

Supporting Information

**Copper-catalyzed asymmetric cyclization of alkenyl diynes: method development  
and new mechanistic insights**

Xin-Qi Zhu,<sup>#</sup> Pan Hong,<sup>#</sup> Yan-Xin Zheng, Ying-Ying Zhen, Feng-Lin Hong, Xin Lu\* and  
Long-Wu Ye\*

State Key Laboratory of Physical Chemistry of Solid Surfaces, Key Laboratory of  
Chemical Biology of Fujian Province, and College of Chemistry and Chemical  
Engineering, Xiamen University, Xiamen 361005, China  
E-mail: [longwuye@xmu.edu.cn](mailto:longwuye@xmu.edu.cn); [xinlu@xmu.edu.cn](mailto:xinlu@xmu.edu.cn)

<b>Content</b>	<b>Page Number</b>
<b>General</b>	2
<b>More Reaction Condition, Scope and Mechanism Studies</b>	3
<b>Preparation of Starting Materials</b>	4
<b>General Procedure: Copper Catalysis</b>	31
<b>Crystal Data</b>	67
<b>Computational Studies</b>	69
<b>HPLC Chromatograms</b>	243
<b><sup>1</sup>H and <sup>13</sup>C NMR Spectra</b>	292

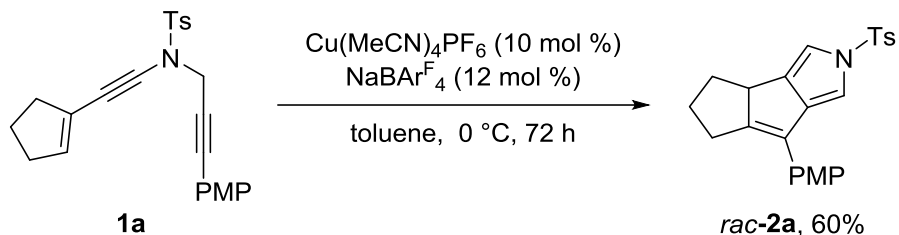
**General Information.** Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1,2-dichloroethane (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter ( $\text{cm}^{-1}$ ). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

$^1\text{H}$  NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform- $\text{d}_3$ . Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant(s) in Hz, integration).

$^{13}\text{C}$  NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform- $\text{d}_3$ . Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

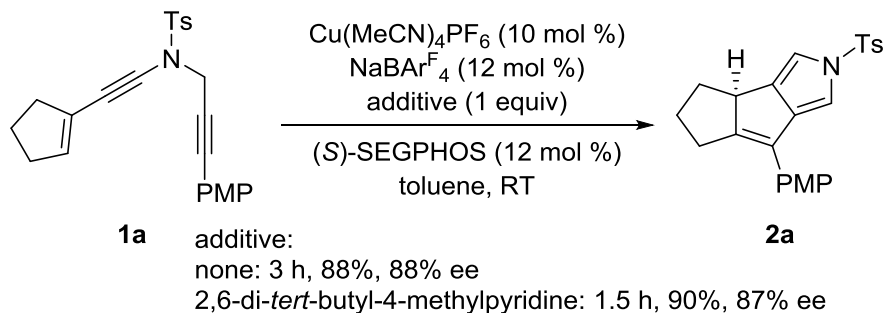
## More Reaction Condition, Scope and Mechanism Studies

1. The reaction of model substrate **1a** in the absence of the chiral ligand gave the desired tricyclic pyrrole *rac*-**2a** in 60% NMR yield.



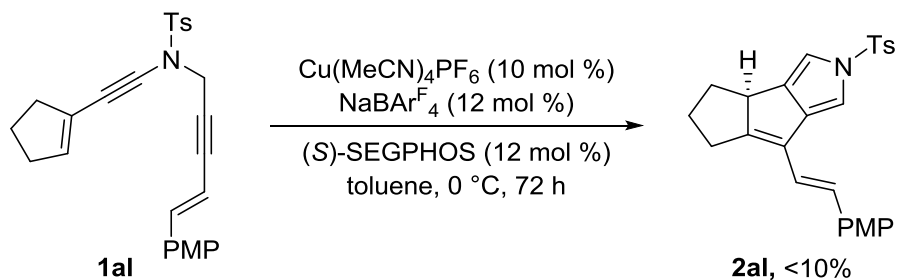
**Supplementary Figure 1.** Reaction of substrate **1a** in the absence of the chiral ligand.

2. The use of 2,6-di-*tert*-butyl-4-methylpyridine as base with large steric hindrance substantially accelerated the reaction (1.5 h vs 3 h).



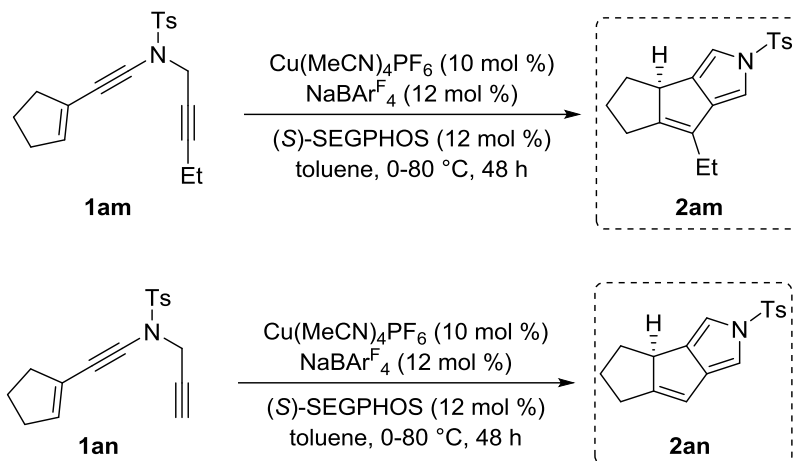
**Supplementary Figure 2.** Reaction of substrate **1a** in the presence of 2,6-di-*tert*-butyl-4-methylpyridine as base.

3. Attempted to extend the reaction to the alkenyl-substituted ynamide **1al** only led to the formation of the corresponding pyrrole product in very low yield (<10%).



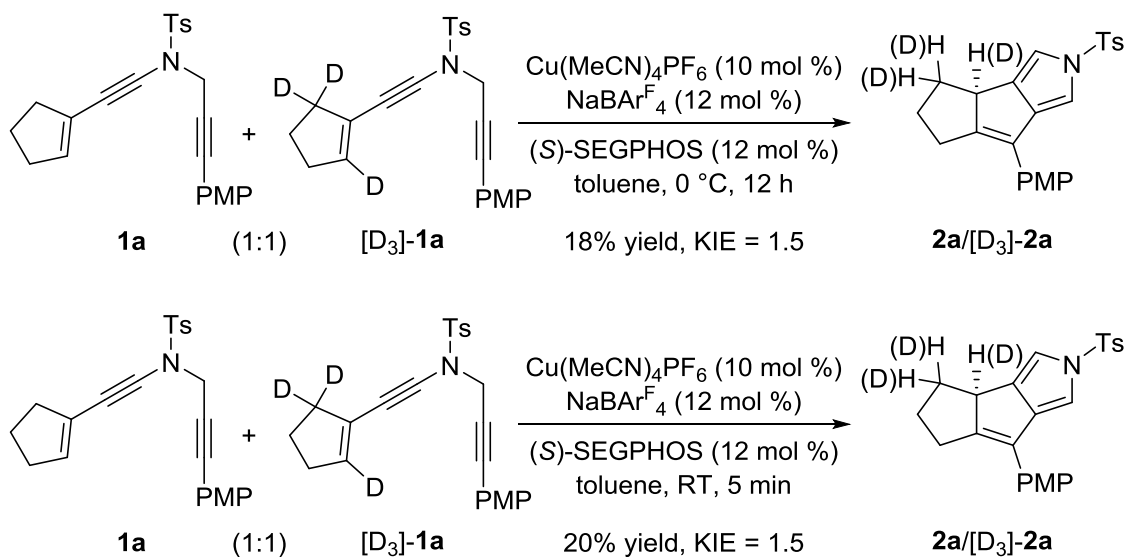
**Supplementary Figure 3.** Cu-catalyzed cascade cyclization of ynamide **1al**.

4. Attempted to extend the reaction to the alkyl-substituted and terminal ynamides **1am** and **1an** only gave a complicated mixture of products, and no desired **2am** and **2an** were obtained.



**Supplementary Figure 4.** Cu-catalyzed cascade cyclization of ynamides **1am** and **1an**.

5. The mixture of substrates **1a** and  $[\text{D}_3]\text{-1a}$  (1 : 1 ratio) was used to probe the intermolecular isotope effect (0 °C:  $k_{\text{H}}/k_{\text{D}} = 1.5$ ; rt:  $k_{\text{H}}/k_{\text{D}} = 1.5$ ). These KIE data suggest that the cleavage of vinylic  $\text{C}(\text{sp}^2)\text{-H}$  bond is not the rate-determining step.

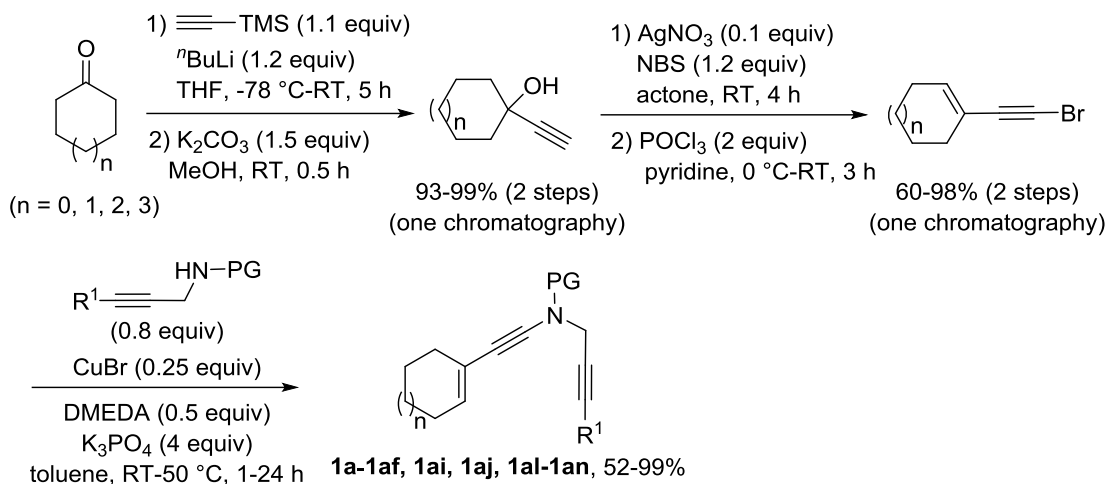


**Supplementary Figure 5.** KIE experiment.

### Representative synthetic procedures for the preparation of ynamides **1**:

General procedure A (**1a-1af**, **1ai**, **1aj**, **1al-1an**):





