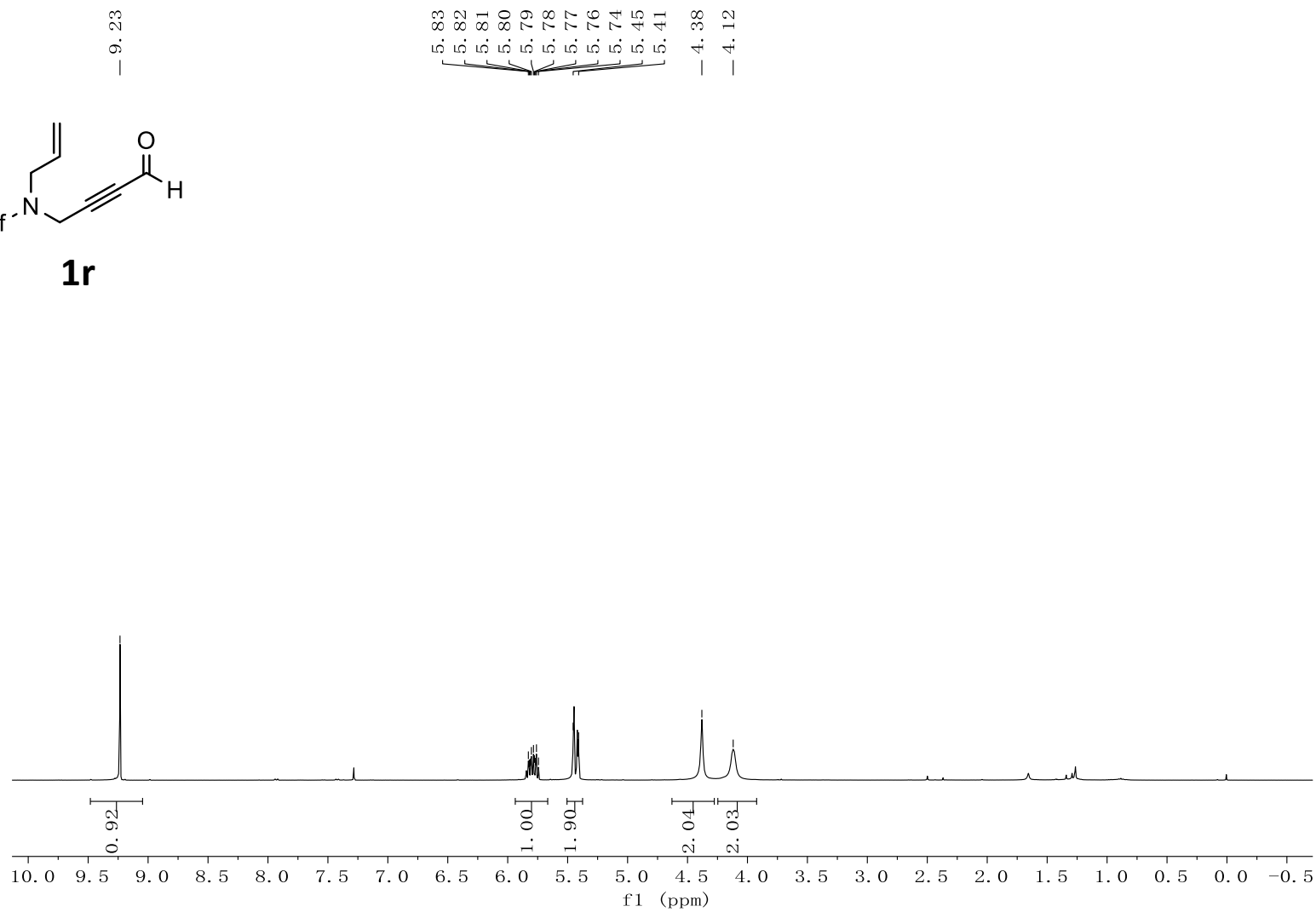


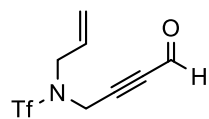
**1q**



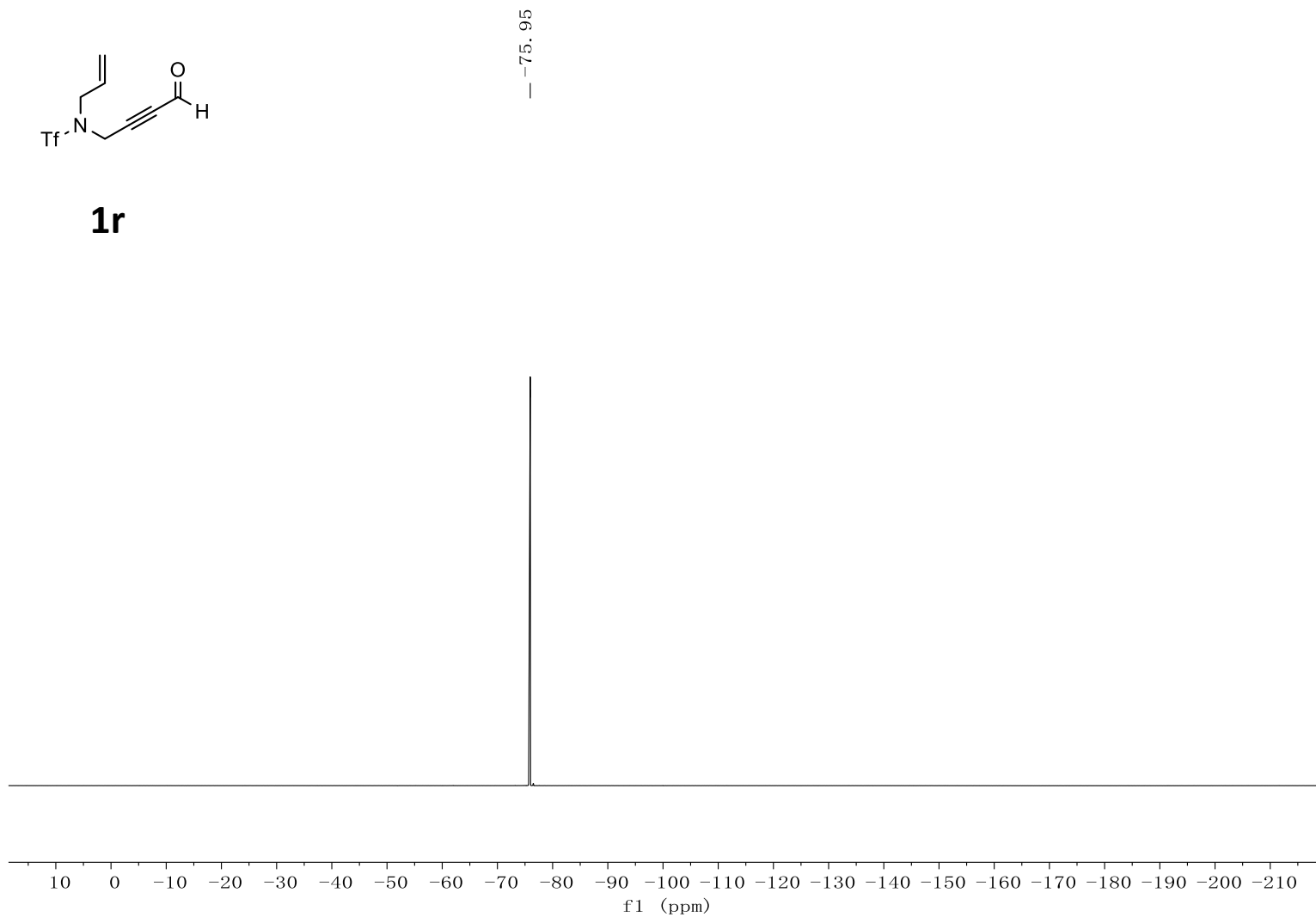


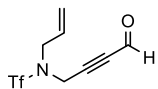
**1r**





**1r**





**1r**

— 175.55

— 129.95

— 122.21

— 121.26

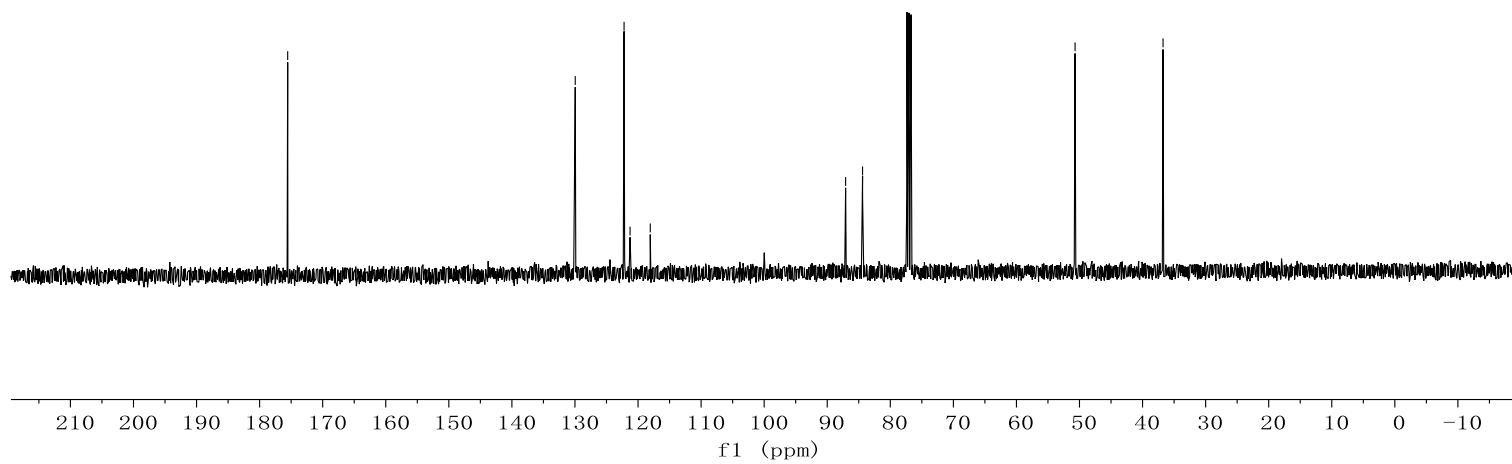
— 118.06

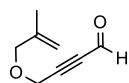
— 87.08

— 84.40

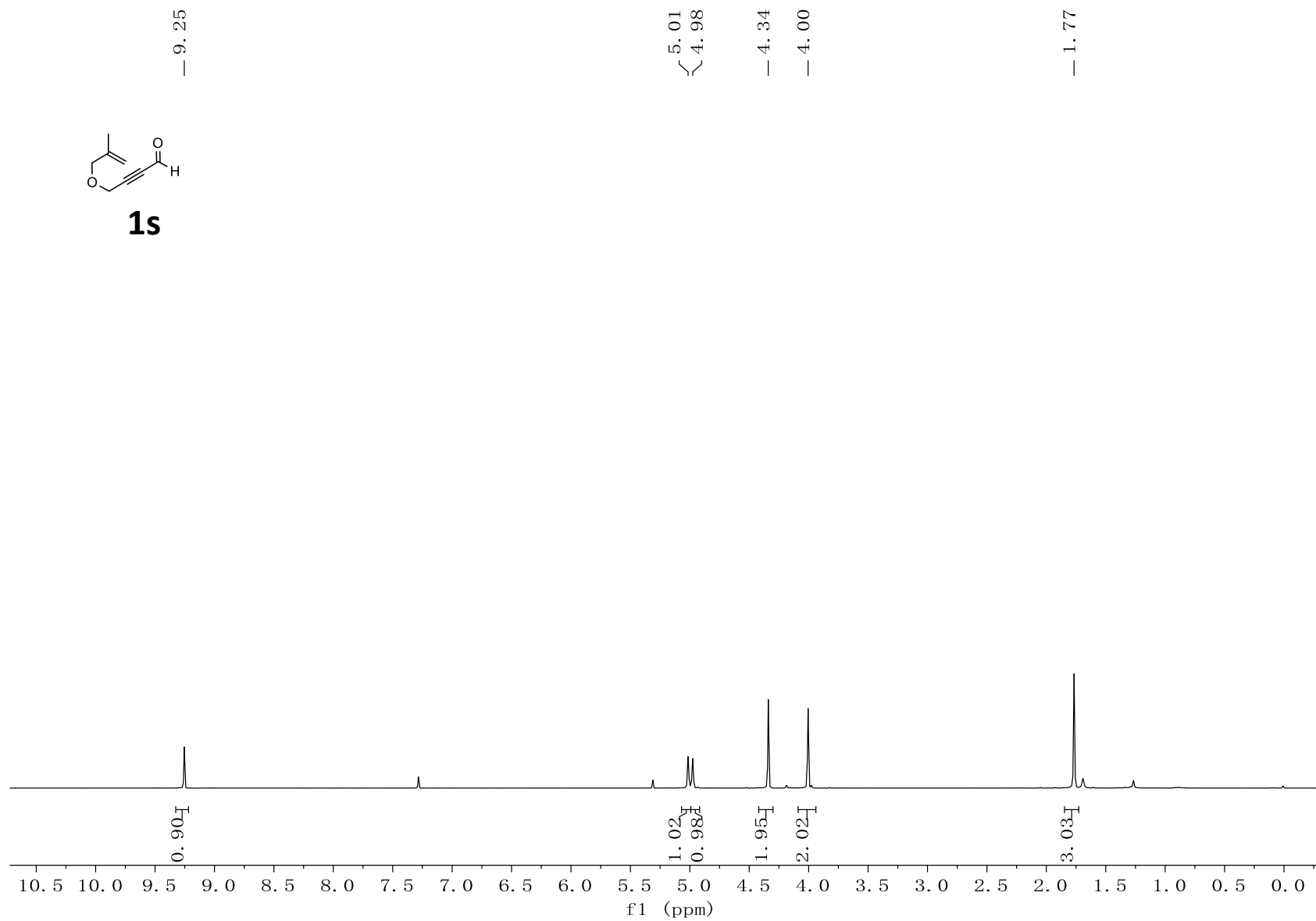
— 50.70

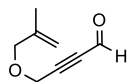
— 36.75





**1s**





**1s**

— 176.22

— 140.76

— 113.72

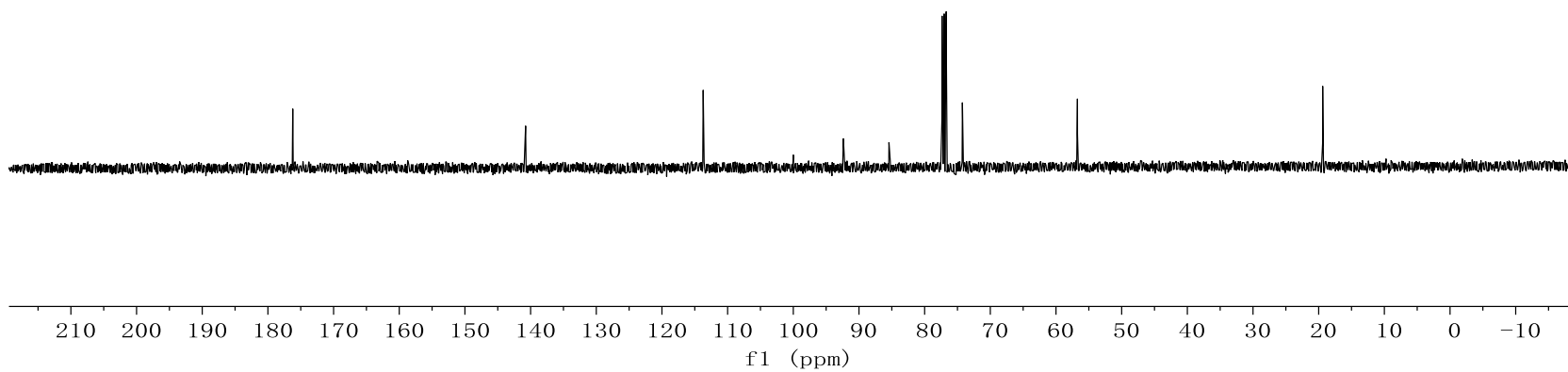
— 92.38

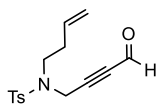
— 85.43

— 74.25

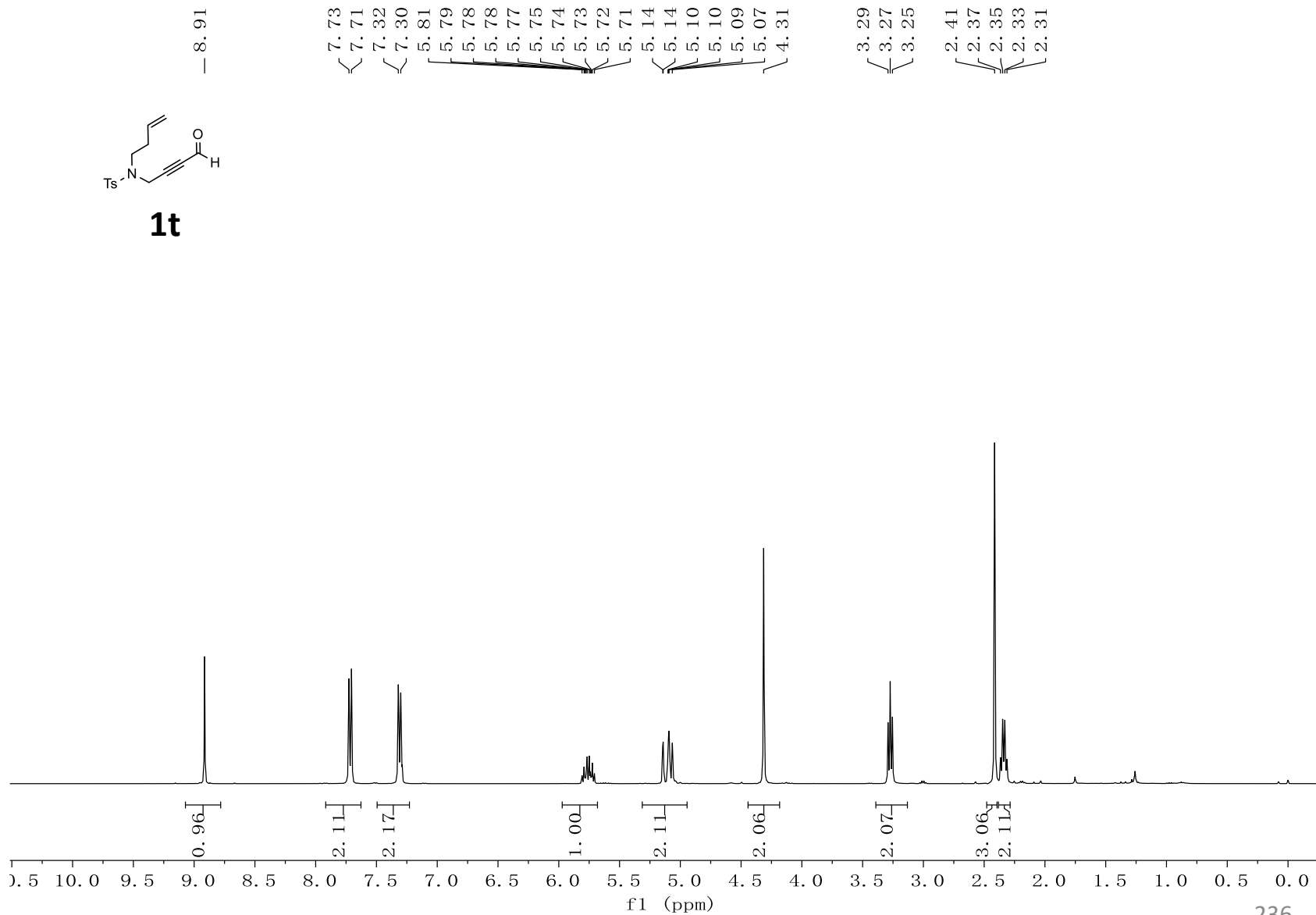
— 56.74

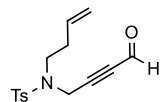
— 19.39



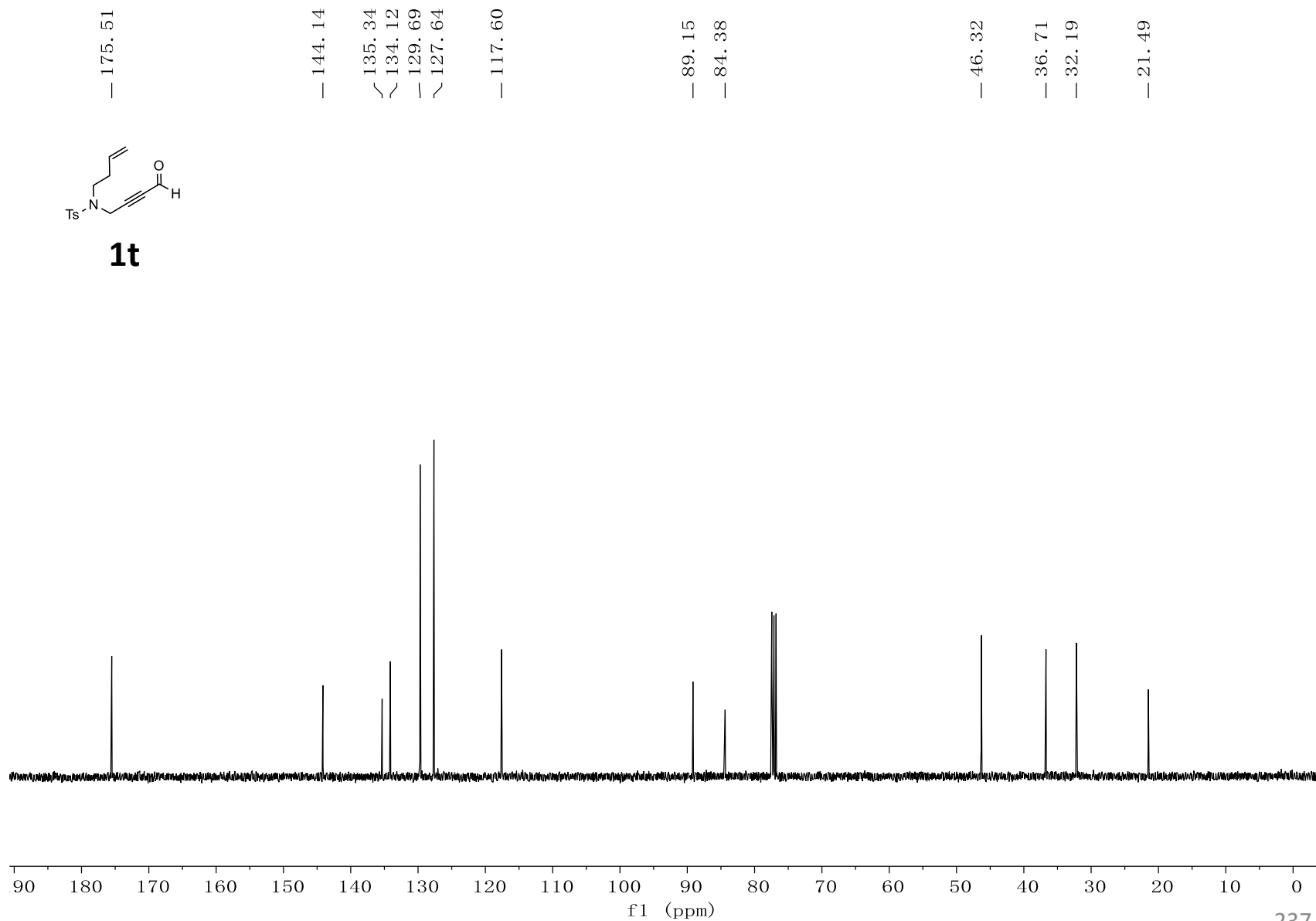


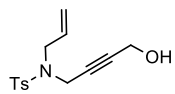
**1t**



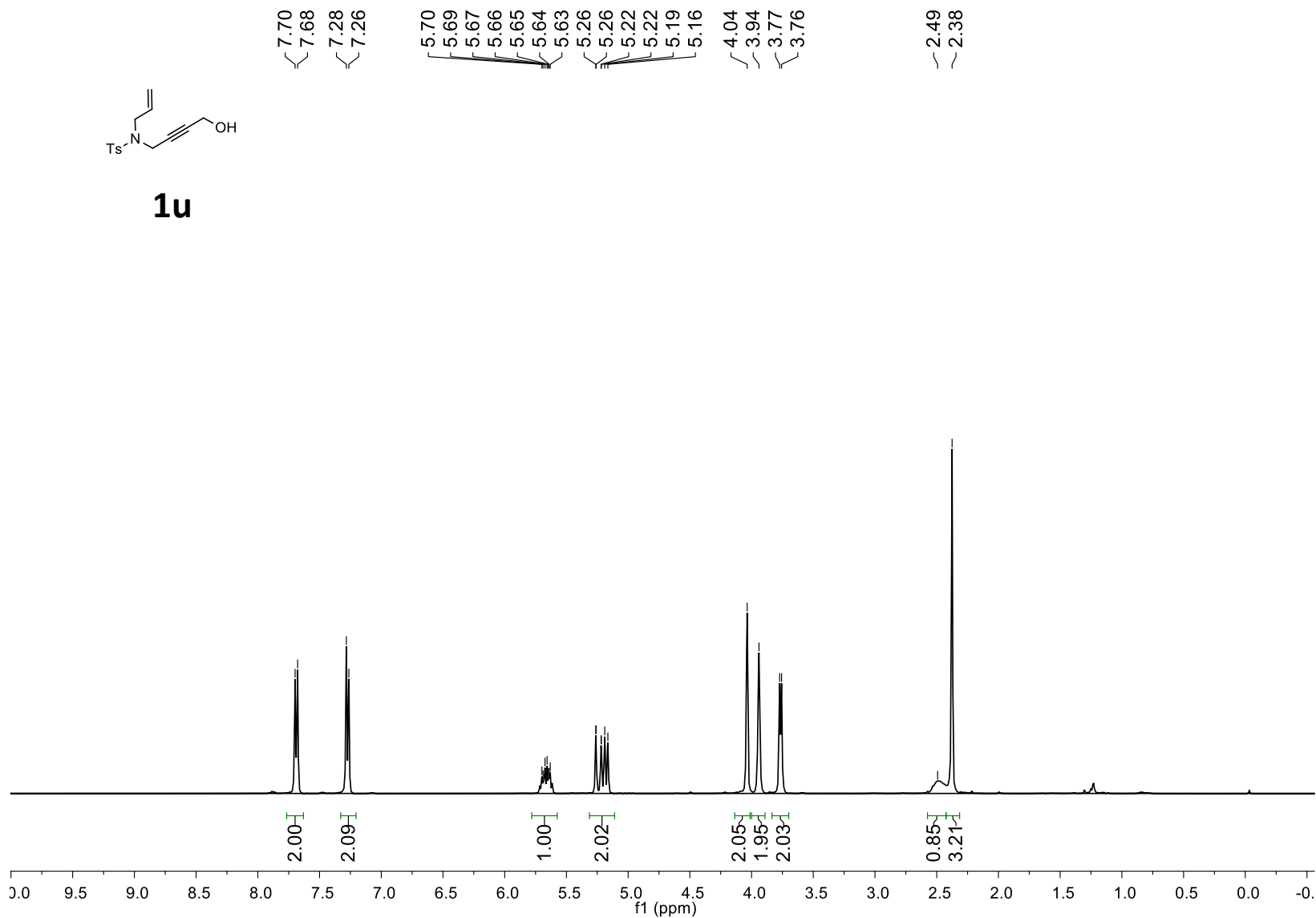


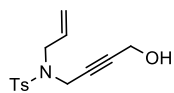
**1t**



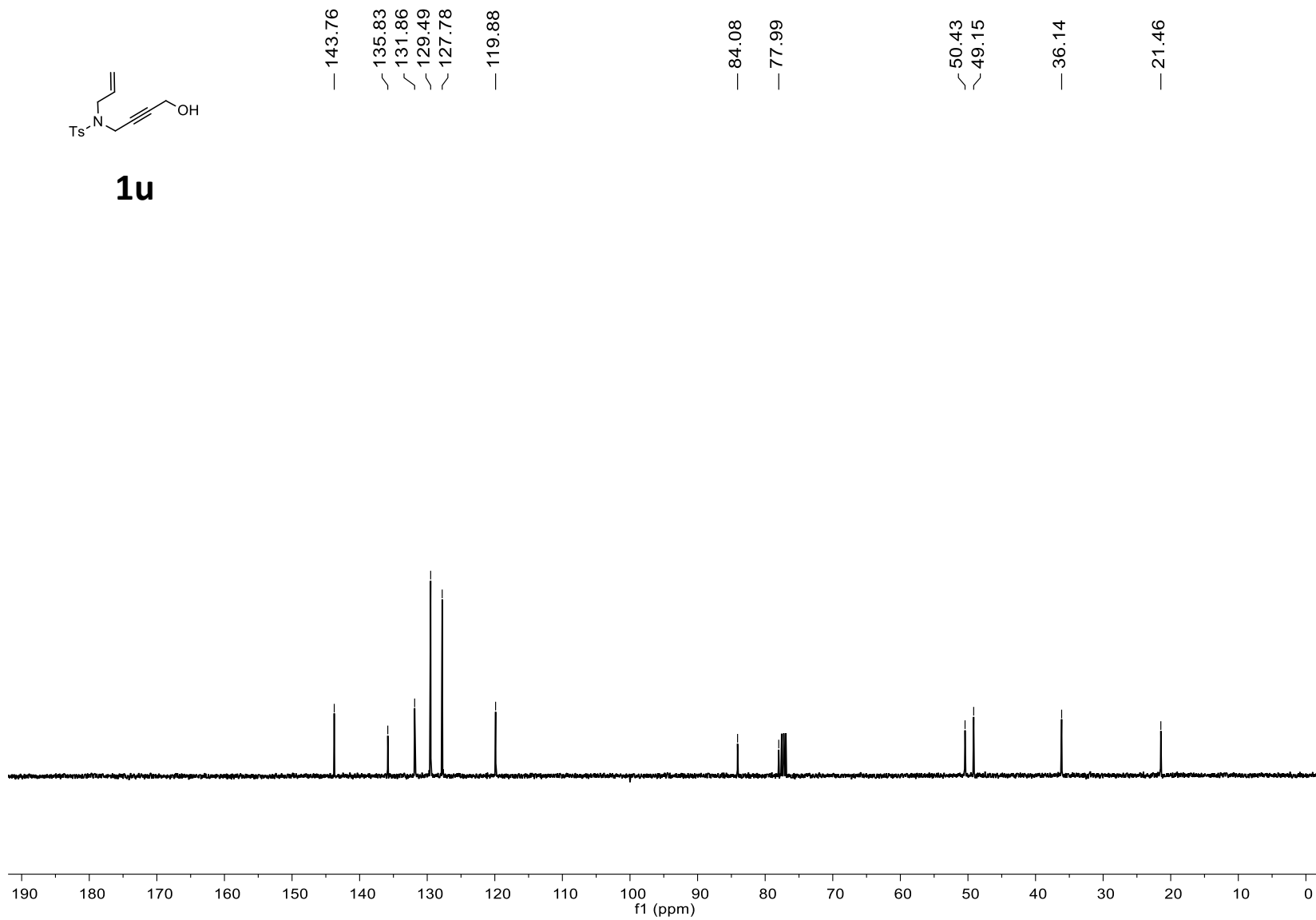


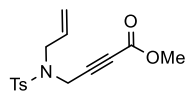
**1u**



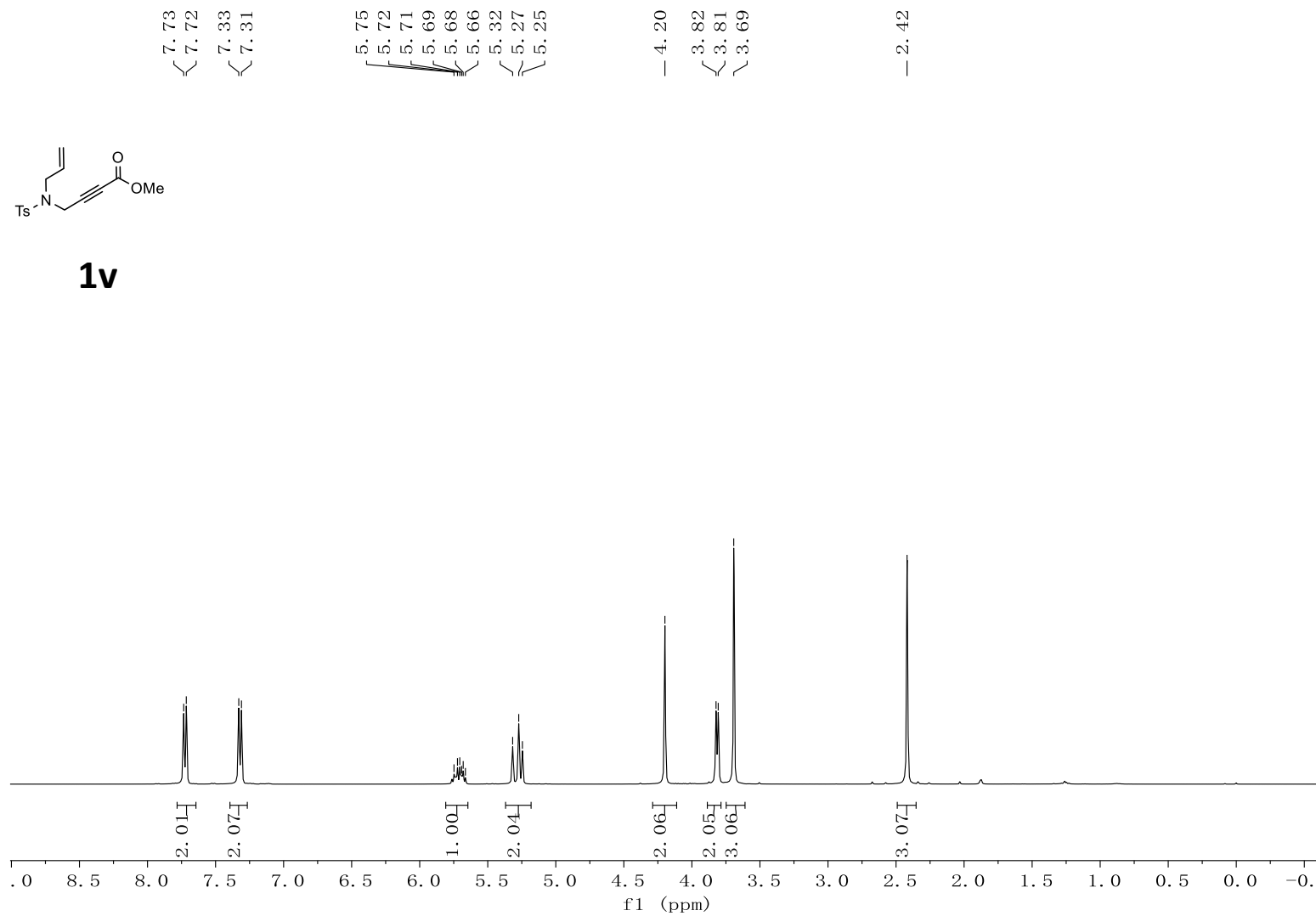


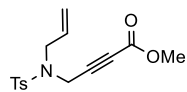
**1u**



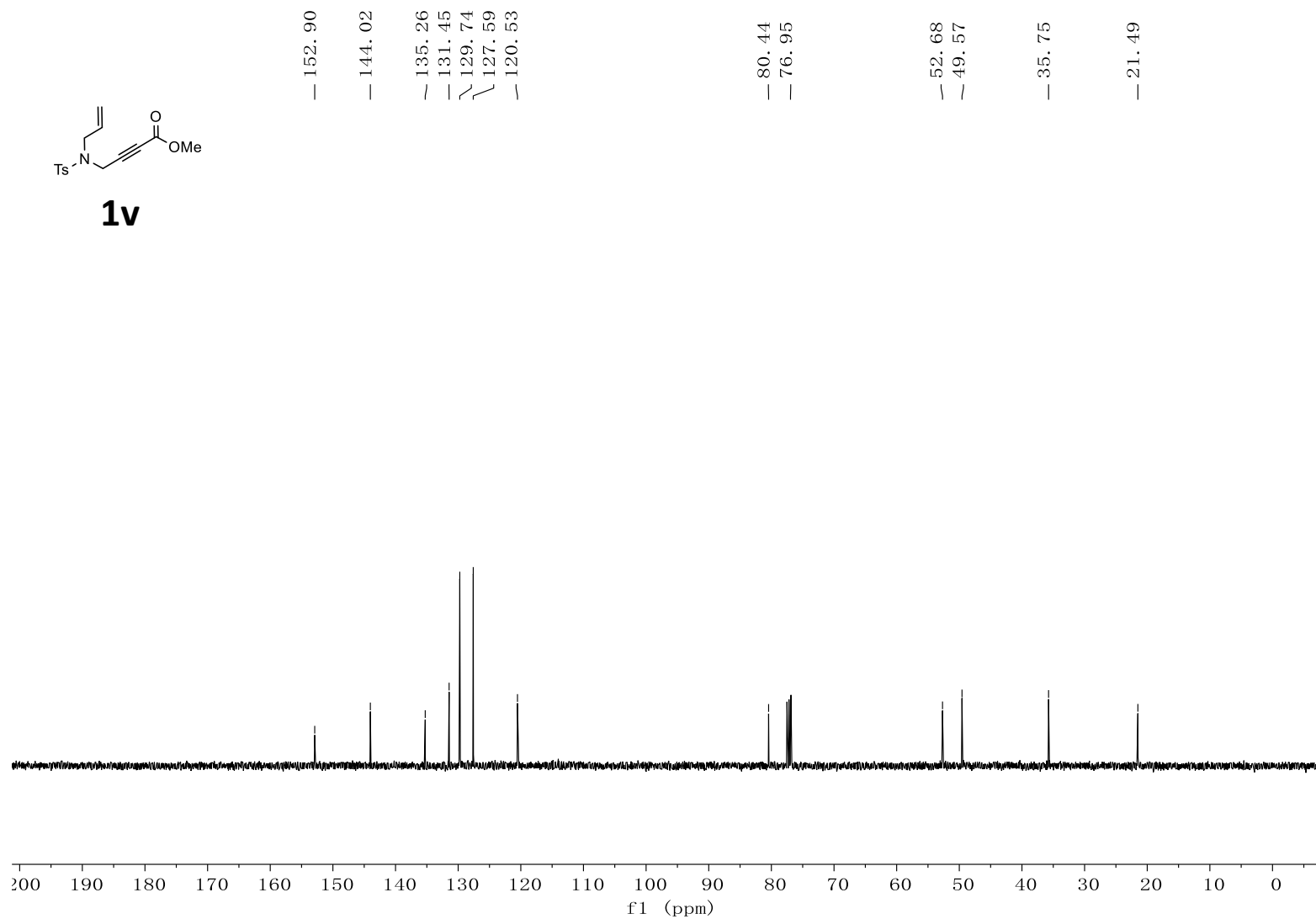


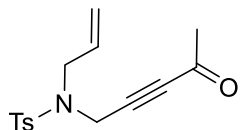
**1v**



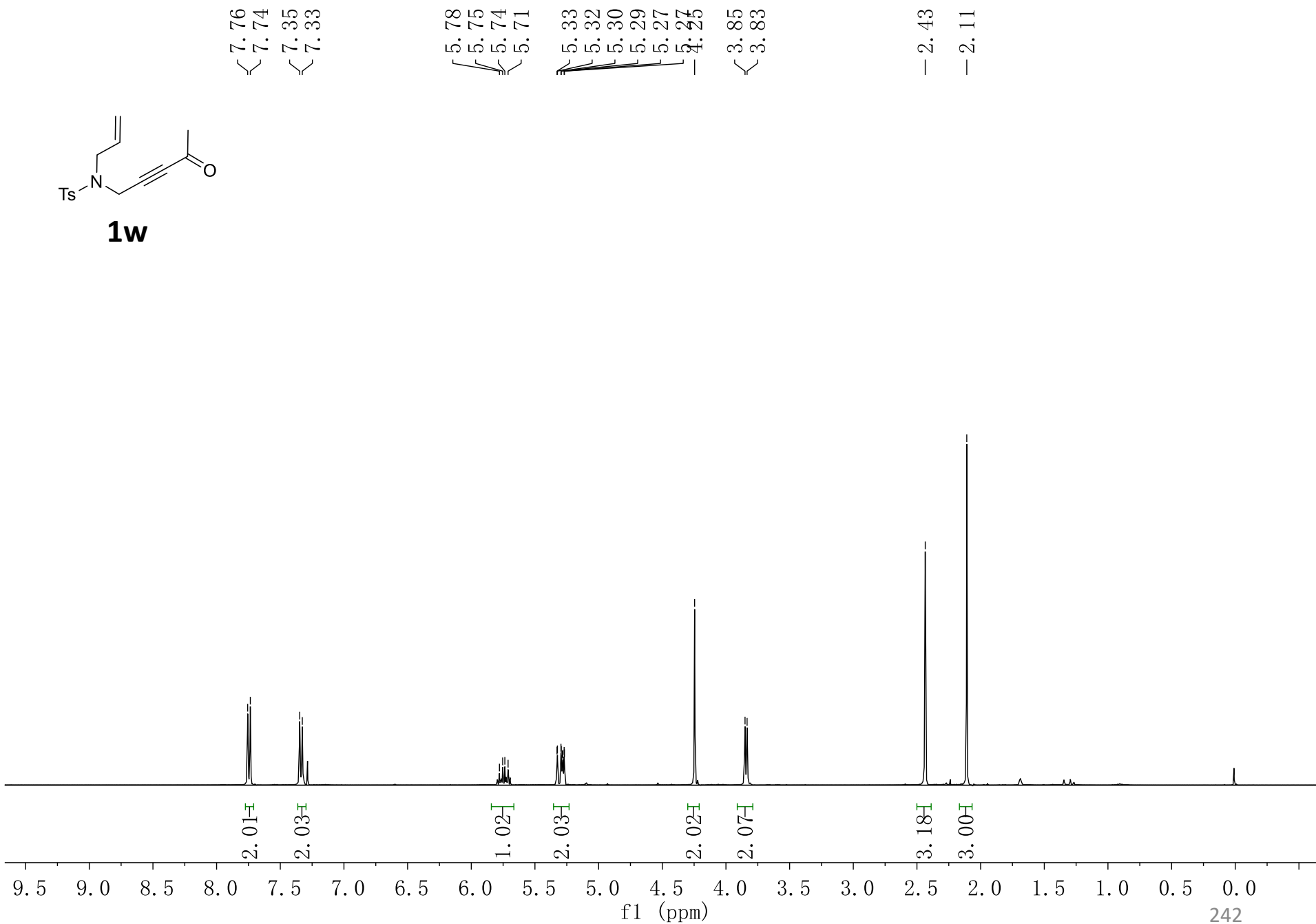


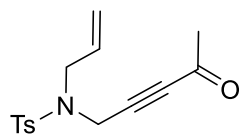
**1v**





**1w**





**1w**

— 183.214

— 144.078

~ 135.537

~ 131.527

~ 129.762

~ 127.731

~ 120.538

< 84.705

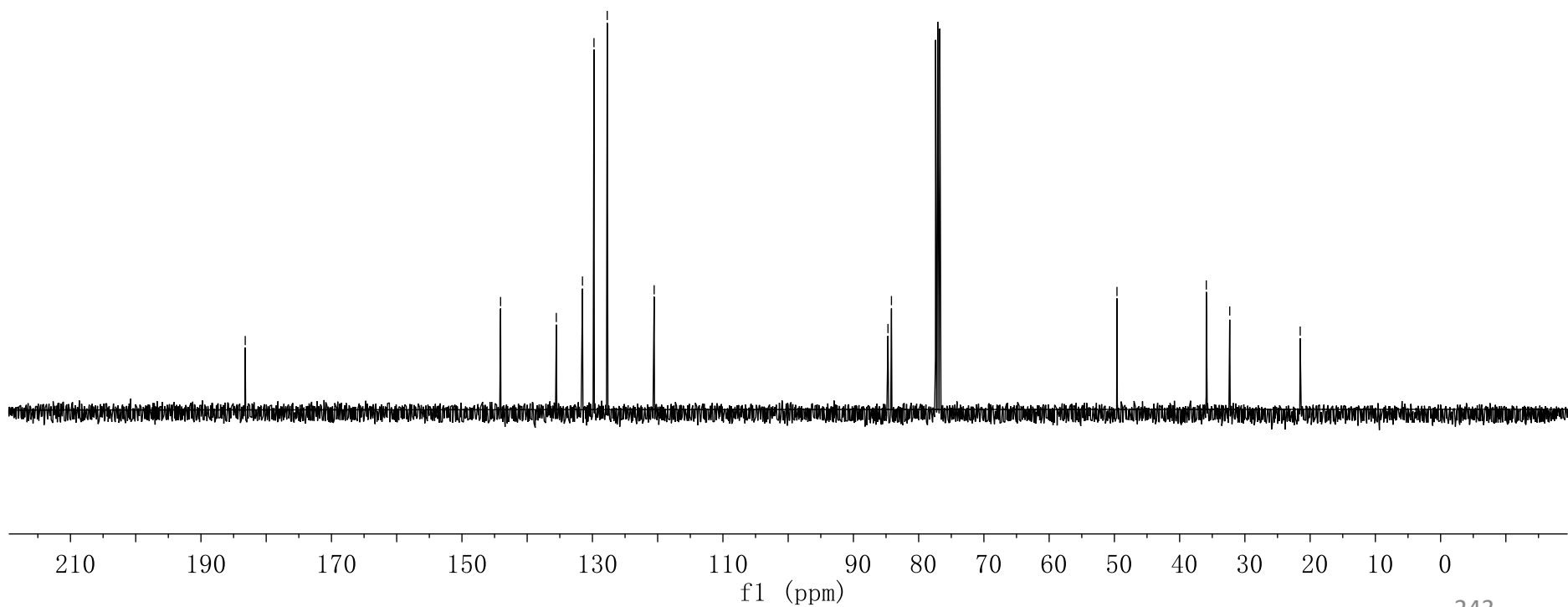