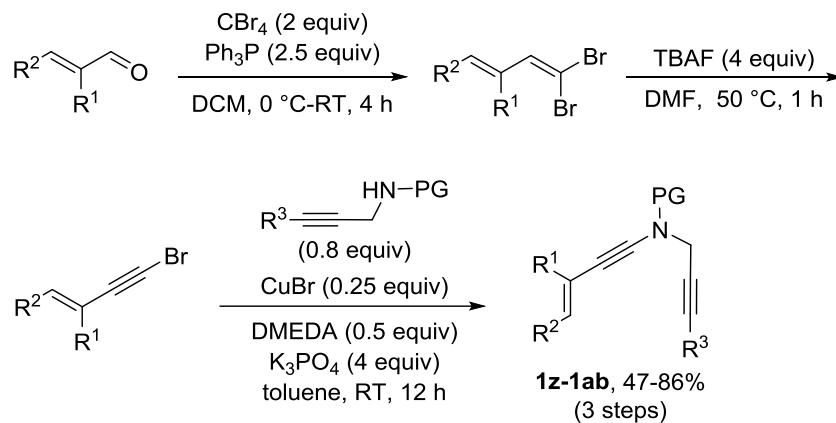
To a solution of trimethylsilyl acetylene (33 mmol, 3.23 g) in 30 mL THF, *n*-butyllithium (36 mmol, 14 mL of 2.5 M solution in hexane) was added dropwise at  $-78\text{ }^\circ\text{C}$ . The mixture was stirred at the same temperature for 0.5 h, then the cyclohexenone (30 mmol) was added dropwise. The resulting solution was warmed up to room temperature and stirred for 5 h. The reaction mixture was then quenched with saturated  $\text{NH}_4\text{Cl}$  (aq.), and the aqueous layer was extracted with  $\text{Et}_2\text{O}$  ( $3 \times 30\text{ mL}$ ). The combined organic extracts were washed with brine and water, dried over  $\text{MgSO}_4$ , filtered and the solvent was removed under reduced pressure to afford the crude alcohol, which was engaged in the next step without purification. To a solution of the crude propargyl alcohol (30 mmol) in 60 mL MeOH was added  $\text{K}_2\text{CO}_3$  (45 mmol, 6.21 g). After stirring for 0.5 h at room temperature, about 90% of the solvent was removed under reduced pressure, and the resulting solution was diluted with 30 mL of water and 30 mL of  $\text{Et}_2\text{O}$ . The aqueous layer was extracted with  $\text{Et}_2\text{O}$  ( $3 \times 30\text{ mL}$ ) and the combined organic extracts were washed with brine and water, dried over  $\text{MgSO}_4$  and evaporated under reduced pressure to afford the pure alcohol (93-99% yields over two steps).

$\text{NBS}$  (36 mmol, 6.41 g) and  $\text{AgNO}_3$  (3.0 mmol, 0.51 g) were added to propargyl alcohol (30 mmol) in actone (60 mL) successively at room temperature. Then, the reaction mixture was stirred at room temperature for 4 h. Upon completion, the mixture was filtered through a pad of celite and then concentrated in vacuum. The crude brominated alkyne was used in the next step without purification.  $\text{POCl}_3$  (60 mmol, 9.20 g) was added dropwise to the crude chlorinated alkyne (30 mmol) in 60 mL pyridine at  $0\text{ }^\circ\text{C}$ , then the mixture was allowed to warm to room temperature and the progress of the

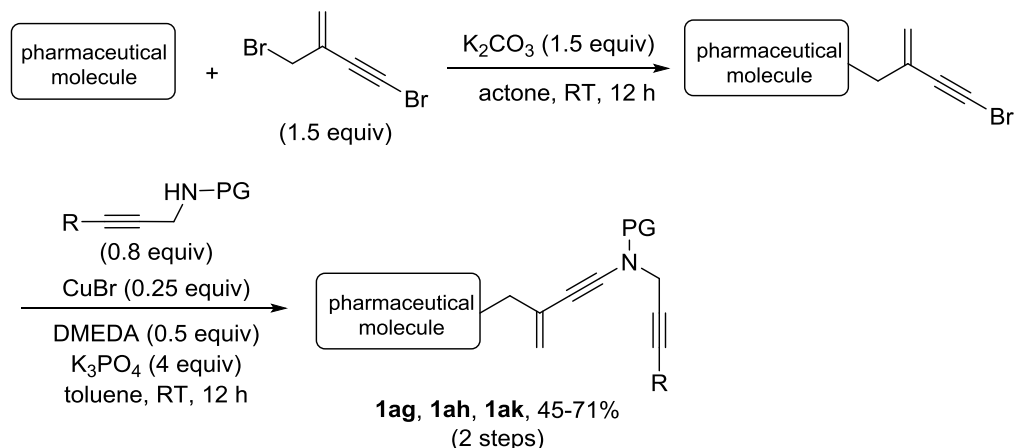
reaction was monitored by TLC. Upon completion, water was added dropwise at 0 °C to quench the reaction, the mixture was then extracted with ether (3 × 30 mL) and the combined organic extracts were washed with brine and water, dried over MgSO<sub>4</sub>, filtered and concentrated in vacuum. The residue was purified by flash chromatography on silica gel to afford 3-en-1-brominated alkyne (60-98% yields over two steps).

To a solution of brominated alkyne (1.0 mmol) in toluene (8 mL) was added copper bromide (0.25 mmol, 36 mg), DMEDA (0.5 mmol, 44 mg), K<sub>3</sub>PO<sub>4</sub> (4 mmol, 0.85 g), protected propargylamide derivative (0.8 mmol). The reaction was stirred at rt or 50 °C for 1-24 h and the progress of the reaction was monitored by TLC. Upon completion, the solution was then filtered and concentrated under a reduced pressure. The residue was purified by silica gel column chromatography (eluent: hexanes/EtOAc, 52-99%).

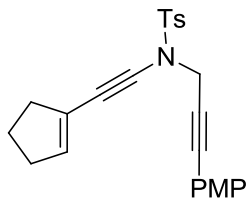
General procedure B (**1z-1ab**)<sup>1</sup>:



General procedure C (**1ag, 1ah and 1ak**)<sup>2</sup>:



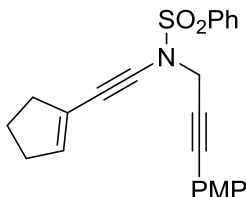
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1a)**



**1a**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 – 7.83 (m, 2H), 7.31 – 7.25 (m, 2H), 7.14 – 7.08 (m, 2H), 6.82 – 6.74 (m, 2H), 5.97 – 5.94 (m, 1H), 4.46 (s, 2H), 3.79 (s, 3H), 2.45 – 2.38 (m, 4H), 2.36 (s, 3H), 1.92 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 144.6, 136.7, 134.3, 133.1, 129.4, 128.2, 123.6, 114.2, 113.7, 86.3, 83.0, 79.8, 68.5, 55.2, 42.9, 36.5, 33.2, 23.2, 21.5; IR (neat): 2945, 2216, 2004, 1712, 1653, 1525, 1323, 1267, 1052, 837, 663, 542; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 428.1291, found 428.1290.

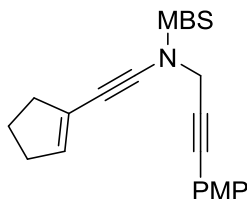
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (1b)**



**1b**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 – 7.95 (m, 2H), 7.61 – 7.45 (m, 3H), 7.12 (d,  $J = 8.8$  Hz, 2H), 6.77 (d,  $J = 8.8$  Hz, 2H), 6.01 – 5.93 (m, 1H), 4.49 (s, 2H), 3.78 (s, 3H), 2.46 – 2.35 (m, 4H), 1.93 – 1.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.8, 137.2, 136.9, 133.6, 133.1, 128.8, 128.1, 123.5, 114.0, 113.7, 86.4, 82.7, 79.7, 68.6, 55.2, 43.0, 36.4, 33.2, 23.1; IR (neat): 2964, 2231, 2014, 1686, 1554, 1324, 1133, 1014, 834, 757, 546; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{21}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 414.1134, found 414.1134.

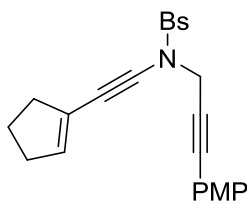
***N*-(cyclopent-1-en-1-ylethynyl)-4-methoxy-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (1c)**



**1c**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 – 7.87 (m, 2H), 7.16 – 7.09 (m, 2H), 6.96 – 6.89 (m, 2H), 6.82 – 6.74 (m, 2H), 5.98 – 5.92 (m, 1H), 4.46 (s, 2H), 3.79 (s, 3H), 3.78 (s, 3H), 2.47 – 2.37 (m, 4H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  163.7, 159.7, 136.7, 133.1, 130.4, 128.8, 123.6, 114.2, 114.0, 113.7, 86.3, 83.1, 79.9, 68.5, 55.5, 55.2, 42.9, 36.5, 33.2, 23.2; IR (neat): 2943, 2242, 2011, 1772, 1571, 1334, 1121, 1004, 814, 612, 571; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 444.1240, found 444.1242.

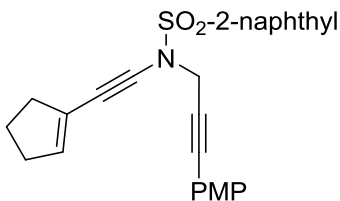
***4*-bromo-*N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (1d)**



**1d**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 – 7.80 (m, 2H), 7.67 – 7.56 (m, 2H), 7.11 – 7.05 (m, 2H), 6.85 – 6.76 (m, 2H), 6.02 – 5.94 (m, 1H), 4.49 (s, 2H), 3.80 (s, 3H), 2.49 – 2.36 (m, 4H), 1.95 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.9, 137.5, 136.3, 133.1, 132.1, 129.7, 128.9, 123.3, 113.9, 113.8, 86.7, 82.4, 79.5, 68.8, 55.3, 43.2, 36.5, 33.2, 23.2; IR (neat): 2911, 2247, 2074, 1747, 1521, 1377, 1286, 1193, 1068, 835, 536; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{20}\text{BrNNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 492.0239, found 492.0238.