< 84.170

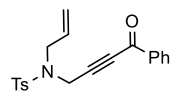
— 49.605

~ 35.913

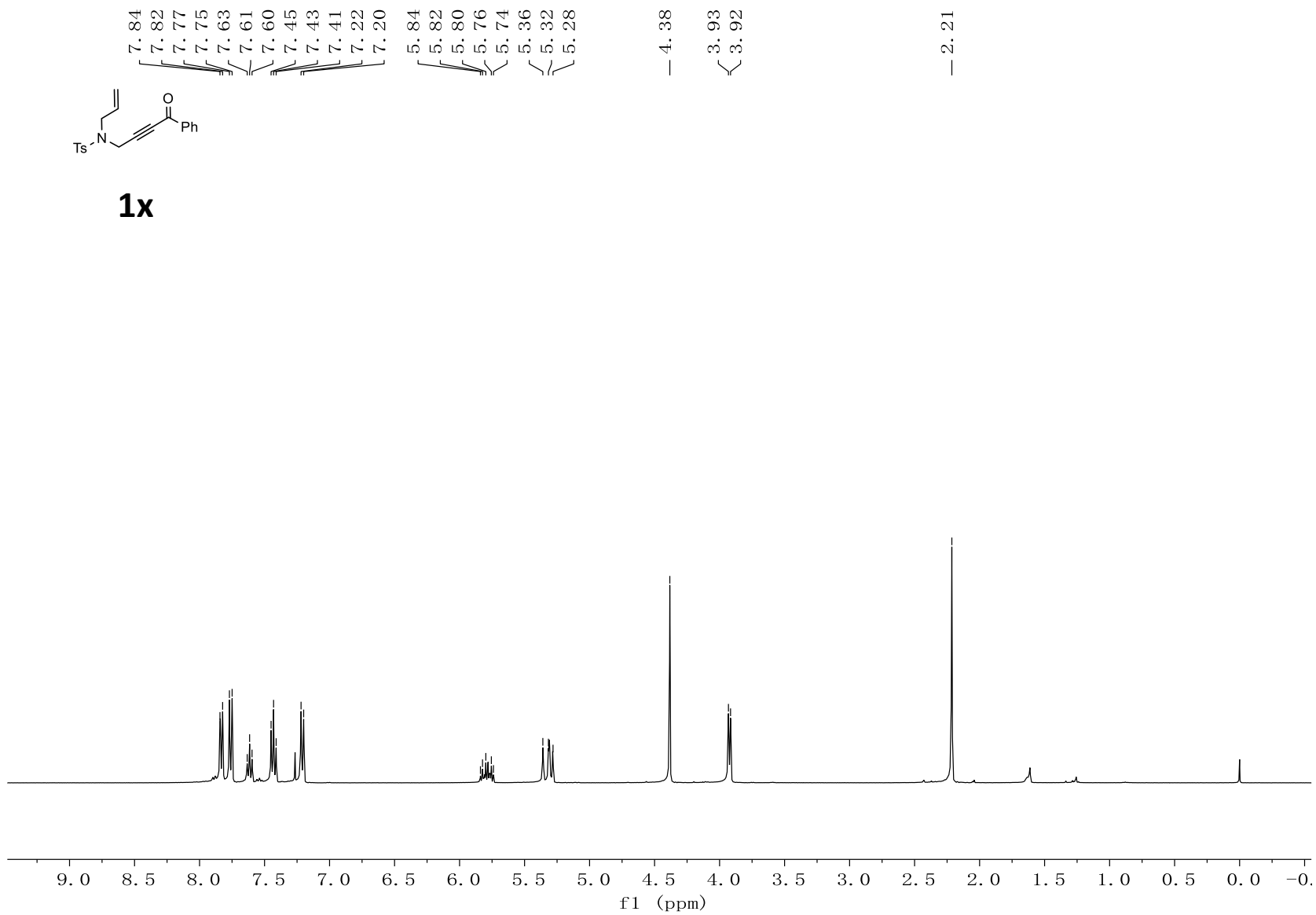
~ 32.323

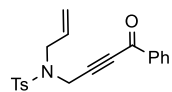
— 21.522



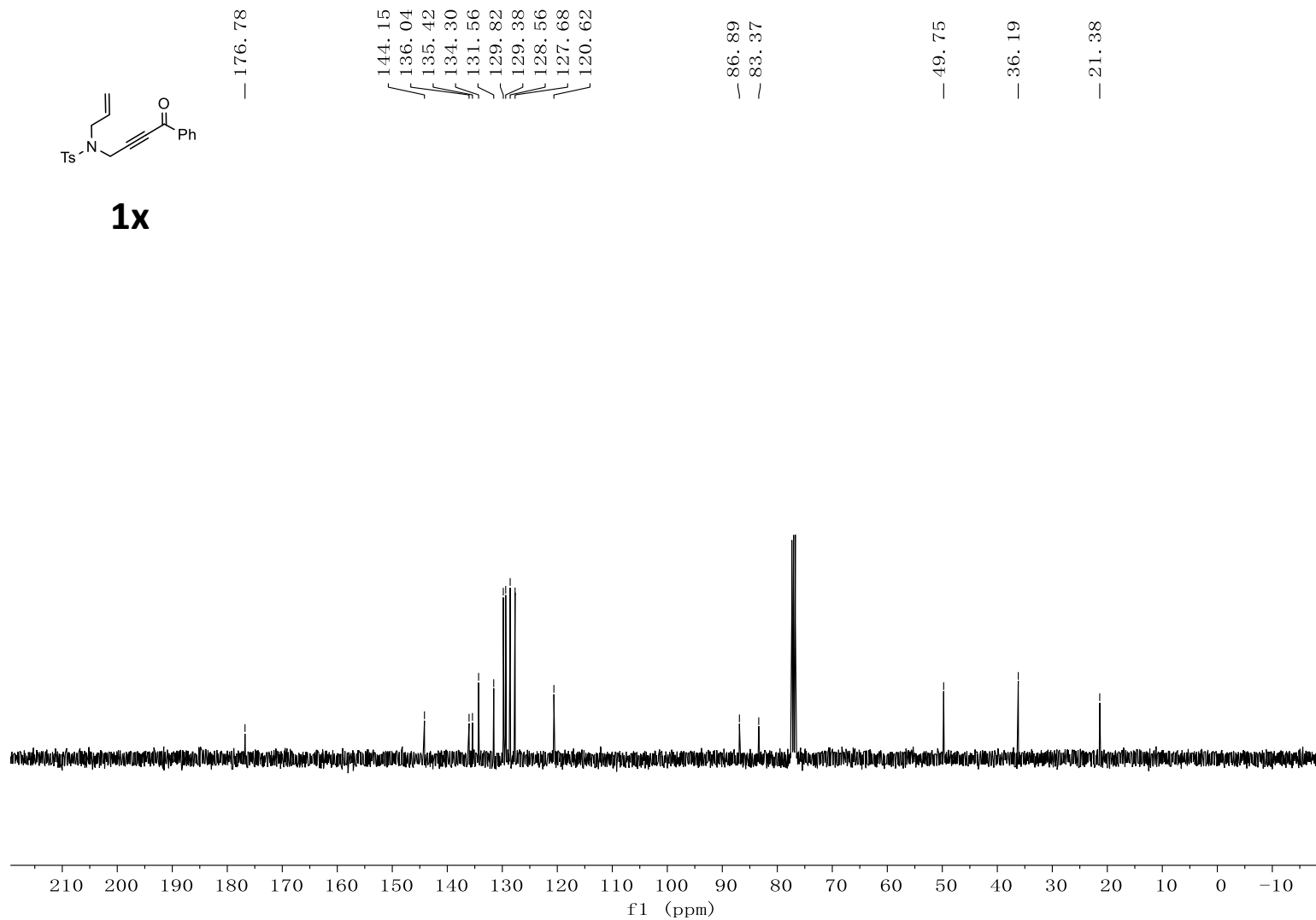


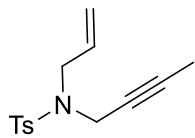
**1x**



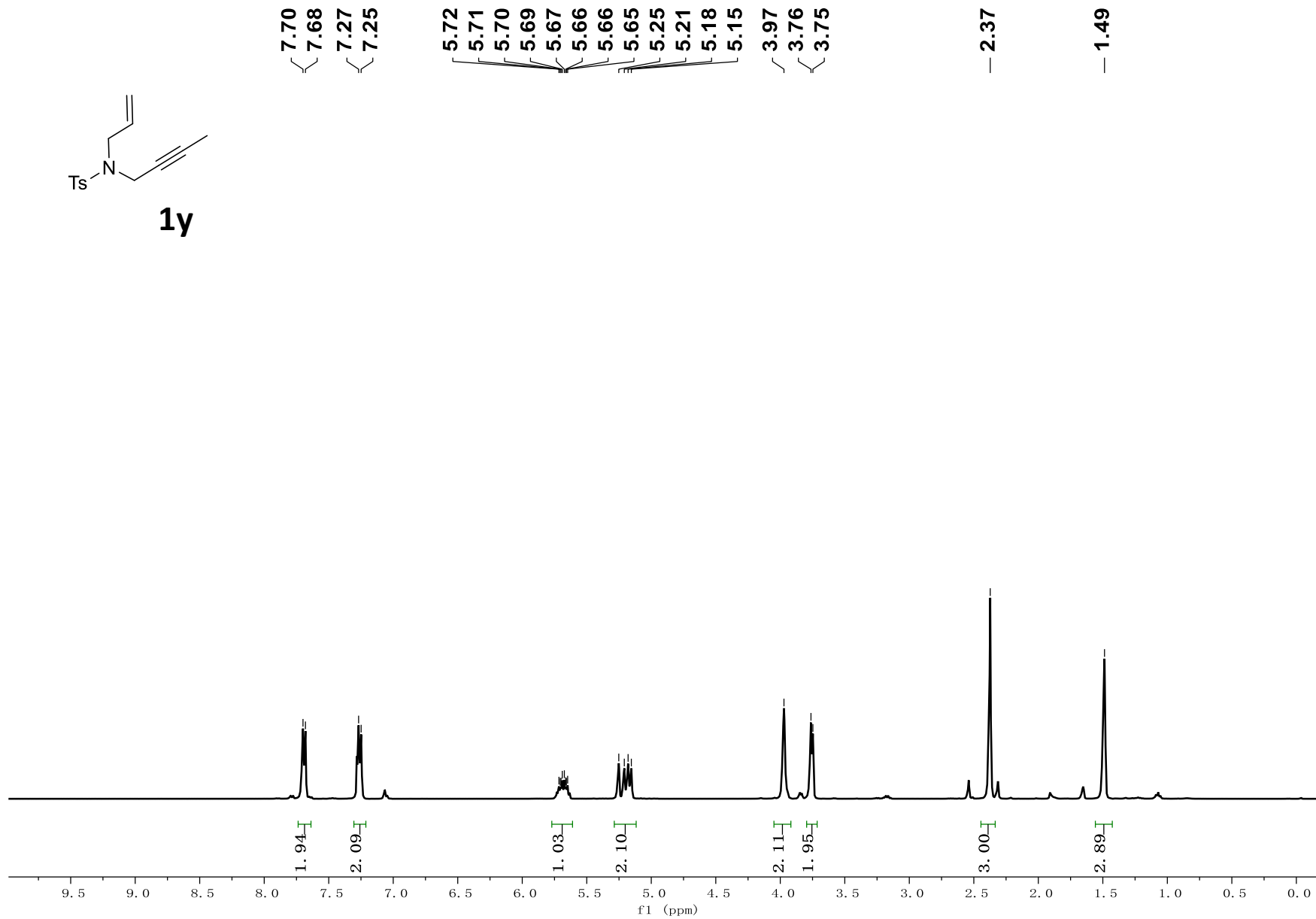


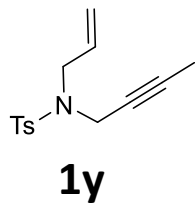
**1x**





**1y**





— 143.31  
 — 136.08  
 — 132.19  
 — 129.26  
 — 127.80  
 — 119.49

— 81.63

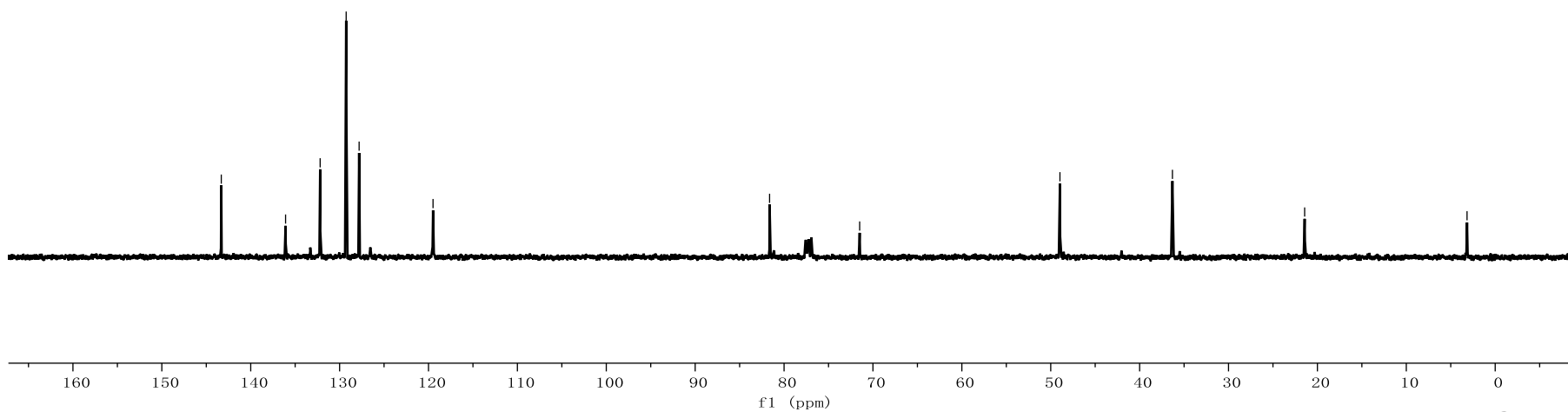
— 71.49

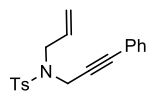
— 48.97

— 36.31

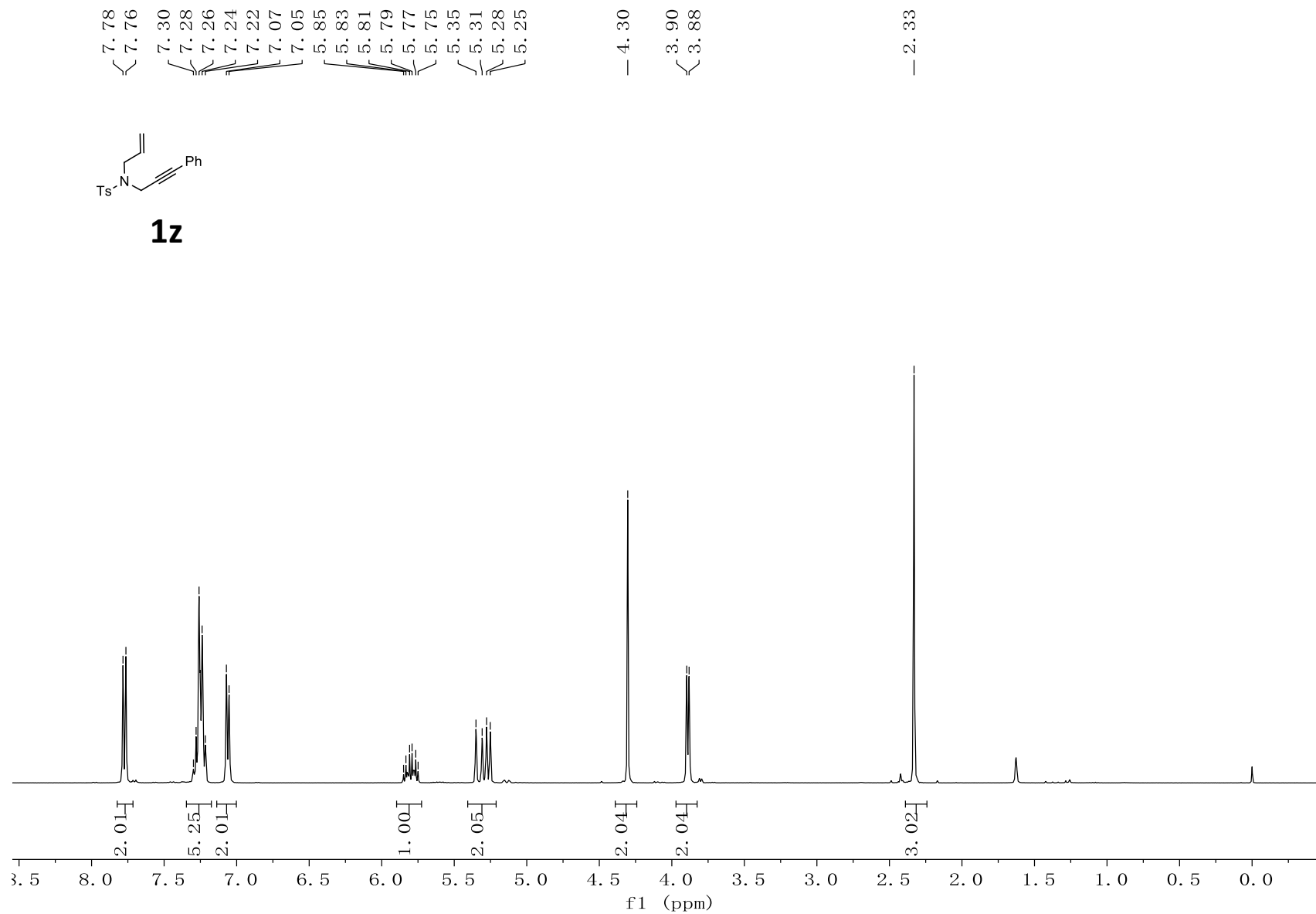
— 21.44

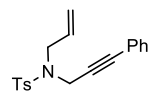
— 3.17



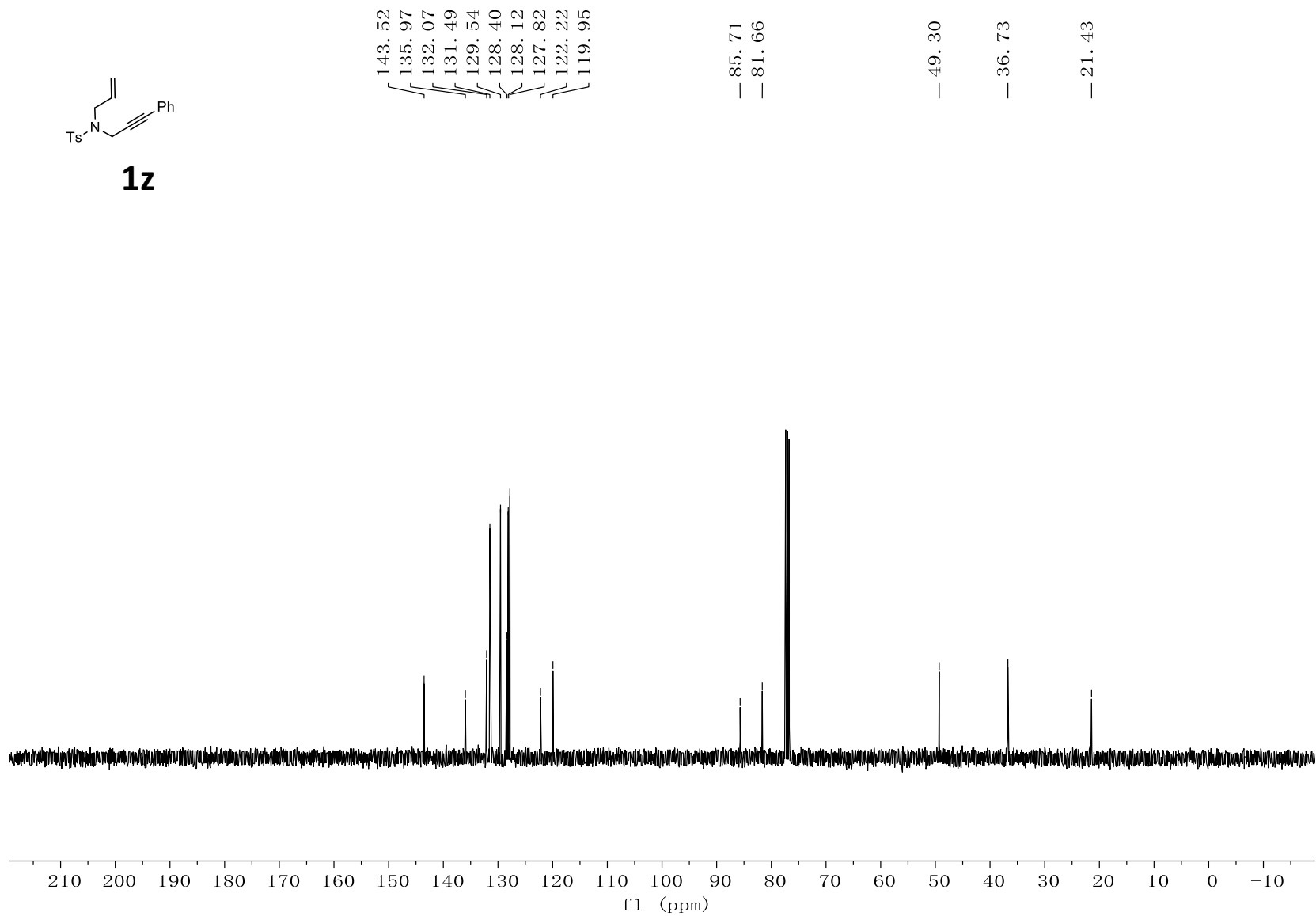


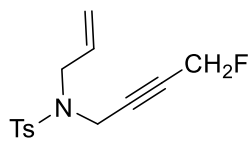
**1z**





**1z**





**1aa**

7.754  
7.733  
7.331  
7.311

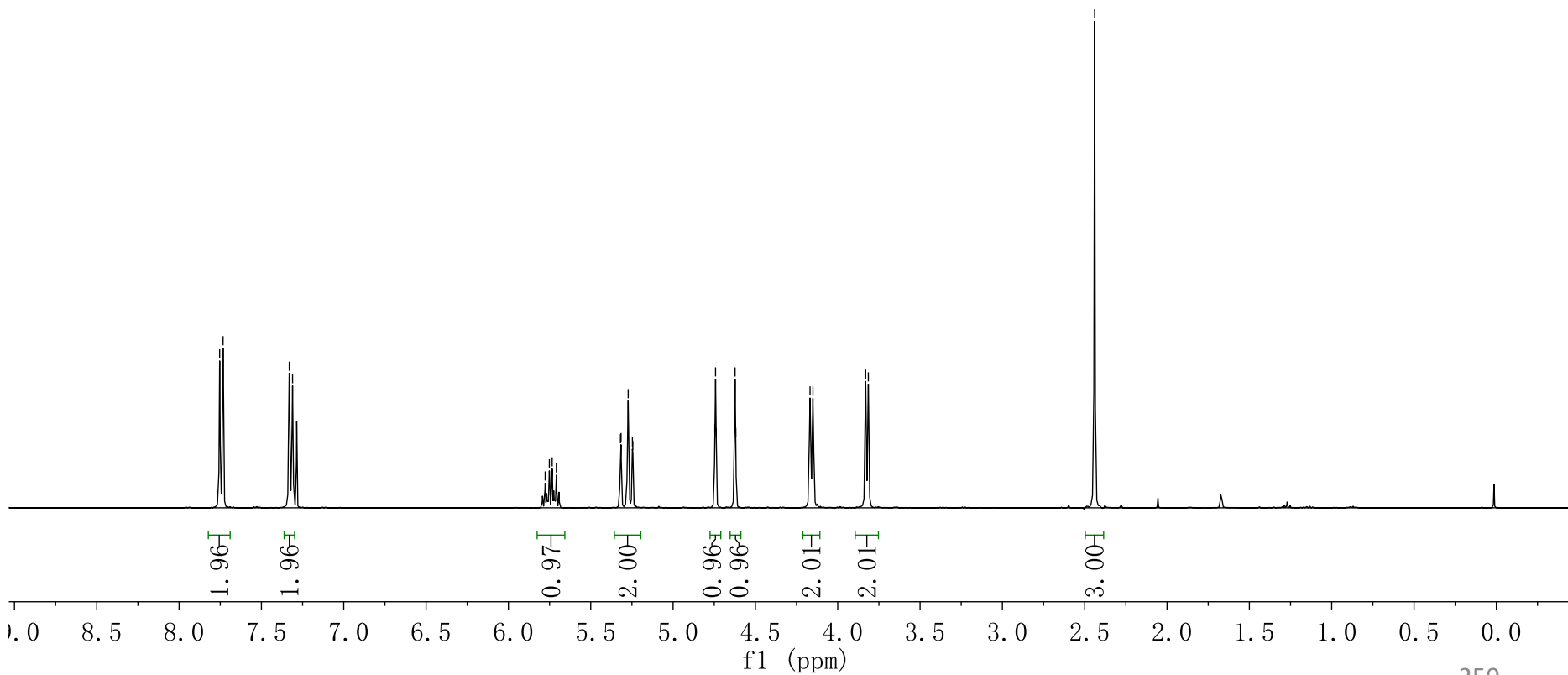
5.777  
5.751  
5.734  
5.709

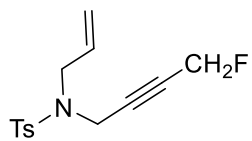
5.319  
5.316  
5.273

4.746  
4.742  
4.628

4.623  
4.618  
4.151  
3.830  
3.814

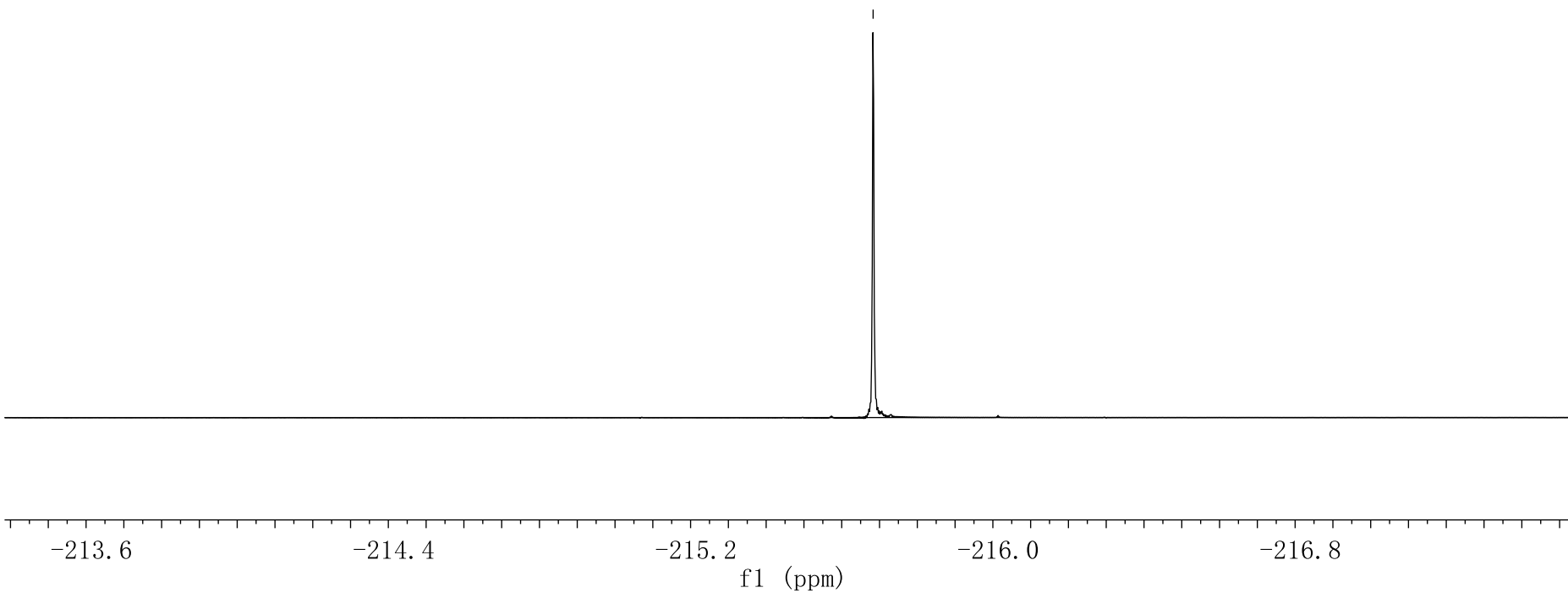
2.440

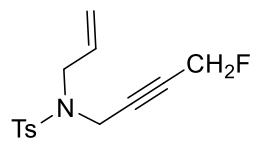




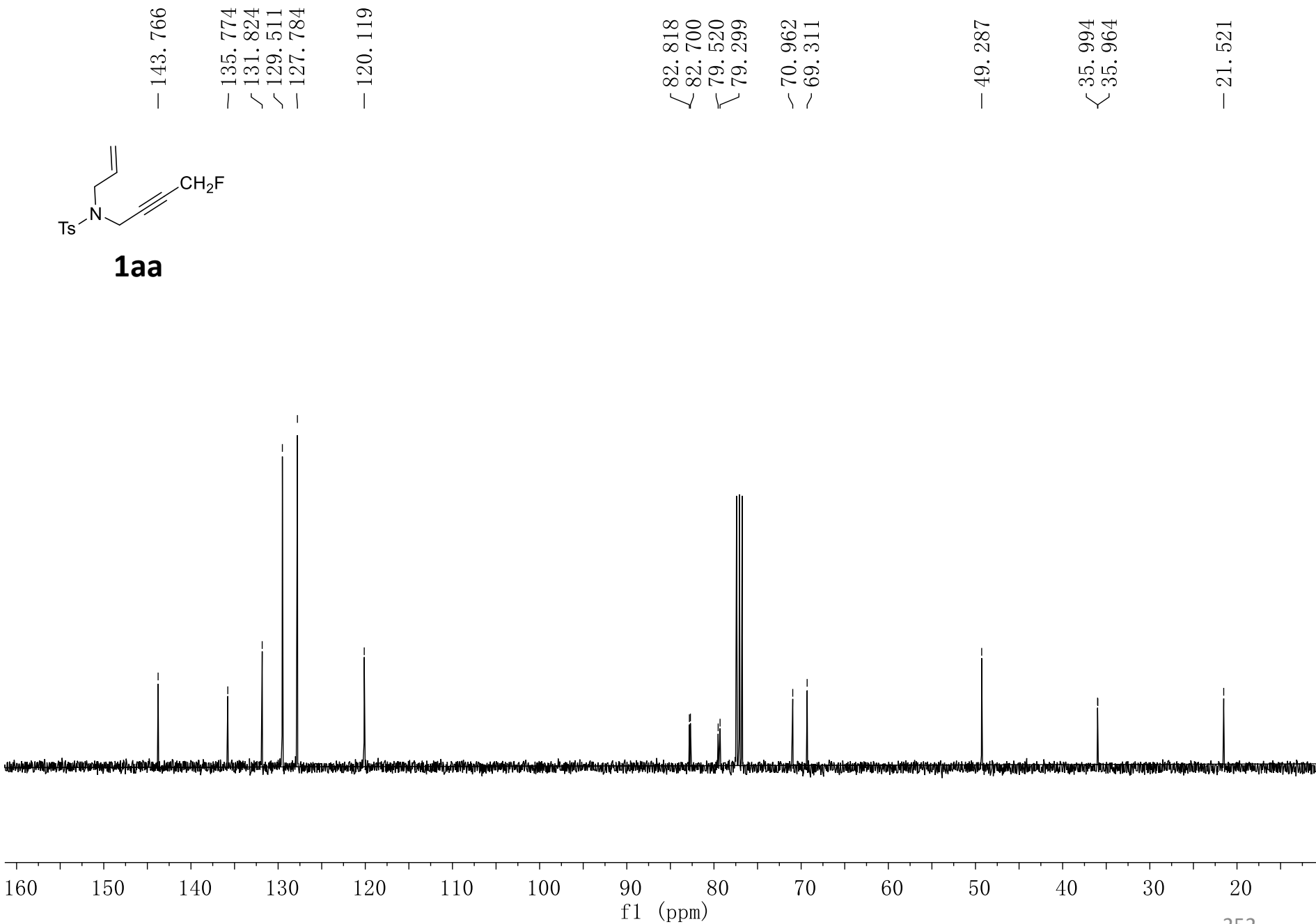
**1aa**

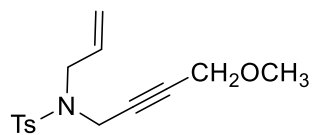
— -215.683



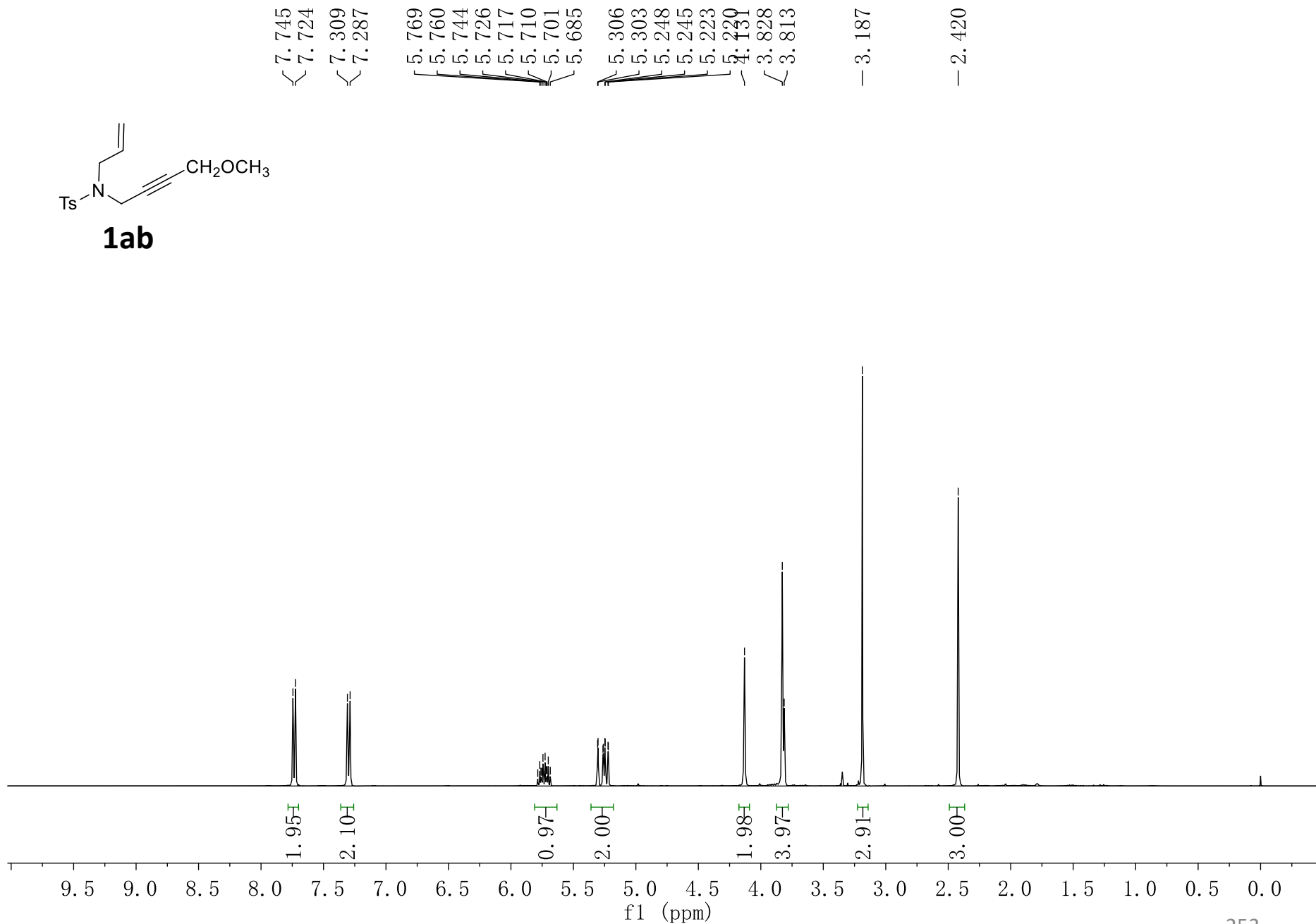


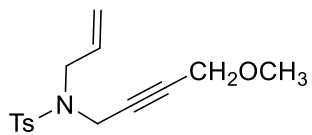
**1aa**





**1ab**





**1ab**

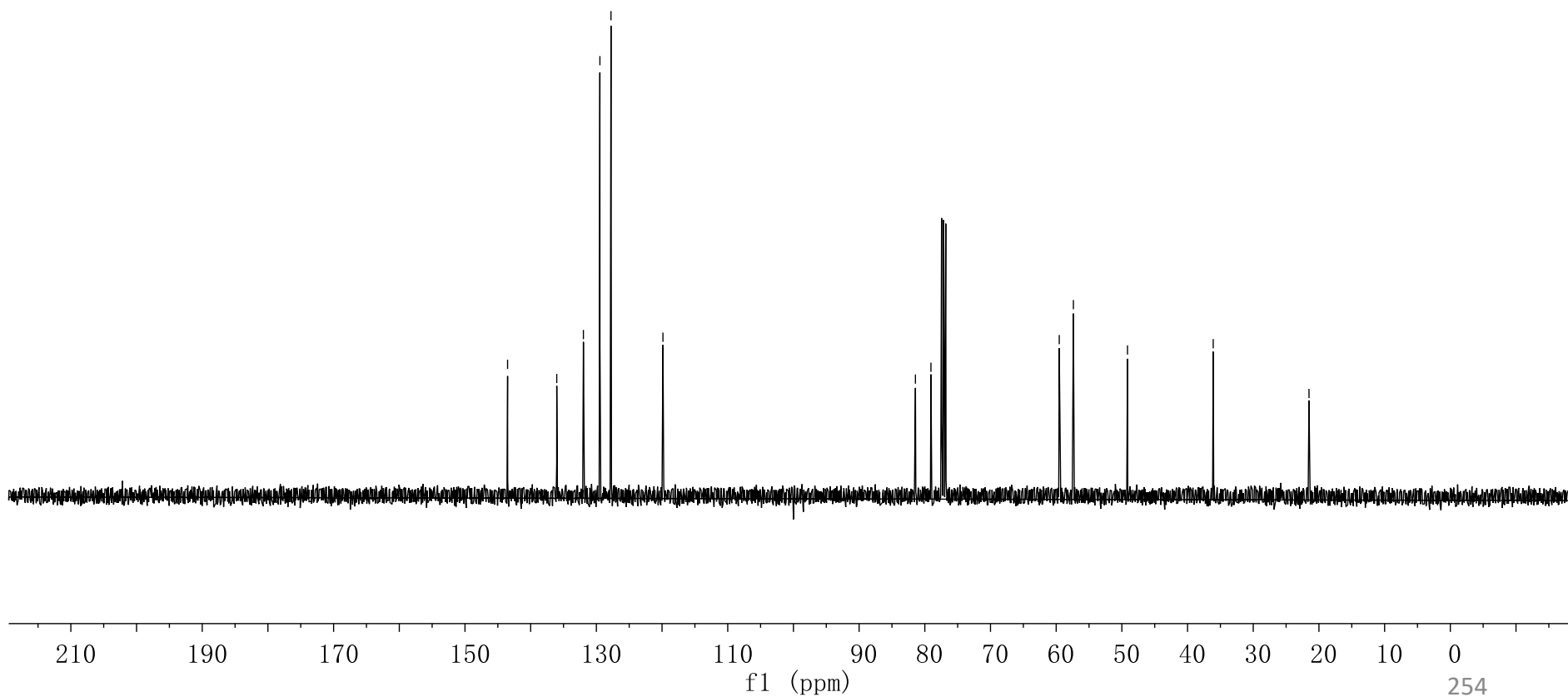
~143.515  
 ~136.029  
 ~131.972  
 ~129.462  
 ~127.772  
 ~119.865

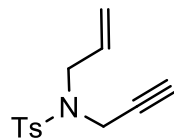
~81.427  
 ~79.065

~59.533  
 ~57.381  
 ~49.144

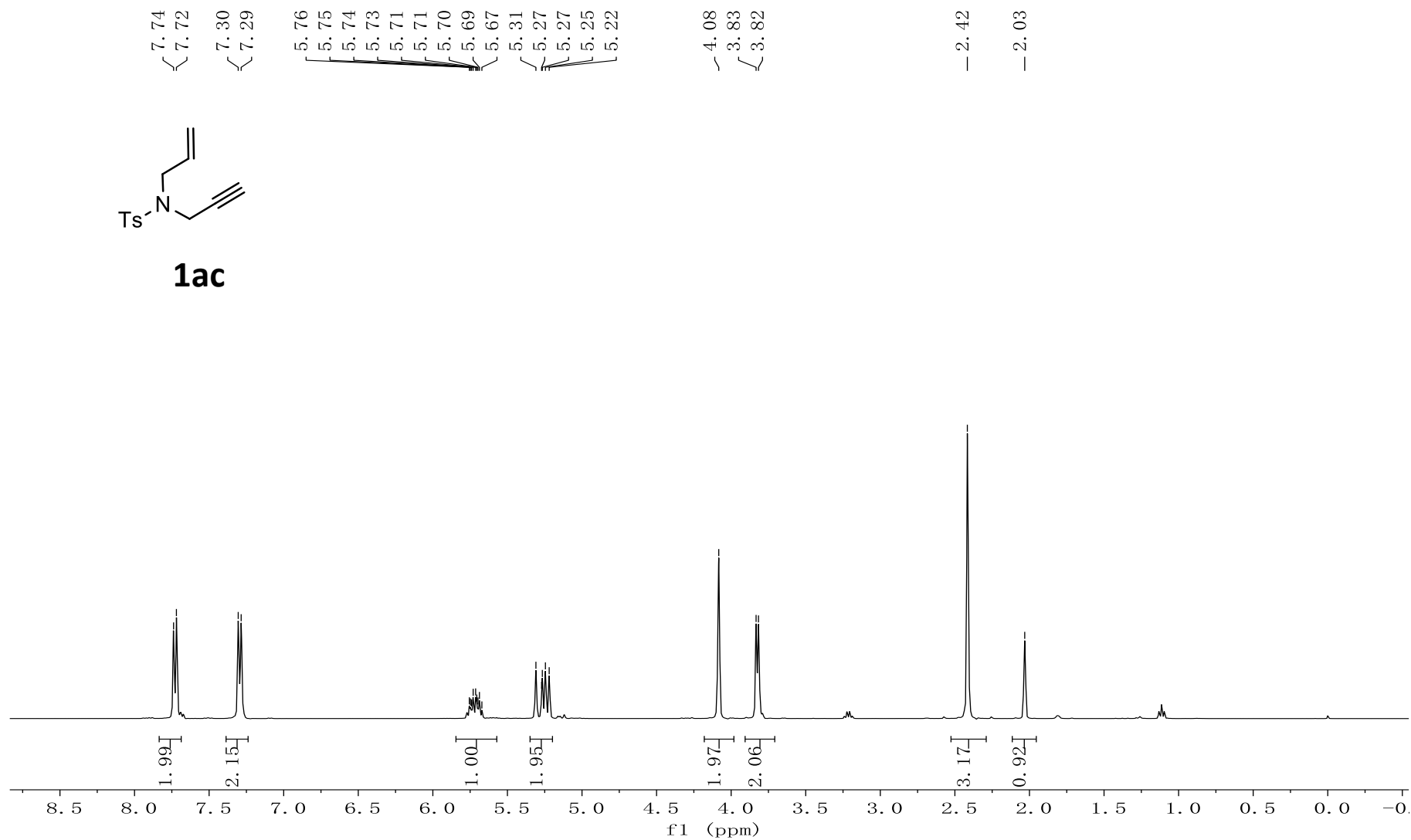
—36.094

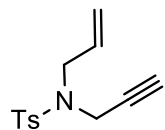
—21.512



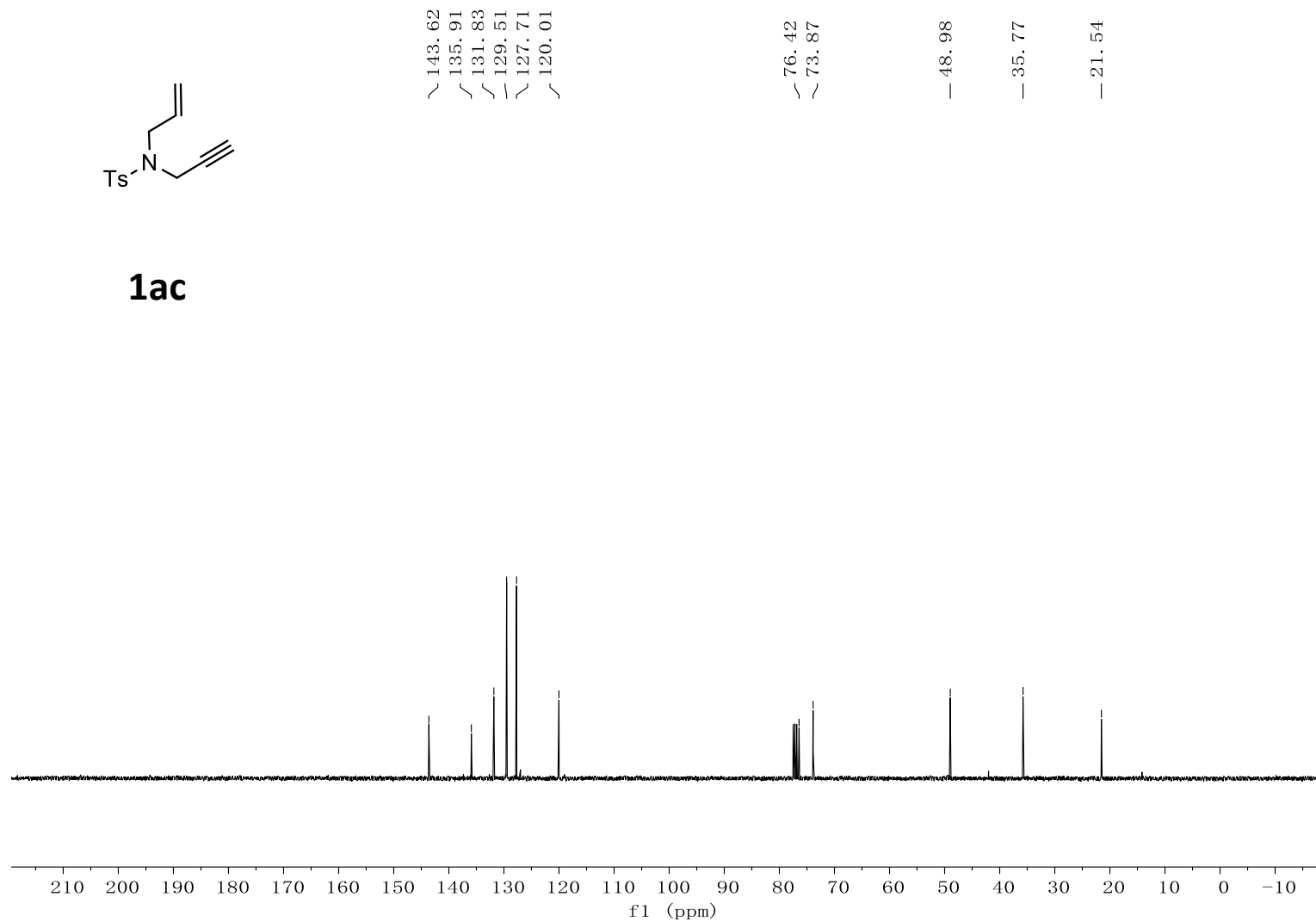


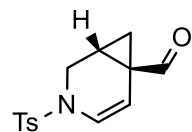
**1ac**



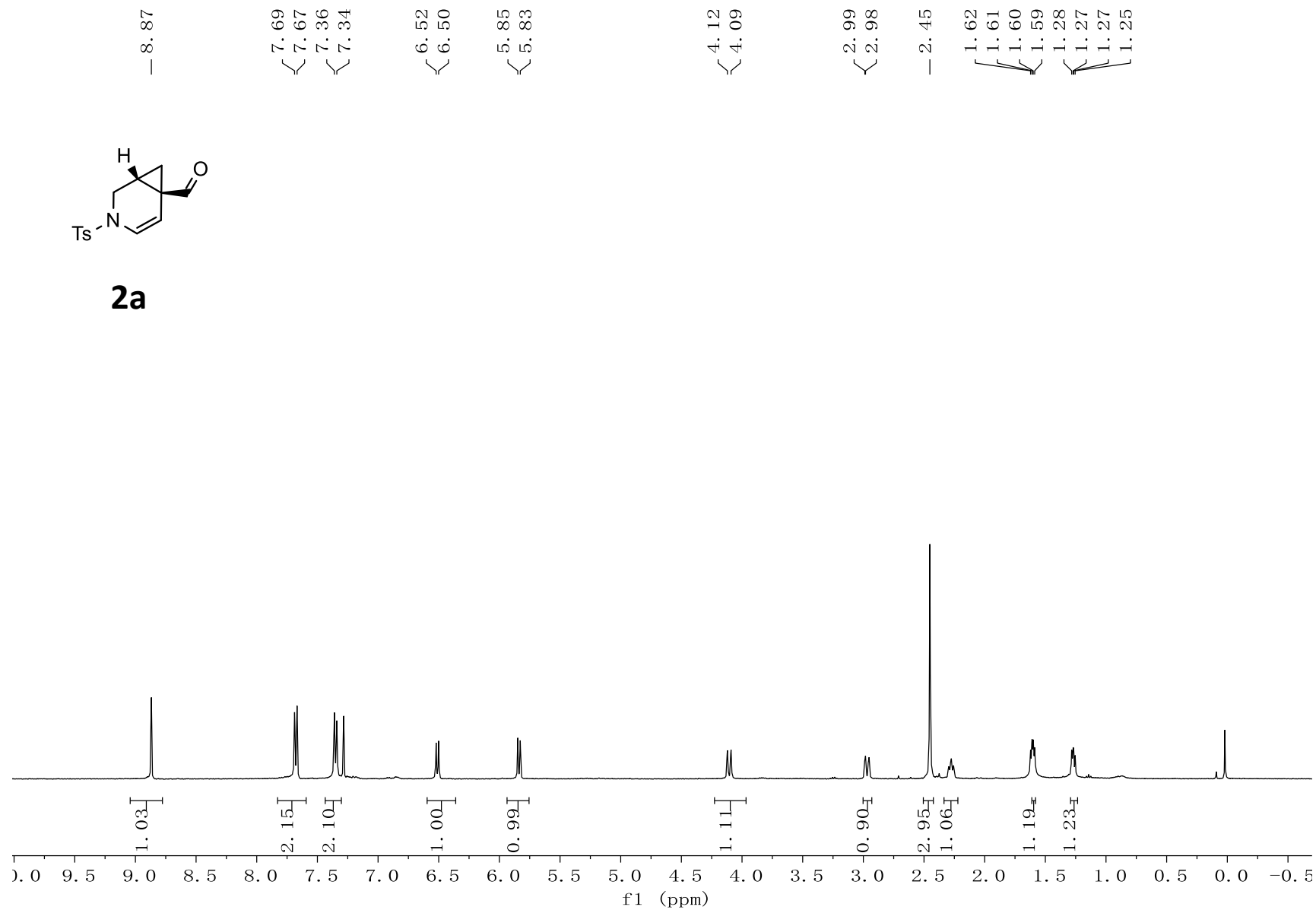


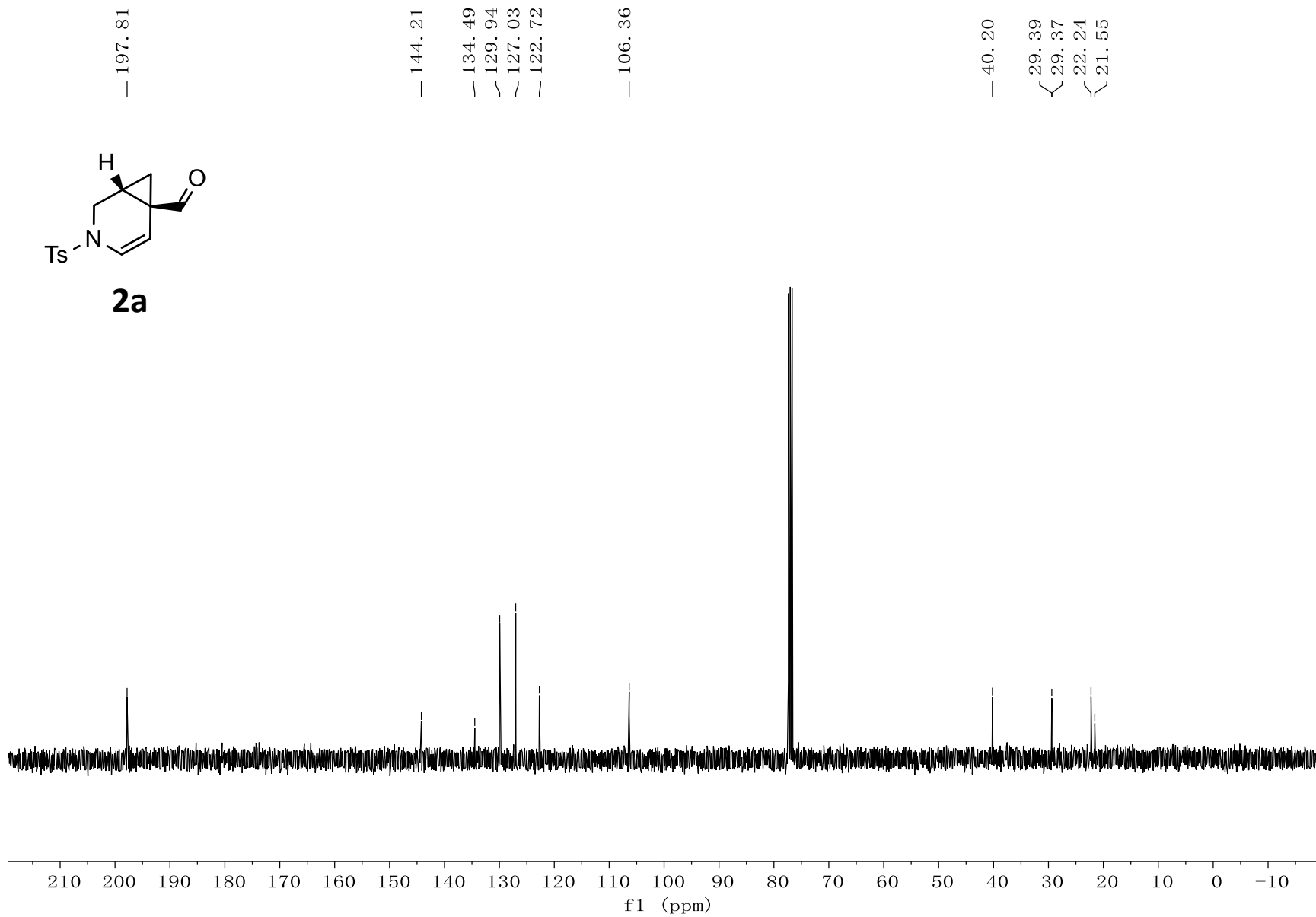
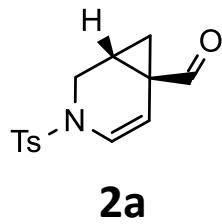
**1ac**

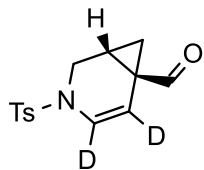




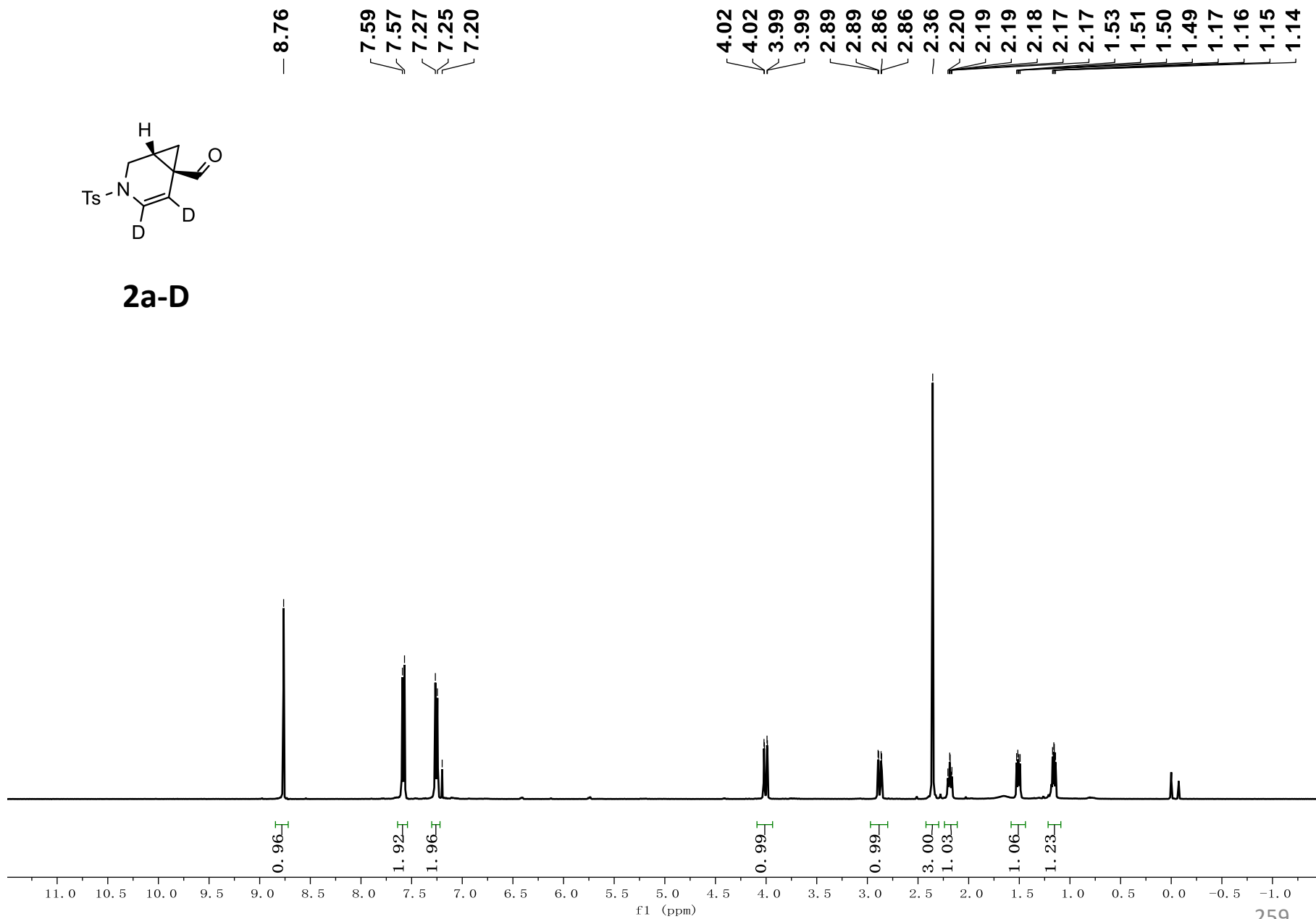
**2a**

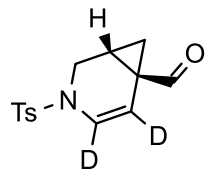




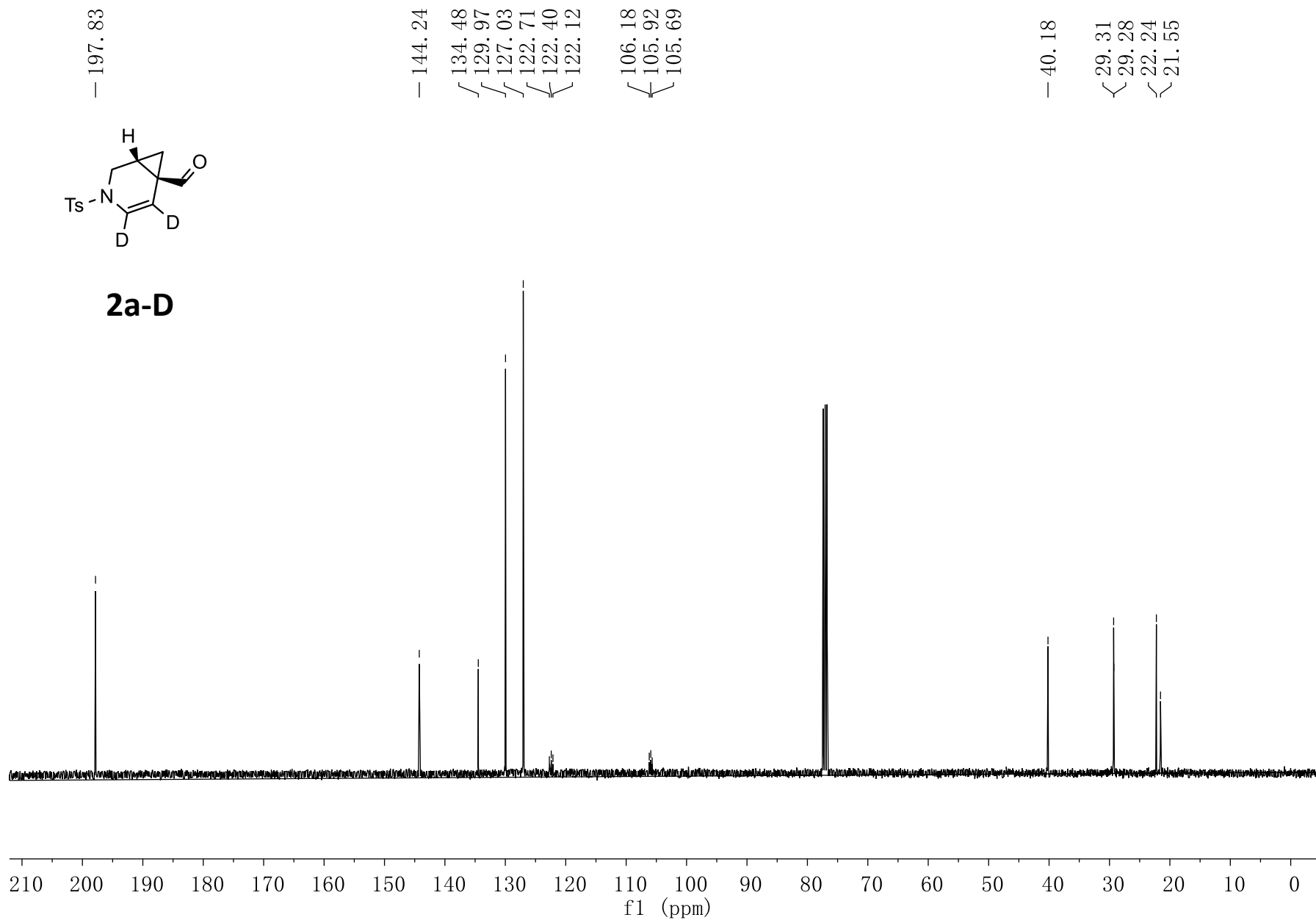


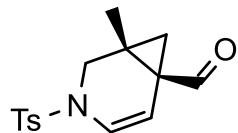
**2a-D**



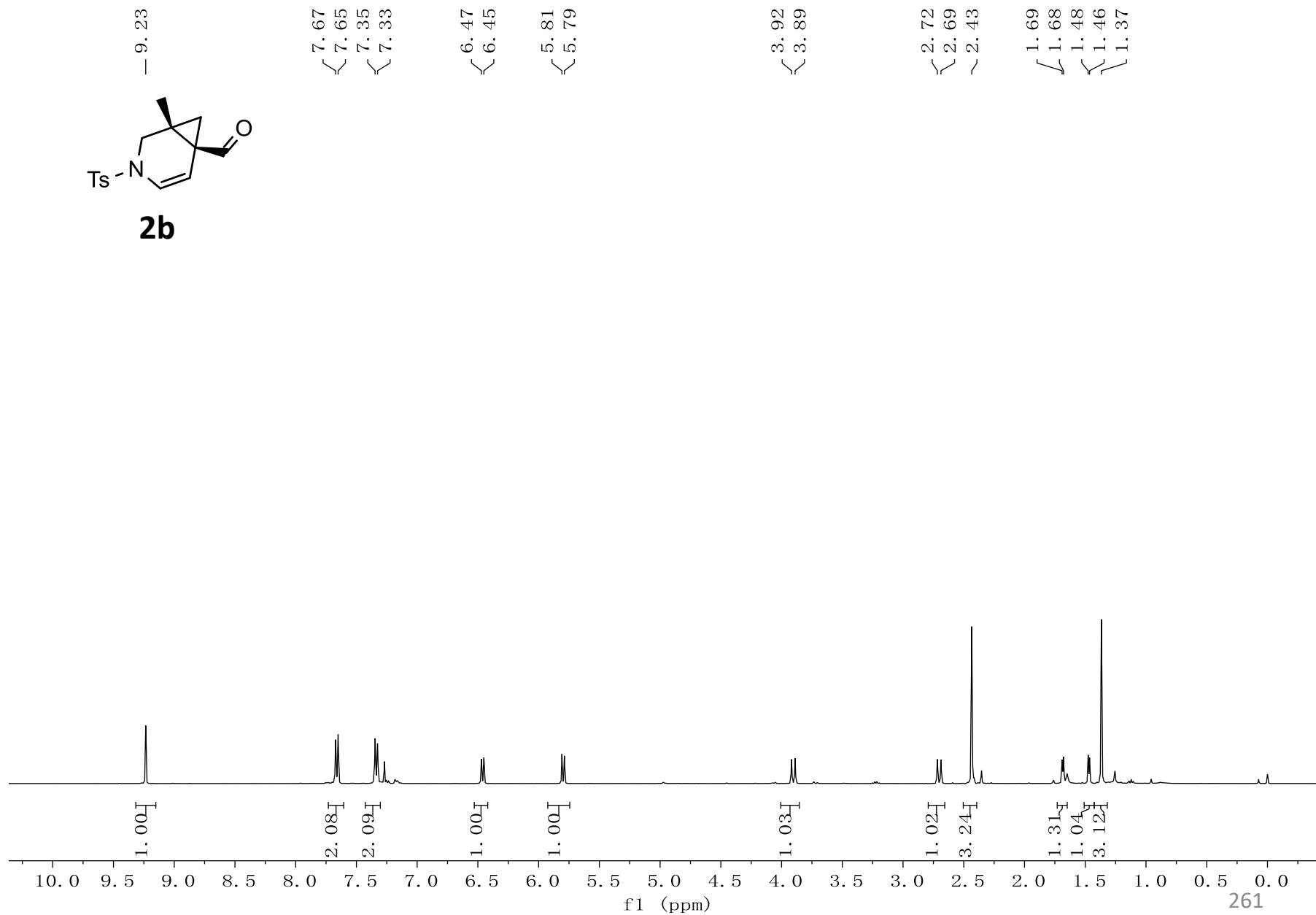


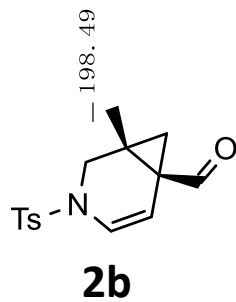
**2a-D**





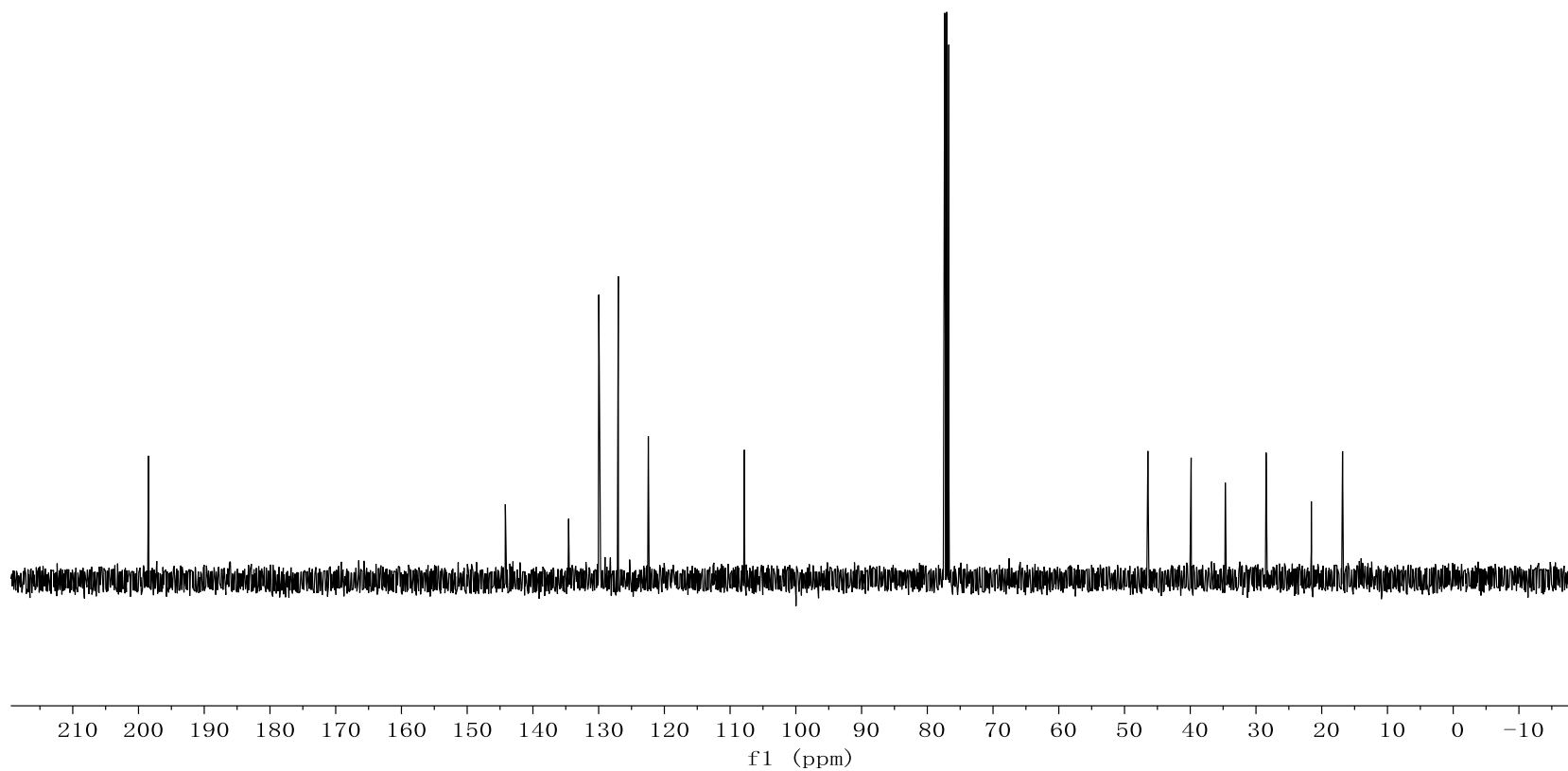
**2b**

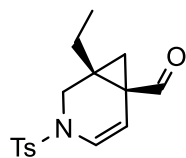




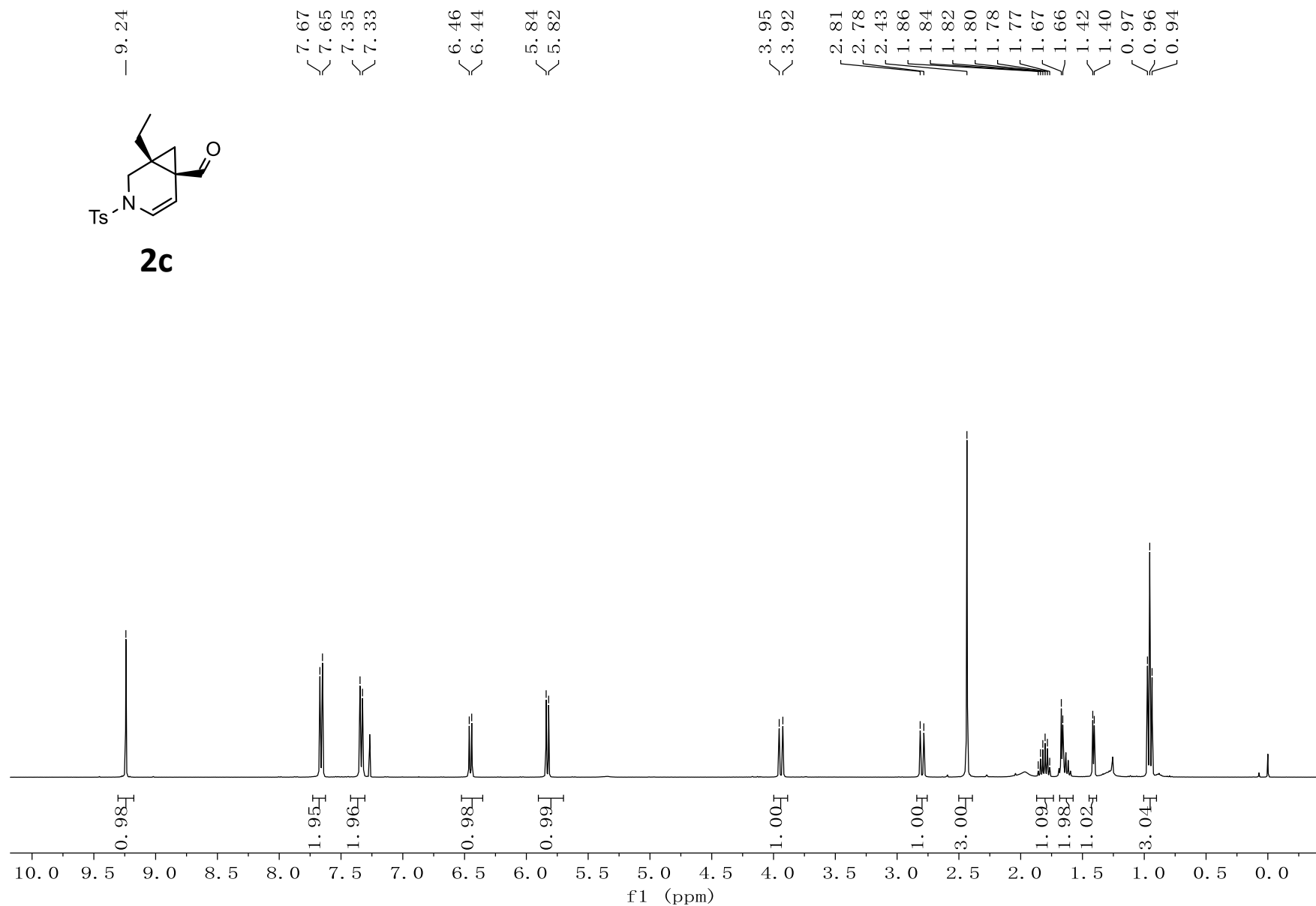
— 144.19  
 — 134.57  
 ~ 129.98  
 ~ 127.01  
 — 122.44  
 — 107.84

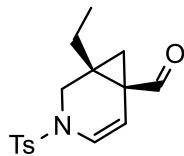
\ 46.45  
 \ 39.86  
 ~ 34.67  
 ~ 28.46  
 ~ 21.58  
 / 16.83



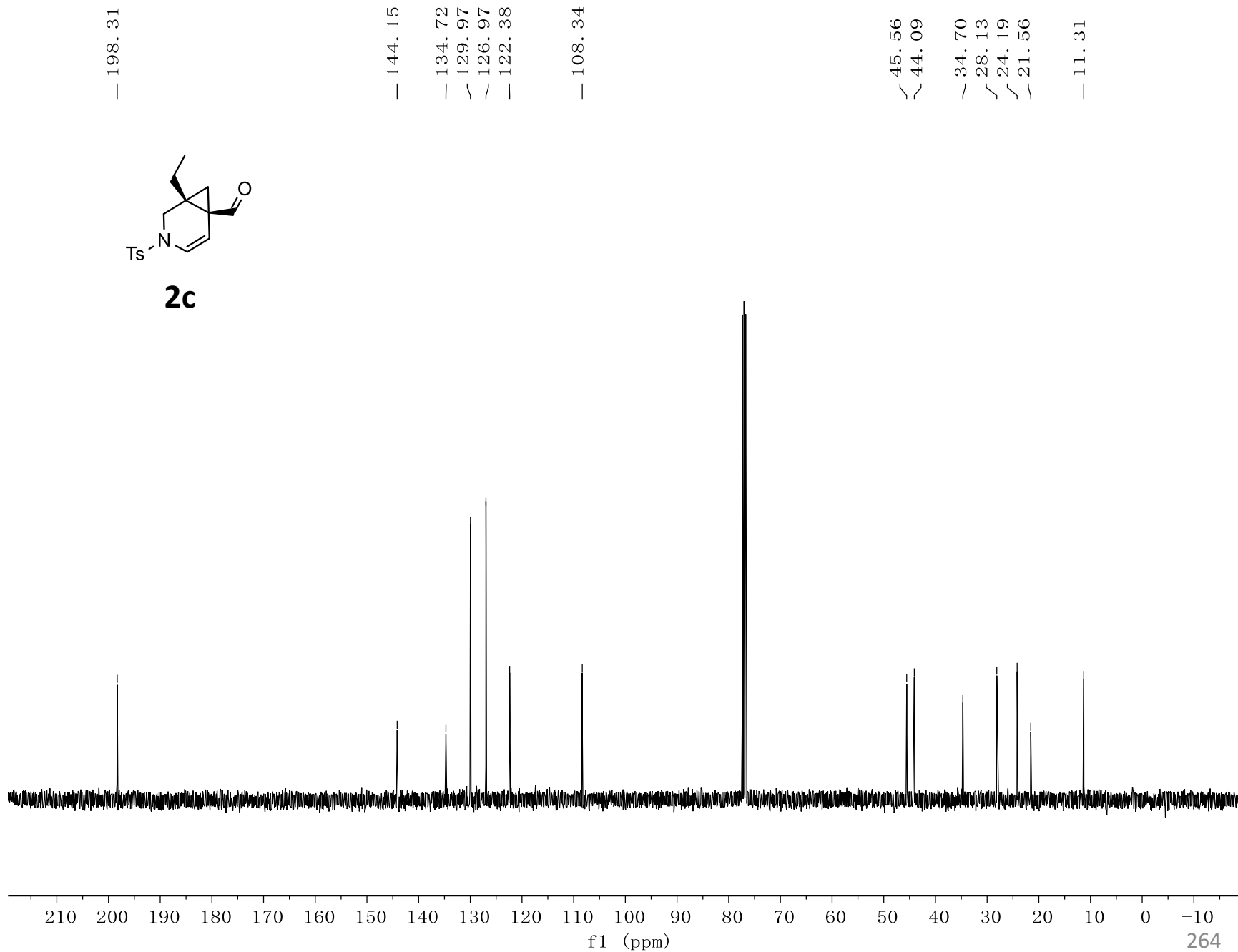


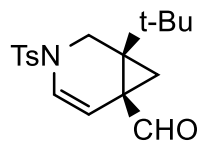
**2c**



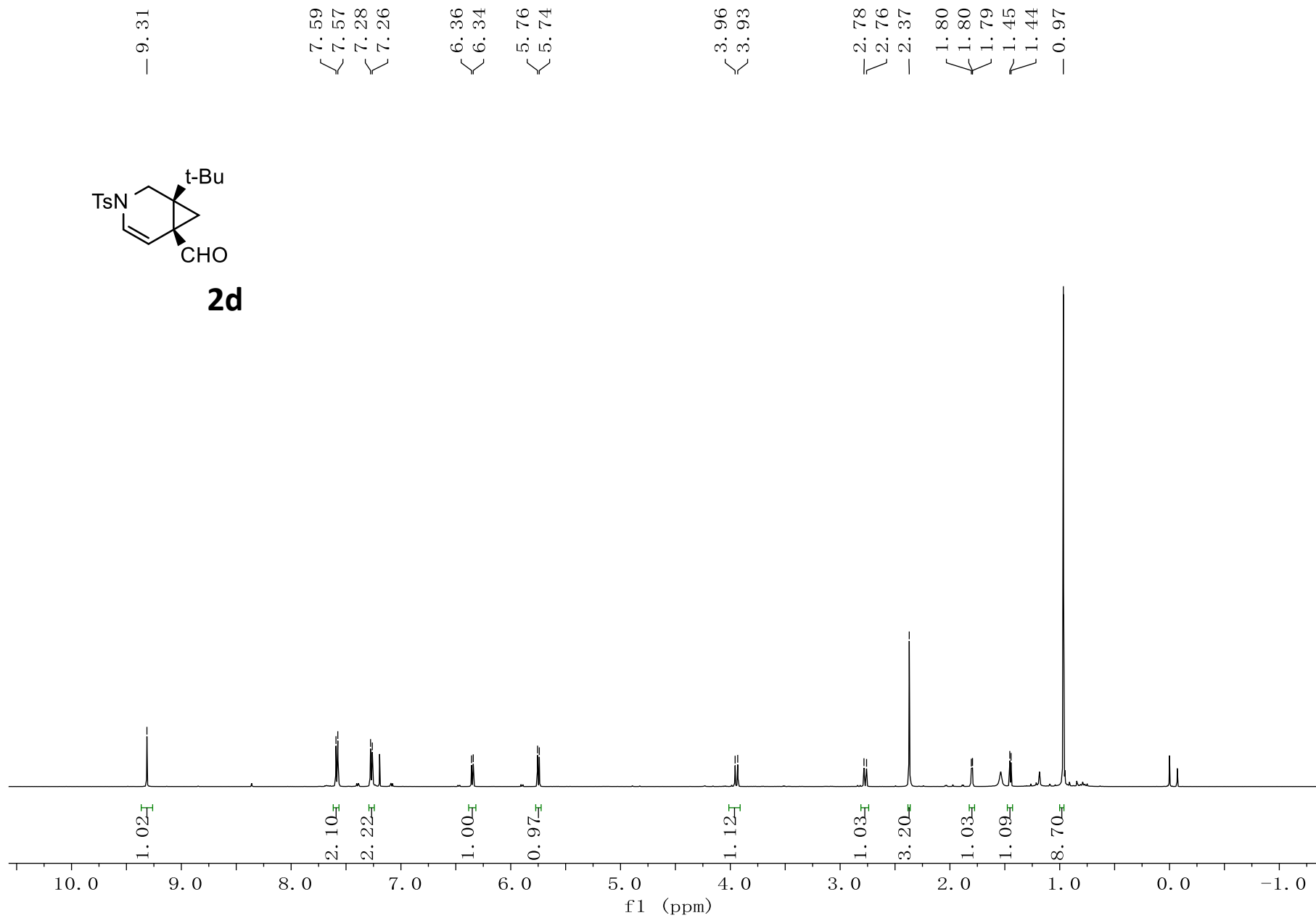


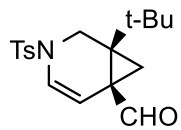
**2c**



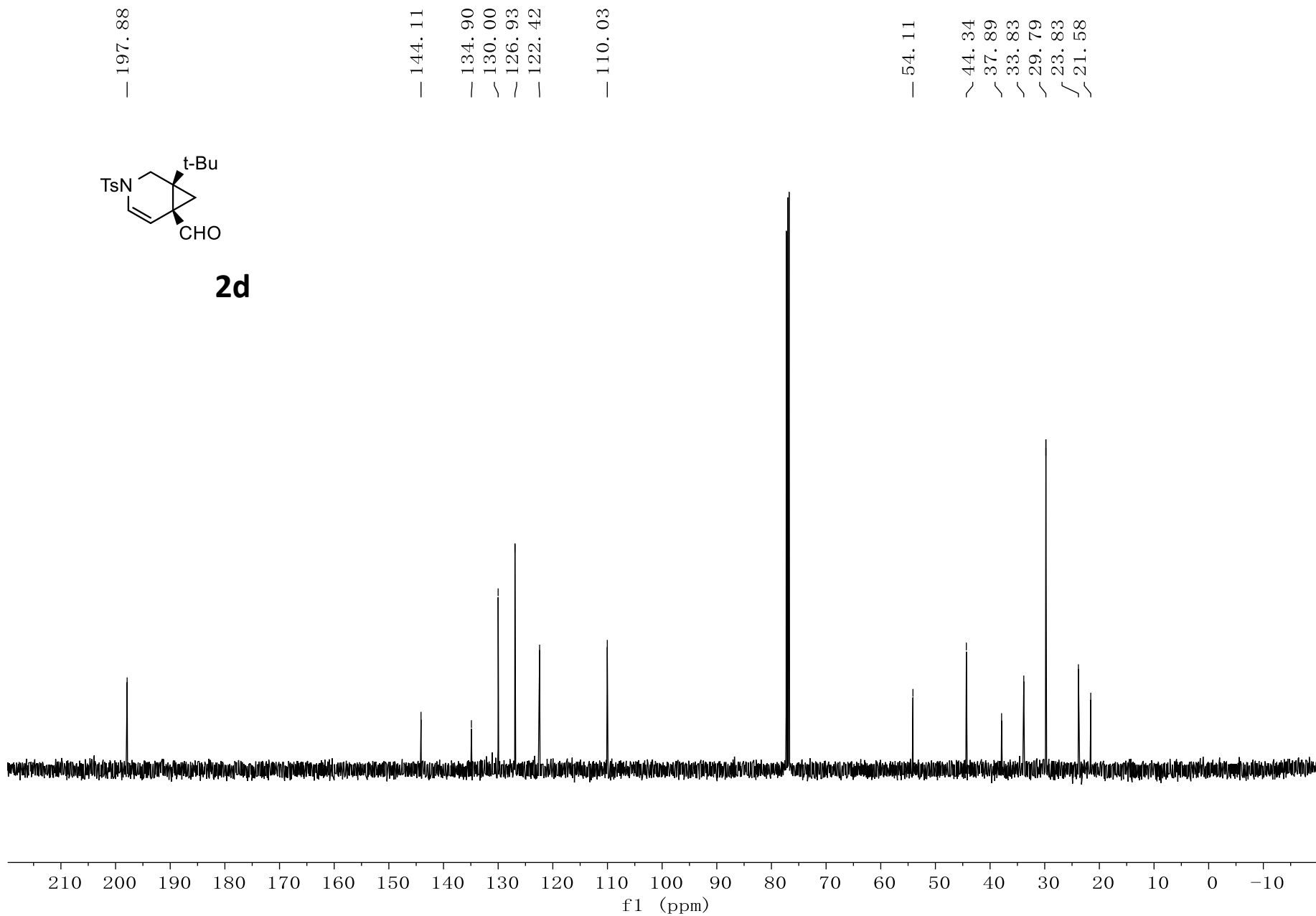


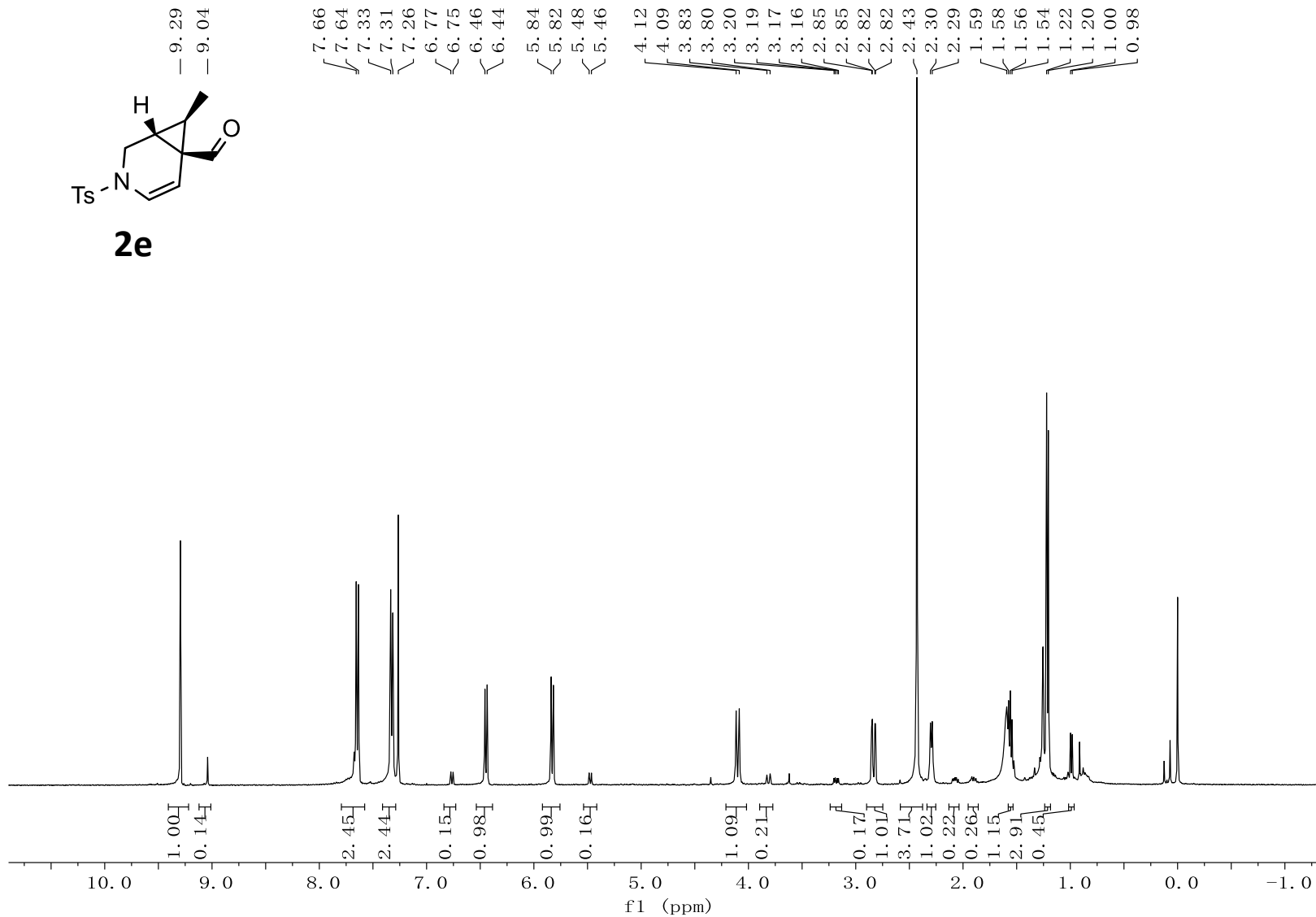
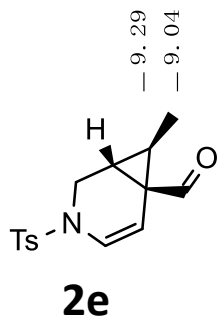
**2d**