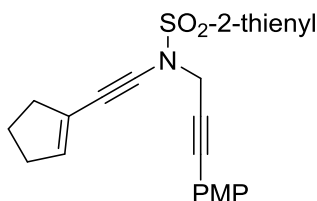
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)naphthalene-2-sulfonamide (1e)**



**1e**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.55 (s, 1H), 7.98 (d,  $J = 8.4$  Hz, 1H), 7.93 – 7.81 (m, 3H), 7.64 – 7.50 (m, 2H), 6.82 (d,  $J = 8.8$  Hz, 2H), 6.59 (d,  $J = 8.8$  Hz, 2H), 6.05 – 5.89 (m, 1H), 4.53 (s, 2H), 3.72 (s, 3H), 2.49 – 2.30 (m, 4H), 1.93 – 1.75 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.5, 136.9, 135.2, 134.2, 132.8, 131.8, 129.8, 129.3, 129.0, 128.9, 127.9, 127.4, 123.4, 123.0, 113.7, 113.5, 86.4, 82.9, 79.6, 68.6, 55.1, 43.1, 36.4, 33.1, 23.1; IR (neat): 2946, 2223, 2017, 1678, 1525, 1379, 1267, 1033, 856, 724, 667; HRESIMS Calcd for  $[\text{C}_{27}\text{H}_{23}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 464.1291, found 464.1292.

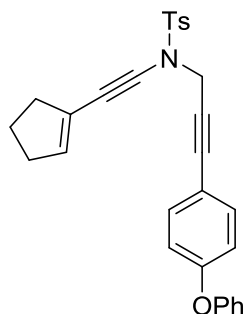
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)thiophene-2-sulfonamide (1f)**



**1f**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 – 7.74 (m, 1H), 7.66 – 7.60 (m, 1H), 7.22 – 7.16 (m, 2H), 7.11 – 7.06 (m, 1H), 6.82 – 6.76 (m, 2H), 6.03 – 5.96 (m, 1H), 4.50 (s, 2H), 3.79 (s, 3H), 2.48 – 2.37 (m, 4H), 1.95 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.8, 137.4, 136.6, 134.0, 133.5, 133.1, 127.3, 123.4, 114.1, 113.8, 86.5, 82.2, 79.3, 69.5, 55.2, 43.2, 36.5, 33.2, 23.2; IR (neat): 2945, 2245, 2074, 1663, 1444, 1424, 1234, 1056, 712, 612, 556; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{19}\text{NNaO}_3\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 420.0699, found 420.0699.

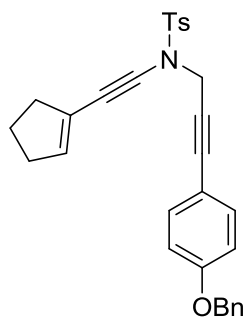
***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-(4-phenoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (1g)**



**1g**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.38 – 7.32 (m, 2H), 7.30 – 7.26 (m, 2H), 7.17 – 7.10 (m, 3H), 7.03 – 6.97 (m, 2H), 6.88 – 6.83 (m, 2H), 5.98 – 5.93 (m, 1H), 4.47 (s, 2H), 2.46 – 2.37 (m, 4H), 2.36 (s, 3H), 1.96 – 1.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.8, 156.2, 144.6, 136.8, 134.3, 133.2, 129.9, 129.4, 128.2, 123.9, 123.6, 119.4, 118.0, 116.6, 85.9, 82.9, 80.6, 68.6, 42.9, 36.5, 33.2, 23.2, 21.5; IR (neat): 2953, 2224, 2014, 1614, 1511, 1434, 1145, 822, 589, 574; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{25}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 490.1447, found 490.1448.

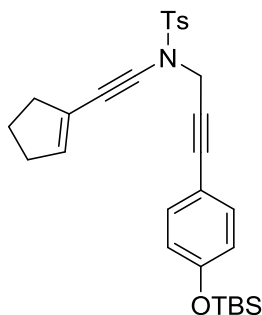
***N*-(3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)-*N*-(cyclopent-1-en-1-ylethynyl)-4-methylbenzenesulfonamide (1h)**



**1h**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.43 – 7.31 (m, 5H), 7.25 – 7.23 (m, 2H), 7.10 (d,  $J = 8.8$  Hz, 2H), 6.84 (d,  $J = 8.8$  Hz, 2H), 5.97 – 5.91 (m, 1H), 5.04 (s, 2H), 4.45 (s, 2H), 2.46 – 2.37 (m, 4H), 2.34 (s, 3H), 1.93 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 144.6, 136.7, 136.4, 134.3, 133.1, 129.4, 128.6, 128.2, 128.0, 127.4, 123.5, 114.6, 114.4, 86.2, 82.9, 79.9, 69.9, 68.5, 42.9, 36.5, 33.2, 23.2, 21.5; IR (neat): 2954, 2262, 2078, 1614, 1544, 1441, 1157, 893, 532, 545; HRESIMS Calcd for  $[\text{C}_{30}\text{H}_{27}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 504.1604, found 504.1604.

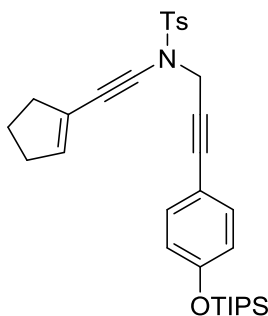
***N*-(3-(4-((*tert*-butyldimethylsilyl)oxy)phenyl)prop-2-yn-1-yl)-*N*-(cyclopent-1-en-1-ylethynyl)-4-methylbenzenesulfonamide (1i)**



**1i**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.27 (d,  $J = 8.0$  Hz, 2H), 7.08 – 7.02 (m, 2H), 6.74 – 6.67 (m, 2H), 6.01 – 5.92 (m, 1H), 4.46 (s, 2H), 2.47 – 2.37 (m, 4H), 2.36 (s, 3H), 1.94 – 1.82 (m, 2H), 0.97 (s, 9H), 0.19 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.1, 144.6, 136.7, 134.3, 133.1, 129.4, 128.2, 123.6, 119.9, 114.8, 86.3, 83.0, 79.9, 68.5, 42.9, 36.5, 33.2, 25.6, 23.2, 21.5, 18.2, -4.5; IR (neat): 2910, 2255, 2017, 1641, 1571, 1304, 1276, 1124, 1082, 804, 771, 573; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{35}\text{NNaO}_3\text{SSi}]^+$  ( $\text{M} + \text{Na}^+$ ) 528.1999, found 528.2004.

***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-(4-((*triisopropylsilyl*)oxy)phenyl)prop-2-yn-1-yl)benzenesulfonamide (1j)**

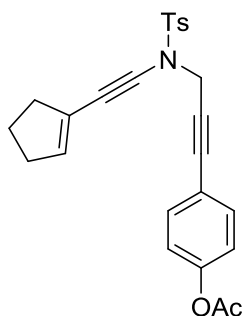


**1j**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.30 – 7.26 (m, 2H), 7.07 – 6.99 (m, 2H), 6.78 – 6.71 (m, 2H), 5.98 – 5.92 (m, 1H), 4.46 (s, 2H), 2.47 – 2.38 (m, 4H), 2.36 (s, 3H), 1.94 – 1.84 (m, 2H), 1.31 – 1.18 (m, 3H), 1.09 (d,  $J = 7.2$  Hz, 18H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.5, 144.6, 136.7, 134.3, 133.1, 129.4, 128.2,

123.6, 119.7, 114.5, 86.4, 83.0, 79.9, 68.5, 43.0, 36.5, 33.2, 23.2, 21.5, 17.8, 12.6; IR (neat): 2911, 2244, 2020, 1641, 1541, 1444, 1182, 814, 592, 582; HRESIMS Calcd for  $[\text{C}_{32}\text{H}_{41}\text{NNaO}_3\text{SSi}]^+$  ( $\text{M} + \text{Na}^+$ ) 570.2469, found 570.2467.

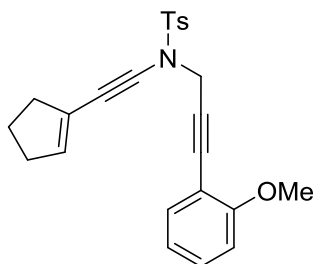
**4-(3-((*N*-(cyclopent-1-en-1-ylethynyl)-4-methylphenyl)sulfonamido)prop-1-yn-1-yl)phenyl acetate (1k)**



**1k**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.27 (d,  $J = 8.0$  Hz, 2H), 7.19 – 7.13 (m, 2H), 7.02 – 6.95 (m, 2H), 5.99 – 5.92 (m, 1H), 4.47 (s, 2H), 2.47 – 2.39 (m, 4H), 2.35 (s, 3H), 2.28 (s, 3H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.0, 150.6, 144.7, 136.9, 134.2, 132.7, 129.4, 128.1, 123.4, 121.4, 119.6, 85.4, 82.8, 81.3, 68.5, 42.7, 36.4, 33.1, 23.1, 21.5, 21.0; IR (neat): 2947, 2810, 2220, 2017, 1689(s), 1647, 1514, 1341, 1117, 1010, 871, 512; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{23}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 456.1240, found 456.1244.

***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(2-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1l)**



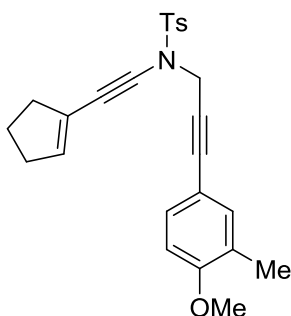
**1l**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.27 – 7.23 (m, 3H), 7.06 – 7.00 (m, 1H), 6.86 – 6.78 (m, 2H), 5.98 – 5.92 (m, 1H), 4.54 (s, 2H), 3.82 (s,



3H), 2.46 – 2.40 (m, 4H), 2.34 (s, 3H), 1.97 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.0, 144.5, 136.6, 134.2, 133.8, 130.0, 129.4, 128.2, 123.6, 120.2, 111.3, 110.6, 85.2, 82.9, 82.8, 68.6, 55.7, 43.1, 36.5, 33.2, 23.2, 21.5; IR (neat): 2910, 2200, 2025, 1601, 1344, 1118, 1044, 714, 667, 578, 541; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 428.1291, found 428.1291.