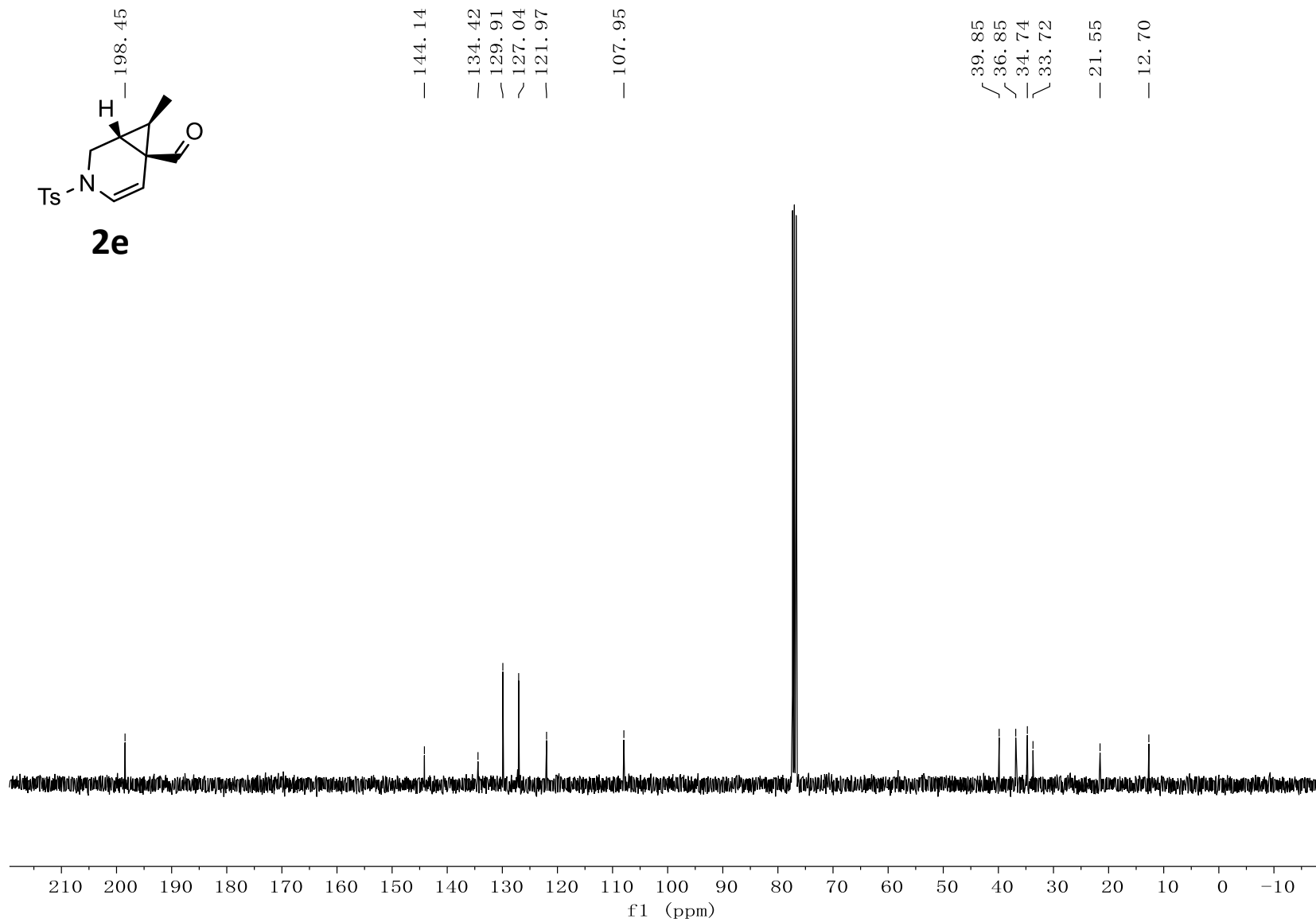
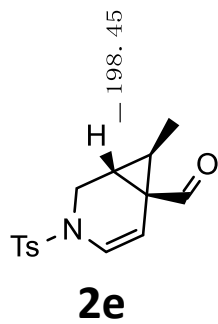


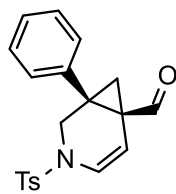


**2d**

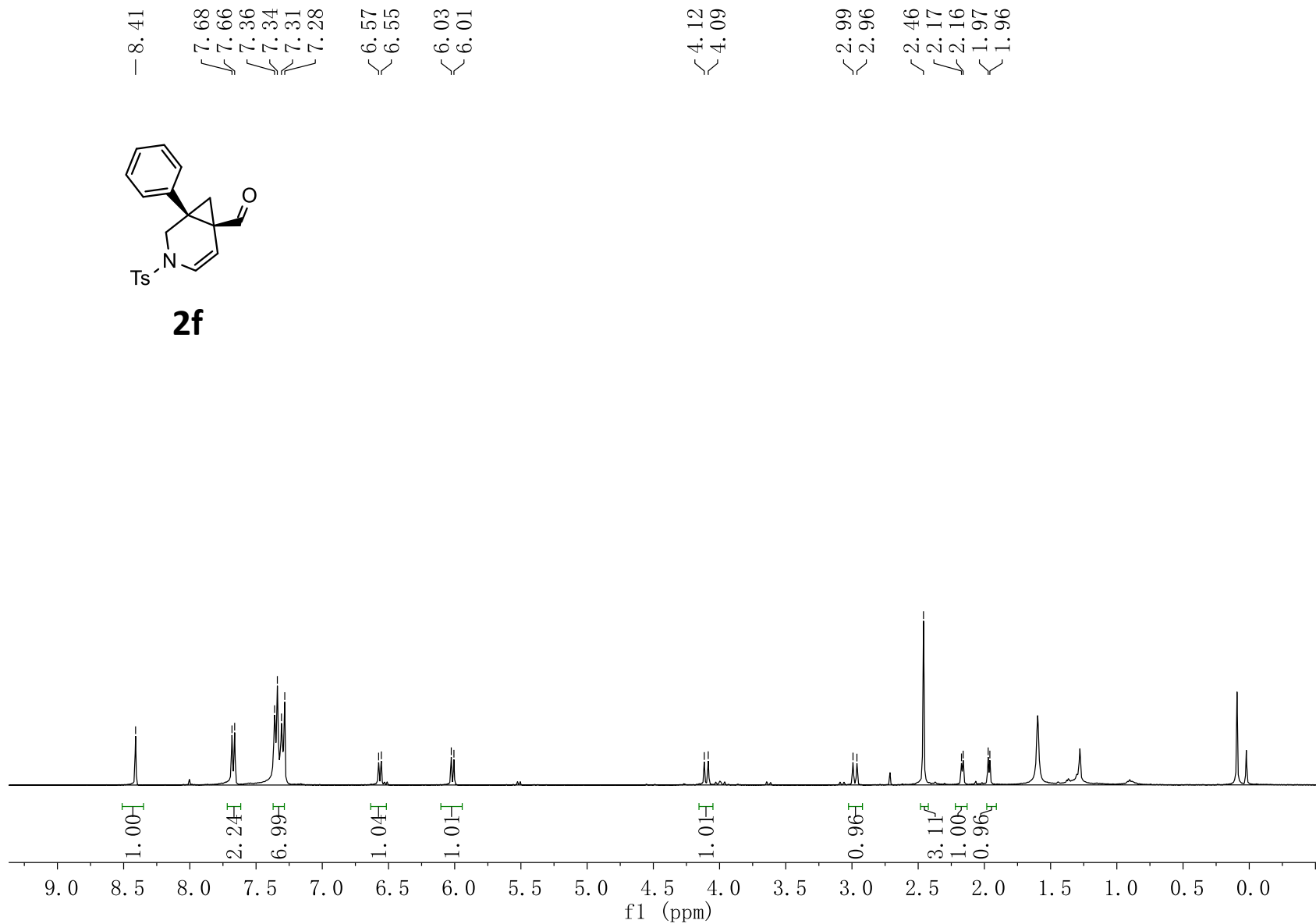


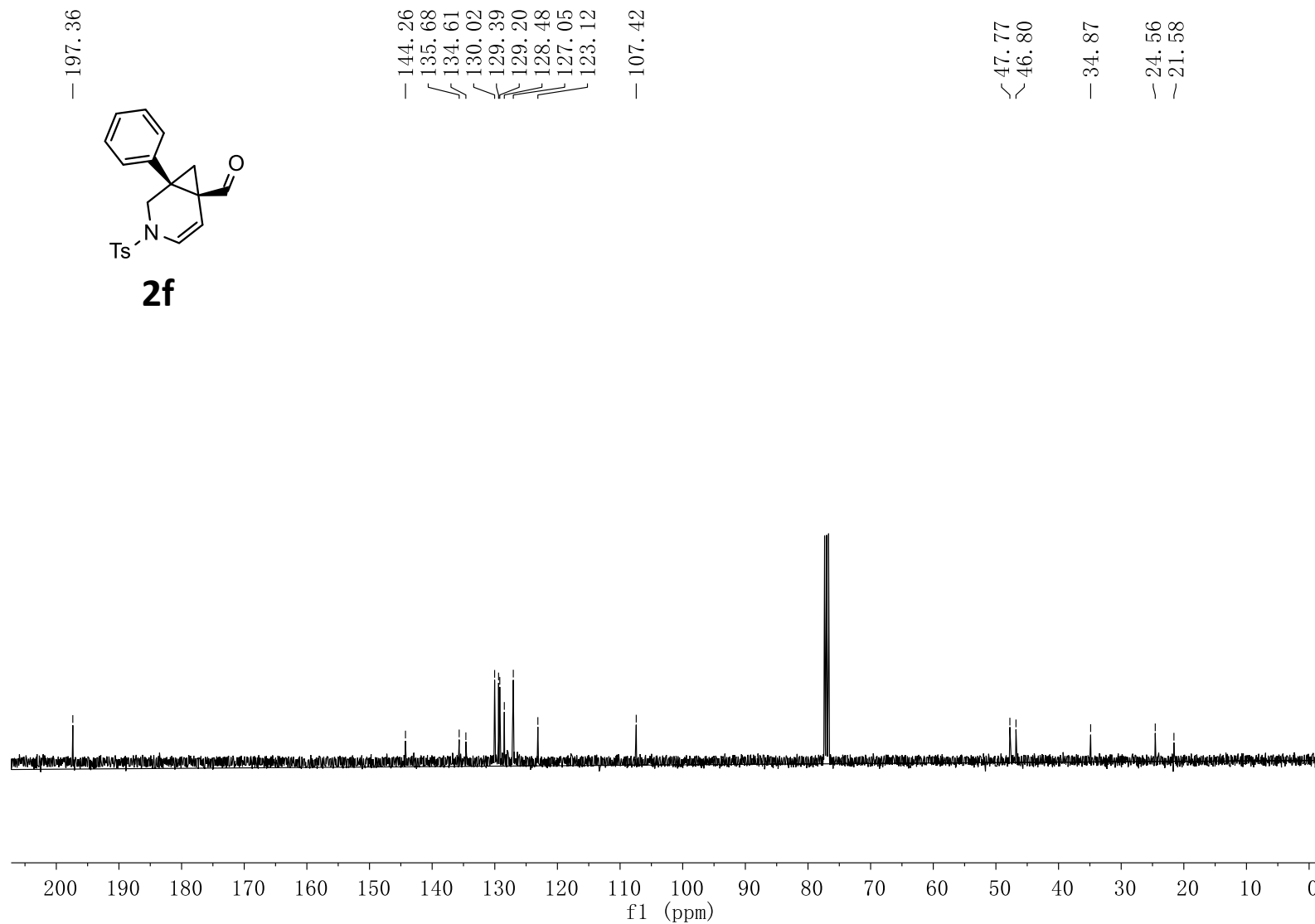
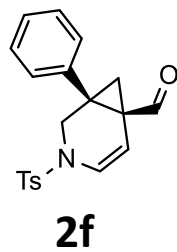


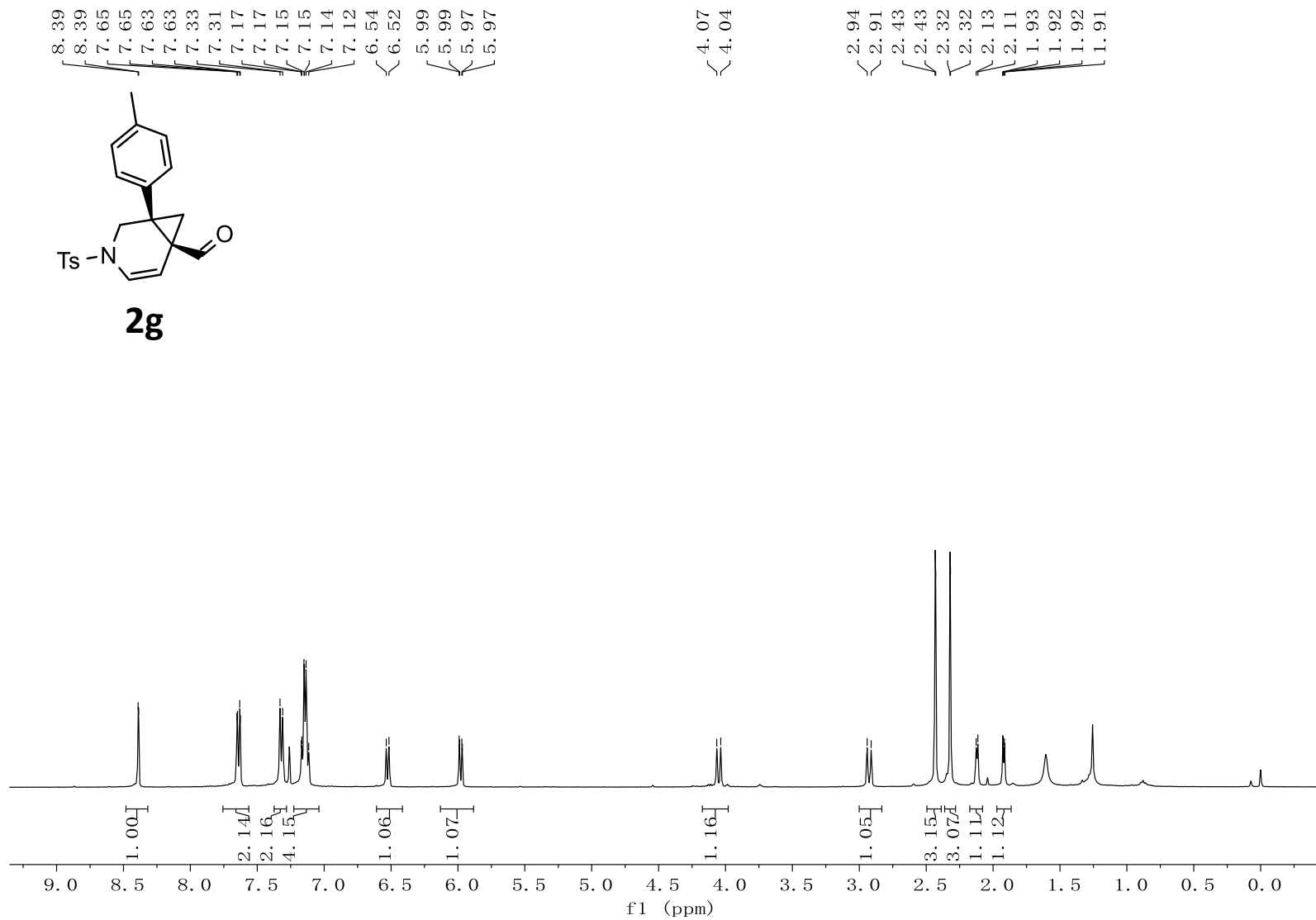
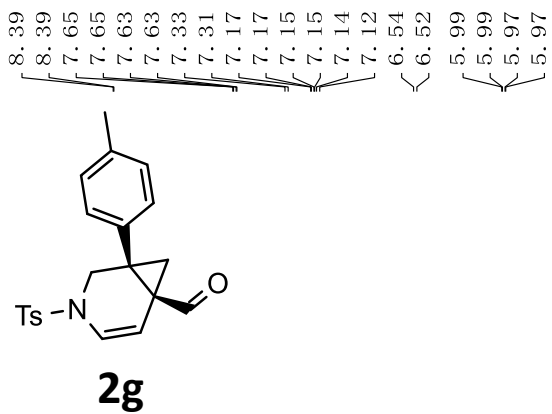


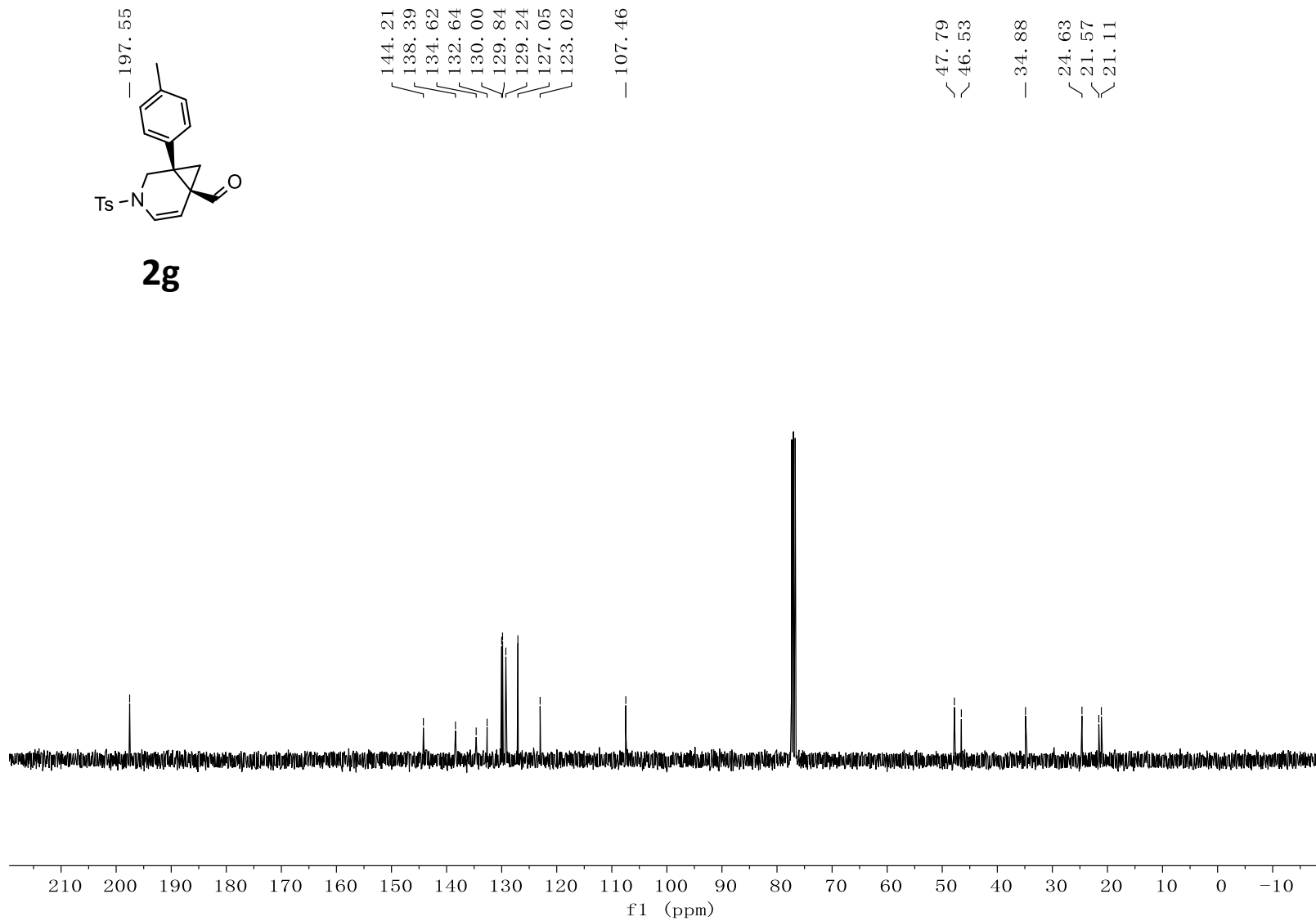
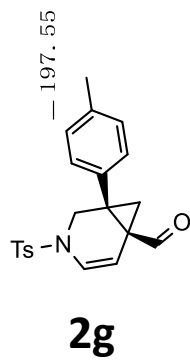


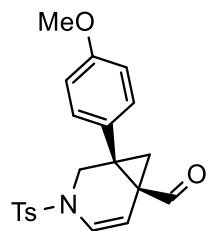
**2f**



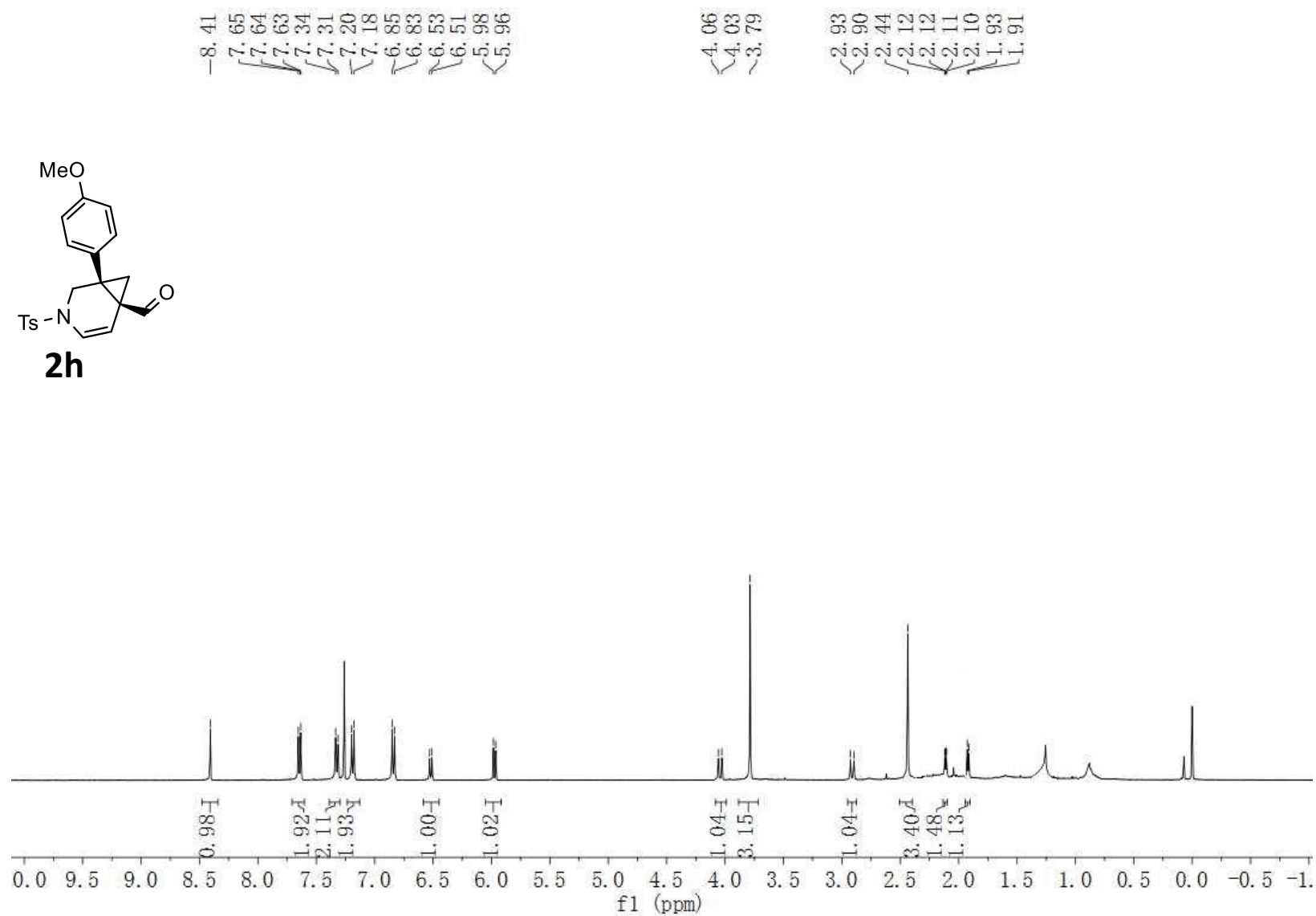


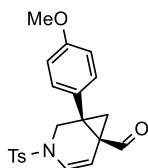




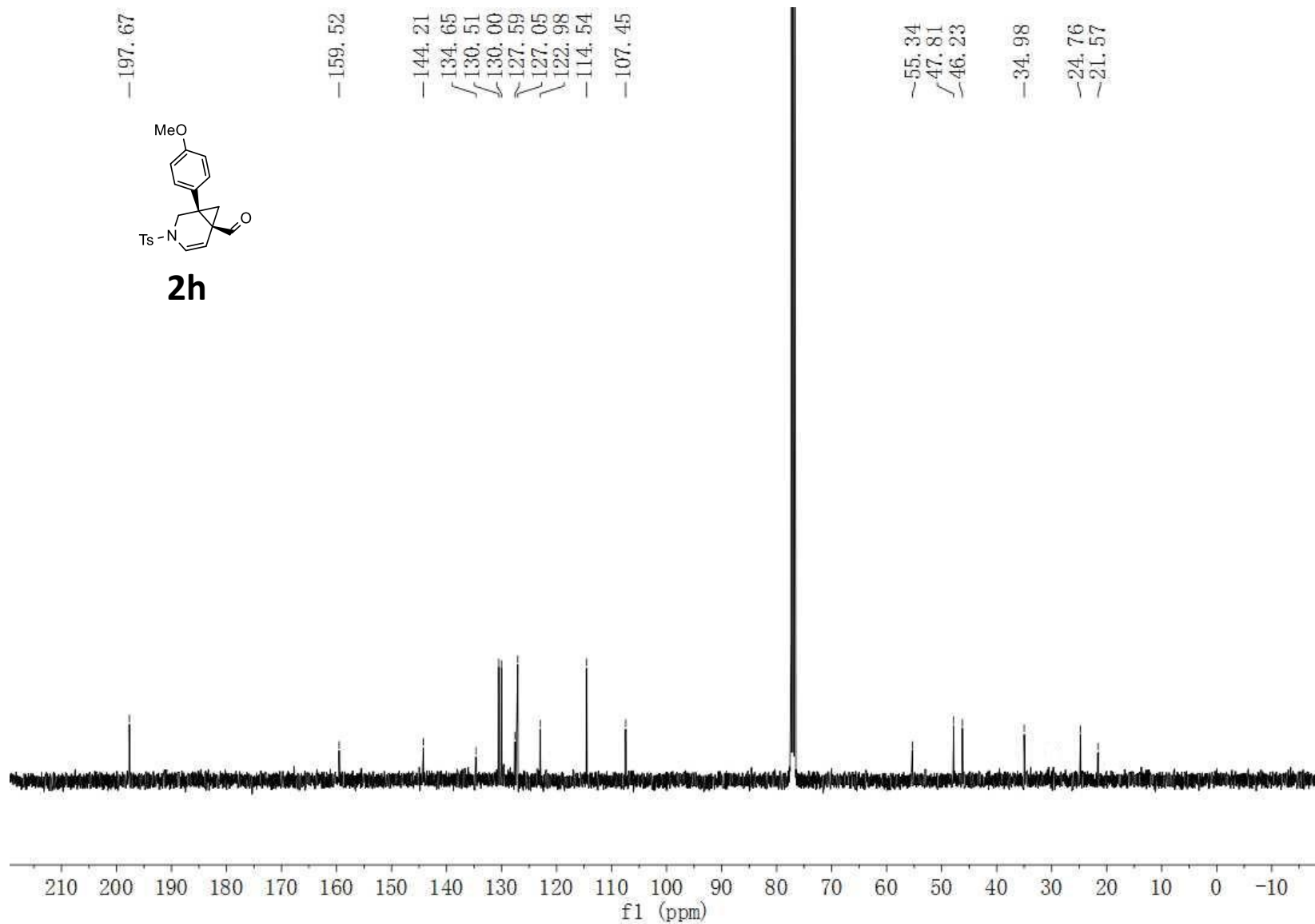


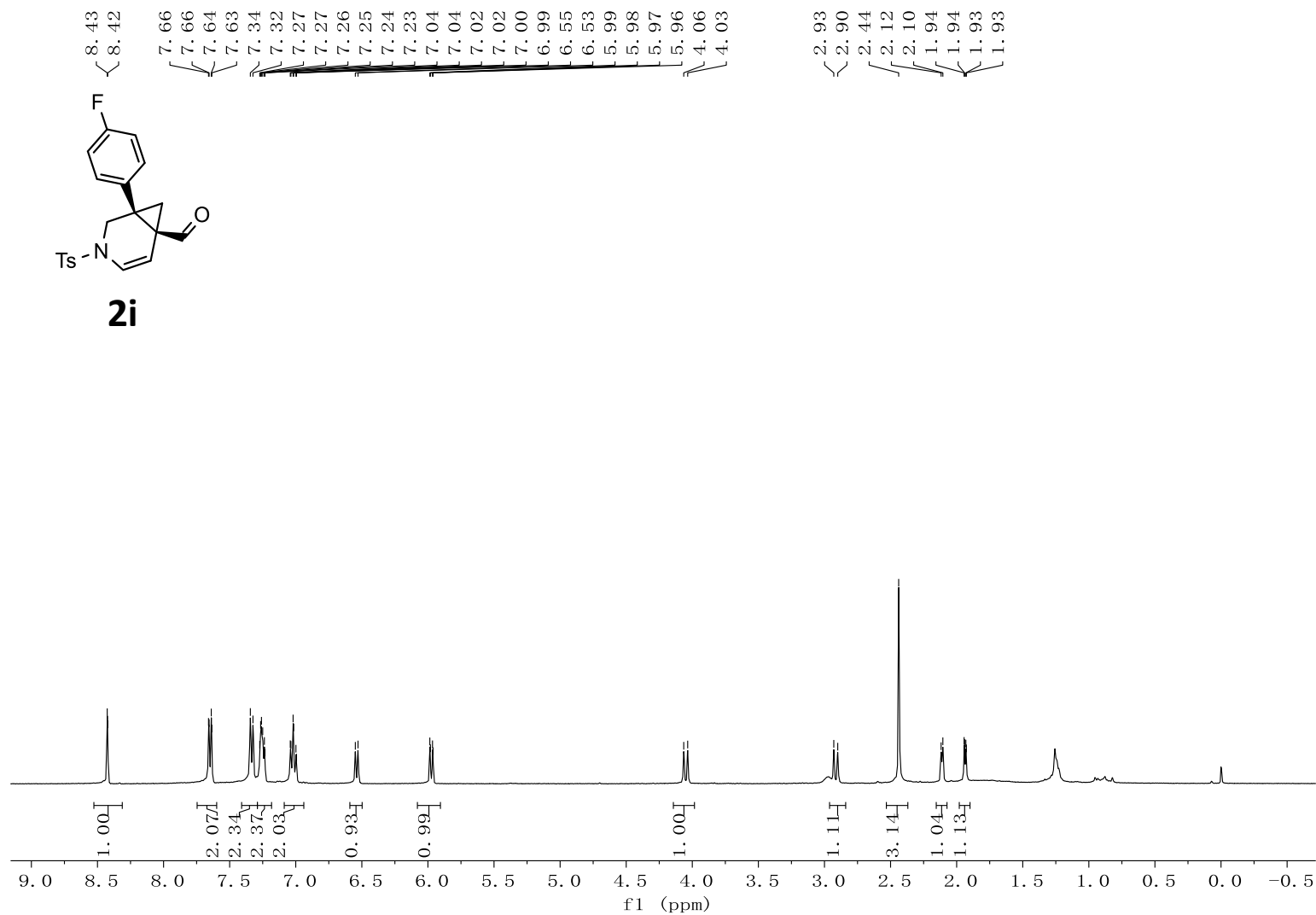
**2h**

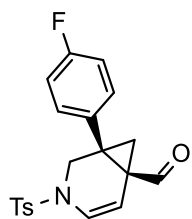




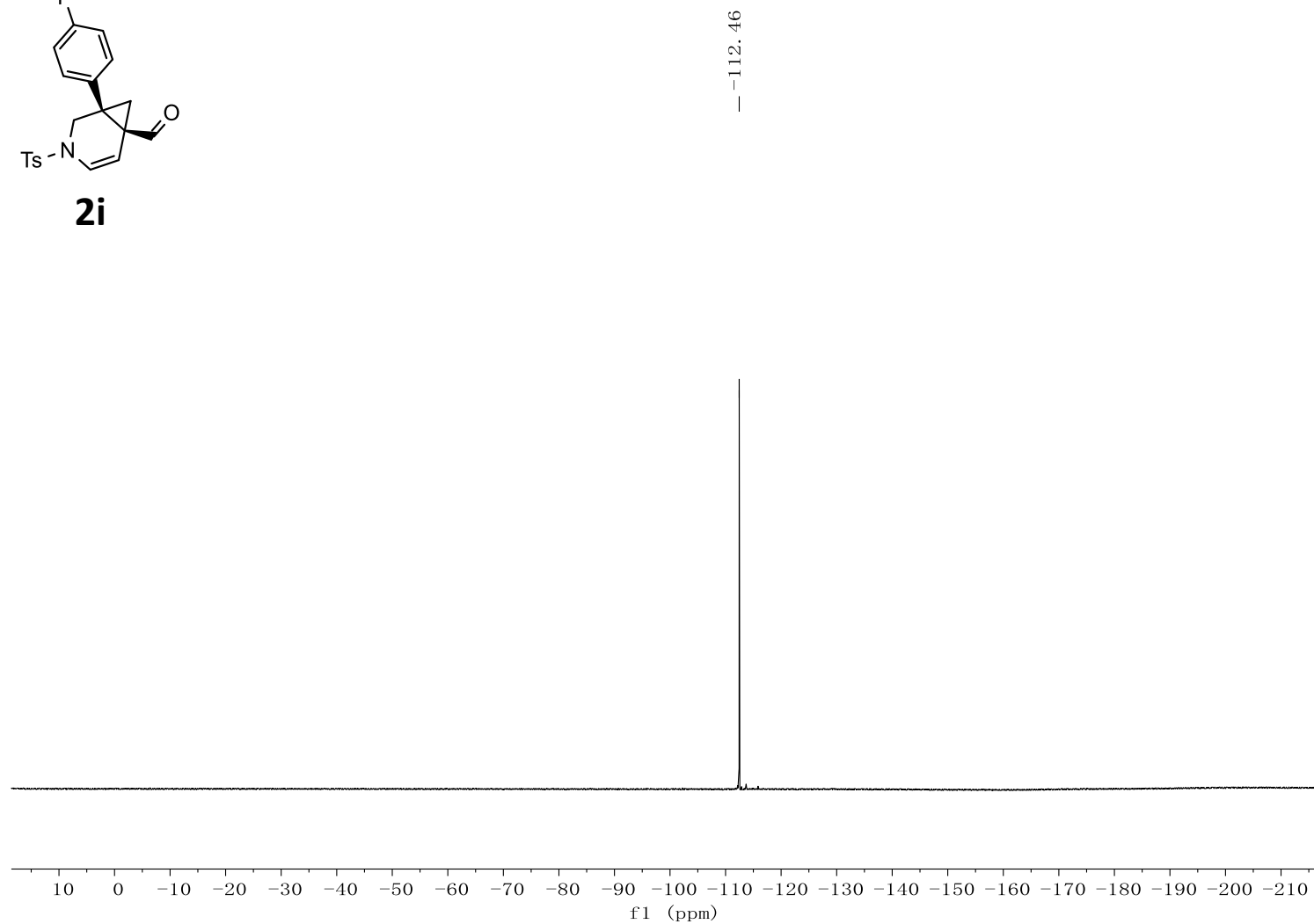
**2h**

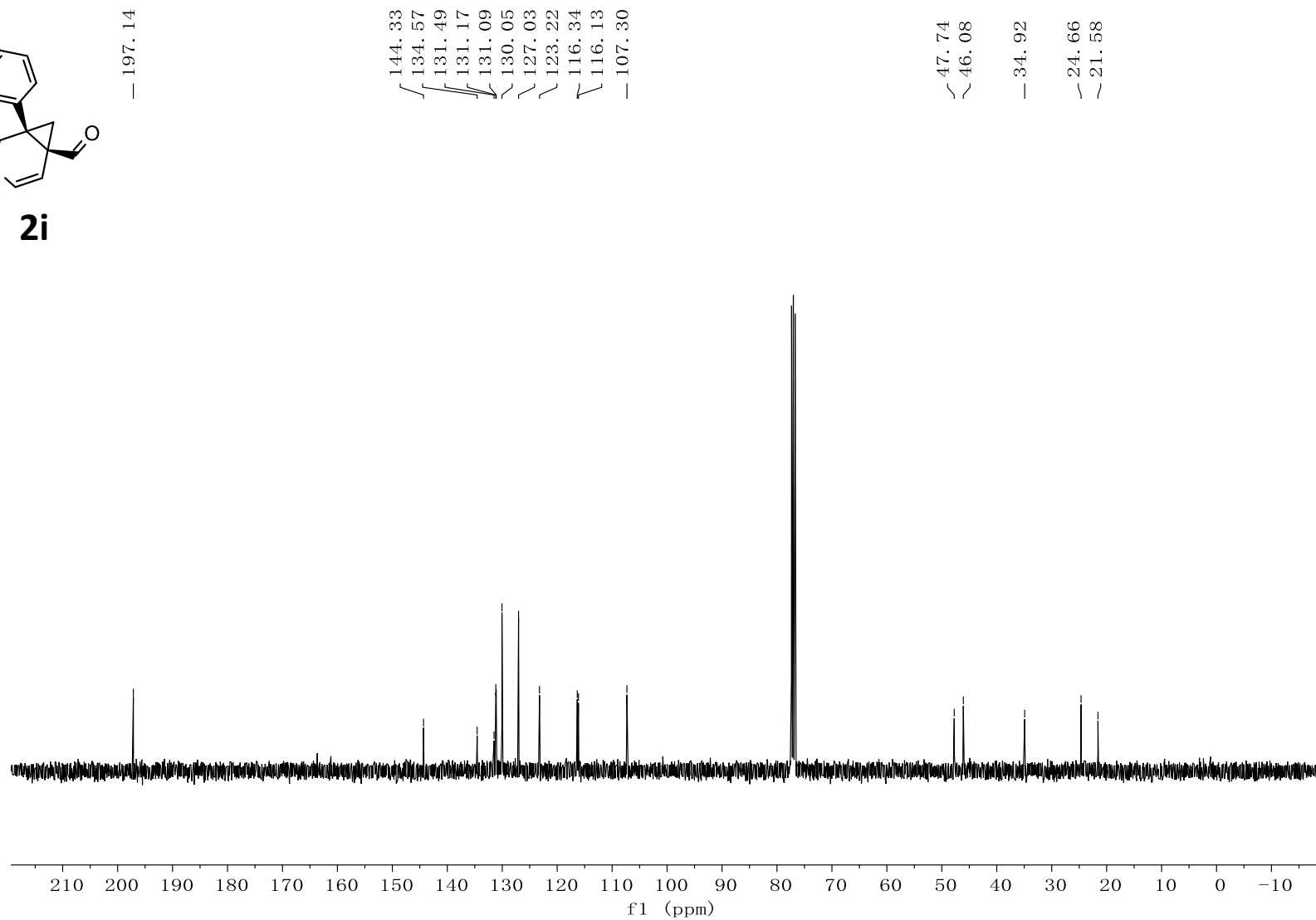
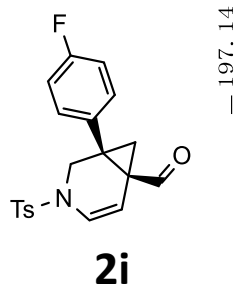


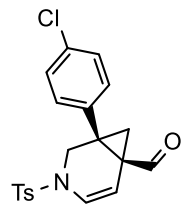




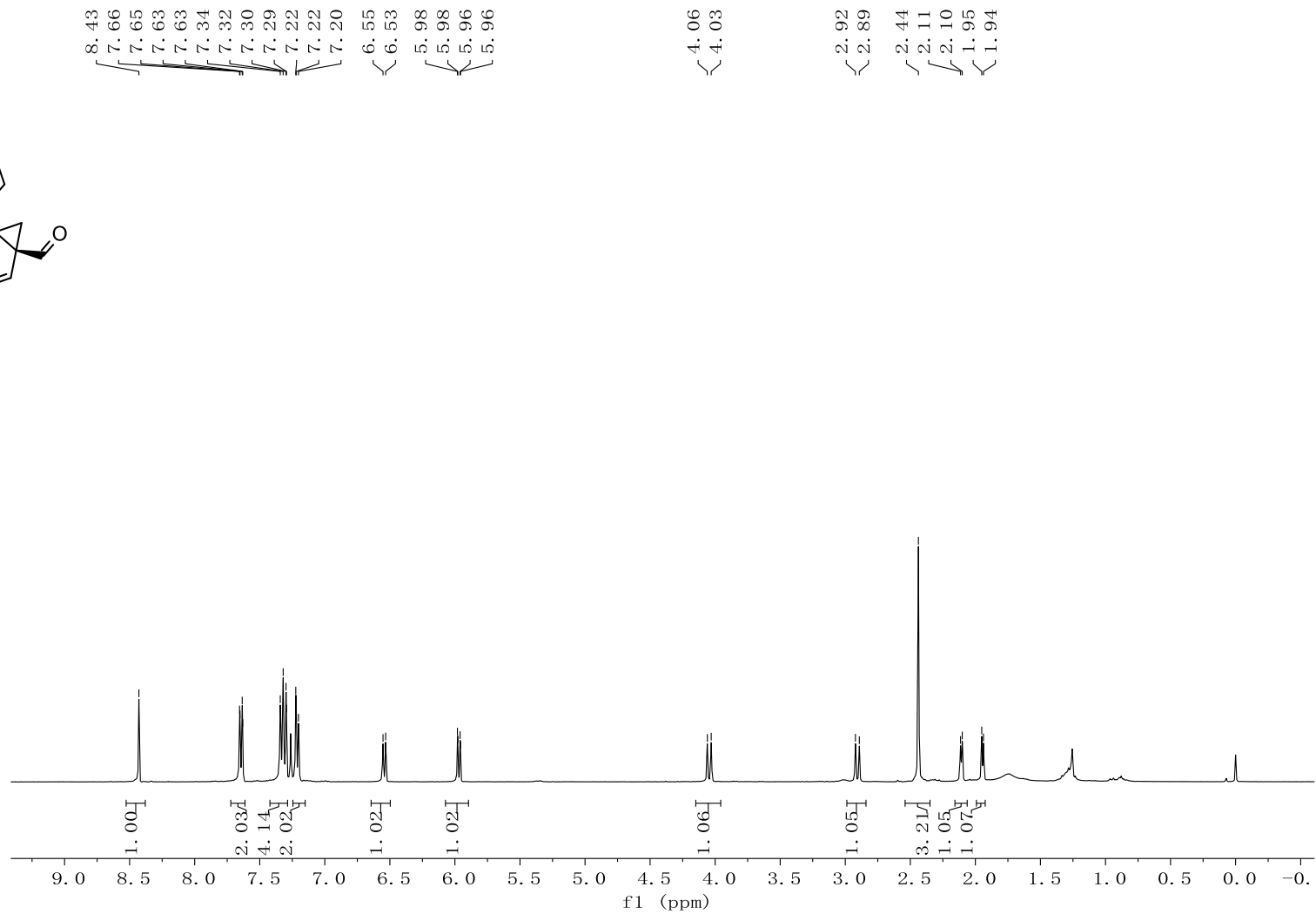
**2i**

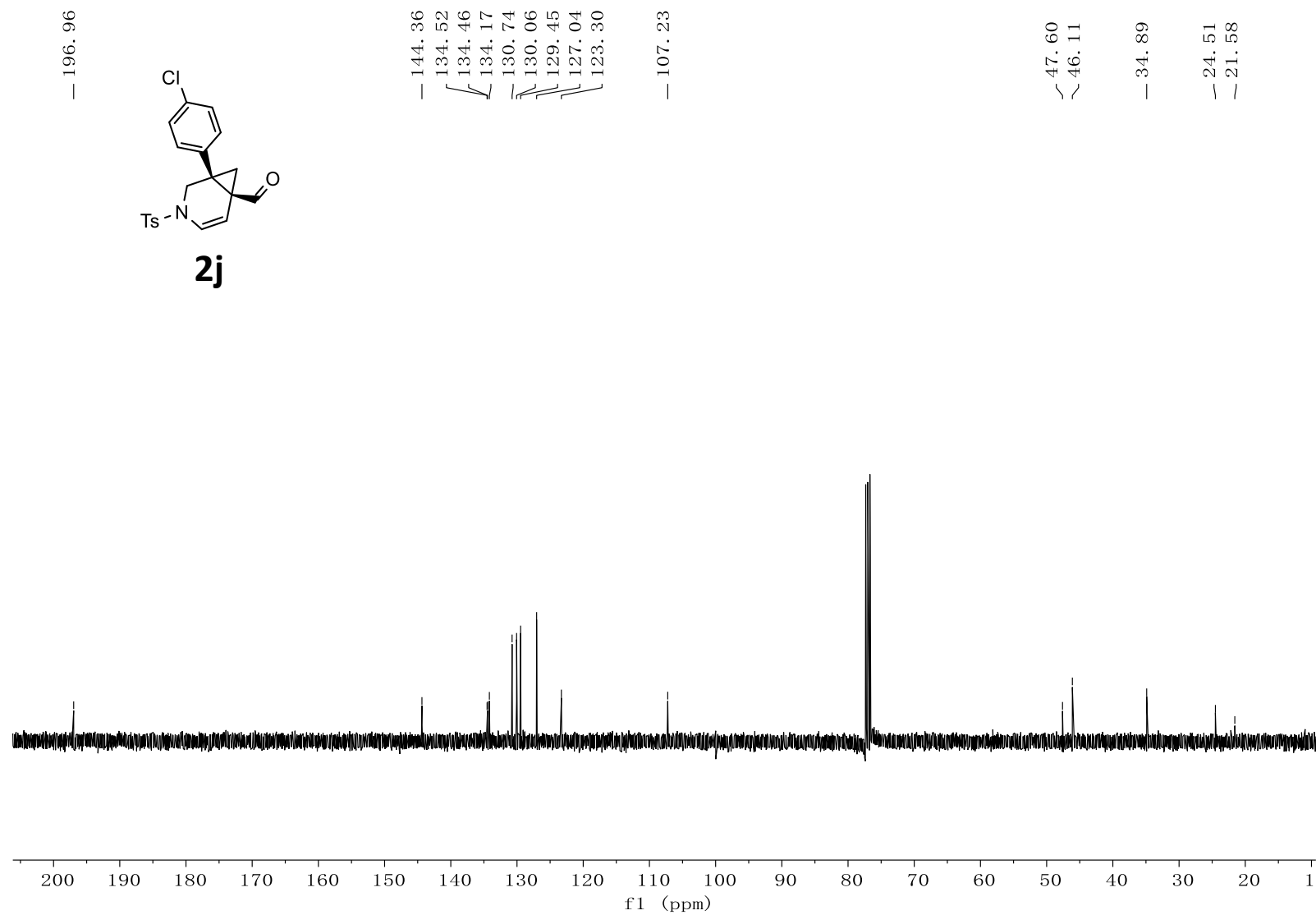


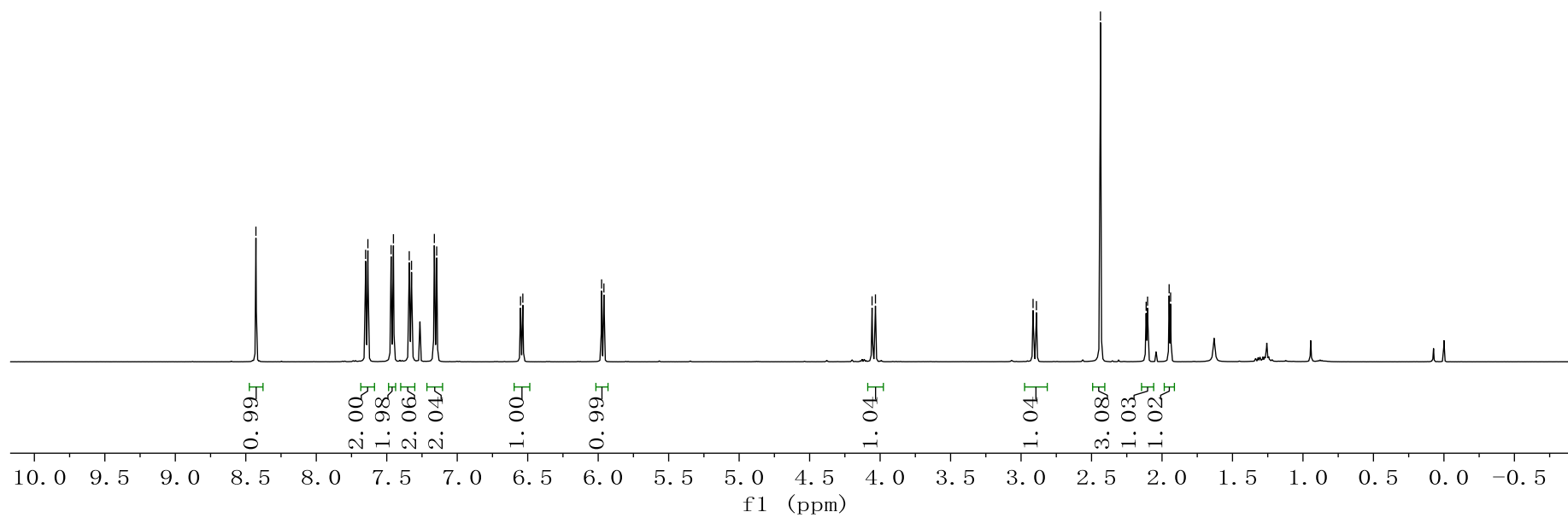
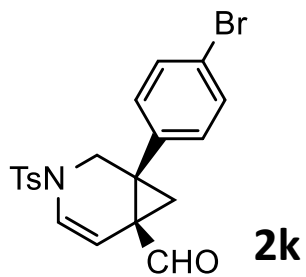


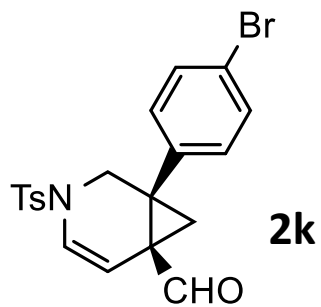


**2j**









— 196.97

— 144.39

134.72

134.50

132.44

131.08

130.09

127.05

123.32

122.57

— 107.23

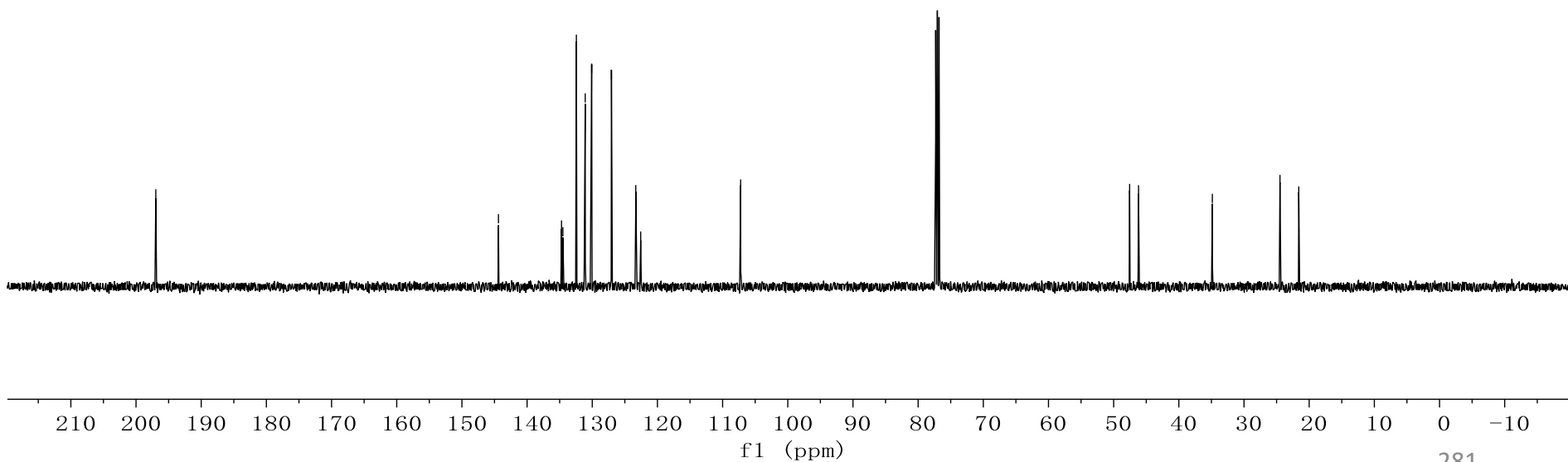
47.55

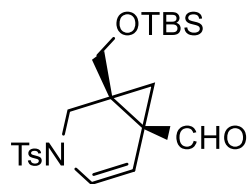
46.18

— 34.86

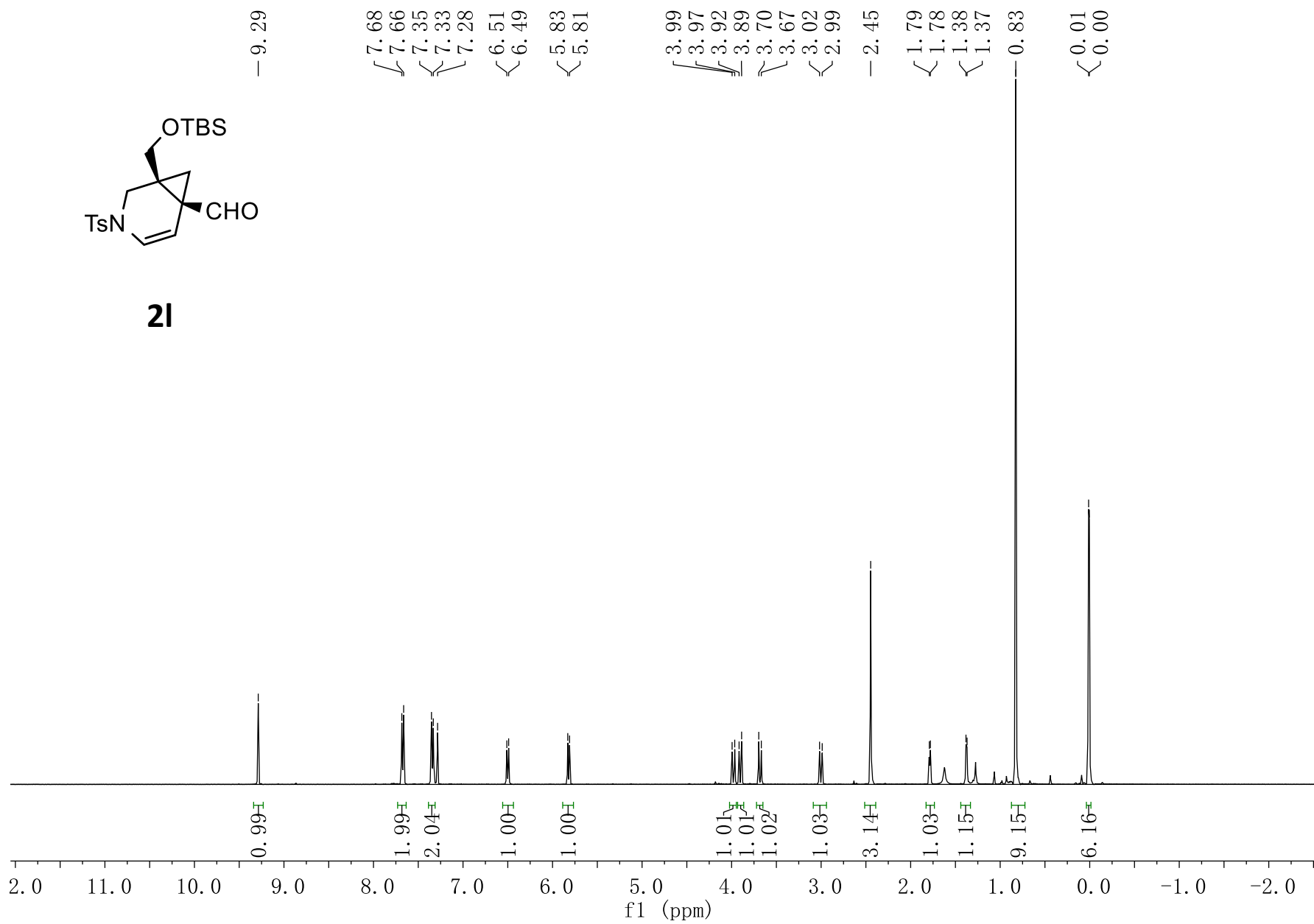
24.48

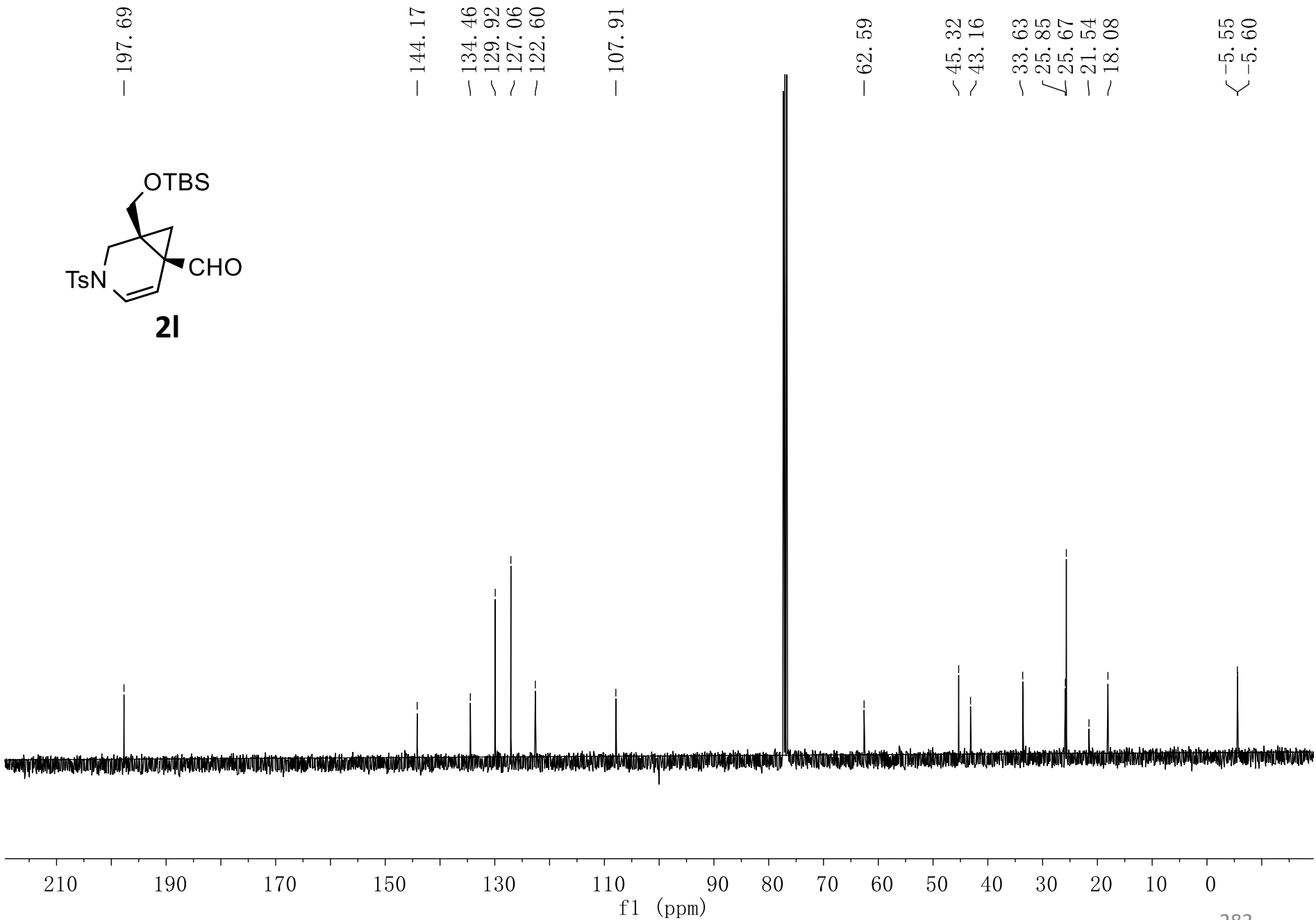
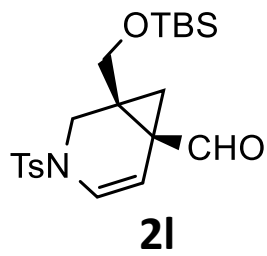
21.60

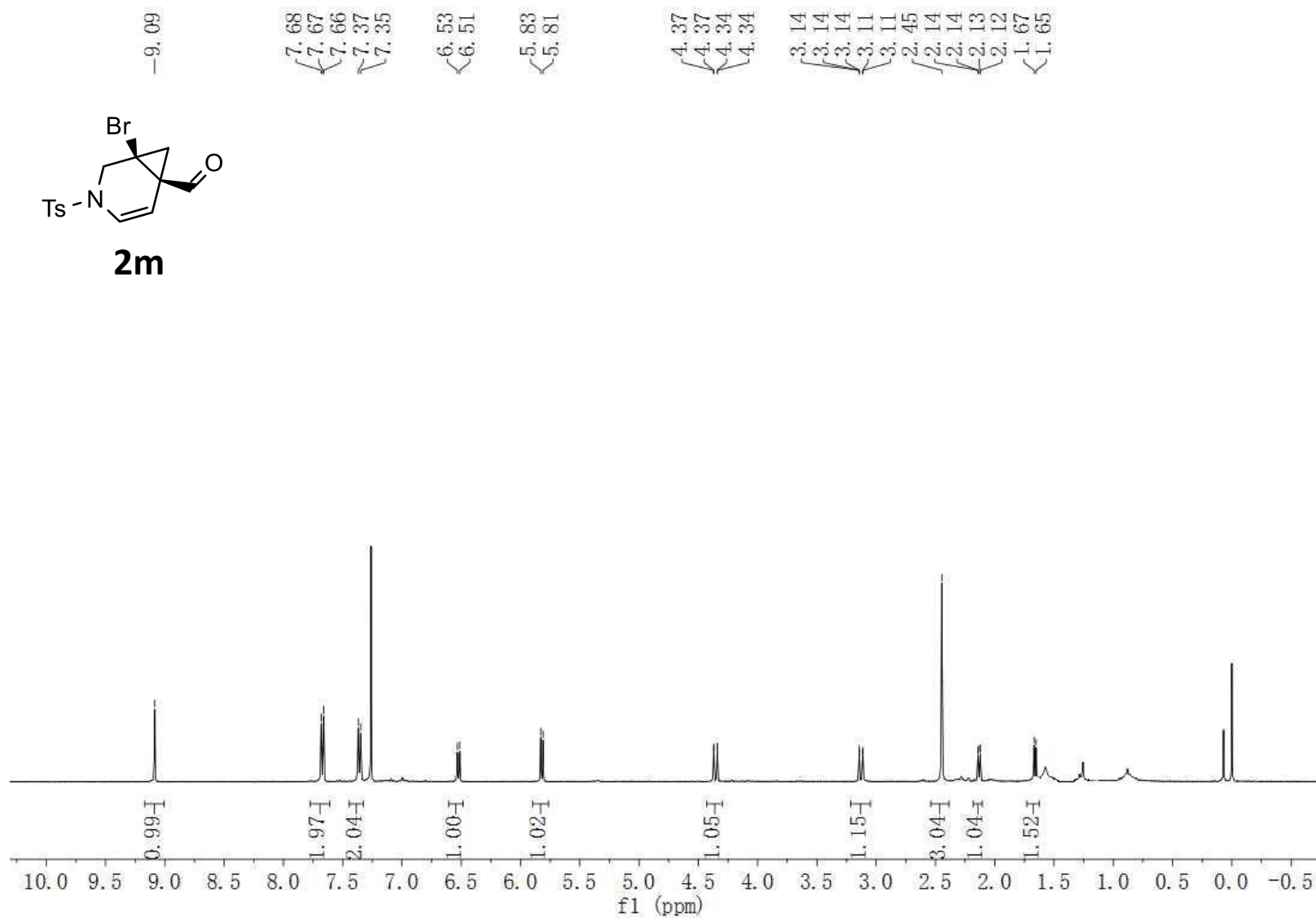
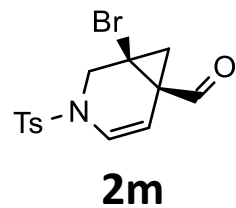