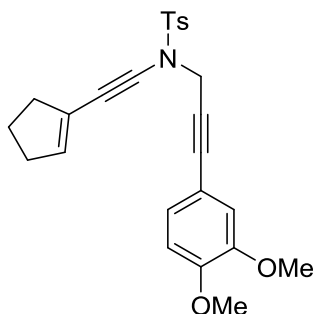
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-methoxy-3-methylphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1m)**



**1m**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.29 – 7.25 (m, 2H), 7.04 – 6.92 (m, 2H), 6.68 (d,  $J = 8.8$  Hz, 1H), 5.98 – 5.92 (m, 1H), 4.46 (s, 2H), 3.81 (s, 3H), 2.46 – 2.39 (m, 4H), 2.37 (s, 3H), 2.15 (s, 3H), 1.93 – 1.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 144.5, 136.7, 134.4, 133.8, 130.6, 129.4, 128.2, 126.5, 123.6, 113.6, 109.5, 86.6, 83.0, 79.4, 68.5, 55.3, 43.0, 36.5, 33.2, 23.2, 21.5, 15.9; IR (neat): 2944, 2240, 2019, 1671, 1371, 1110, 1004, 710, 604, 511; ESIMS Calcd for  $[\text{C}_{25}\text{H}_{25}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 442.1447, found 442.1441.

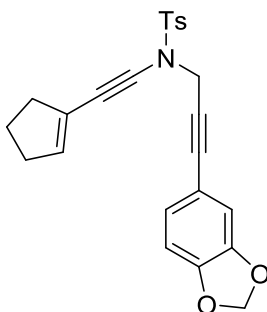
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(3,4-dimethoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1n)**



### 1n

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.28 (d,  $J = 8.0$  Hz, 2H), 6.83 – 6.77 (m, 1H), 6.77 – 6.71 (m, 2H), 5.98 – 5.92 (m, 1H), 4.47 (s, 2H), 3.87 (s, 3H), 3.83 (s, 3H), 2.47 – 2.39 (m, 4H), 2.37 (s, 3H), 1.93 – 1.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.6, 148.4, 144.6, 136.7, 134.2, 129.3, 128.1, 125.0, 123.5, 114.3, 114.2, 110.7, 86.4, 82.9, 79.7, 68.5, 55.8, 42.8, 36.4, 33.1, 23.1, 21.5; IR (neat): 2944, 2229, 2028, 1344, 1111, 1022, 910, 810, 771, 644, 510; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{25}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 458.1397, found 458.1391.

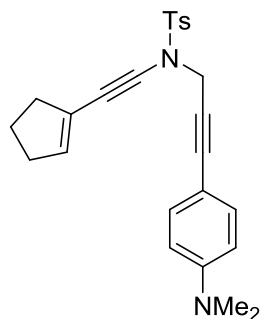
### *N*-(3-(benzo[*d*][1,3]dioxol-5-yl)prop-2-yn-1-yl)-*N*-(cyclopent-1-en-1-ylethynyl)-4-methylbenzenesulfonamide (1o)



### 1o

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.29 (d,  $J = 8.0$  Hz, 2H), 6.73 – 6.65 (m, 2H), 6.57 – 6.54 (m, 1H), 5.98 – 5.92 (m, 3H), 4.45 (s, 2H), 2.47 – 2.40 (m, 4H), 2.39 (s, 3H), 1.94 – 1.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.0, 147.2, 144.7, 136.9, 134.3, 129.5, 128.2, 126.3, 123.5, 115.3, 111.6, 108.2, 101.3, 86.2, 82.9, 79.6, 68.5, 42.9, 36.5, 33.2, 23.2, 21.5; IR (neat): 2920, 2201, 2035, 1510, 1344, 1111, 746, 664, 611, 545; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{21}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 442.1083, found 442.1080.

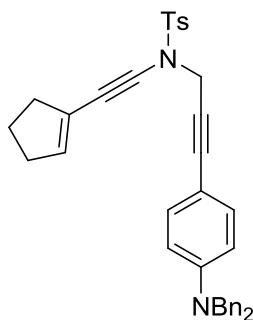
### *N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1p)



**1p**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.27 (d,  $J = 8.0$  Hz, 2H), 7.08 – 7.01 (m, 2H), 6.57 – 6.50 (m, 2H), 5.97 – 5.92 (m, 1H), 4.47 (s, 2H), 2.94 (s, 6H), 2.45 – 2.38 (m, 4H), 2.37 (s, 3H), 1.93 – 1.81 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 144.5, 136.5, 134.3, 132.7, 129.4, 128.1, 123.6, 111.4, 108.7, 87.4, 83.1, 78.8, 68.5, 43.2, 40.0, 36.4, 33.1, 23.1, 21.5; IR (neat): 2944, 2247, 2021, 1711, 1611, 1514, 1311, 1220, 1034, 831, 664, 518; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{26}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 441.1607, found 441.1607.

***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(3-(4-(dibenzylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1q)**

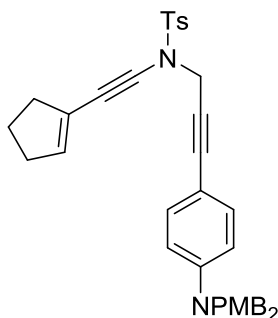


**1q**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (d,  $J = 8.4$  Hz, 2H), 7.32 – 7.29 (m, 3H), 7.26 – 7.16 (m, 9H), 6.96 (d,  $J = 8.8$  Hz, 2H), 6.56 (d,  $J = 9.2$  Hz, 2H), 5.94 – 5.89 (m, 1H), 4.62 (s, 4H), 4.41 (s, 2H), 2.44 – 2.33 (m, 4H), 2.27 (s, 3H), 1.90 – 1.79 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.9, 144.5, 137.7, 136.5, 134.3, 132.8, 129.3, 128.6, 128.0, 127.0, 126.3, 123.5, 111.7, 109.4, 87.2, 83.0, 78.9, 68.4, 54.0, 43.1, 36.4, 33.1, 23.1, 21.4 ; IR (neat): 2978, 2247, 2022, 1712, 1614, 1524, 1325,

1221, 1032, 878, 612, 527; HRESIMS Calcd for  $[C_{37}H_{34}N_2NaO_2S]^+$  ( $M + Na^+$ ) 593.2233, found 593.2234.

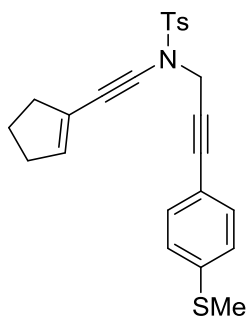
***N*-(3-(4-(bis(4-methoxybenzyl)amino)phenyl)prop-2-yn-1-yl)-*N*-(cyclopent-1-en-1-ylethynyl)-4-methylbenzenesulfonamide (1r)**



**1r**

Pale yellow oil.  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.83 (d,  $J = 8.0$  Hz, 2H), 7.22 (d,  $J = 8.4$  Hz, 2H), 7.09 (d,  $J = 8.4$  Hz, 4H), 6.96 (d,  $J = 8.8$  Hz, 2H), 6.87 – 6.81 (m, 4H), 6.58 (d,  $J = 9.2$  Hz, 2H), 5.95 – 5.90 (m, 1H), 4.53 (s, 4H), 4.42 (s, 2H), 3.75 (s, 6H), 2.43 – 2.33 (m, 4H), 2.29 (s, 3H), 1.90 – 1.80 (m, 2H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  158.6, 149.0, 144.4, 136.5, 134.2, 132.8, 129.6, 129.3, 128.0, 127.6, 123.5, 114.0, 111.8, 109.2, 87.2, 83.0, 78.8, 68.4, 55.1, 53.3, 43.0, 36.4, 33.1, 23.1, 21.4; IR (neat): 2948, 2241, 2020, 1701, 1611, 1514, 1357, 1278, 1051, 812, 678, 578; HRESIMS Calcd for  $[C_{39}H_{38}N_2NaO_4S]^+$  ( $M + Na^+$ ) 653.2444, found 653.2447.

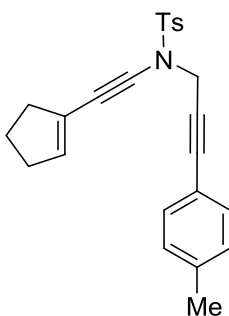
***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-(4-(methylthio)phenyl)prop-2-yn-1-yl)benzenesulfonamide (1s)**



**1s**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.27 (d,  $J = 8.4$  Hz, 2H), 7.13 – 7.03 (m, 4H), 5.98 – 5.94 (m, 1H), 4.47 (s, 2H), 2.49 – 2.39 (m, 7H), 2.36 (s, 3H), 1.93 – 1.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.6, 139.7, 136.8, 134.2, 131.8, 129.4, 128.1, 125.4, 123.5, 118.2, 86.1, 82.9, 81.2, 68.5, 42.8, 36.4, 33.1, 23.1, 21.5, 15.2; IR (neat): 2922, 2210, 2011, 1610, 1600, 1500, 1377, 1272, 1042, 824, 641, 544; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_2\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 444.1062, found 444.1070.

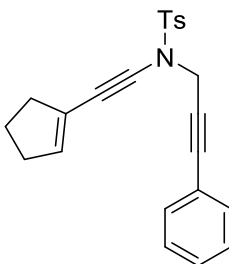
***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)benzenesulfonamide (1t)**



**1t**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.27 (d,  $J = 8.4$  Hz, 2H), 7.10 – 7.02 (m, 4H), 5.98 – 5.94 (m, 1H), 4.47 (s, 2H), 2.47 – 2.38 (m, 4H), 2.36 (s, 3H), 2.32 (s, 3H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.6, 138.6, 136.8, 134.3, 131.5, 129.4, 128.8, 128.2, 123.6, 119.0, 86.5, 82.9, 80.5, 68.6, 42.9, 36.5, 33.2, 23.2, 21.5, 21.4; IR (neat): 2974, 2212, 2074, 1610, 1505, 1371, 1112, 1005, 840, 740, 547; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 412.1342, found 412.1340.

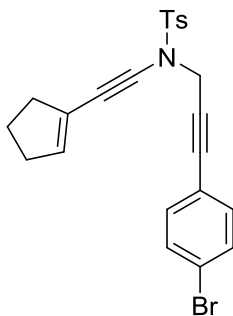
***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1u)**



**1u**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.31 – 7.27 (m, 3H), 7.26 – 7.21 (m, 2H), 7.19 – 7.12 (m, 2H), 5.99 – 5.95 (m, 1H), 4.49 (s, 2H), 2.47 – 2.38 (m, 4H), 2.35 (s, 3H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.7, 136.9, 134.3, 131.6, 129.5, 128.5, 128.2, 128.1, 123.6, 122.1, 86.3, 82.9, 81.3, 68.6, 42.9, 36.5, 33.2, 23.2, 21.5; IR (neat): 2970, 2271, 2004, 1773, 1688, 1572, 1372, 1217, 1027, 817, 620, 544; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{21}\text{NNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 398.1185, found 398.1187.

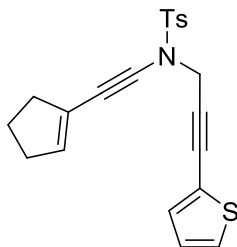
***N*-(3-(4-bromophenyl)prop-2-yn-1-yl)-*N*-(cyclopent-1-en-1-ylethynyl)-4-methylbenzenesulfonamide (1v)**



**1v**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.45 – 7.39 (m, 1H), 7.30 (d,  $J = 8.0$  Hz, 2H), 7.24 – 7.20 (m, 1H), 7.16 – 7.08 (m, 2H), 6.01 – 5.96 (m, 1H), 4.48 (s, 2H), 2.48 – 2.40 (m, 4H), 2.39 (s, 3H), 1.95 – 1.84 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.9, 137.1, 134.4, 131.6, 130.0, 129.5, 128.2, 124.0, 123.4, 121.8, 84.7, 82.8, 82.7, 68.6, 42.7, 36.5, 33.2, 23.2, 21.6; IR (neat): 2950, 2247, 2047, 1740, 1571, 1320, 1105, 1025, 843, 664, 597; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{20}\text{BrNNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 476.0290, found 476.0291.

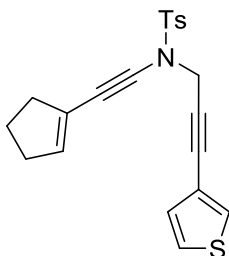
***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-(thiophen-2-yl)prop-2-yn-1-yl)benzenesulfonamide (1w)**



**1w**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 7.24 – 7.19 (m, 1H), 7.01 (d,  $J = 2.8$  Hz, 1H), 6.94 – 6.89 (m, 1H), 5.99 – 5.95 (m, 1H), 4.50 (s, 2H), 2.47 – 2.39 (m, 4H), 2.38 (s, 3H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.8, 137.0, 134.1, 132.5, 129.5, 128.1, 127.5, 126.8, 123.5, 121.9, 85.2, 82.8, 79.6, 68.7, 43.0, 36.5, 33.2, 23.2, 21.6; IR (neat): 2944, 2241, 2042, 1612, 1641, 1504, 1373, 1141, 840, 671, 571, 542; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{19}\text{NNaO}_2\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 404.0749, found 404.0747.

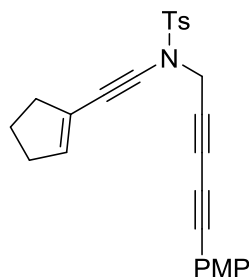
***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(3-(thiophen-3-yl)prop-2-yn-1-yl)benzenesulfonamide (1x)**



**1x**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 – 7.83 (m, 2H), 7.28 (d,  $J = 8.0$  Hz, 2H), 7.24 – 7.18 (m, 2H), 6.89 – 6.85 (m, 1H), 5.99 – 5.93 (m, 1H), 4.46 (s, 2H), 2.46 – 2.39 (m, 4H), 2.37 (s, 3H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.7, 136.8, 134.2, 129.6, 129.4, 129.2, 128.2, 125.1, 123.5, 121.1, 82.9, 81.5, 80.9, 68.6, 42.8, 36.5, 33.2, 23.2, 21.5; IR (neat): 2941, 2225, 2027, 1640, 1671, 1510, 1173, 810, 618, 547; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{19}\text{NNaO}_2\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 404.0749, found 404.0747.

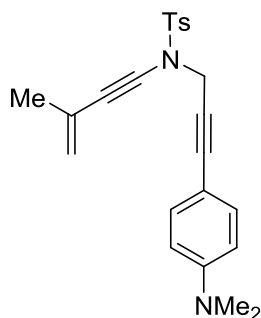
***N*-(cyclopent-1-en-1-ylethynyl)-*N*-(5-(4-methoxyphenyl)penta-2,4-diyn-1-yl)-4-methylbenzenesulfonamide (1y)**



**1y**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (d,  $J = 8.0$  Hz, 2H), 7.42 – 7.33 (m, 4H), 6.84 (d,  $J = 8.4$  Hz, 2H), 6.05 – 5.96 (m, 1H), 4.41 (s, 2H), 3.81 (s, 3H), 2.54 – 2.33 (m, 7H), 1.94 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5, 145.0, 137.0, 134.2, 133.9, 129.5, 128.2, 123.4, 114.1, 112.9, 82.6, 78.4, 74.0, 71.9, 71.2, 68.8, 55.3, 43.0, 36.4, 33.2, 23.2, 21.7; IR (neat): 2973, 2274, 2078, 1615, 1551, 1444, 1128, 827, 580, 544; HRESIMS Calcd for  $[\text{C}_{26}\text{H}_{23}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 452.1291, found 452.1291.

***N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methyl-*N*-(3-methylbut-3-en-1-yn-1-yl)benzenesulfonamide (1z)**

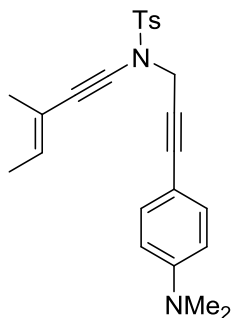


**1z**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.4$  Hz, 2H), 7.28 (d,  $J = 8.0$  Hz, 2H), 7.11 – 6.99 (m, 2H), 6.58 – 6.47 (m, 2H), 5.19 (dd,  $J = 2.0, 0.8$  Hz, 1H), 5.13 (dd,  $J = 3.2, 1.6$  Hz, 1H), 4.47 (s, 2H), 2.95 (s, 6H), 2.37 (s, 3H), 1.87 (t,  $J = 1.2$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.2, 144.6, 134.2, 132.7, 129.4, 128.1, 126.0, 119.9, 111.4, 108.7, 87.5, 81.5, 78.7, 72.6, 43.1, 40.1, 23.5, 21.6; IR (neat): 2924, 2242, 2078, 1541, 1341, 1119, 726, 648, 624, 526, 505; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{24}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 415.1451, found 415.1456.



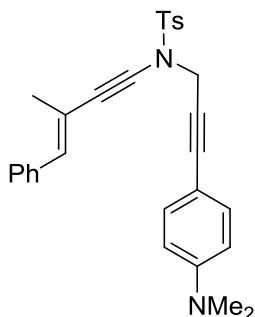
**(E)-N-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methyl-N-(3-methylpent-3-en-1-yn-1-yl)benzenesulfonamide (1aa)**



**1aa**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 – 7.83 (m, 2H), 7.27 (d,  $J = 8.0$  Hz, 2H), 7.07 – 7.02 (m, 2H), 6.57 – 6.51 (m, 2H), 5.89 – 5.81 (m, 1H), 4.45 (s, 2H), 2.94 (s, 6H), 2.36 (s, 3H), 1.77 – 1.73 (m, 3H), 1.69 – 1.63 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 144.4, 134.3, 132.7, 131.9, 129.3, 128.1, 117.6, 111.4, 108.8, 87.3, 78.8, 78.6, 73.9, 43.2, 40.0, 21.5, 17.1, 14.0; IR (neat): 2902, 2201, 2078, 1610, 1510, 1311, 1241, 1124, 1010, 804, 744, 513; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{26}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 429.1607, found 429.1607.

**(E)-N-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methyl-N-(3-methyl-4-phenylbut-3-en-1-yn-1-yl)benzenesulfonamide (1ab)**

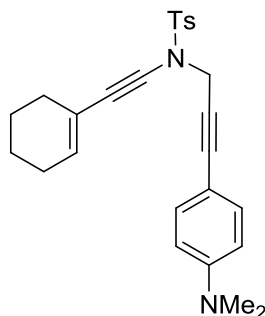


**1ab**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 8.4$  Hz, 2H), 7.33 – 7.26 (m, 4H), 7.24 – 7.18 (m, 3H), 7.10 – 7.05 (m, 2H), 6.73 (s, 1H), 6.57 – 6.51 (m, 2H), 4.50 (s, 2H), 2.93 (s, 6H), 2.37 (s, 3H), 2.04 (d,  $J = 1.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.2, 144.6, 136.8, 134.5, 134.3, 132.7, 129.5, 128.8, 128.1, 126.9, 119.2, 111.4, 108.7, 87.6, 81.5, 78.8, 75.0, 43.2, 40.0, 21.6, 19.3; IR (neat): 2977, 2211, 2068, 1611, 1311,

1110, 1041, 710, 641, 542, 510; HRESIMS Calcd for  $[C_{29}H_{28}N_2NaO_2S]^+$  ( $M + Na^+$ ) 491.1764, found 491.1771.

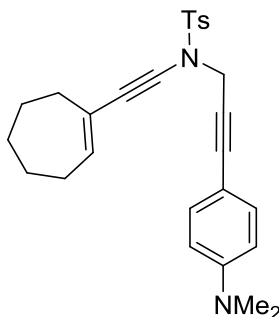
***N*-(cyclohex-1-en-1-ylethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1ac)**



**1ac**

Pale yellow oil.  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.86 (d,  $J = 8.0$  Hz, 2H), 7.27 (d,  $J = 8.0$  Hz, 2H), 7.04 (d,  $J = 9.2$  Hz, 2H), 6.54 (d,  $J = 8.8$  Hz, 2H), 6.05 – 6.01 (m, 1H), 4.45 (s, 2H), 2.95 (s, 6H), 2.37 (s, 3H), 2.12 – 2.05 (m, 4H), 1.65 – 1.53 (m, 4H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  150.1, 144.4, 134.3, 132.7, 129.3, 128.1, 119.8, 111.4, 108.9, 87.3, 79.6, 78.8, 72.6, 43.2, 40.1, 29.4, 25.6, 22.3, 21.5, 21.4; IR (neat): 2914, 2202, 2087, 1640, 1640, 1571, 1372, 1210, 1070, 810, 640, 510; HRESIMS Calcd for  $[C_{26}H_{28}N_2NaO_2S]^+$  ( $M + Na^+$ ) 455.1764, found 455.1769.