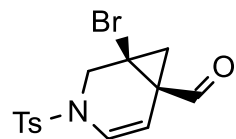


**2l**

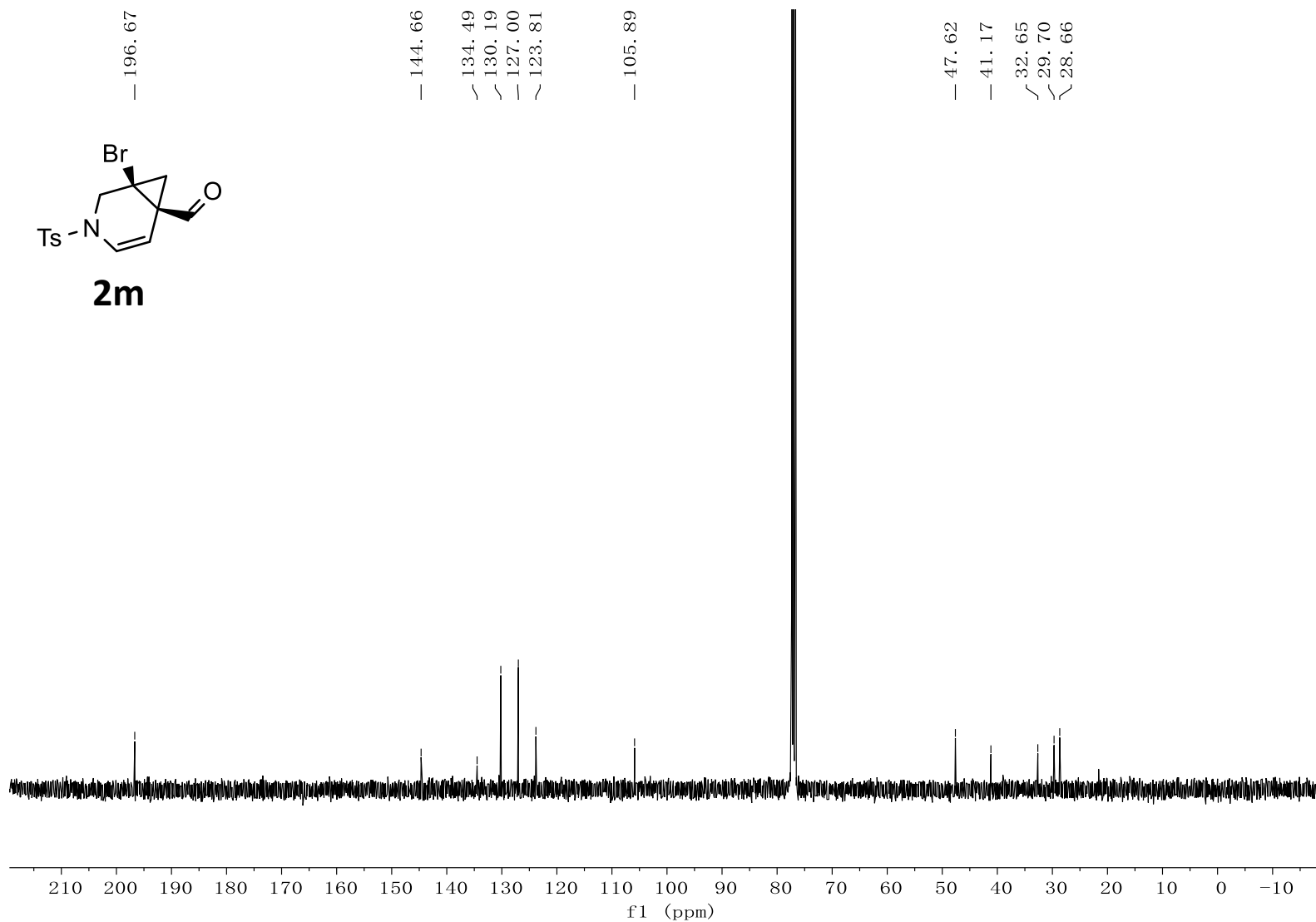


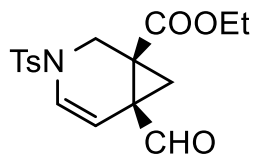




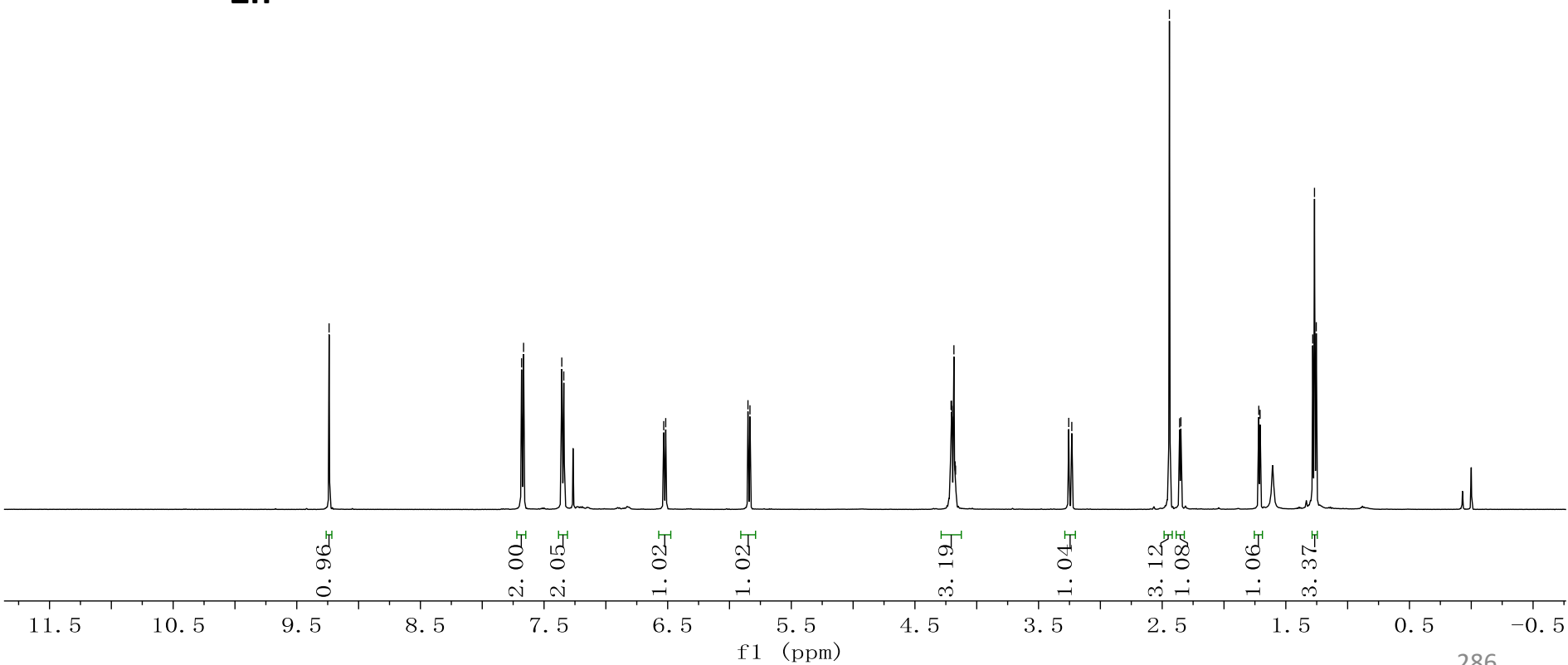


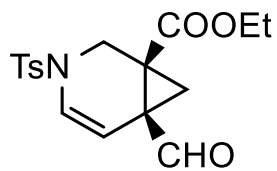
**2m**



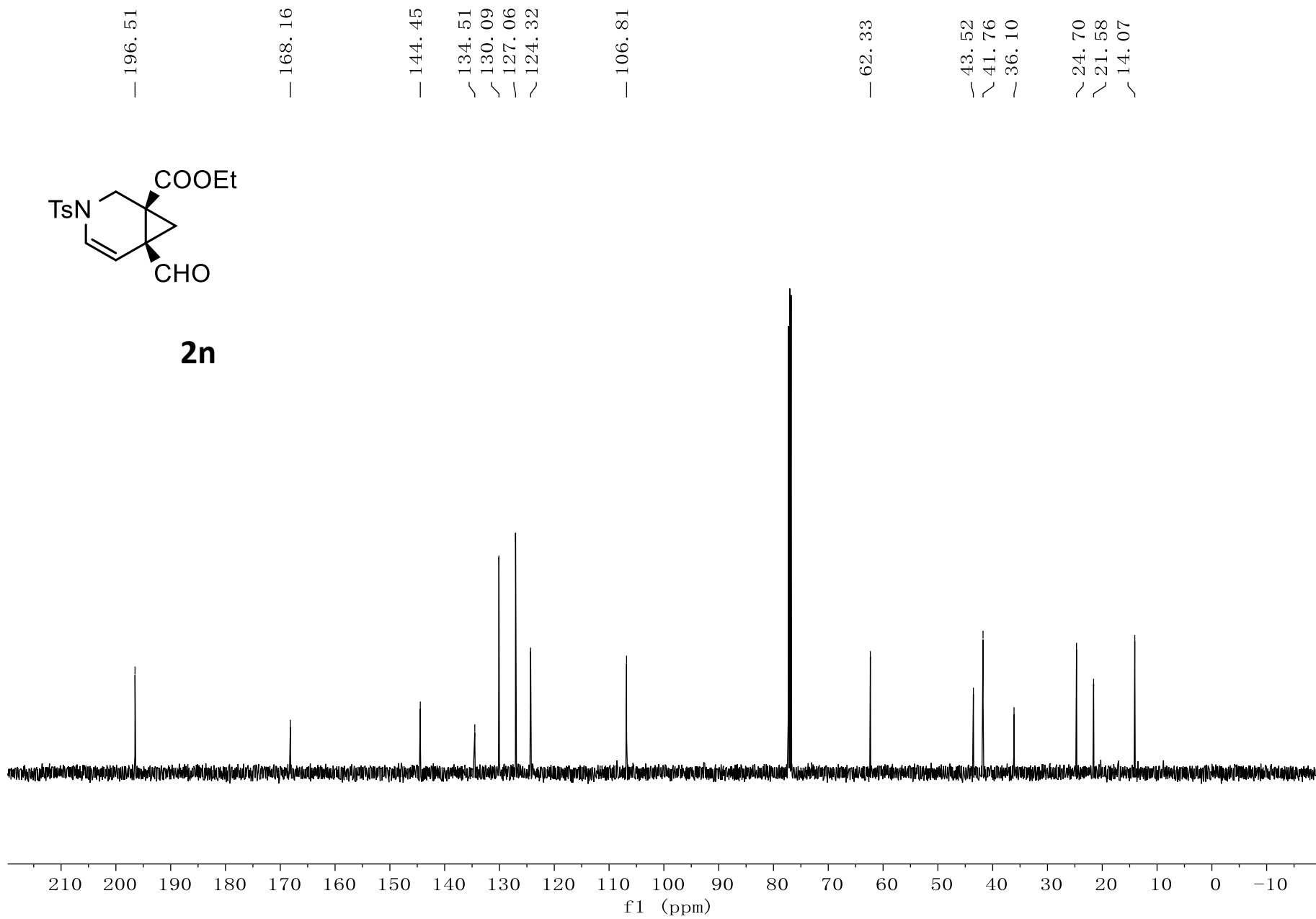


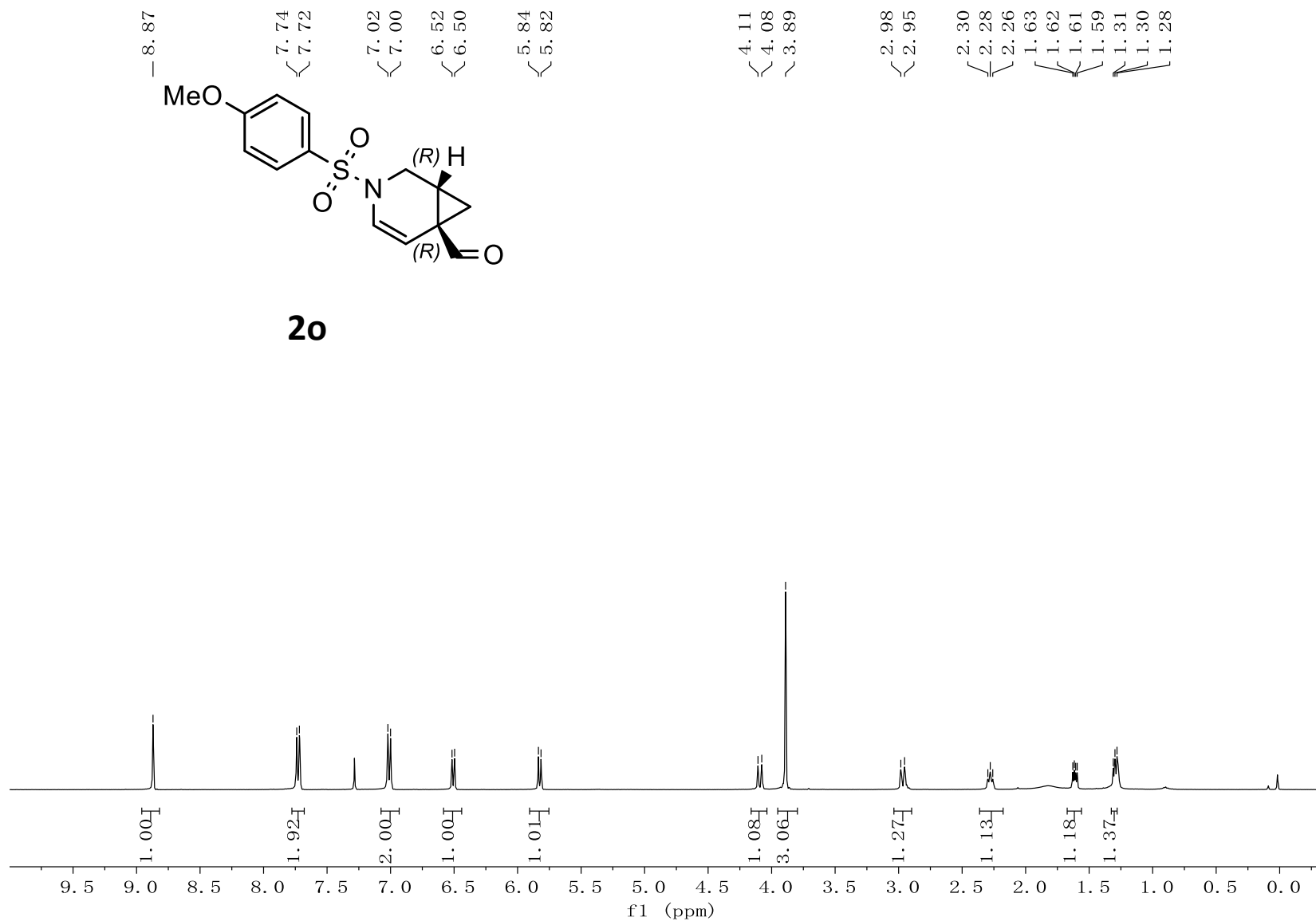
**2n**

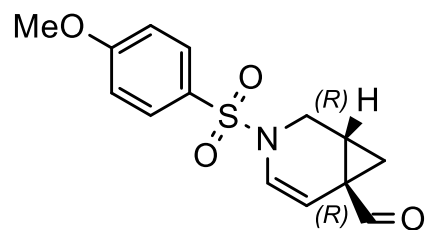




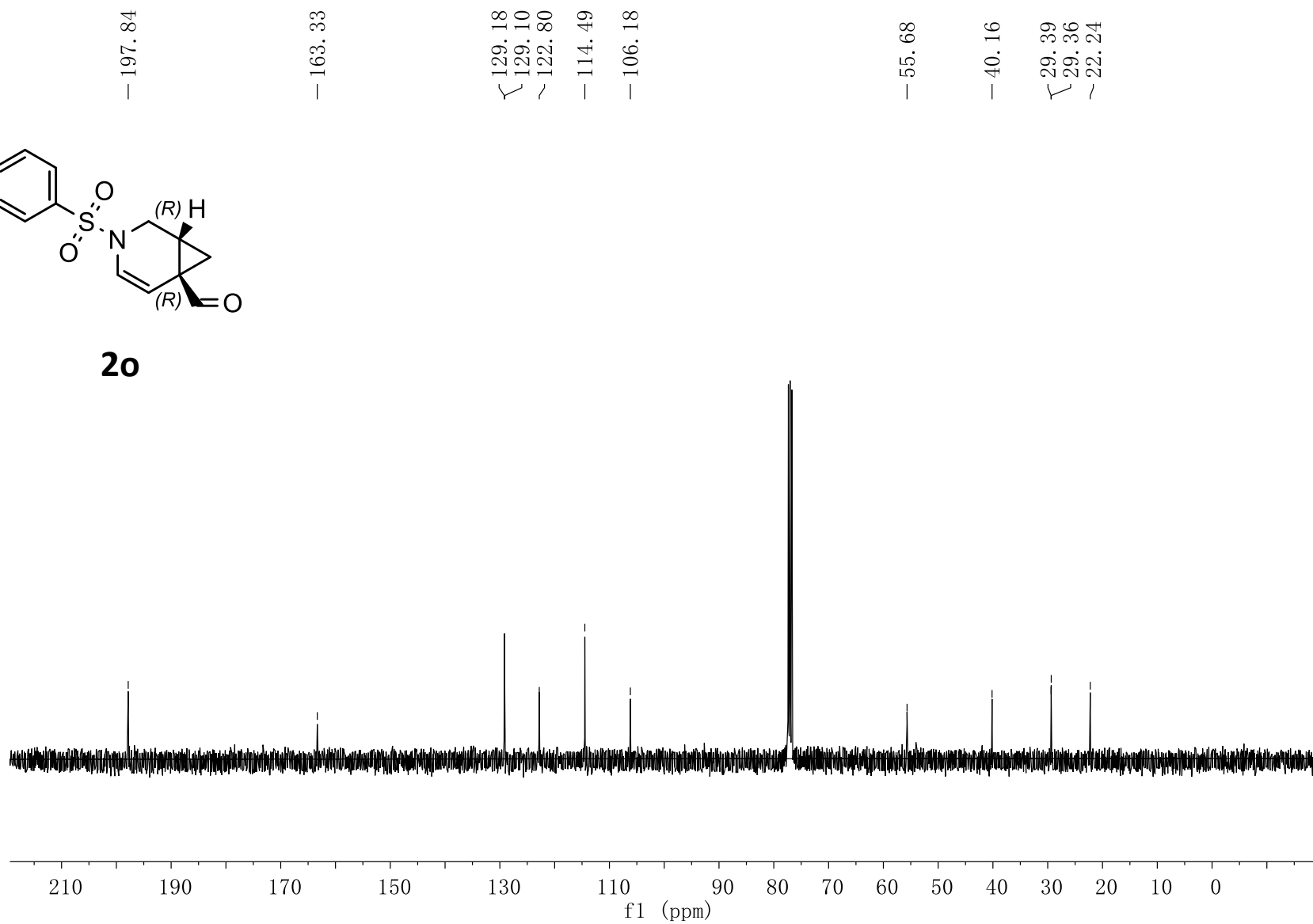
**2n**

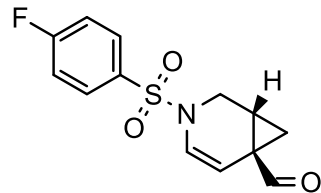




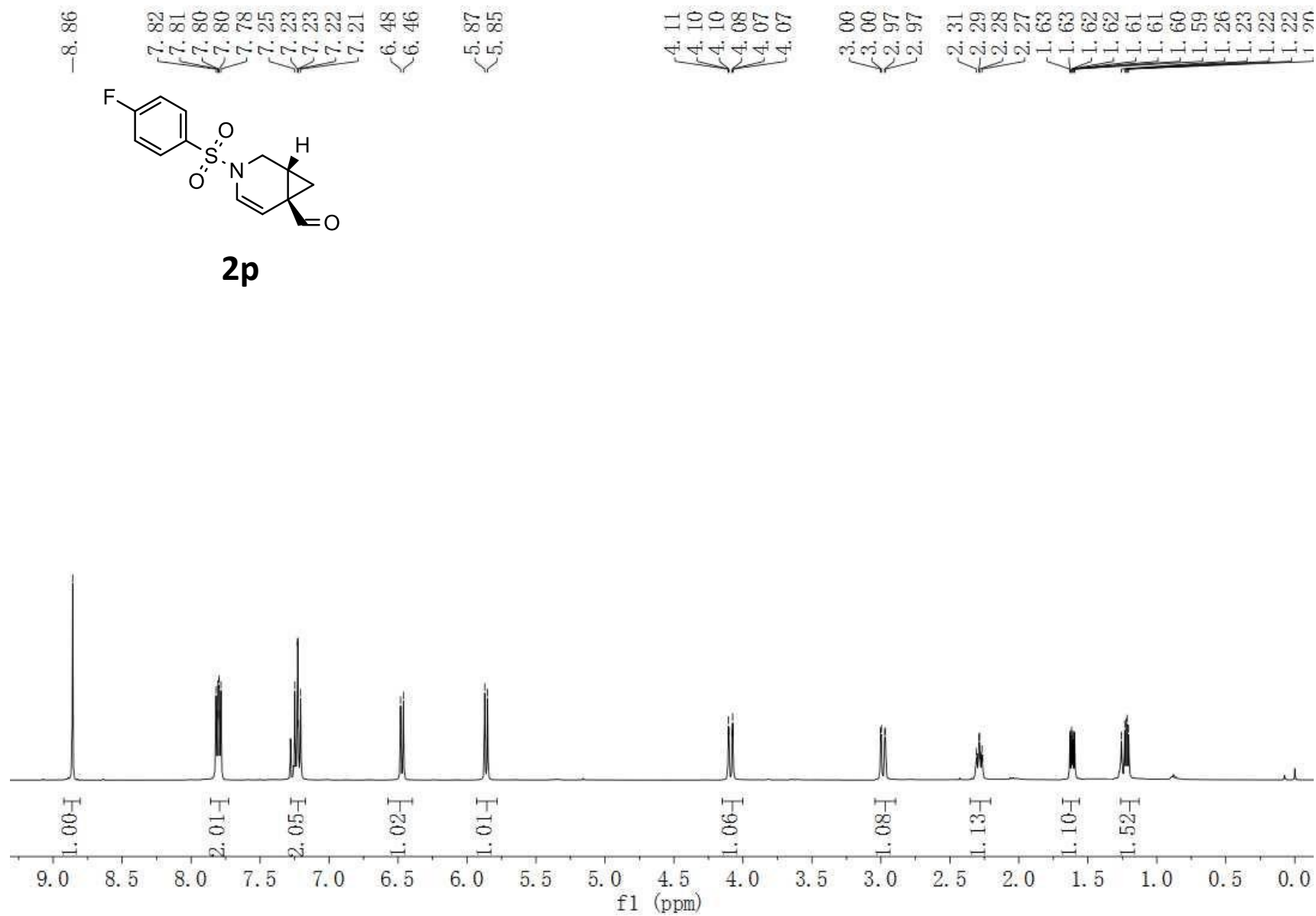


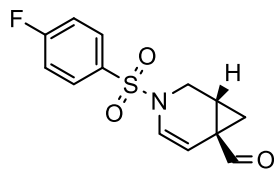
**2o**



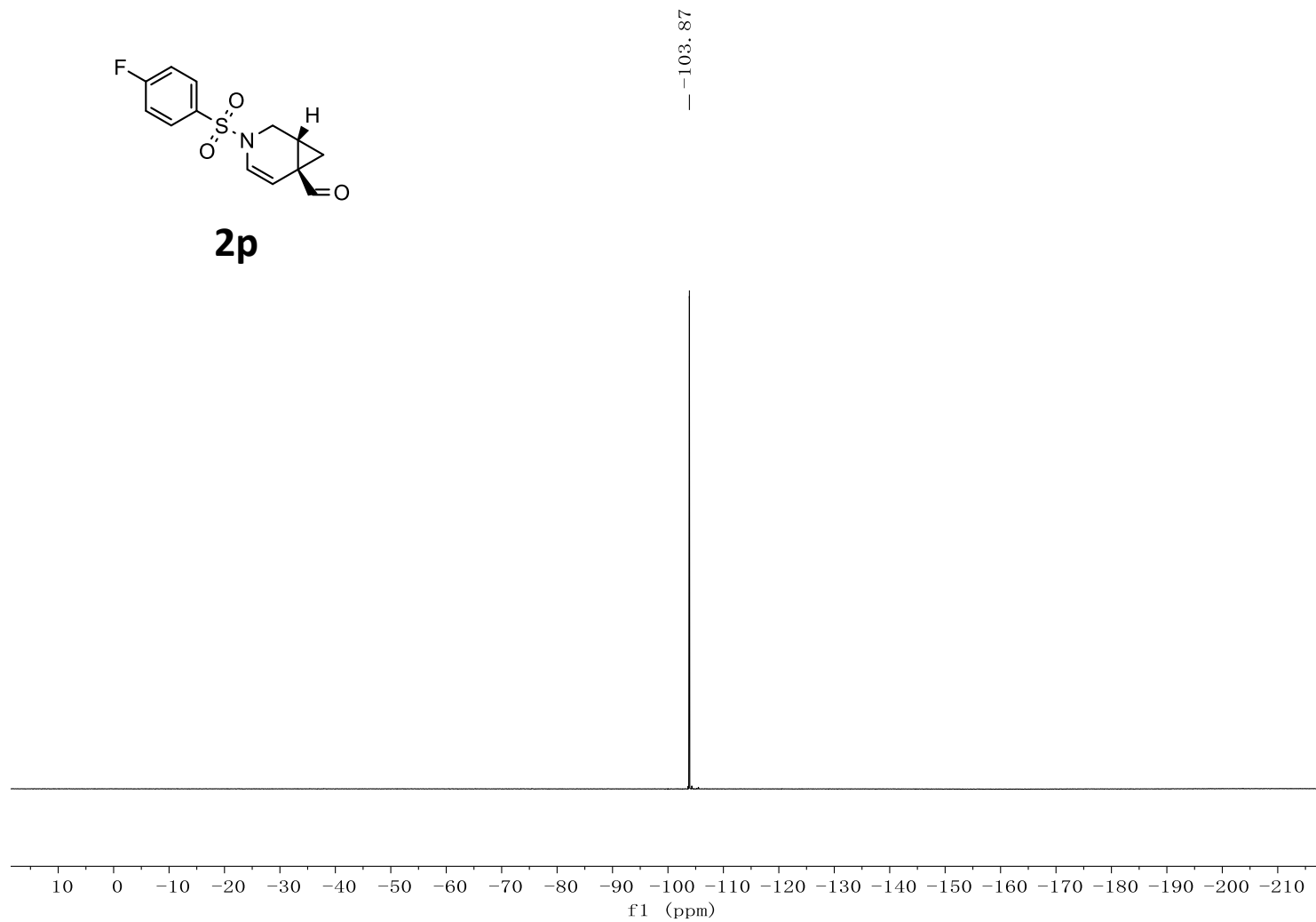


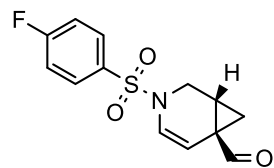
**2p**



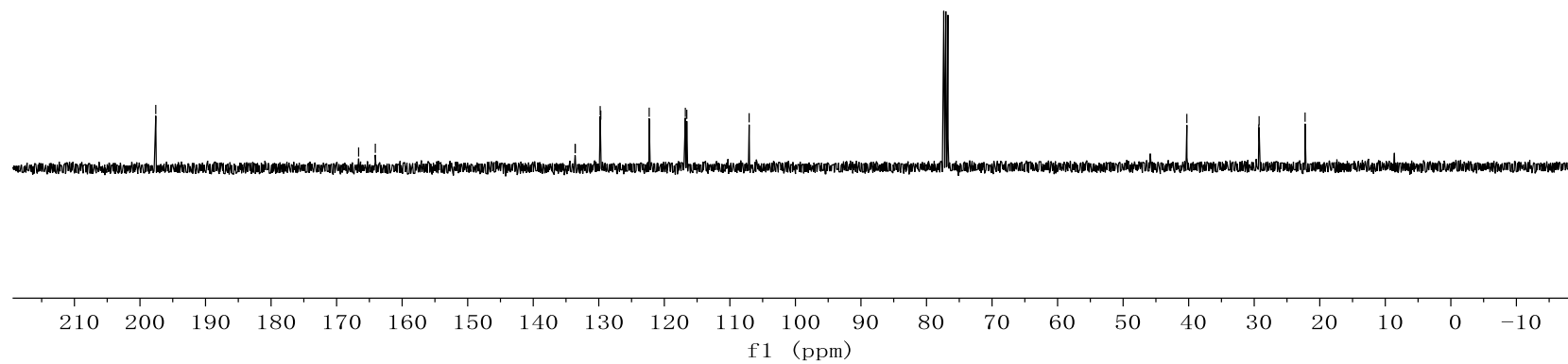


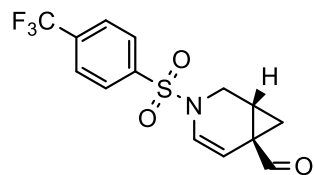
**2p**



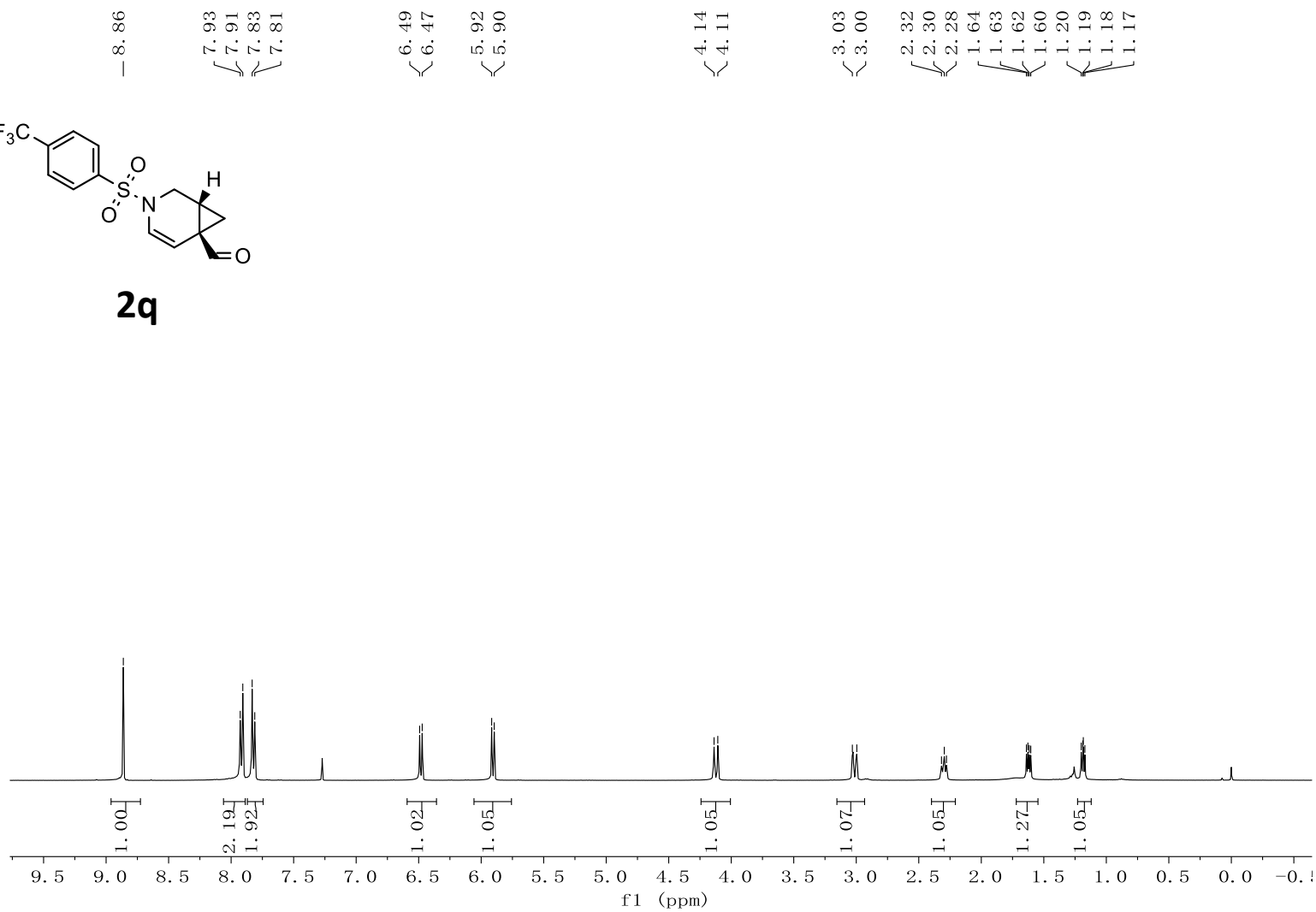


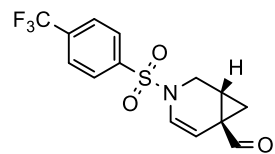
**2p**





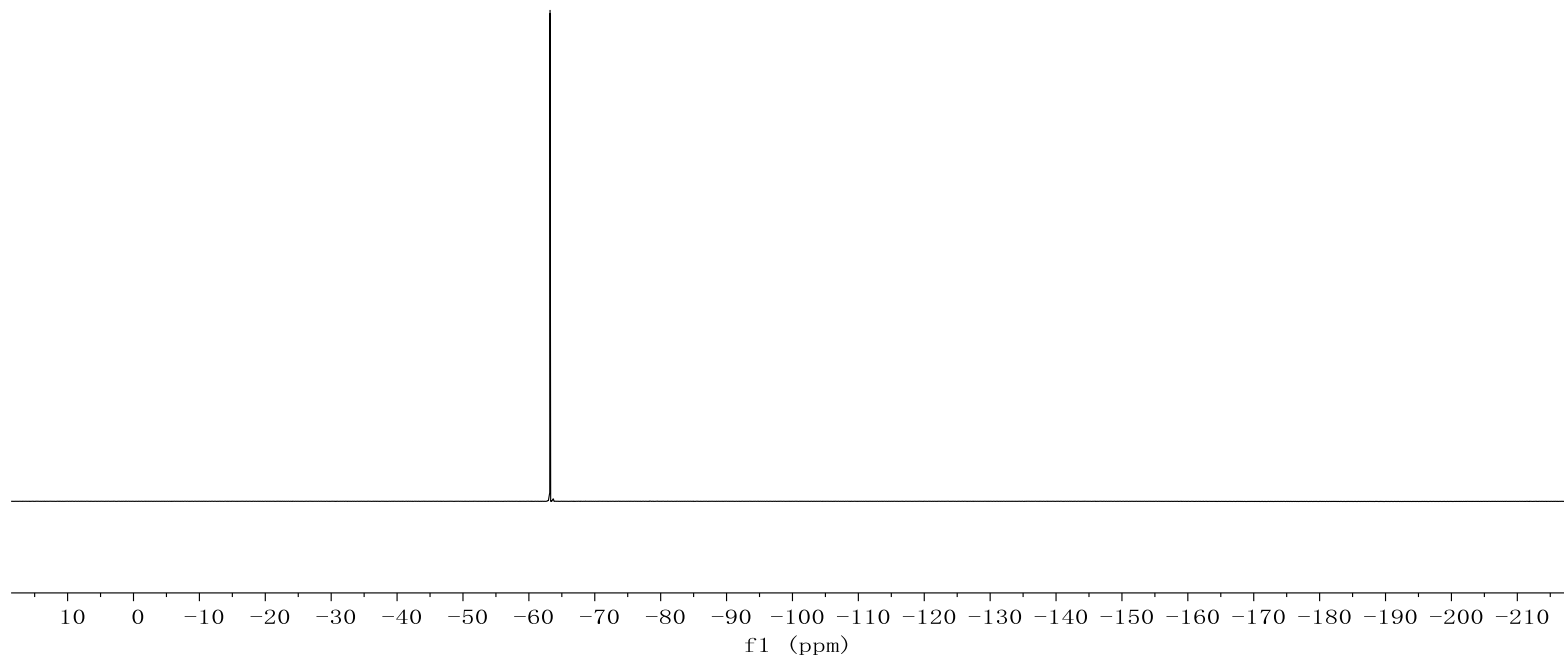
**2q**

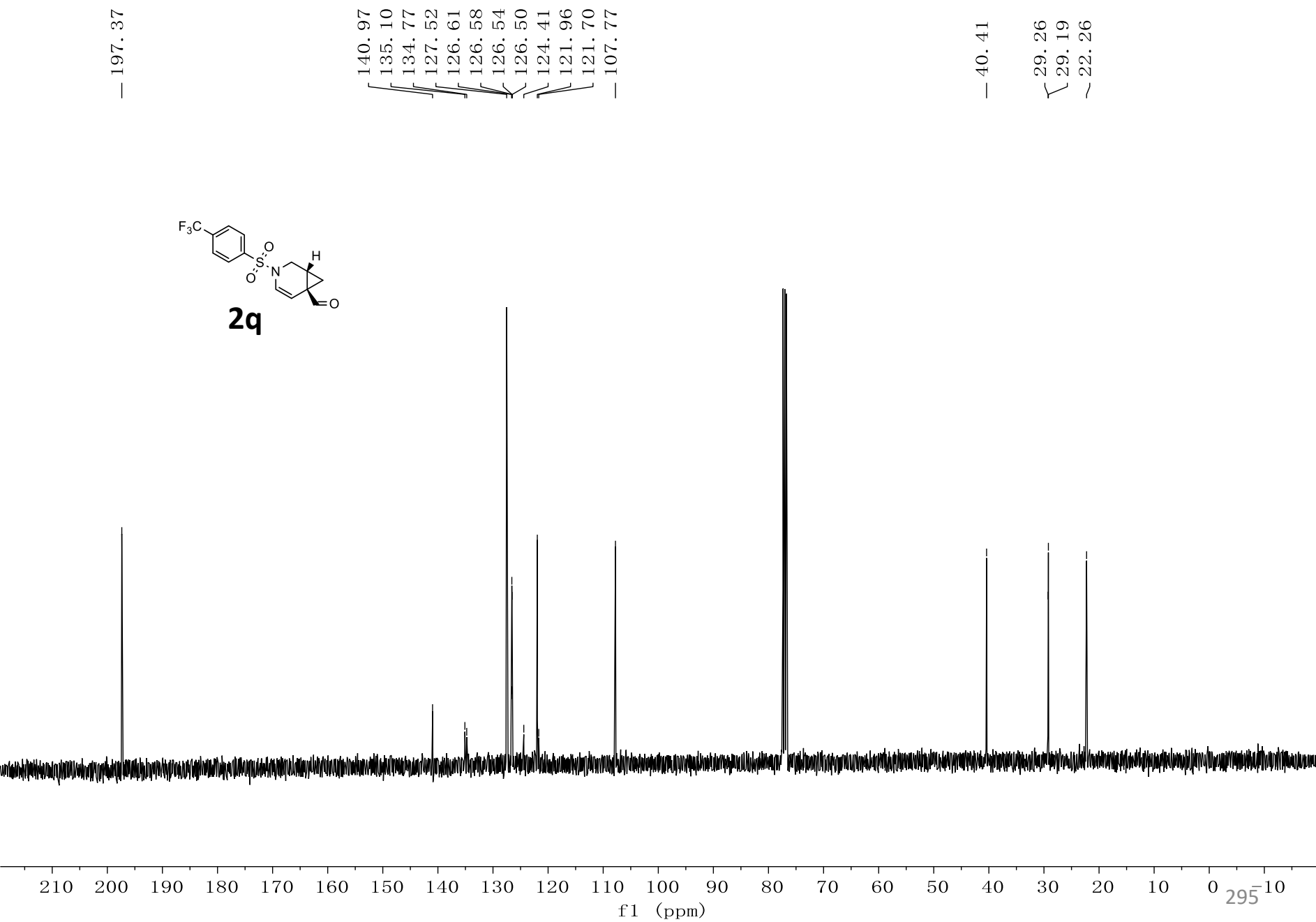
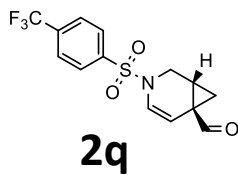


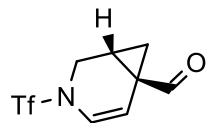


**2q**

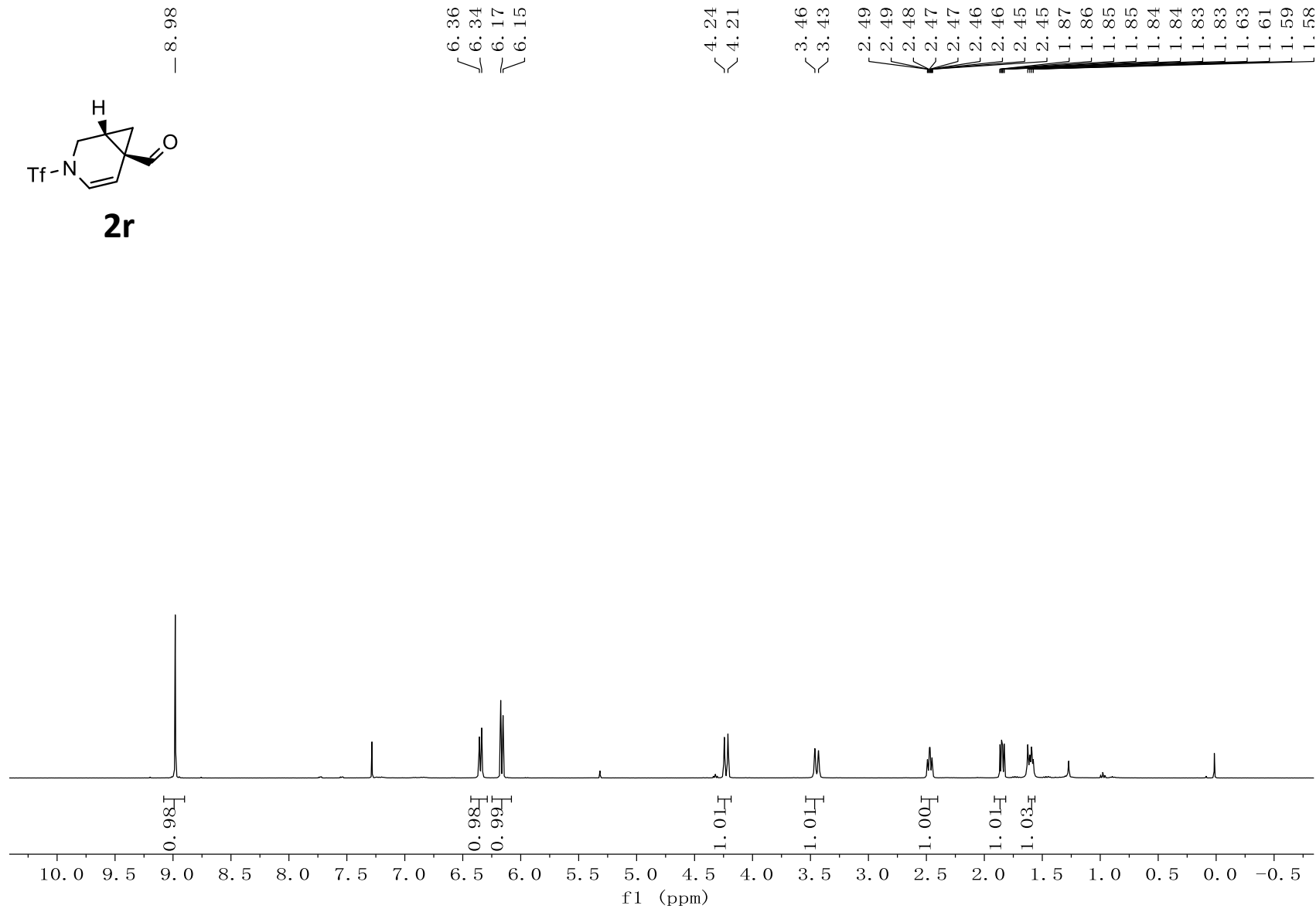
— -63.21

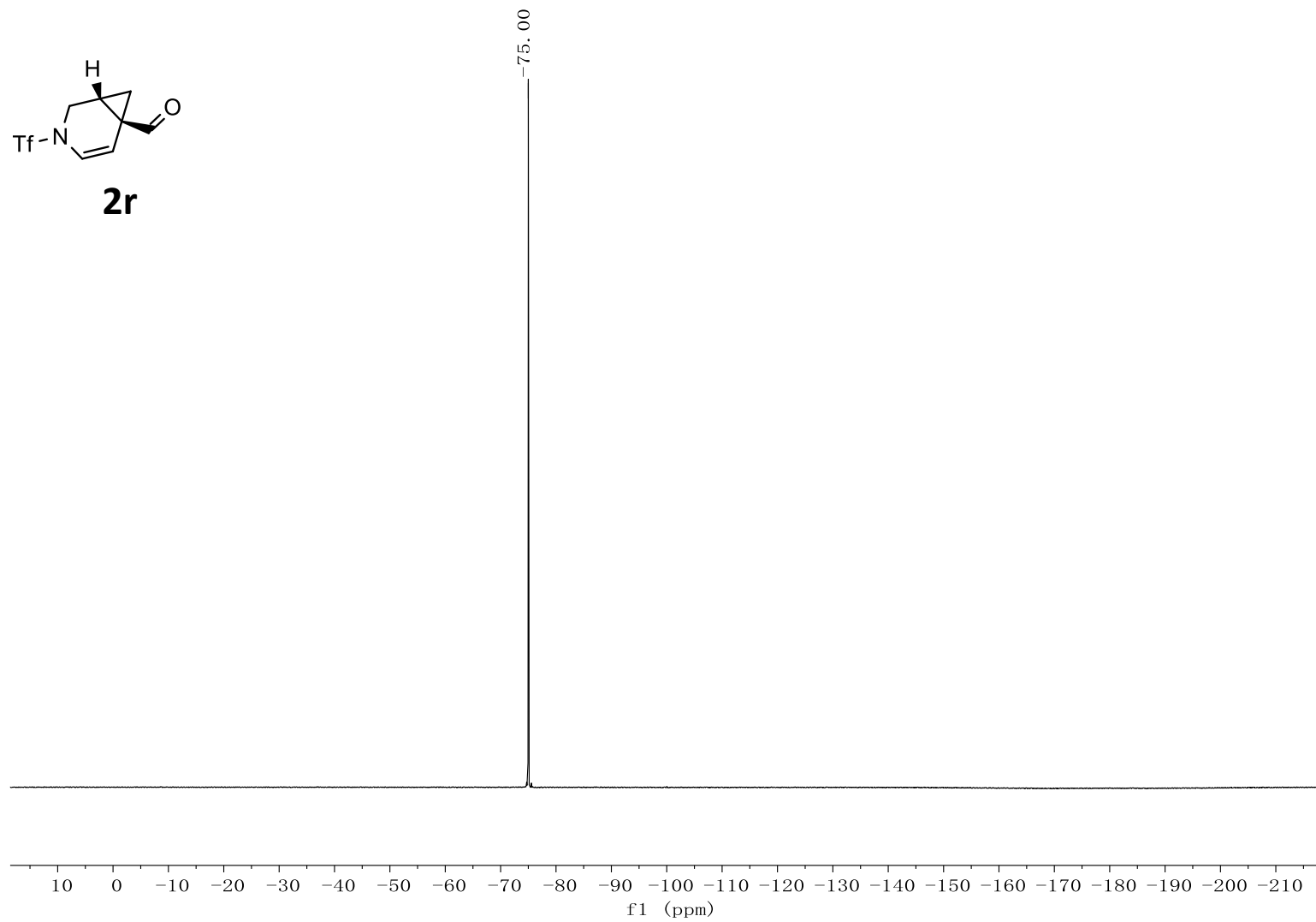
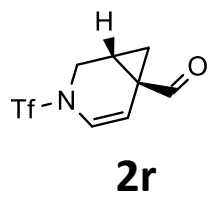


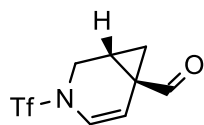




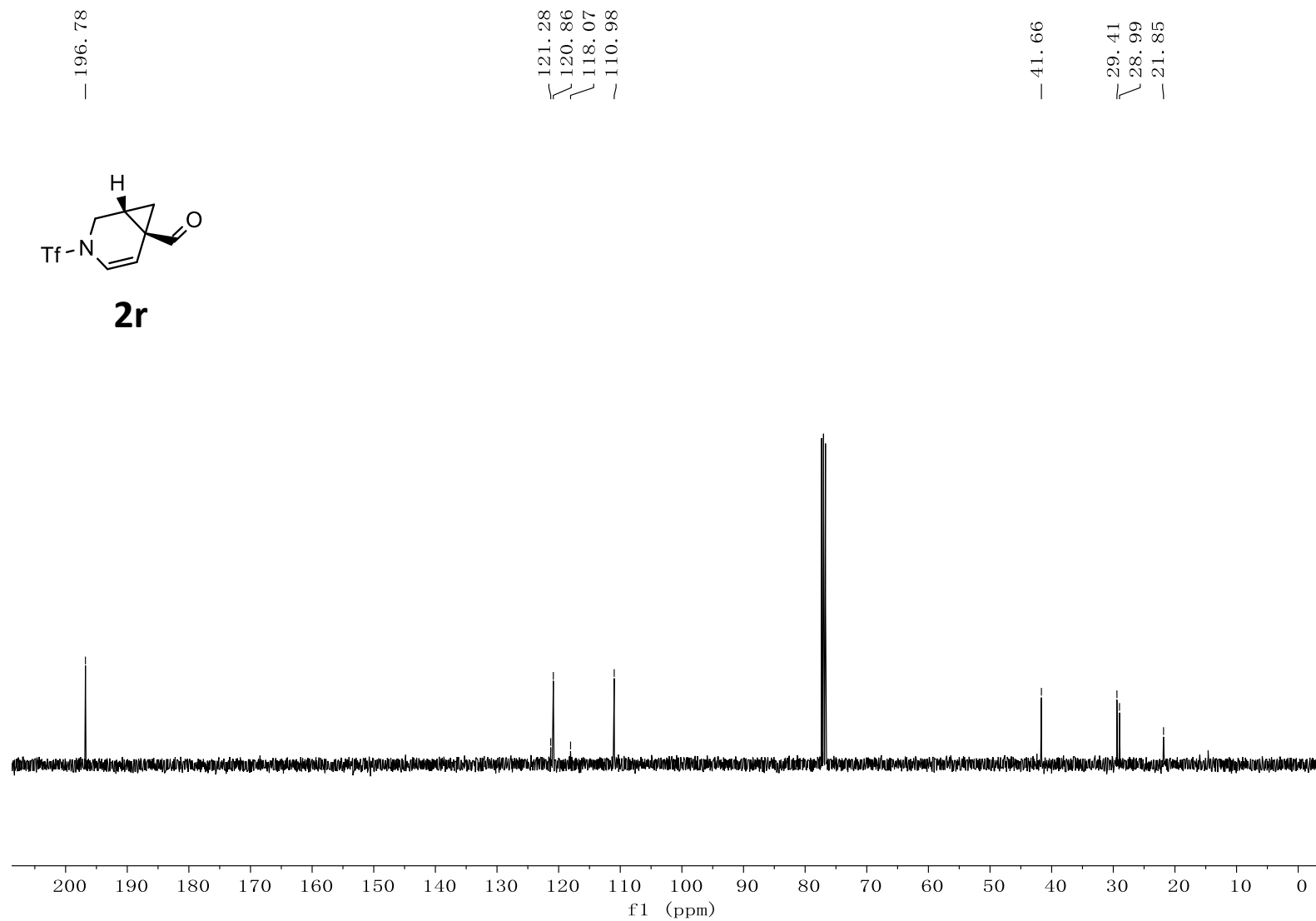
**2r**

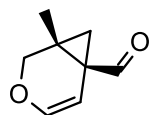




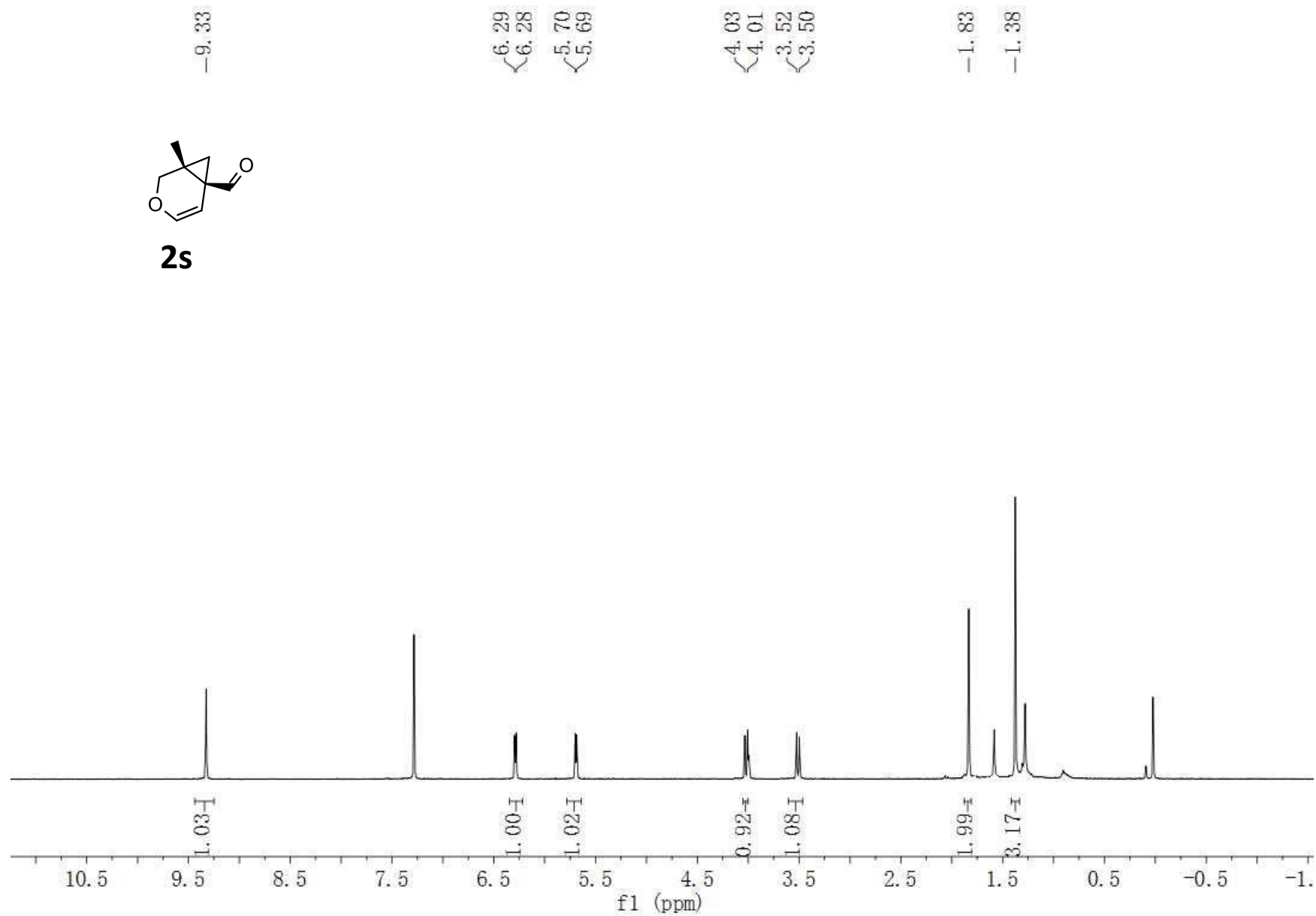


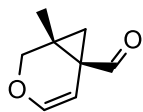
**2r**



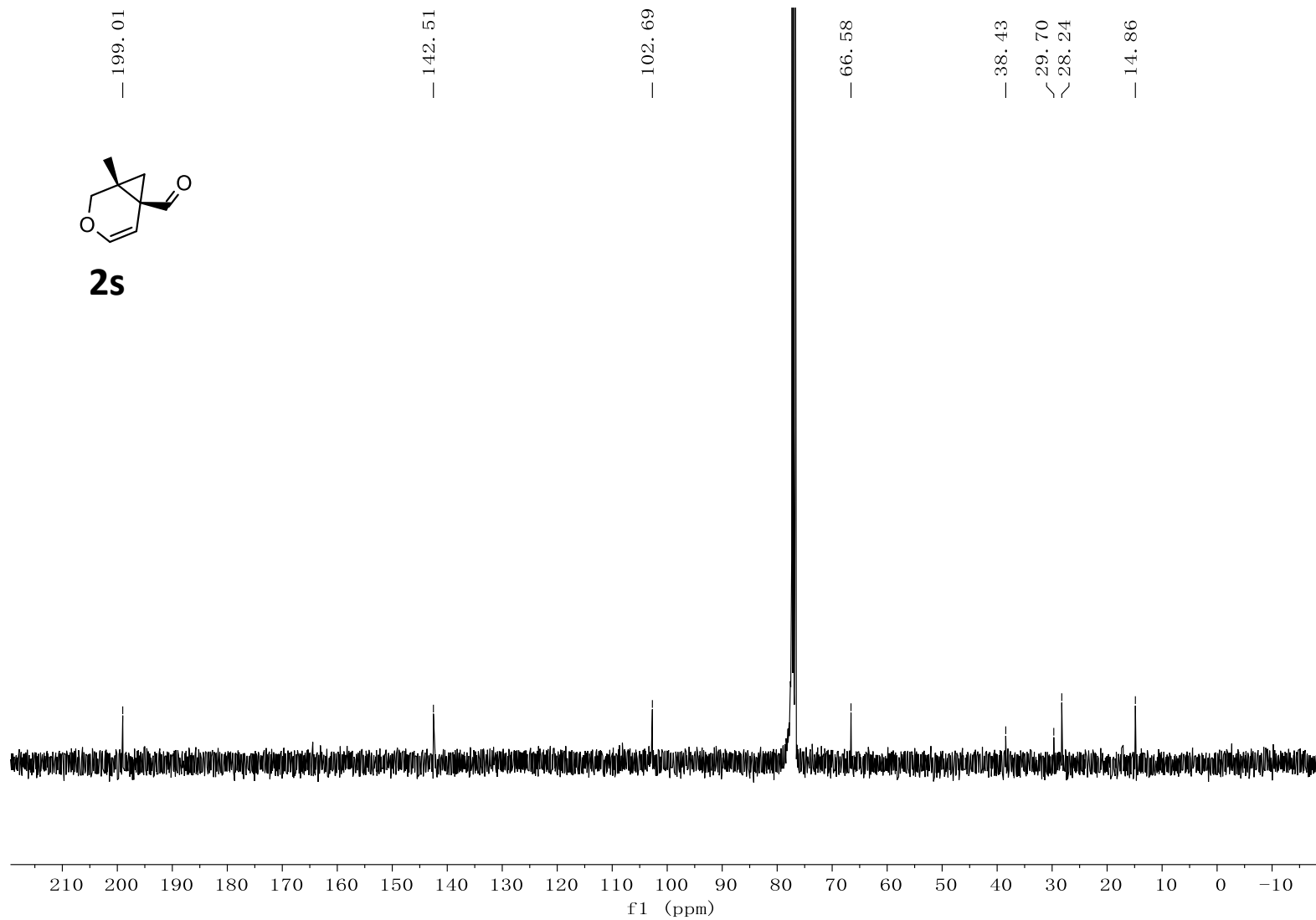


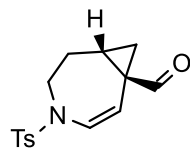
**2s**



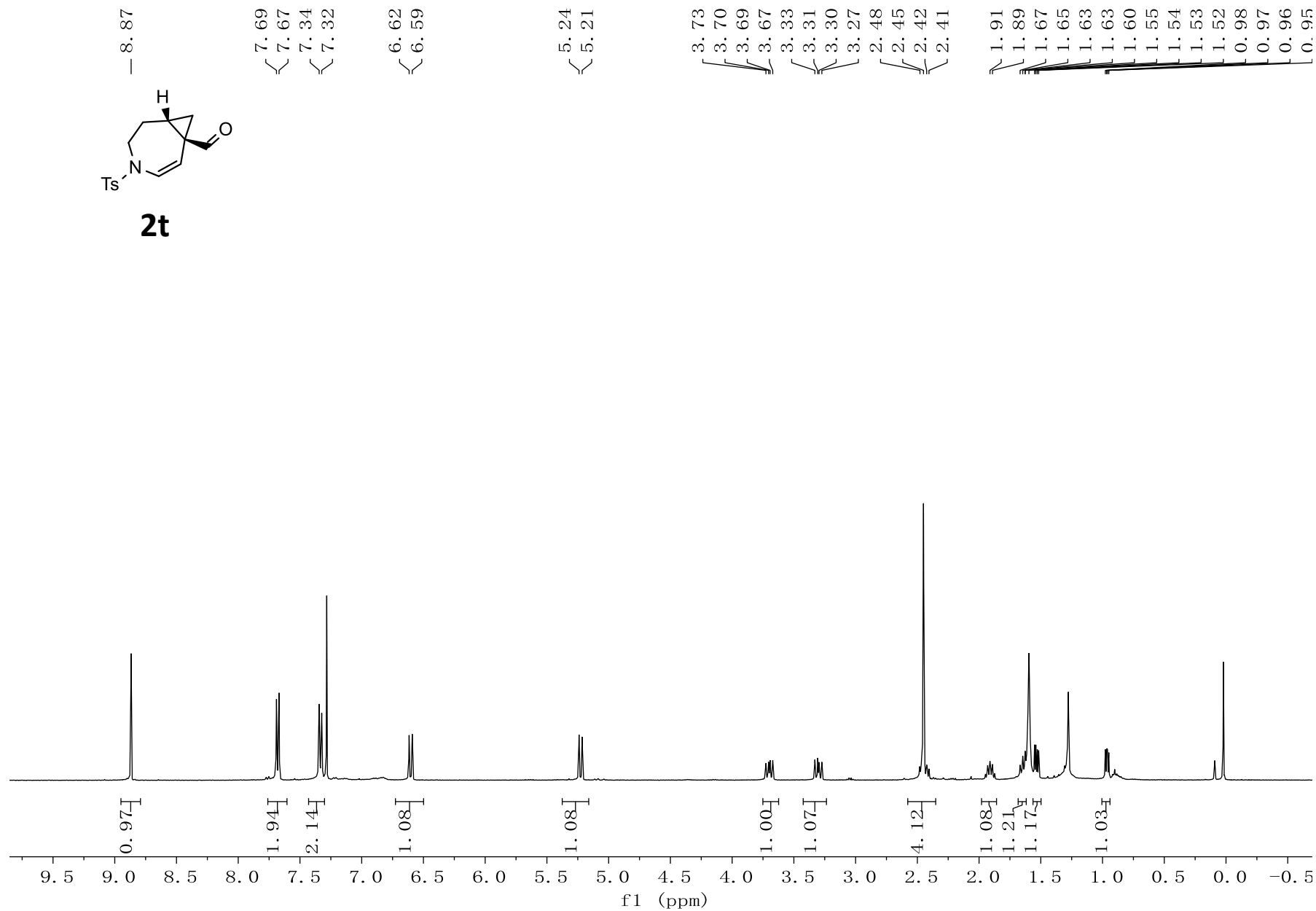


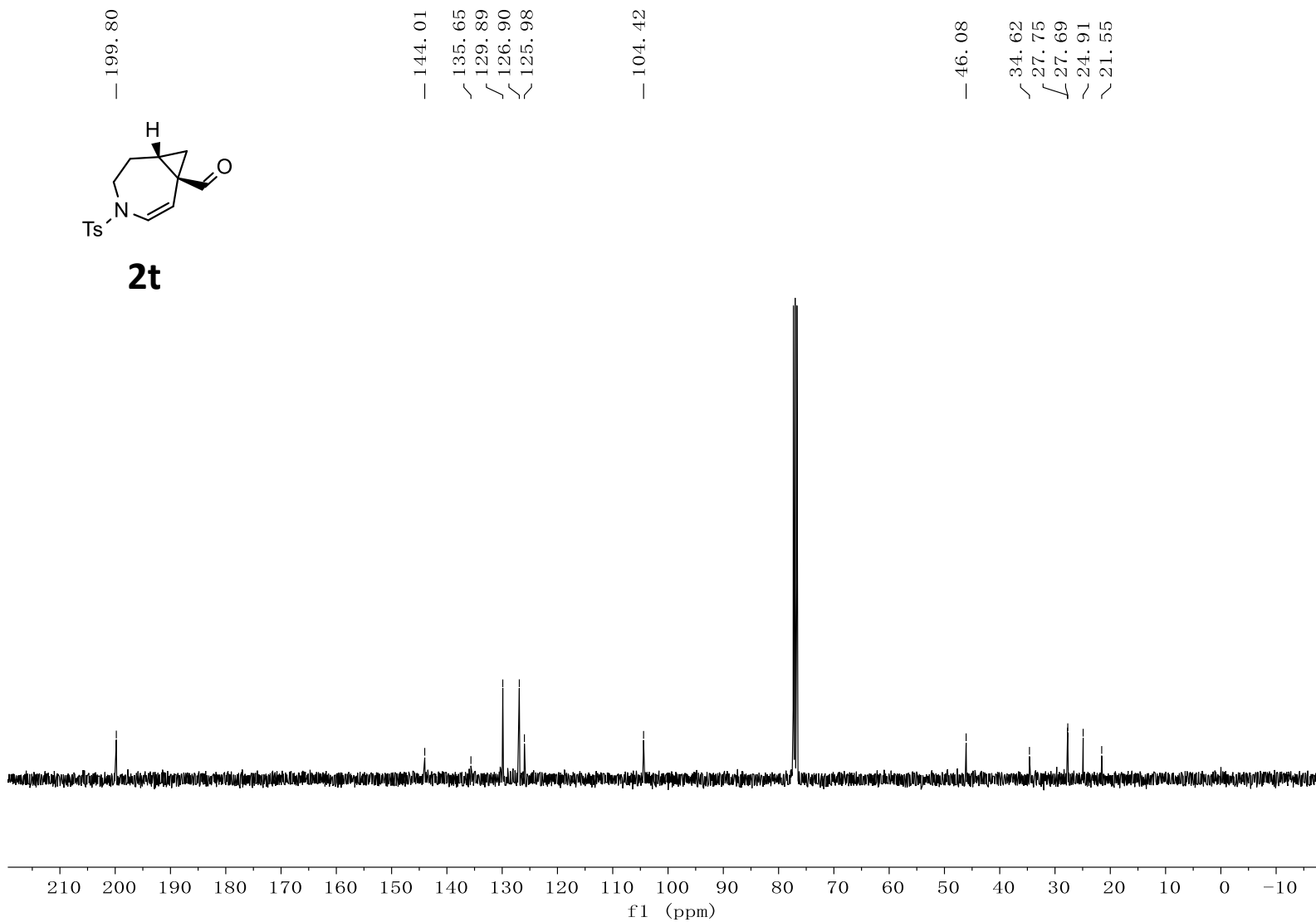
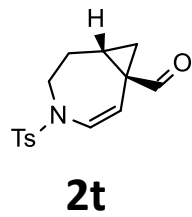
**2s**