***N*-(cyclohept-1-en-1-ylethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1ad)**

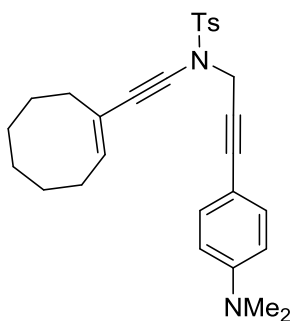


**1ad**

Pale yellow oil.  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.85 (d,  $J = 8.0$  Hz, 2H), 7.26 (d,  $J = 8.0$  Hz, 2H), 7.07 – 7.01 (m, 2H), 6.54 (d,  $J = 8.8$  Hz, 2H), 6.19 (t,  $J = 6.8$  Hz, 1H), 4.44 (s,

2H), 2.94 (s, 6H), 2.36 (s, 3H), 2.32 – 2.26 (m, 2H), 2.19 – 2.12 (m, 2H), 1.76 – 1.66 (m, 2H), 1.59 – 1.44 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 144.4, 138.8, 134.3, 132.7, 129.3, 128.1, 125.9, 111.4, 108.8, 87.3, 79.7, 78.8, 74.3, 43.2, 40.0, 34.4, 32.0, 29.0, 26.5, 26.4, 21.5; IR (neat): 2910, 2210, 2078, 1647, 1370, 1275, 1166, 1065, 932, 745, 532; HRESIMS Calcd for  $[\text{C}_{27}\text{H}_{30}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 469.1920, found 469.1911.

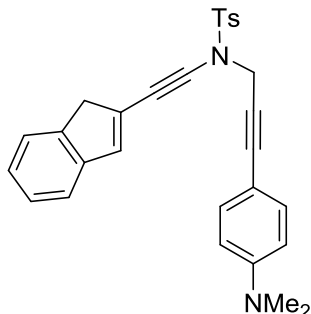
***N*-(cyclooct-1-en-1-ylethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1ae)**



**1ae**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (d,  $J = 8.4$  Hz, 2H), 7.26 (d,  $J = 8.0$  Hz, 2H), 7.06 – 7.01 (m, 2H), 6.53 (d,  $J = 9.2$  Hz, 2H), 6.01 (t,  $J = 8.4$  Hz, 1H), 4.45 (s, 2H), 2.94 (s, 6H), 2.36 (s, 3H), 2.29 – 2.21 (m, 2H), 2.18 – 2.09 (m, 2H), 1.54 – 1.43 (m, 8H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 144.4, 136.7, 134.2, 132.7, 129.3, 128.2, 122.8, 111.4, 108.8, 87.4, 79.4, 78.8, 73.3, 43.2, 40.1, 30.1, 29.7, 28.2, 26.9, 26.3, 25.7, 21.5; IR (neat): 2914, 2220, 2084, 1614, 1510, 1472, 1340, 1140, 845, 649, 544; HRESIMS Calcd for  $[\text{C}_{28}\text{H}_{32}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 483.2077, found 483.2079.

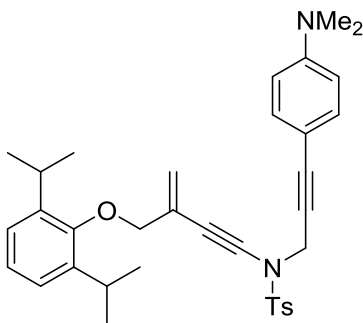
***N*-((1*H*-inden-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1af)**



### 1af

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (d,  $J = 8.4$  Hz, 2H), 7.35 – 7.23 (m, 5H), 7.20 – 7.14 (m, 1H), 7.09 – 7.03 (m, 2H), 6.96 (s, 1H), 6.53 (d,  $J = 8.8$  Hz, 2H), 4.53 (s, 2H), 3.47 (s, 2H), 2.93 (s, 6H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.2, 144.7, 144.1, 142.6, 136.0, 134.3, 132.7, 129.5, 128.1, 126.7, 126.6, 125.3, 123.4, 121.0, 111.4, 108.6, 87.7, 86.7, 78.7, 68.6, 43.2, 42.7, 40.0, 21.5; IR (neat): 2937, 2240, 2087, 1650, 1544, 1352, 1255, 1020, 850, 742, 610; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{26}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 489.1607, found 489.1600.

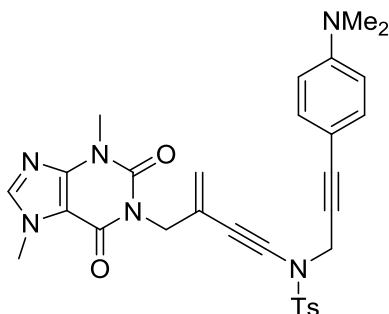
### *N*-(3-((2,6-diisopropylphenoxy)methyl)but-3-en-1-yn-1-yl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1ag)



### 1ag

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.25 (d,  $J = 8.0$  Hz, 2H), 7.14 – 7.06 (m, 3H), 7.05 – 7.00 (m, 2H), 6.50 (d,  $J = 8.8$  Hz, 2H), 5.75 (d,  $J = 2.0$  Hz, 1H), 5.53 (d,  $J = 1.2$  Hz, 1H), 4.48 (s, 2H), 4.23 (s, 2H), 3.36 – 3.25 (m, 2H), 2.93 (s, 6H), 2.34 (s, 3H), 1.21 (d,  $J = 6.8$  Hz, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  152.8, 150.2, 144.7, 141.8, 134.3, 132.7, 129.5, 128.1, 127.1, 124.7, 123.9, 120.1, 111.4, 108.6, 87.7, 83.2, 78.5, 75.5, 69.3, 43.1, 40.1, 26.4, 24.0, 21.5; IR (neat): 2947, 2814, 2221, 2058, 1700, 1578, 1341, 1101, 1037, 787, 617, 510; HRESIMS Calcd for  $[\text{C}_{35}\text{H}_{40}\text{N}_2\text{NaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 591.2652, found 591.2657.

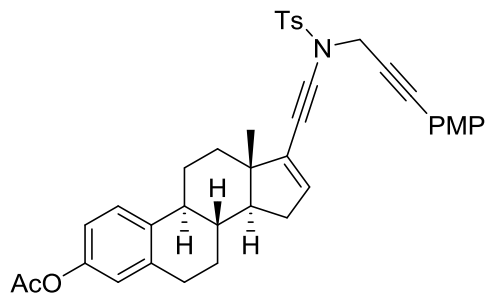
### *N*-(3-((3,7-dimethyl-2,6-dioxo-2,3,6,7-tetrahydro-1*H*-purin-1-yl)methyl)but-3-en-1-yn-1-yl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1ah)



**1ah**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 8.4$  Hz, 2H), 7.46 (s, 1H), 7.25 (d,  $J = 8.4$  Hz, 2H), 6.97 (d,  $J = 8.8$  Hz, 2H), 6.52 (d,  $J = 8.8$  Hz, 2H), 5.36 (d,  $J = 0.8$  Hz, 1H), 5.32 – 5.30 (m, 1H), 4.74 (s, 2H), 4.41 (s, 2H), 3.94 (s, 3H), 3.56 (s, 3H), 2.95 (s, 6H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.8, 151.2, 150.1, 148.8, 144.6, 141.5, 134.3, 132.6, 129.5, 128.0, 126.2, 119.3, 111.4, 108.5, 107.6, 87.4, 83.5, 78.5, 69.3, 44.6, 43.0, 40.0, 33.5, 29.6, 21.5; IR (neat): 2956, 2877, 2213, 2098, 1712(s), 1689(s), 1343, 1182, 1035, 747, 614, 532; HRESIMS Calcd for  $[\text{C}_{30}\text{H}_{30}\text{N}_6\text{NaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 593.1941, found 593.1945.

**(8*S*,9*S*,13*S*,14*S*)-17-(((*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylphenyl)sulfonamido)ethynyl)-13-methyl-7,8,9,11,12,13,14,15-octahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl acetate (1ai)**

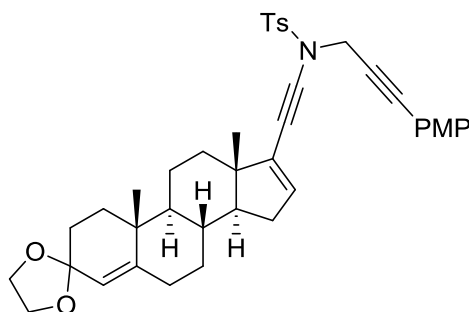


**1ai**

Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -34.5$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.88 (d,  $J = 8.4$  Hz, 2H), 7.28 (d,  $J = 8.0$  Hz, 2H), 7.22 (d,  $J = 8.4$  Hz, 1H), 7.10 (d,  $J = 8.8$  Hz, 2H), 6.86 – 6.74 (m, 4H), 5.98 – 5.94 (m, 1H), 4.55 – 4.42 (m, 2H), 3.79 (s, 3H), 2.92 – 2.85 (m, 2H), 2.38 (s, 3H), 2.32 – 2.20 (m, 6H), 2.11 – 2.02 (m, 1H), 1.94 – 1.83 (m, 2H), 1.60 – 1.39 (m, 5H), 0.80 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.8, 159.7, 148.4, 144.6,

138.1, 136.3, 134.3, 134.2, 133.1, 129.4, 128.2, 126.0, 121.4, 118.5, 114.2, 113.7, 86.3, 85.3, 79.8, 66.9, 55.2, 48.5, 44.4, 43.1, 37.1, 34.5, 31.8, 29.4, 27.5, 26.2, 21.6, 21.1, 16.0; IR (neat): 2944, 2845, 2211, 2074, 1689(s), 1347, 1187, 1085, 787, 664, 644, 544; HRESIMS Calcd for  $[C_{39}H_{39}NNaO_5S]^+$  ( $M + Na^+$ ) 656.2441, found 656.2446.