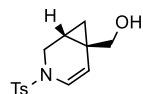


**2t**









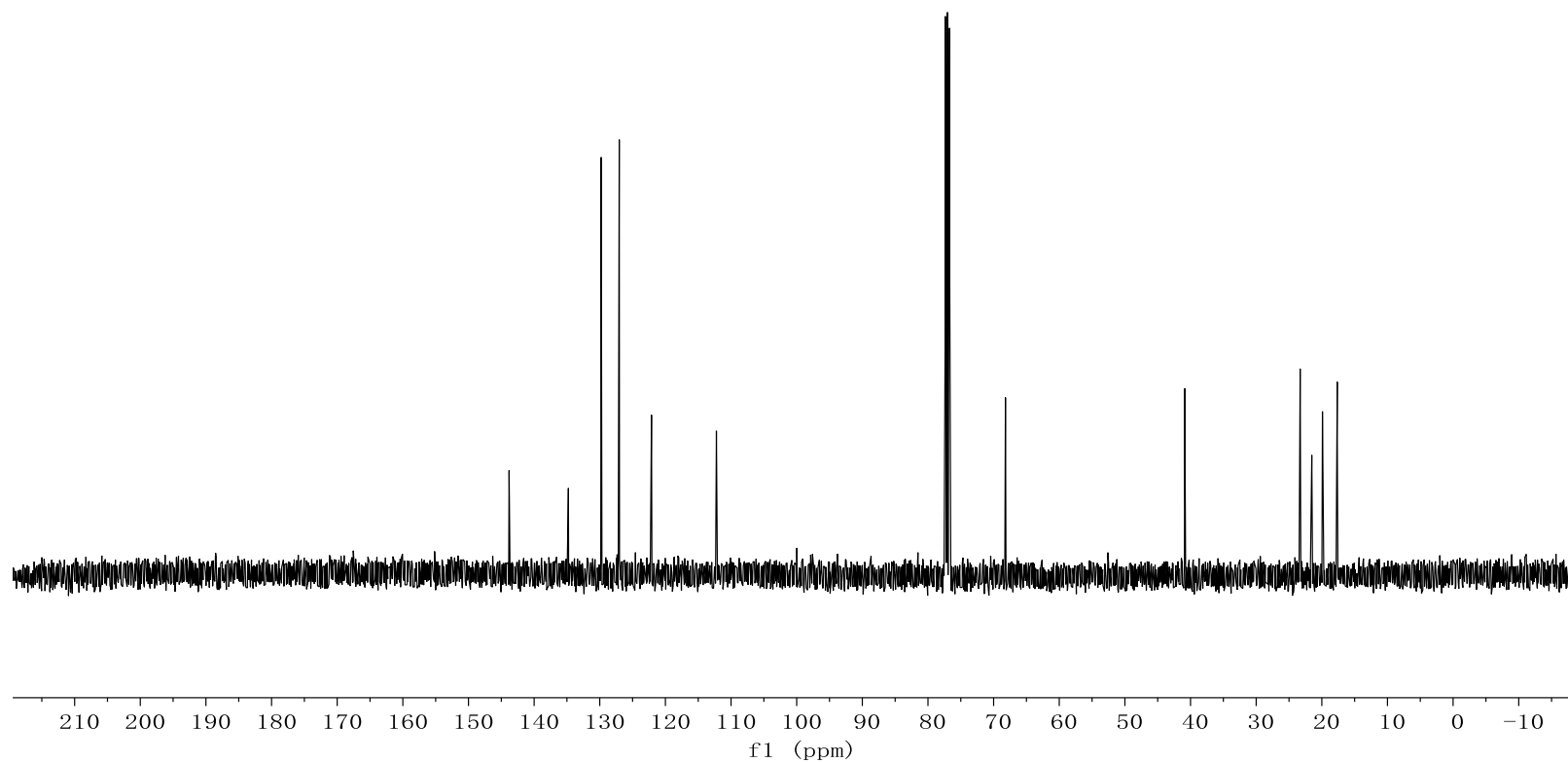
**2u**

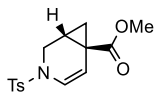
— 143.81  
 ~ 134.78  
 ~ 129.78  
 ~ 127.03  
 ~ 122.12  
 — 112.23

— 68.20

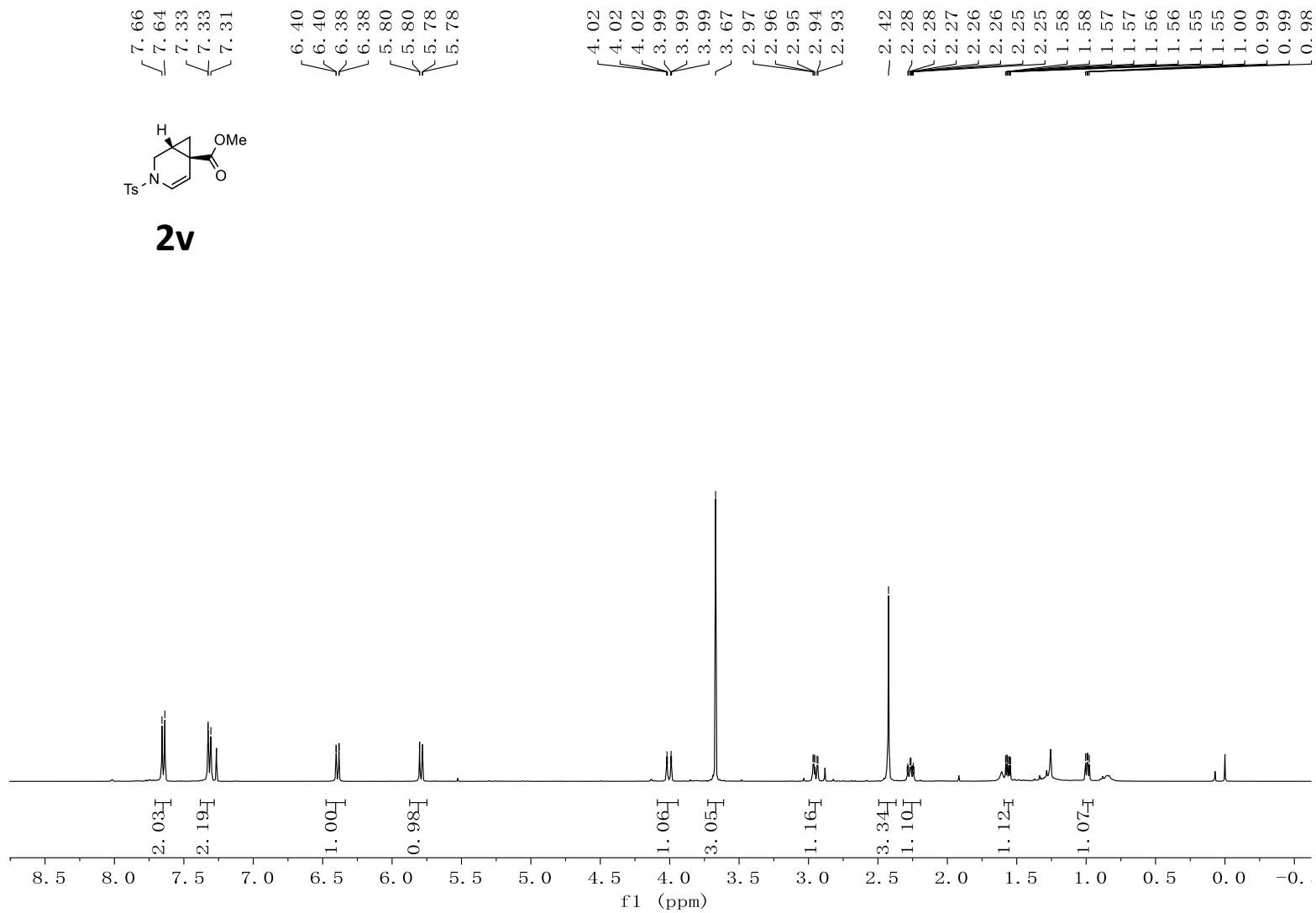
— 40.88

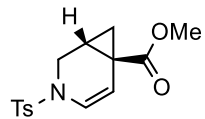
✓ 23.30  
 ✓ 21.53  
 ✓ 19.90  
 ✓ 17.65



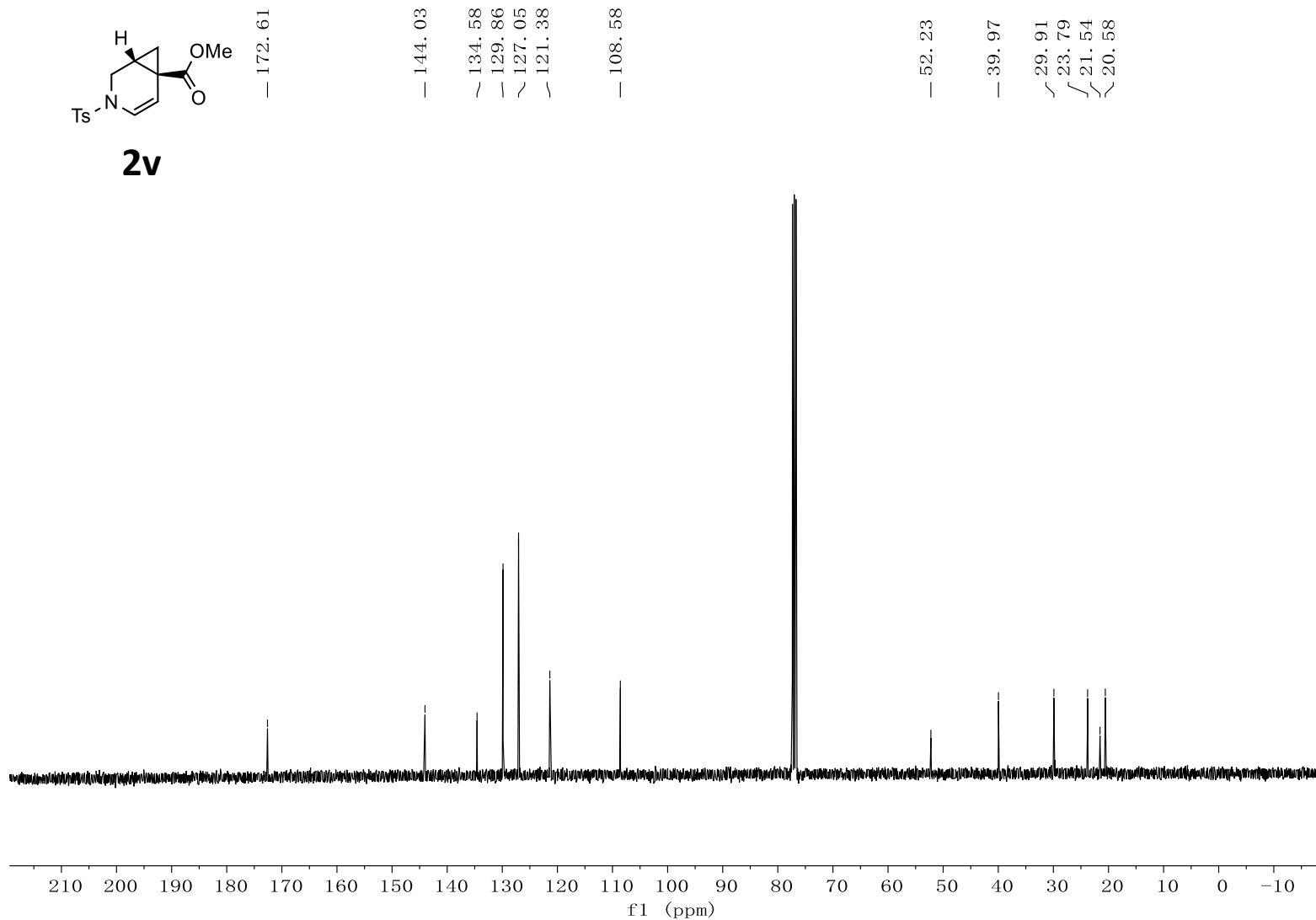


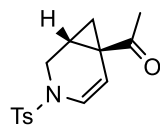
**2v**



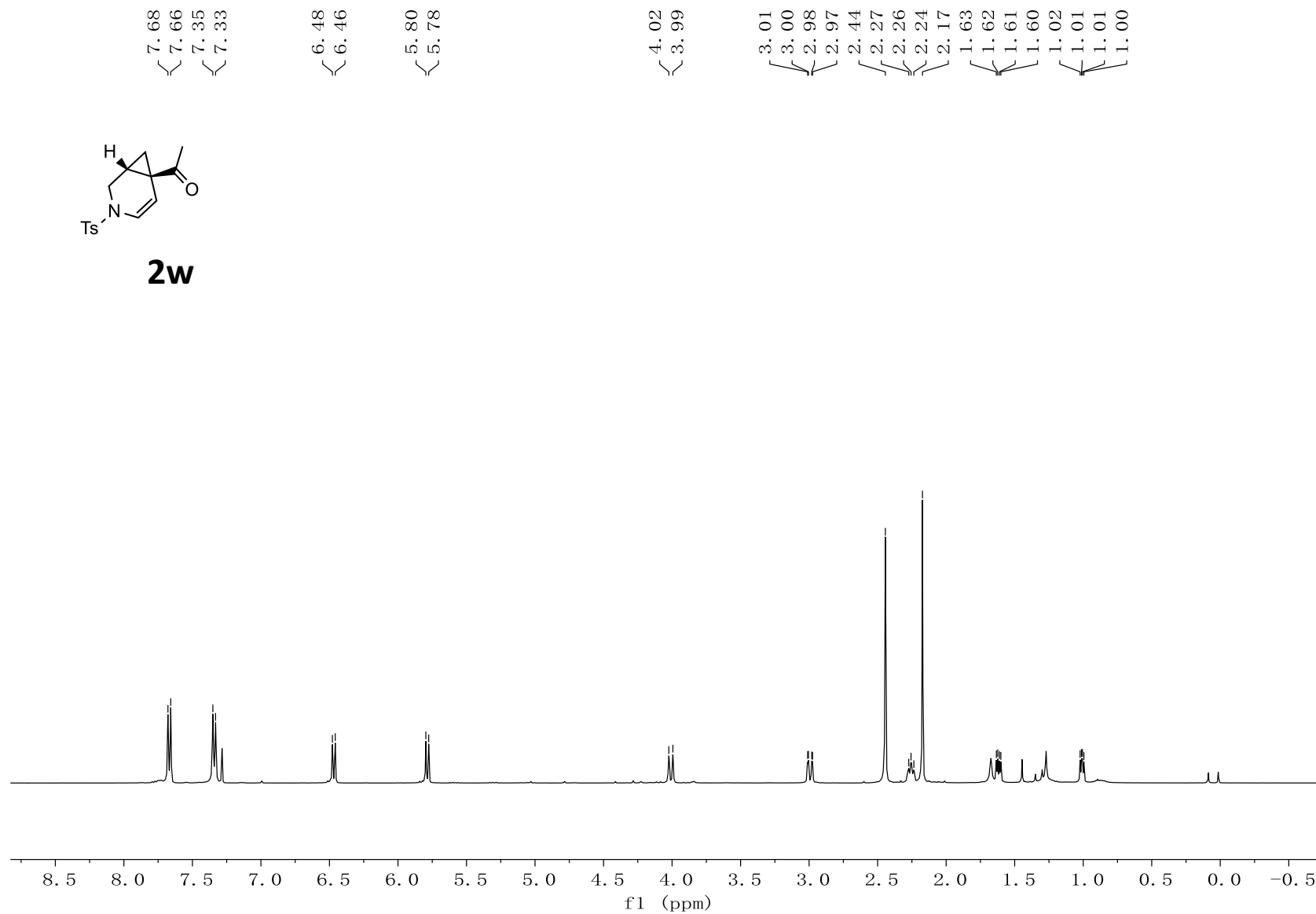


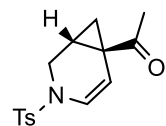
**2v**





**2w**





**2w**

— 205.52

— 144.12

— 134.51

— 129.91

— 127.04

— 121.86

— 108.55

— 40.22

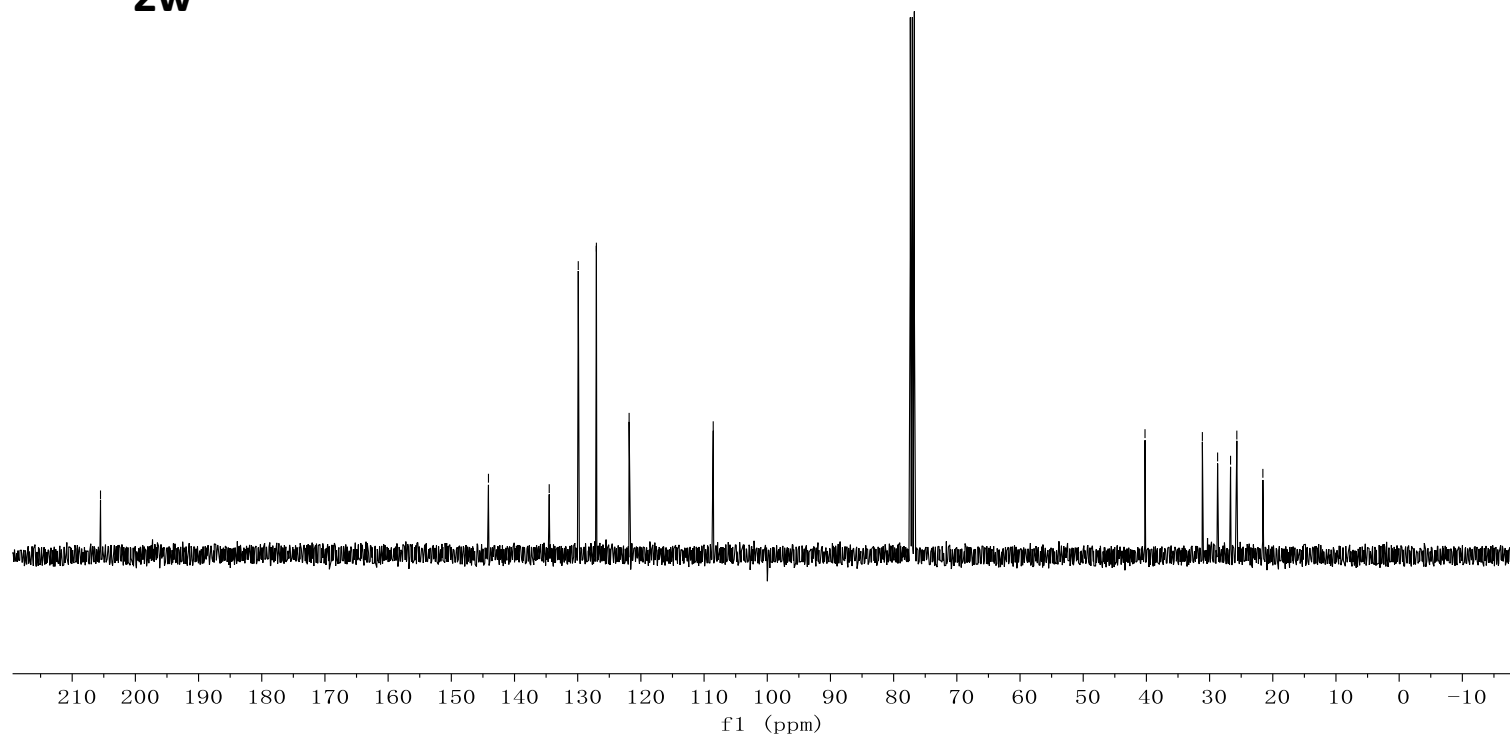
— 31.14

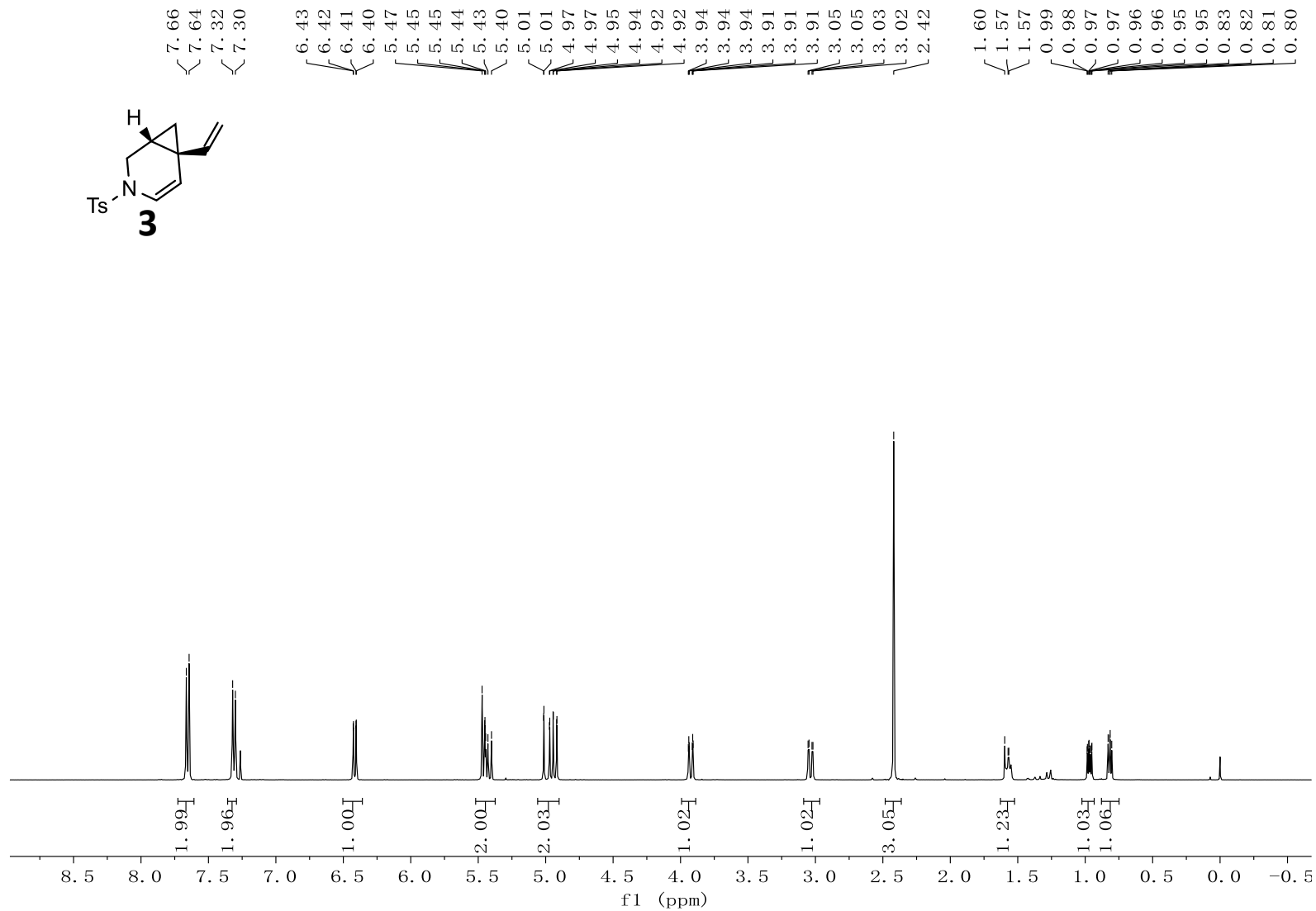
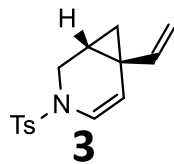
— 28.73

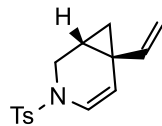
— 26.68

— 25.69

— 21.57



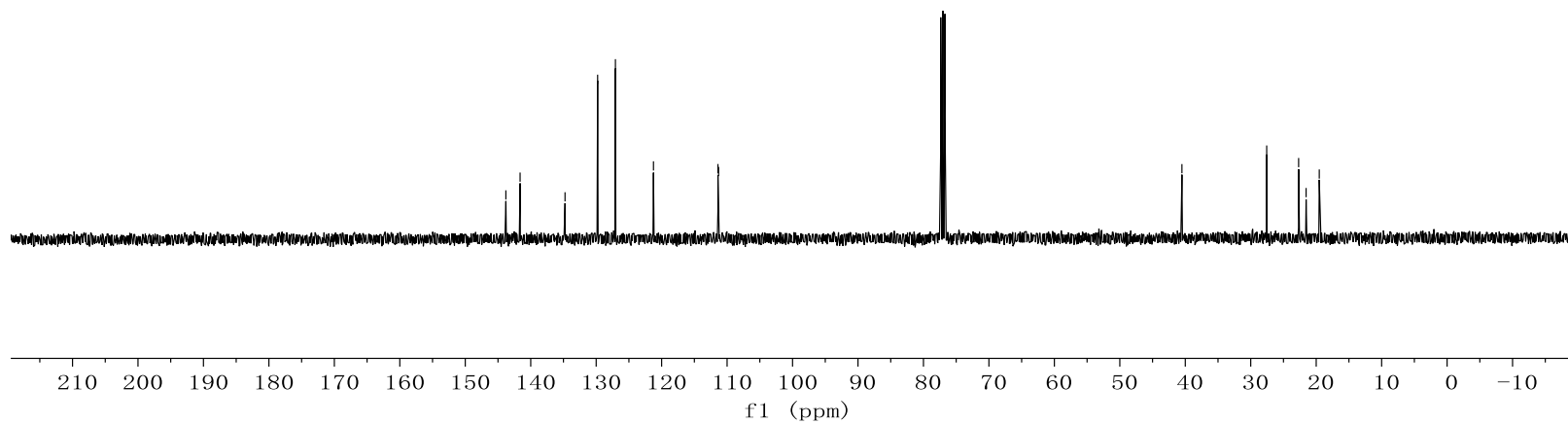


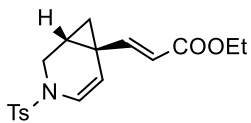


**3**

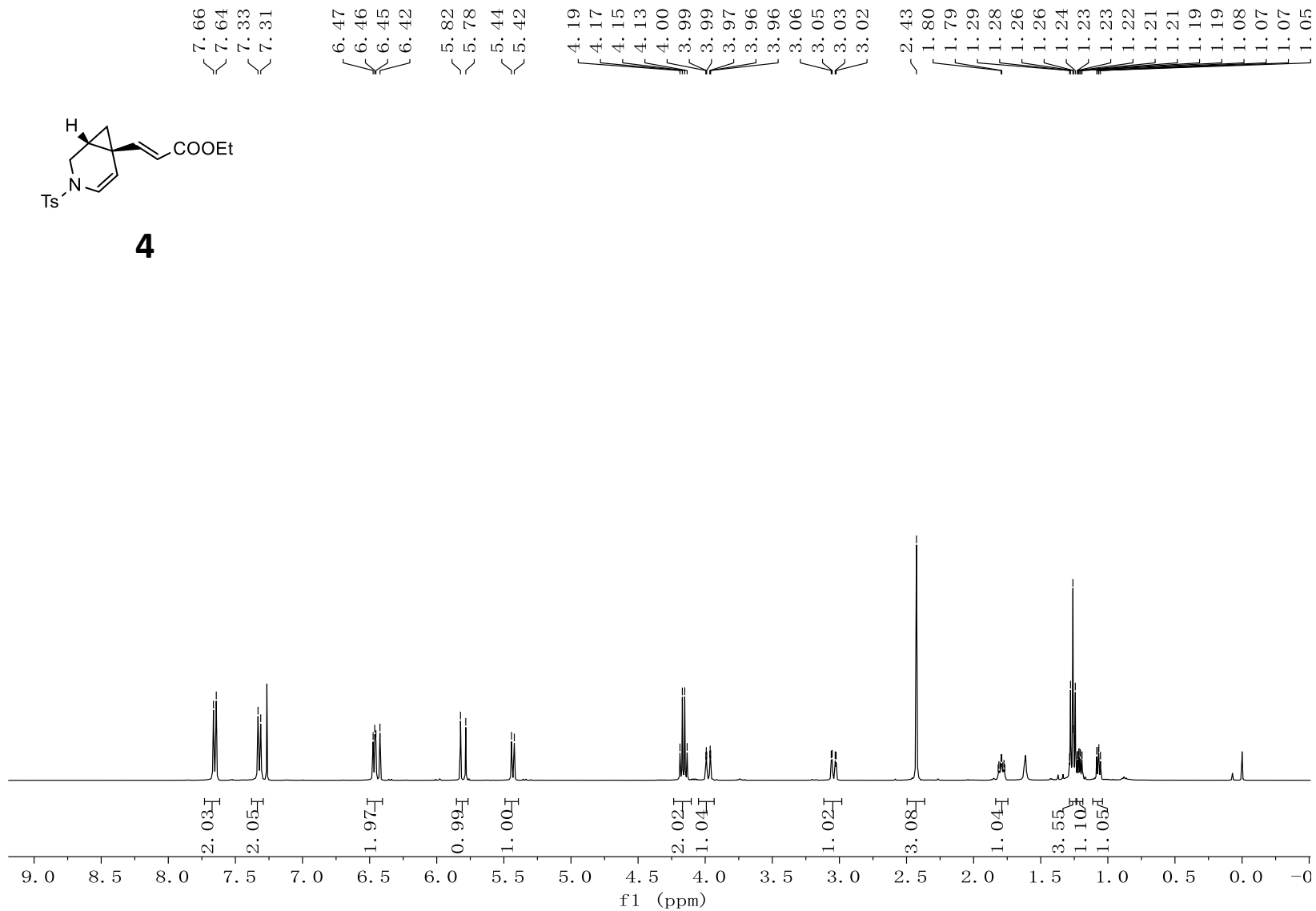
~ 143.80  
 ~ 141.62  
 ~ 134.76  
 ~ 129.78  
 ~ 127.06  
 ~ 121.25  
 ~ 111.39  
 ~ 111.30

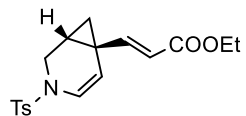
— 40.51  
 ~ 27.56  
 ~ 22.68  
 ~ 21.54  
 ~ 19.53





**4**

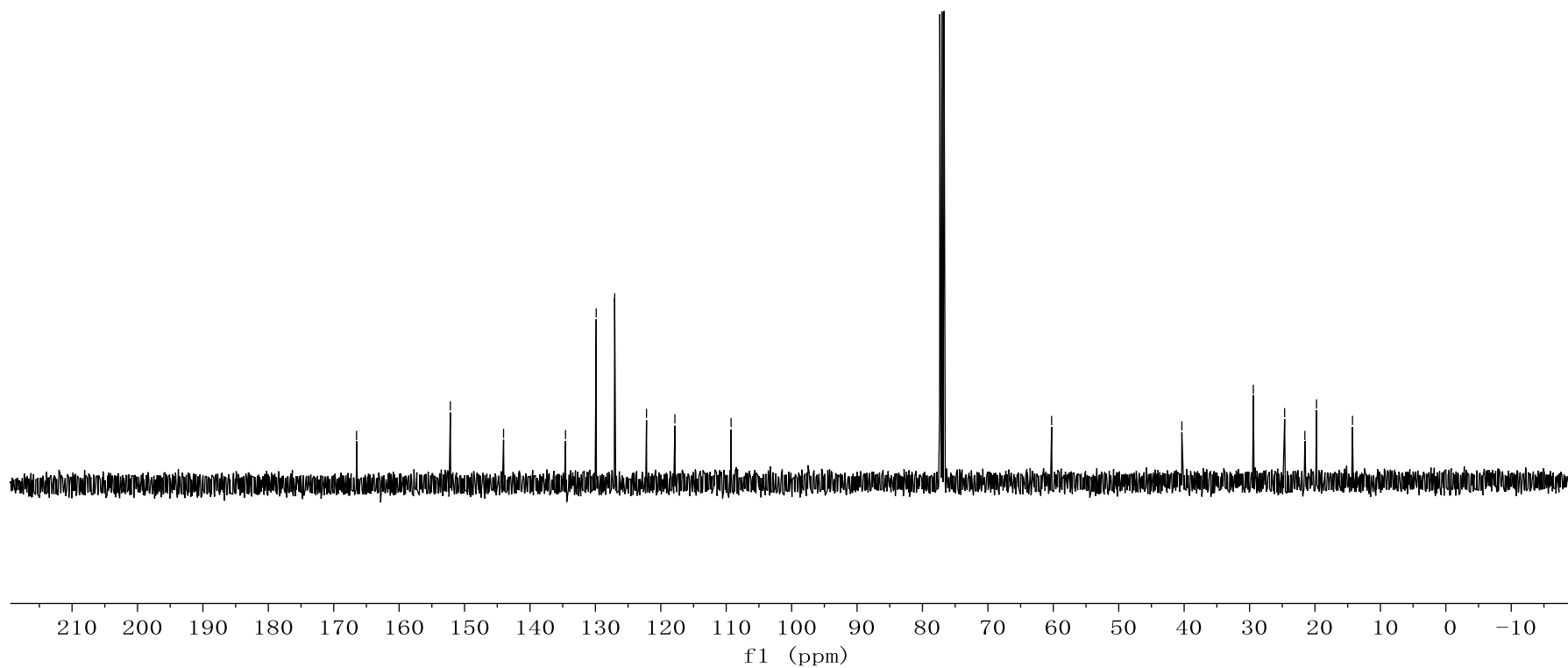


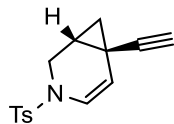


**4**

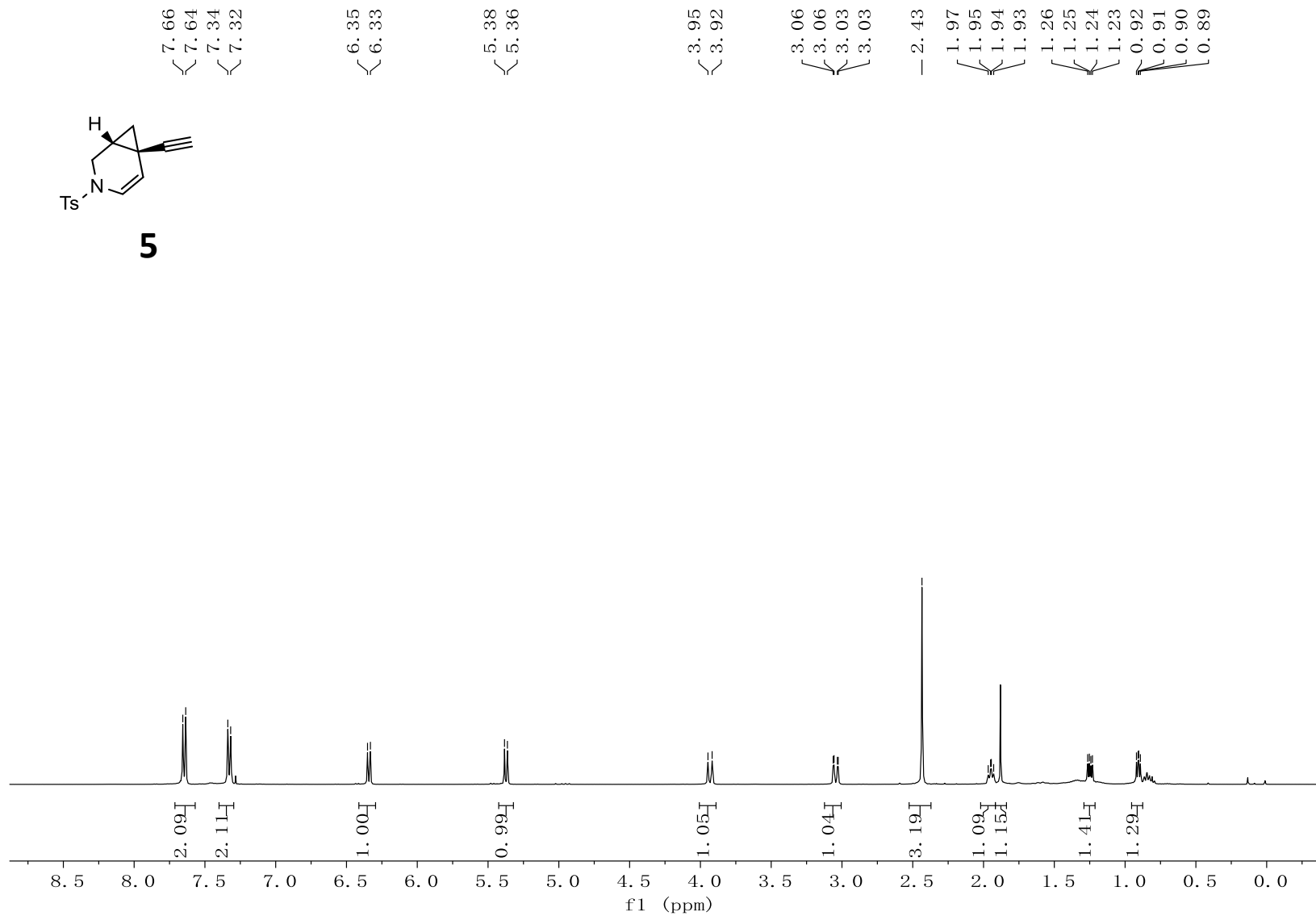
— 166.51      — 152.18      — 144.04      — 134.57      — 129.88      — 127.05      — 122.19      — 117.85      — 109.26

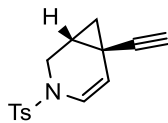
— 60.26      — 40.35      — 29.42      — 24.64      — 21.55      — 19.77      — 14.27



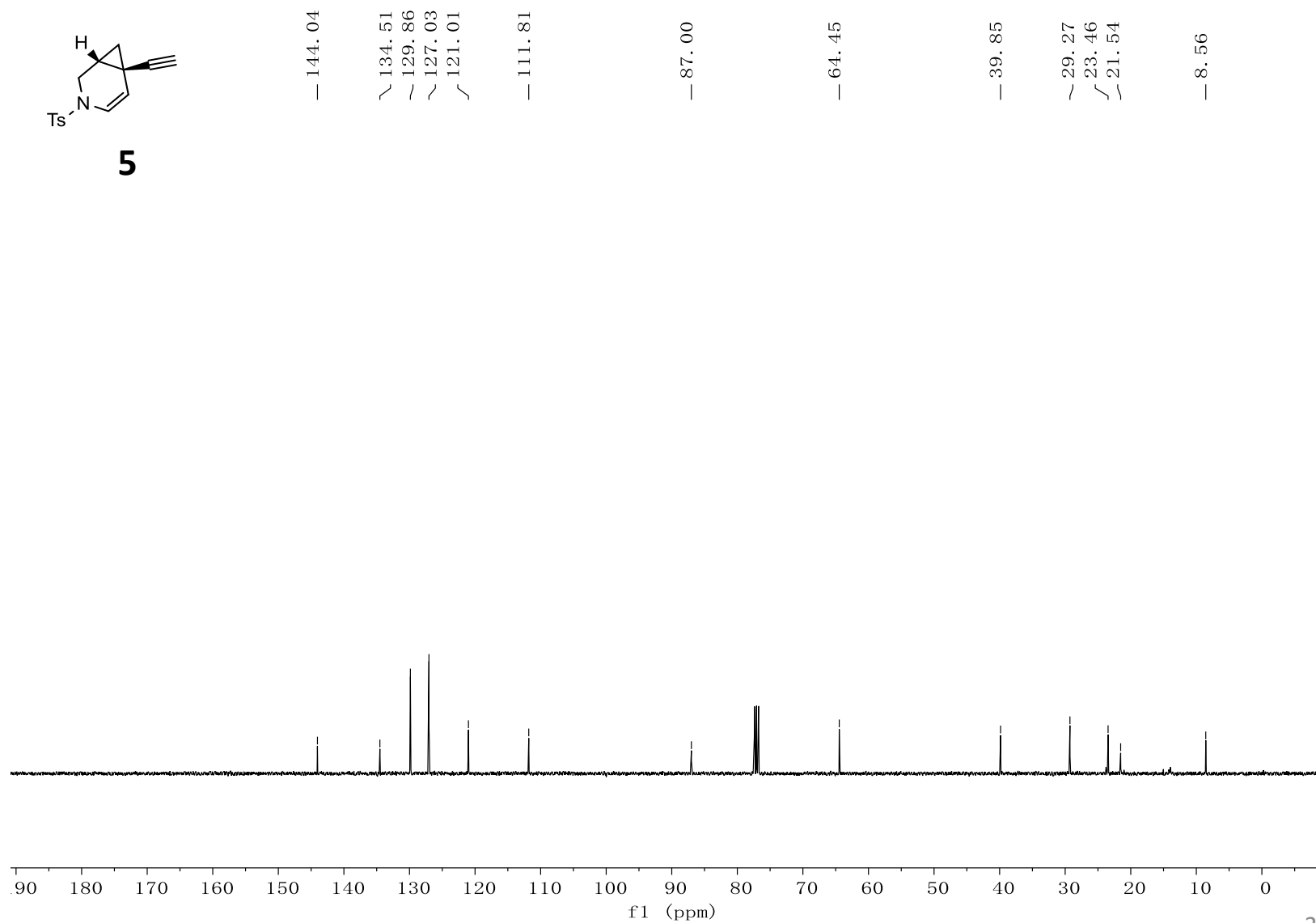


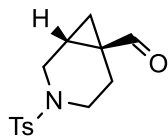
**5**



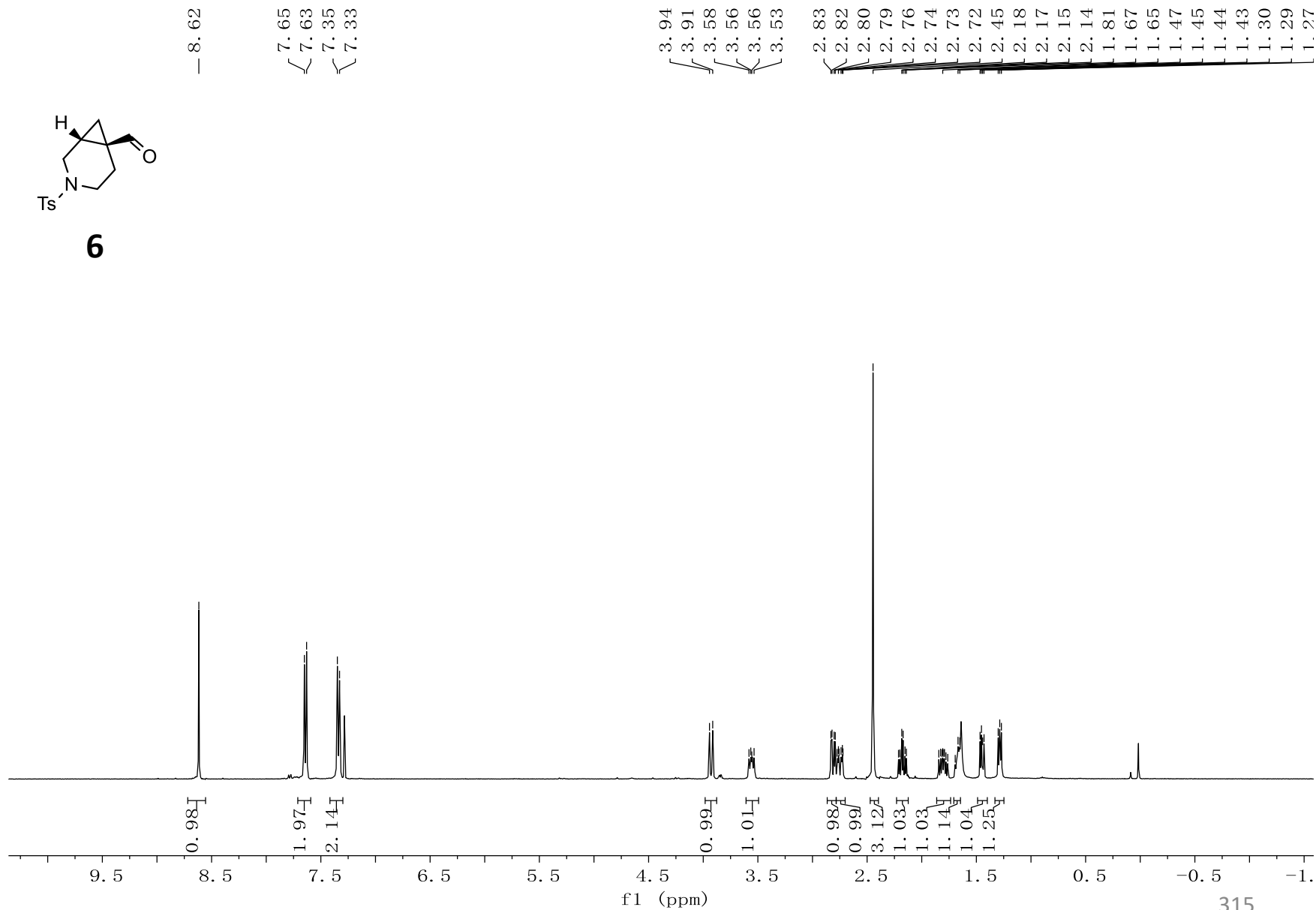


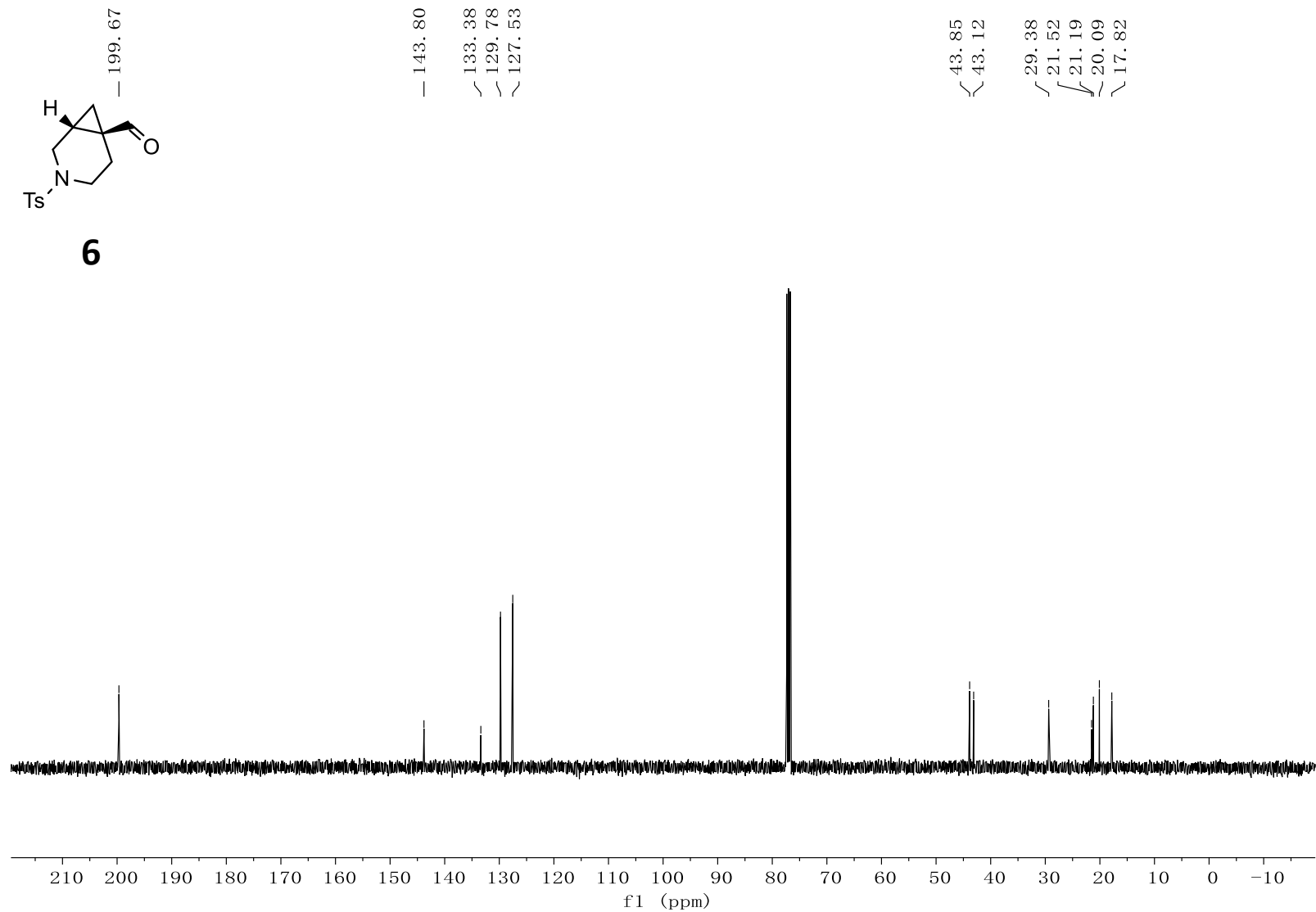
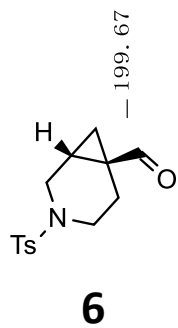
**5**

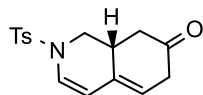




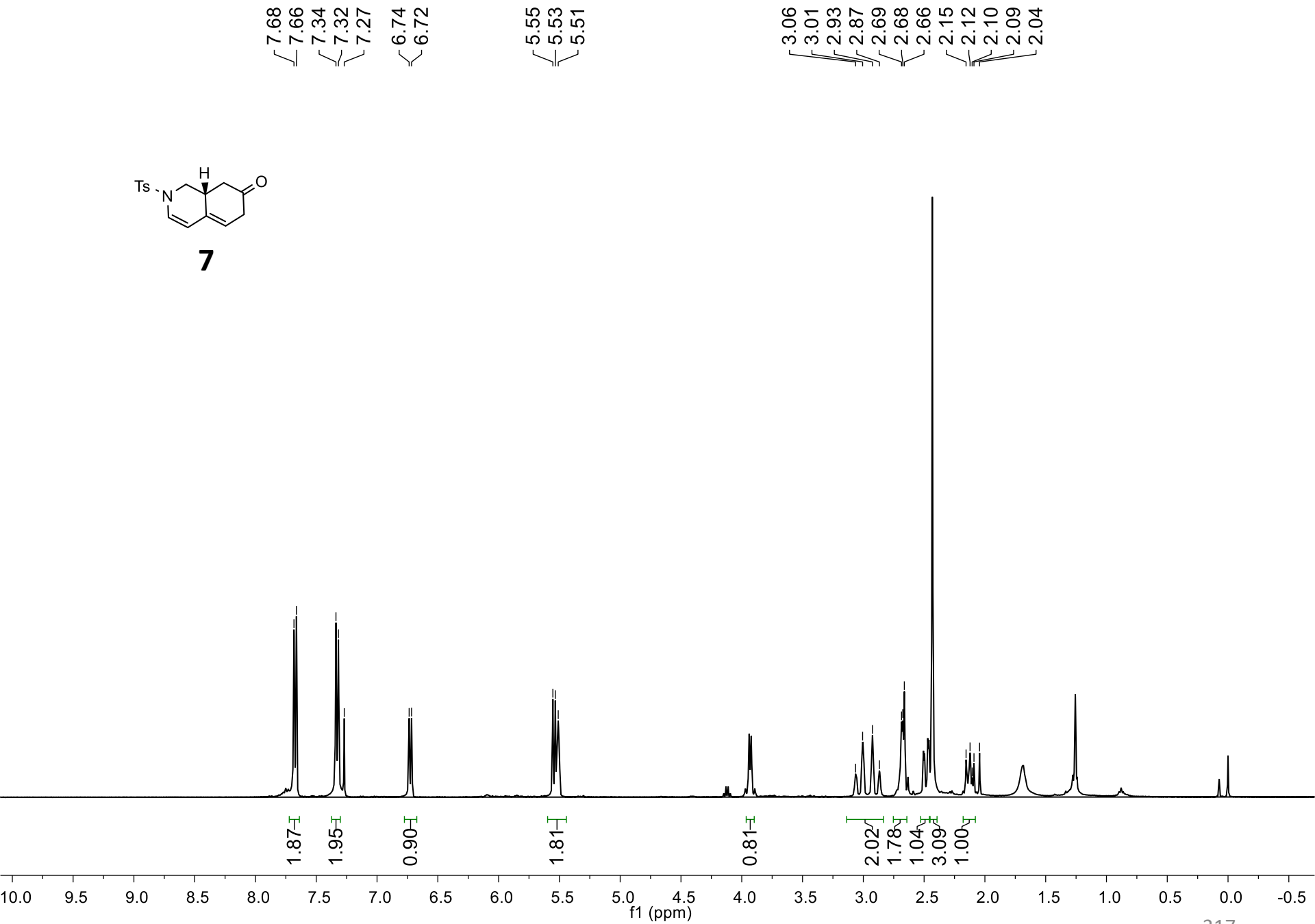
**6**

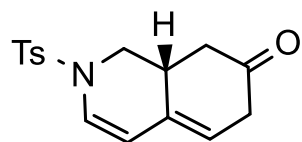




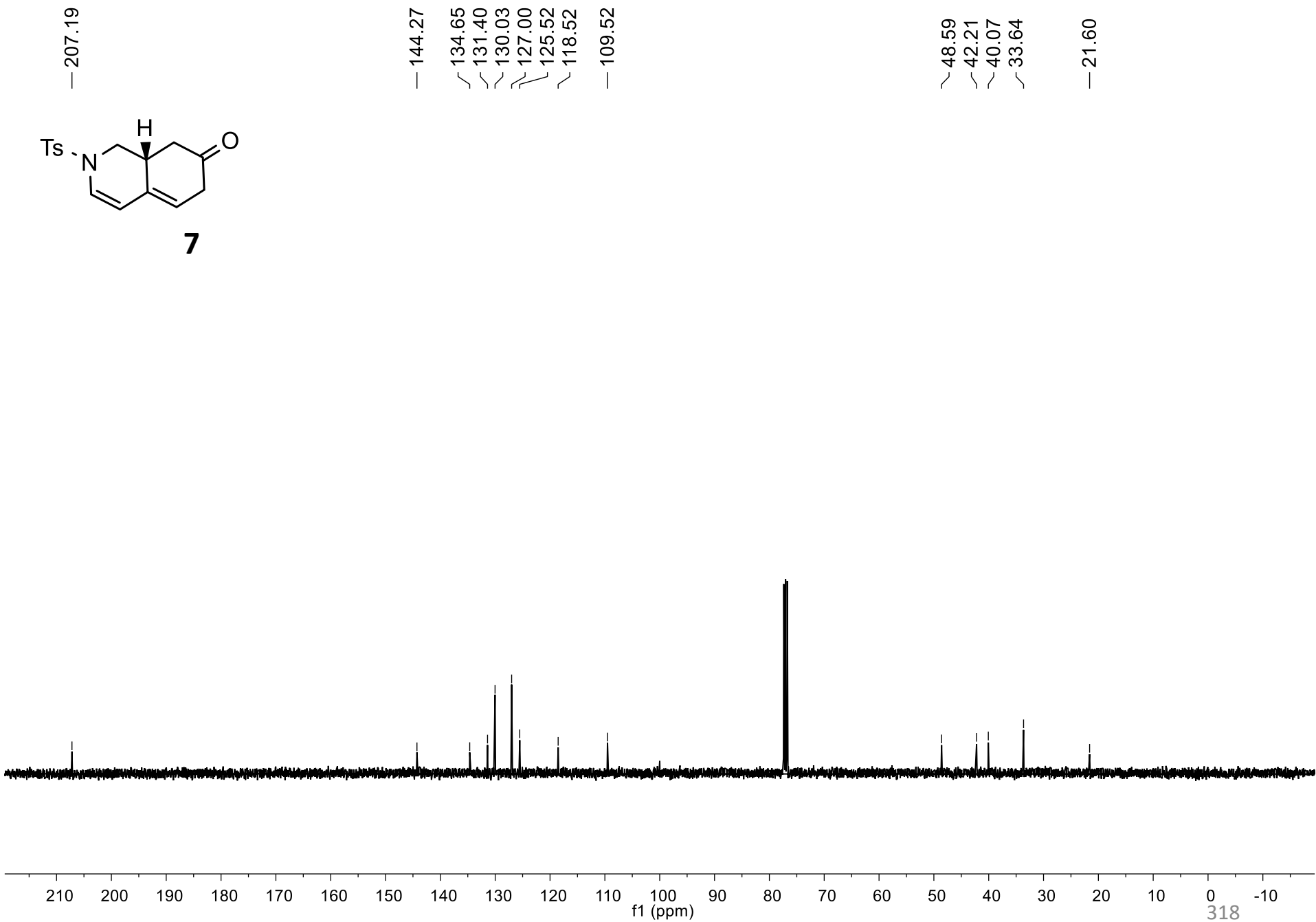


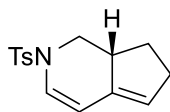
**7**



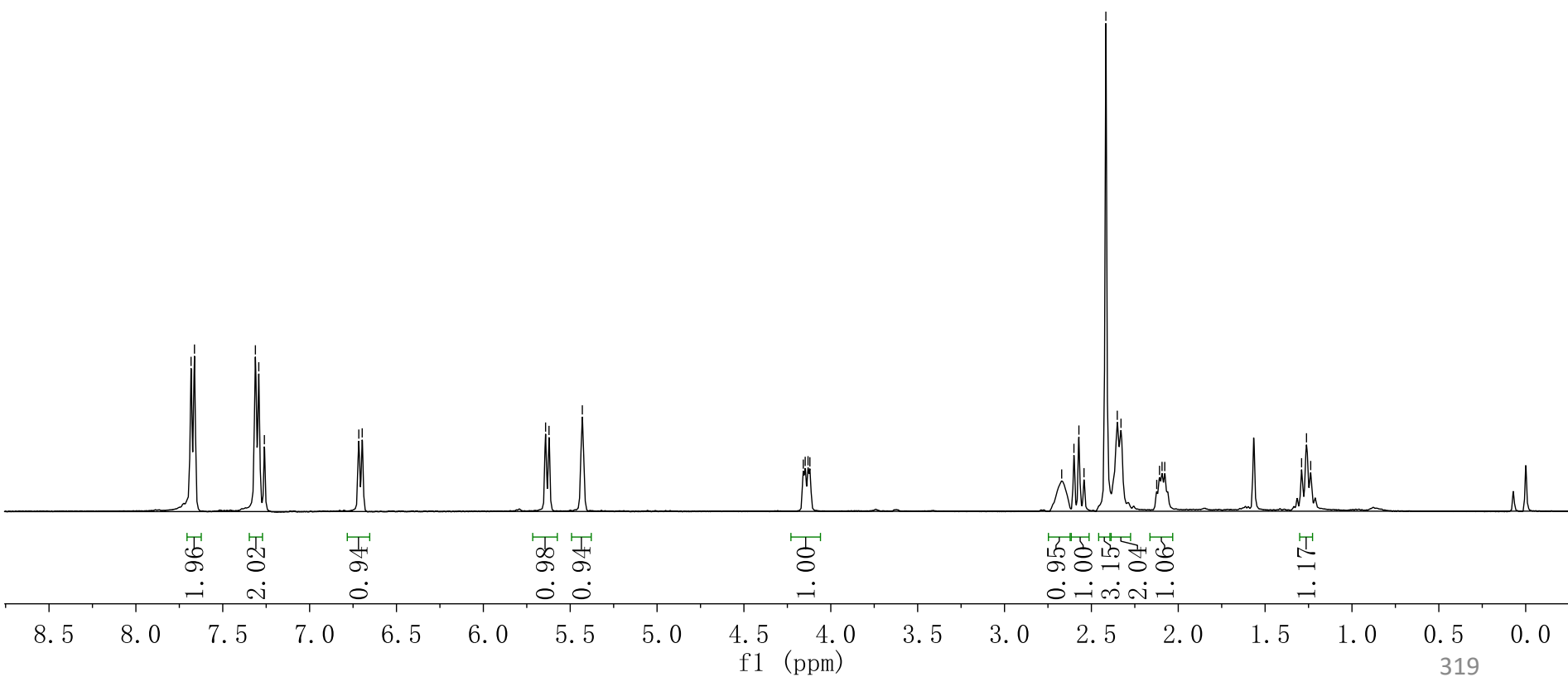


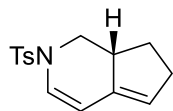
**7**





**8**





**8**

— 143.794

— 136.372

— 135.265

— 129.823

— 126.983

— 126.142

— 122.913

— 105.269

— 50.215

— 41.407

— 31.900

— 29.088

— 21.530

160

150

140

130

120

110

100

90

80

70

60

50

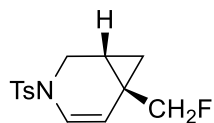
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30

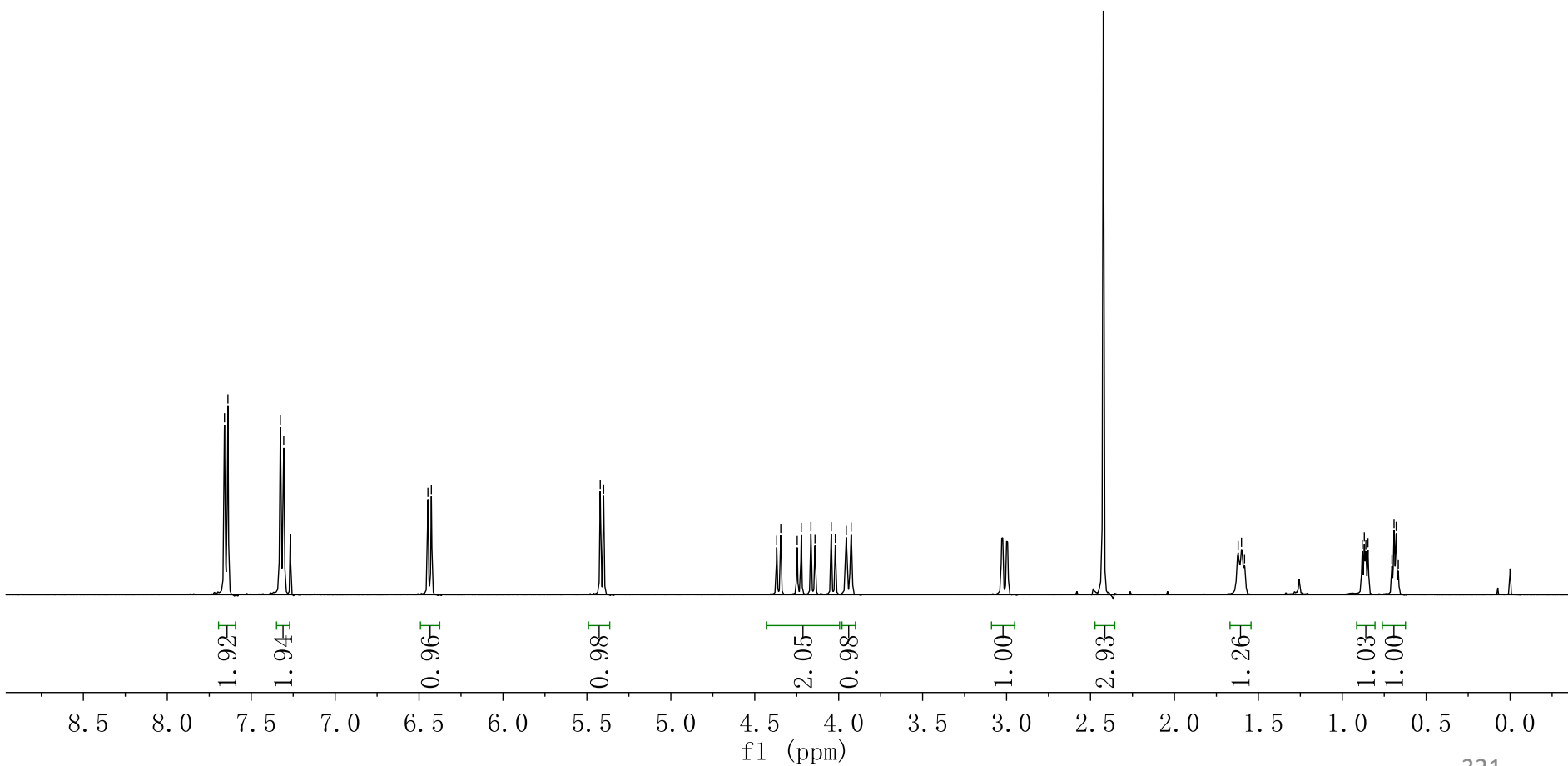
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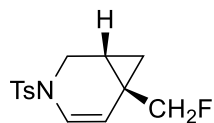
10

f1 (ppm)



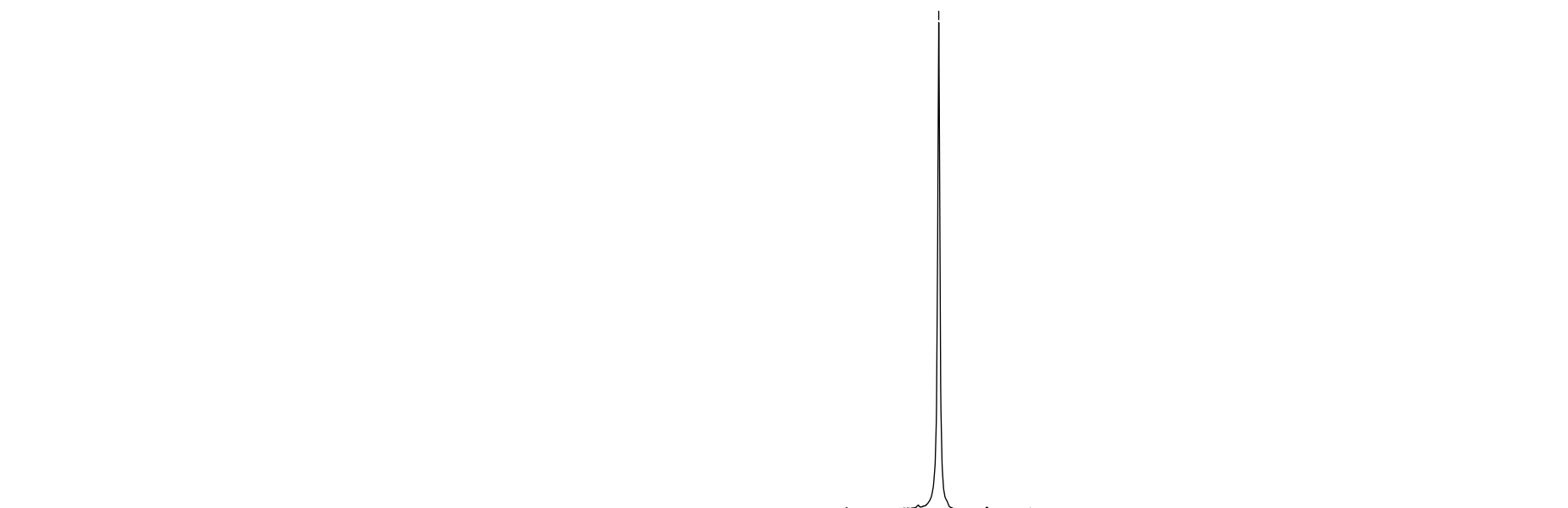
**2aa**





**2aa**

— -214.369



-209.0

-210.0

-211.0

-212.0

-213.0

-214.0

-215.0

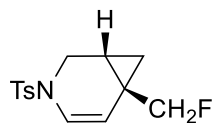
-216.0

-217.0

-218.0

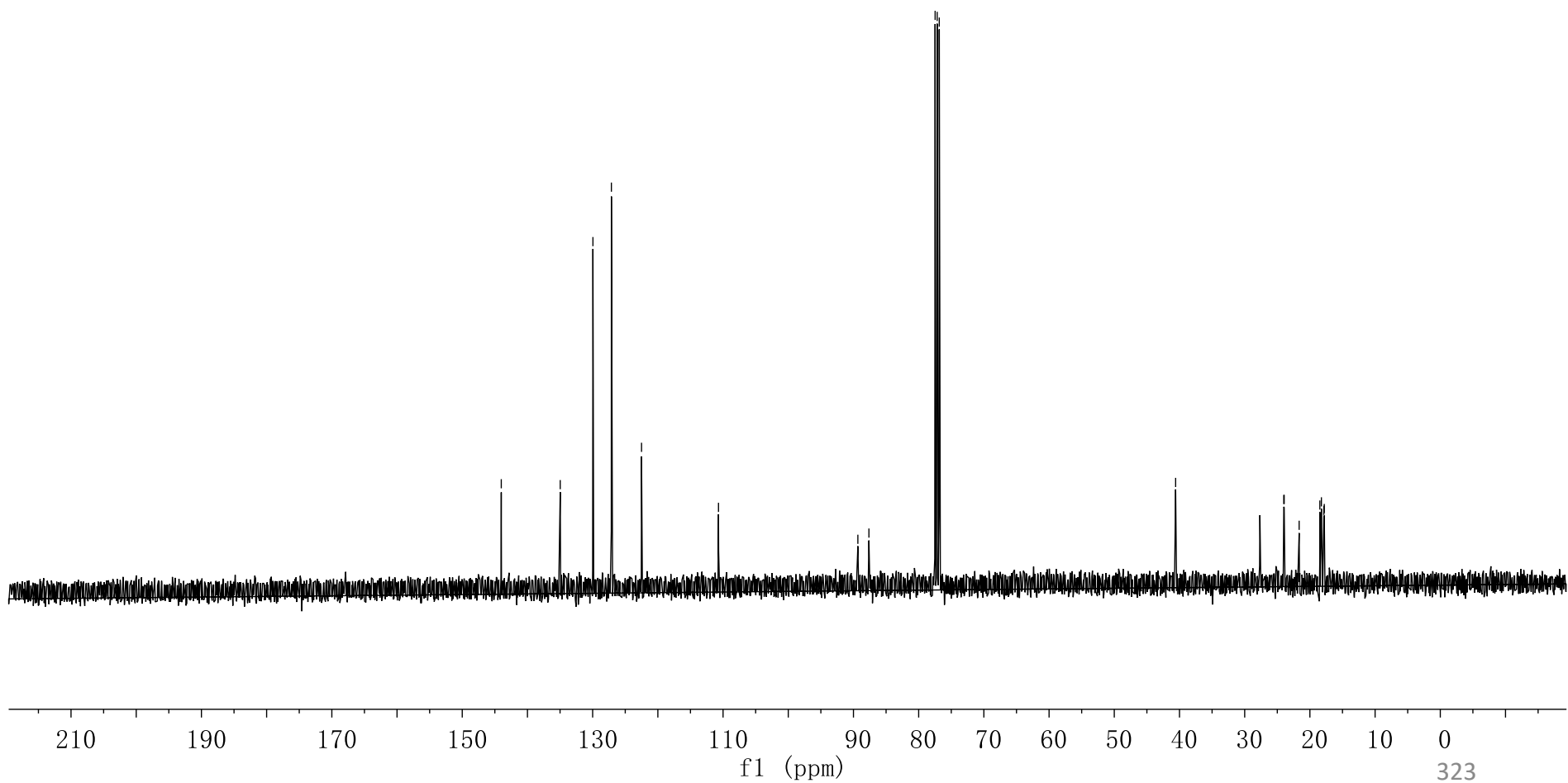
f1 (ppm)

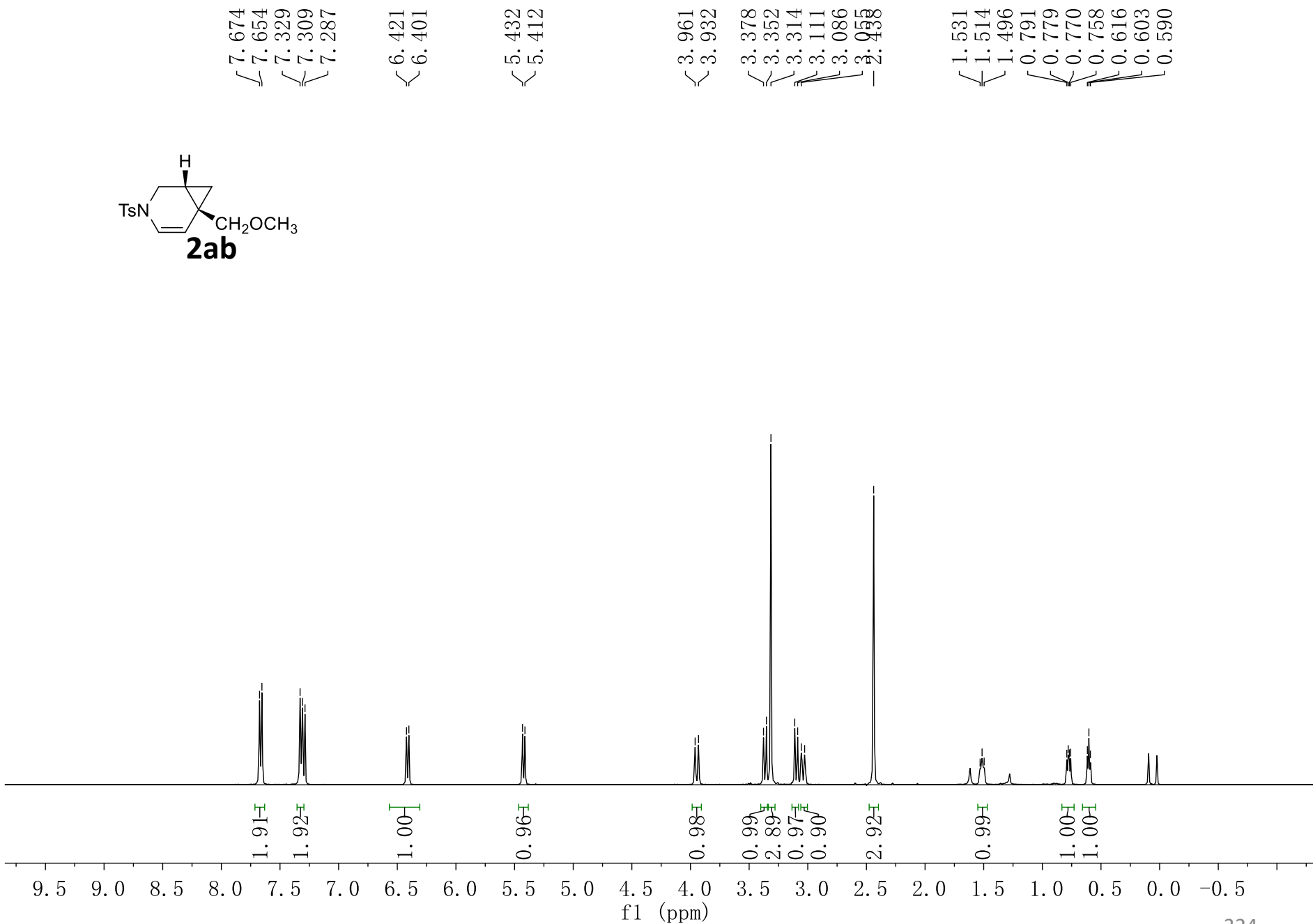
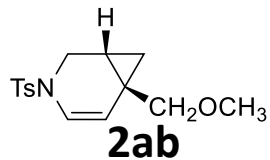
322

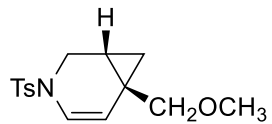


**2aa**

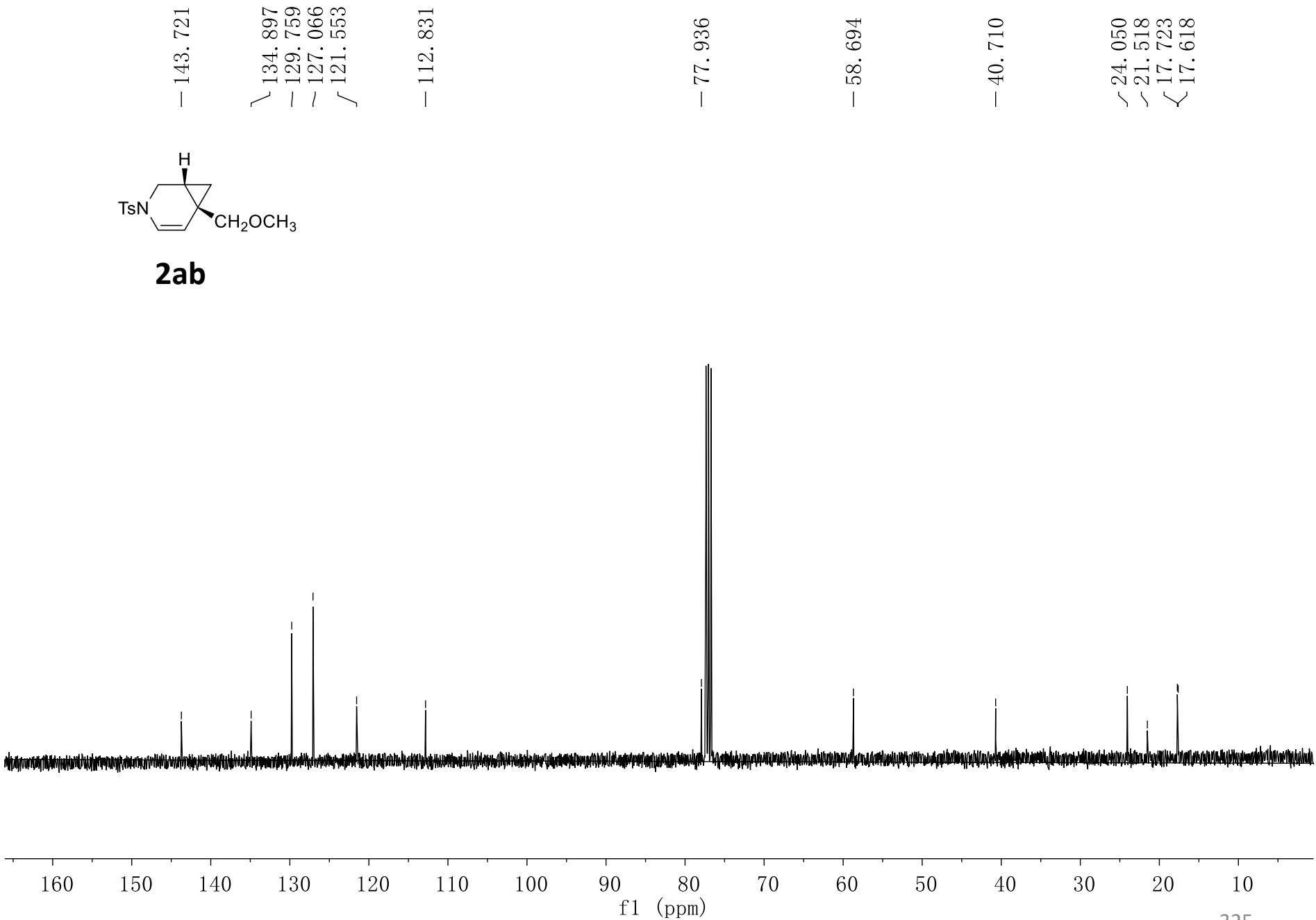
-144.014  
 -134.973  
 -129.956  
 -127.127  
 -122.502  
 -110.700  
 -89.324  
 -87.631  
 -77.477  
 -77.160  
 -76.842  
 -40.590  
 24.003  
 23.942  
 21.649  
 18.472  
 18.235  
 17.860  
 17.794

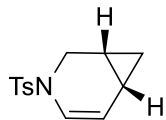




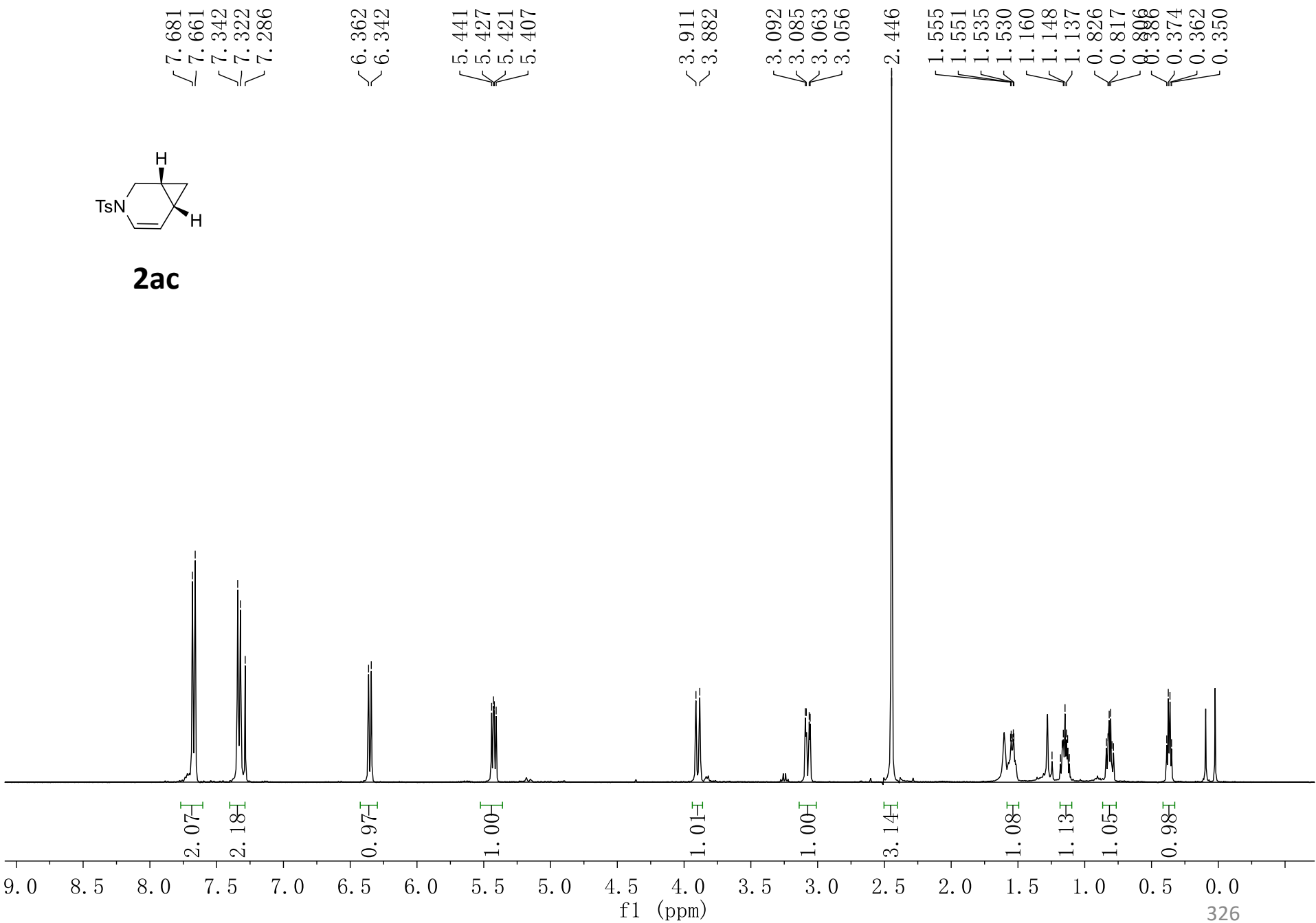


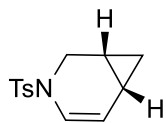
**2ab**





**2ac**





**2ac**

-143.63  
 ~134.88  
 ~129.72  
 ~127.04  
 ~121.09  
 -112.08  
 77.37  
 77.05  
 76.74  
 -40.87  
 ~21.54  
 ~18.48  
 ~13.42  
 ~7.10