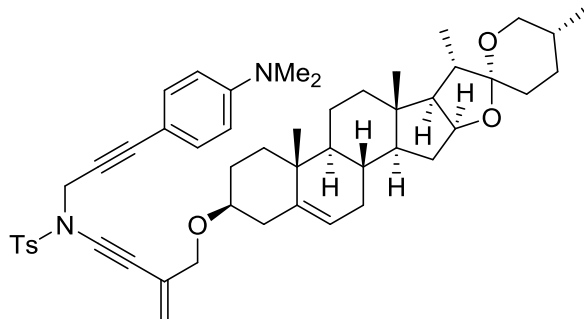
***N*-(((8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-1,2,6,7,8,9,10,11,12,13,14,15-dodecahydrospiro[cyclopenta[*a*]phenanthrene-3,2'-[1,3]dioxolan]-17-yl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1aj)**



**1aj**

Pale yellow oil.  $[\alpha]_D^{20} = -41.2$  (c = 1.0,  $CHCl_3$ ).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.87 (d,  $J = 8.4$  Hz, 2H), 7.28 (d,  $J = 6.4$  Hz, 2H), 7.08 (d,  $J = 8.8$  Hz, 2H), 6.77 (d,  $J = 8.8$  Hz, 2H), 5.95 – 5.90 (m, 1H), 5.37 – 5.32 (m, 1H), 4.54 – 4.26 (m, 2H), 3.99 – 3.88 (m, 4H), 3.79 (s, 3H), 2.61 – 2.53 (m, 1H), 2.37 (s, 3H), 2.20 – 2.08 (m, 2H), 2.05 – 1.95 (m, 2H), 1.83 – 1.62 (m, 6H), 1.56 – 1.29 (m, 5H), 1.18 – 1.08 (m, 1H), 1.04 (s, 3H), 0.81 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  159.7, 144.6, 140.4, 136.1, 134.4, 134.3, 133.1, 129.4, 128.2, 121.7, 114.1, 113.6, 109.3, 86.3, 85.1, 79.8, 66.9, 64.3, 64.2, 56.0, 55.2, 50.1, 48.2, 43.0, 41.7, 36.8, 36.2, 34.4, 32.1, 31.3, 31.0, 30.6, 21.5, 20.6, 18.7, 15.8; IR (neat): 2942, 2846, 2223, 2079, 1671, 1323, 1113, 1025, 747, 614, 600, 548; HRESIMS Calcd for  $[C_{40}H_{45}NNaO_5S]^+$  ( $M + Na^+$ ) 674.2911, found 674.2919.

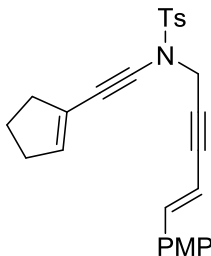
***N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methyl-*N*-(3-(((4*S*,5'*R*,6*aR*,6*bS*,8*aS*,8*bR*,9*S*,10*R*,11*aS*,12*aS*,12*bS*)-5',6*a*,8*a*,9-tetramethyl-1,3,3',4,4',5,5',6,6*a*,6*b*,6',7,8,8*a*,8*b*,9,11*a*,12,12*a*,12*b*-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-*b*]furan-10,2'-pyran]-4-yl)oxy)methyl)but-3-en-1-yn-1-yl)benzenesulfonamide (1ak)**



**1ak**

Pale yellow oil.  $[\alpha]_D^{20} = -88.4$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (d,  $J = 8.4$  Hz, 2H), 7.32 – 7.28 (m, 2H), 7.06 – 7.02 (m, 2H), 6.55 (d,  $J = 9.2$  Hz, 2H), 5.48 (d,  $J = 1.6$  Hz, 1H), 5.40 (d,  $J = 1.6$  Hz, 1H), 5.33 – 5.29 (m, 1H), 4.48 (s, 2H), 4.42 (dd,  $J = 15.0$ , 7.6 Hz, 1H), 4.01 (s, 2H), 3.52 – 3.33 (m, 2H), 3.29 – 3.15 (m, 1H), 2.96 (s, 6H), 2.39 (s, 3H), 2.38 – 2.31 (m, 1H), 2.28 – 2.15 (m, 1H), 2.04 – 1.94 (m, 2H), 1.93 – 1.71 (m, 6H), 1.70 – 1.57 (m, 5H), 1.57 – 1.39 (m, 5H), 1.37 – 1.27 (m, 2H), 1.20 – 1.05 (m, 2H), 1.00 (s, 3H), 0.99 (d,  $J = 7.0$  Hz, 3H), 0.84 – 0.76 (m, 6H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 144.6, 140.8, 134.3, 132.8, 129.5, 128.5, 128.2, 121.2, 119.6, 111.4, 109.2, 108.7, 87.6, 83.0, 80.7, 78.7, 78.6, 69.9, 66.8, 62.1, 56.5, 50.0, 43.1, 41.5, 40.2, 40.1, 39.7, 39.0, 37.1, 36.9, 32.0, 31.8, 31.4, 31.3, 30.2, 28.7, 28.3, 21.6, 20.8, 19.3, 17.1, 16.2, 14.5; IR (neat): 2932, 2901, 2844, 2221, 2089, 1678, 1324, 1117, 1085, 872, 737, 644, 531; HRESIMS Calcd for  $[\text{C}_{50}\text{H}_{64}\text{N}_2\text{NaO}_5\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 827.4428, found 827.4417.

**(*E*)-*N*-(cyclopent-1-en-1-ylethynyl)-*N*-(5-(4-methoxyphenyl)pent-4-en-2-yn-1-yl)-4-methylbenzenesulfonamide (1al)**



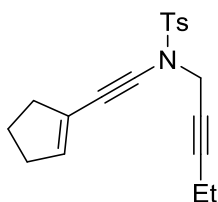
**1al**

Pale yellow oil.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 8.0$  Hz, 2H), 7.25 (d,  $J = 8.8$  Hz, 2H), 6.85 (d,  $J = 8.8$  Hz, 2H), 6.65 (d,  $J = 16.4$  Hz, 1H), 5.98 – 5.95 (m, 1H), 5.82 – 5.75 (m, 1H), 4.43 (d,  $J = 1.6$  Hz, 2H), 3.80 (s, 3H), 2.48 –

2.37 (m, 7H), 1.93 – 1.83 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.3, 144.7, 141.9, 136.8, 134.4, 129.5, 128.7, 128.3, 127.6, 123.6, 114.2, 104.5, 86.0, 83.0, 82.6, 68.6, 55.3, 43.1, 36.6, 33.3, 23.2, 21.7; IR (neat): 2944, 2211, 2020, 1671, 1574, 1327, 1132, 1012, 872, 714, 512; HRESIMS Calcd for  $[\text{C}_{26}\text{H}_{25}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 454.1447, found 454.1447.

***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(pent-2-yn-1-yl)benzenesulfonamide**

**(1am)**

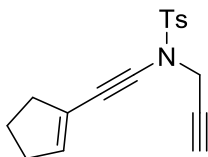


**1am**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (d,  $J = 8.4$  Hz, 2H), 7.33 (d,  $J = 8.4$  Hz, 2H), 6.00 – 5.90 (m, 1H), 4.22 (t,  $J = 2.0$  Hz, 2H), 2.46 – 2.37 (m, 7H), 2.05 – 1.96 (m, 2H), 1.94 – 1.86 (m, 2H), 0.96 (t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 136.5, 134.4, 129.3, 128.2, 123.6, 88.5, 82.9, 71.4, 68.4, 42.5, 36.5, 33.1, 23.1, 21.6, 13.3, 12.2; IR (neat): 2947, 2215, 2055, 1744, 1512, 1374, 1111, 1045, 827, 642, 584; HRESIMS Calcd for  $[\text{C}_{19}\text{H}_{21}\text{NNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 350.1185, found 350.1188.

***N*-(cyclopent-1-en-1-ylethynyl)-4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide**

**(1an)**



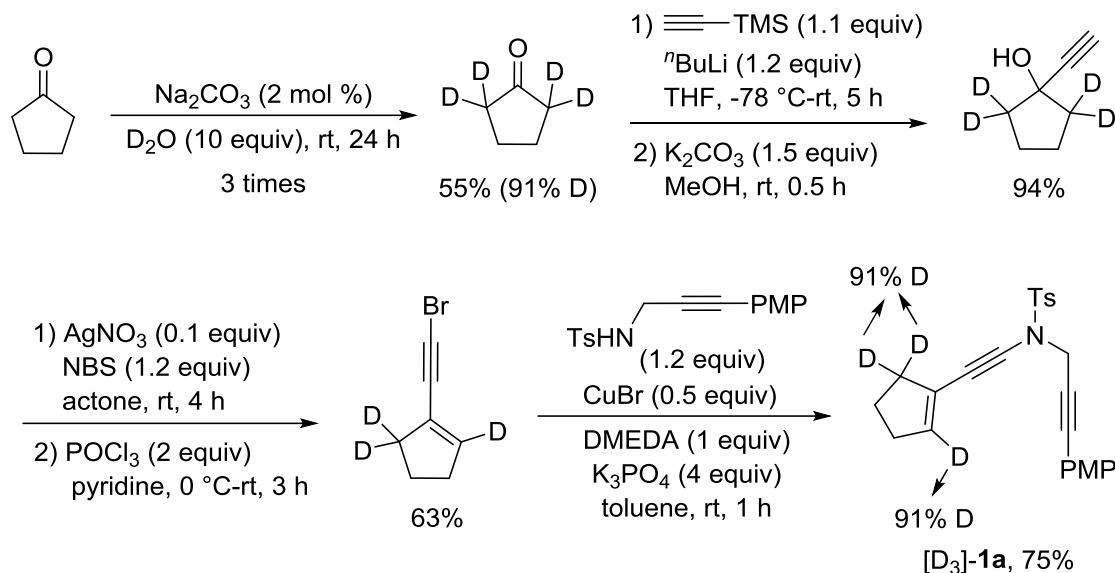
**1an**

Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (d,  $J = 8.0$  Hz, 2H), 7.34 (d,  $J = 8.4$  Hz, 2H), 6.02 – 5.91 (m, 1H), 4.27 (d,  $J = 2.4$  Hz, 2H), 2.45 (s, 3H), 2.43 – 2.37 (m, 4H), 2.20 (t,  $J = 2.4$  Hz, 1H), 1.93 – 1.84 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.8, 136.9, 134.0, 129.5, 128.1, 123.4, 82.4, 75.8, 74.5, 68.7, 41.7, 36.4, 33.2, 23.1, 21.6; IR



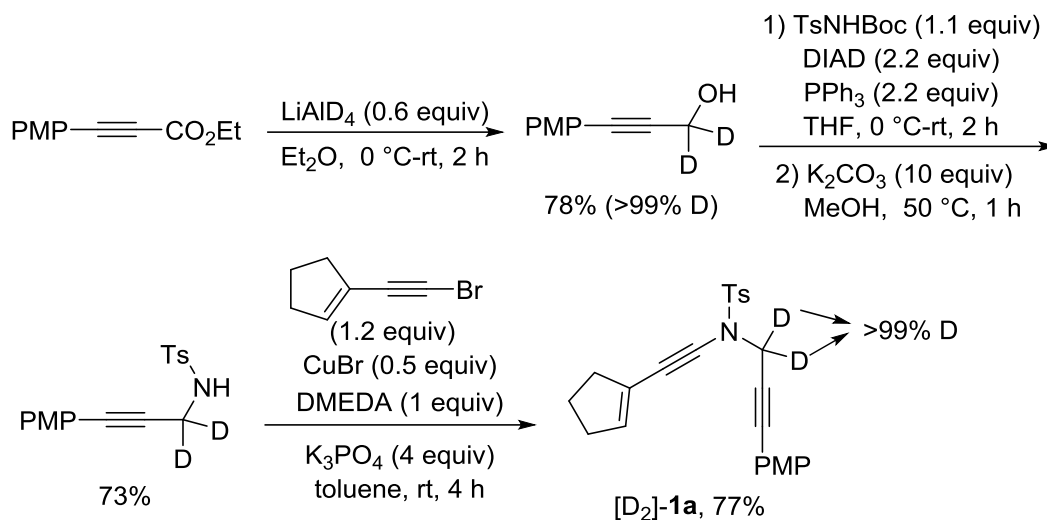
(neat): 3332, 2953, 2255, 2064, 1748, 1561, 1314, 1211, 1172, 1020, 812, 578;  
HRESIMS Calcd for  $[C_{17}H_{17}NNaO_2S]^+$  ( $M + Na^+$ ) 322.0872, found 322.0871.

[D<sub>3</sub>]-**1a** (91% D)



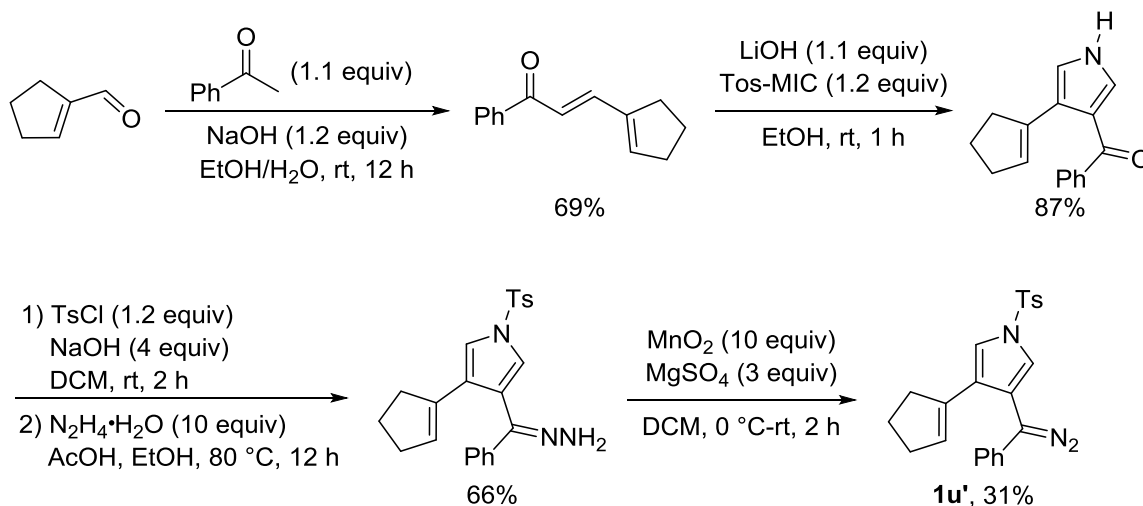
Compound [D<sub>3</sub>]-**1a** was prepared according to the known procedure<sup>3</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.86 (d,  $J$  = 8.0 Hz, 2H), 7.27 (d,  $J$  = 8.4 Hz, 2H), 7.11 (d,  $J$  = 8.8 Hz, 2H), 6.77 (d,  $J$  = 8.8 Hz, 2H), 5.99 – 5.92 (m, 0.09H), 4.46 (s, 2H), 3.79 (s, 3H), 2.50 – 2.39 (m, 2.18H), 2.36 (s, 3H), 1.90 – 1.82 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  159.7, 144.6, 134.2, 133.1, 129.4, 128.1, 123.3, 114.1, 113.7, 86.3, 82.9, 79.8, 68.5, 55.2, 42.9, 33.0, 22.9, 21.5.

[D<sub>2</sub>]-**1a** (>99% D)



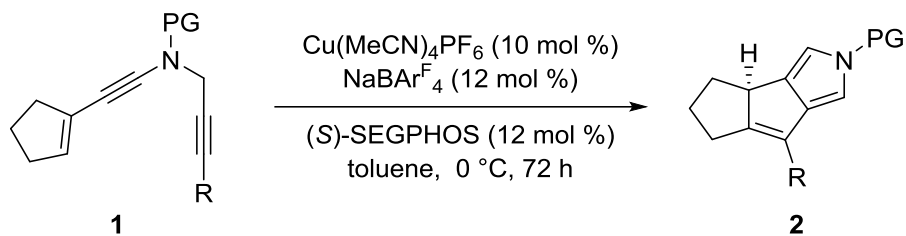
Compound [D<sub>2</sub>]-1a was prepared according to the known procedure<sup>4</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.14 – 7.07 (m, 2H), 6.81 – 6.74 (m, 2H), 5.98 – 5.90 (m, 1H), 3.79 (s, 3H), 2.48 – 2.38 (m, 4H), 2.36 (s, 3H), 1.94 – 1.82 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.7, 144.6, 136.7, 134.2, 133.1, 129.4, 128.1, 123.5, 114.1, 113.7, 86.3, 82.9, 79.7, 68.5, 55.2, 36.4, 33.1, 23.1, 21.5.

### 3-(cyclopent-1-en-1-yl)-4-(diazophenylmethyl)-1-tosyl-1H-pyrrole



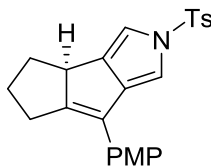
Compound 1u' was prepared according to the known procedures<sup>5,6</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.26 (m, 5H), 7.18 – 7.09 (m, 1H), 7.08 – 6.99 (m, 1H), 6.99 – 6.82 (m, 2H), 5.83 – 5.61 (m, 1H), 2.62 – 2.46 (m, 2H), 2.43 (s, 3H), 2.41 – 2.29 (m, 2H), 1.92 – 1.81 (m, 2H). HRESIMS Calcd for [C<sub>23</sub>H<sub>21</sub>N<sub>3</sub>NaO<sub>2</sub>S]<sup>+</sup> (M + Na<sup>+</sup>) 426.1247, found 426.1249.

## General procedure for the synthesis of chiral pyrroles 2:



The powdered  $\text{Cu}(\text{MeCN})_4\text{PF}_6$  (0.02 mmol, 7.5 mg), (*S*)-SEGPHOS (0.024 mmol, 14.6 mg) and  $\text{NaBAR}_4^{\text{F}}$  (0.024 mmol, 21.3 mg) were introduced into an oven-dried Schlenk tube under argon atmosphere. After toluene (1 mL) was injected into the Schlenk tube, the solution was stirred at rt under the argon atmosphere for 0.5 h. Then the reaction was cooled to 0 °C, *N*-propargyl ynamide **1** (0.2 mmol) in toluene (1 mL) were introduced into the system dropwise. The resulting mixture was stirred at indicating temperature and the progress of the reaction was monitored by TLC. After concentration in vacuo, the residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate) to give chiral pyrrole **2**.

### (*R*)-7-(4-methoxyphenyl)-2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (**2a**)

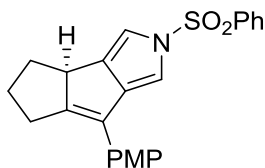


**2a**

Compound **2a** was prepared in 91% yield (73.7 mg) according to the general procedure. White solid (mp 101-102 °C).  $[\alpha]_{\text{D}}^{20} = -74.5^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 93% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 16.02 min (major), 25.00 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.45 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.23 (m, 2H), 7.07 – 6.90 (m, 4H), 3.83 (s, 3H), 3.60 – 3.52 (m, 1H), 2.75 – 2.64 (m, 1H), 2.43 – 2.38 (m, 1H), 2.36 (s, 3H), 2.23 – 2.05 (m, 3H), 1.10 – 0.96 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.7, 157.8, 144.4, 141.5, 136.5, 134.9, 129.8, 128.4, 127.4, 127.3, 126.7, 113.9, 113.2, 107.7, 55.3, 49.6, 29.6, 27.8, 25.0,

21.5; IR (neat): 2999, 1684, 1518, 1290, 1188, 1068, 785, 771, 722, 552; HRESIMS Calcd for  $[C_{24}H_{23}NNaO_3S]^+$  ( $M + Na^+$ ) 428.1291, found 428.1295.

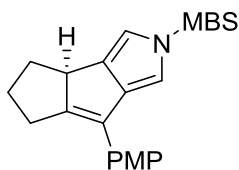
**(R)-7-(4-methoxyphenyl)-2-(phenylsulfonyl)-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2b)**



**2b**

Compound **2b** was prepared in 88% yield (68.8 mg) according to the general procedure. Colorless oil.  $[\alpha]_D^{20} = -18.2^\circ$  ( $c = 1.0$ ,  $CHCl_3$ ). 90% ee (determined by HPLC: Chiralpak ADH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 18.03 min (major), 27.53 min (minor)).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.86 (d,  $J = 7.6$  Hz, 2H), 7.52 – 7.42 (m, 5H), 7.09 – 6.91 (m, 4H), 3.82 (s, 3H), 3.60 – 3.53 (m, 1H), 2.75 – 2.65 (m, 1H), 2.43 – 2.35 (m, 1H), 2.22 – 2.04 (m, 3H), 1.12 – 0.96 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  158.7, 157.9, 141.6, 139.4, 135.1, 133.4, 129.2, 128.4, 127.4, 127.3, 126.6, 113.9, 113.3, 107.8, 55.2, 49.6, 29.5, 27.8, 25.0; IR (neat): 2923, 1610, 1544, 1422, 1342, 1020, 1020, 720, 525; HRESIMS Calcd for  $[C_{23}H_{21}NNaO_3S]^+$  ( $M + Na^+$ ) 414.1134, found 414.1136.

**(R)-7-(4-methoxyphenyl)-2-((4-methoxyphenyl)sulfonyl)-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2c)**

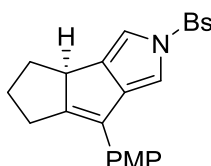


**2c**

Compound **2c** was prepared in 85% yield (71.6 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -57.0^\circ$  ( $c = 1.0$ ,  $CHCl_3$ ). 88% ee (determined by HPLC: Chiralpak IC Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 13.93 min (minor), 15.51 min (major)).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.84 – 7.77 (m, 2H), 7.46 (d,  $J = 8.4$  Hz, 2H), 7.05 (d,  $J = 1.2$  Hz, 1H), 6.98 – 6.88 (m, 5H), 3.83 (s, 3H), 3.81 (s, 3H),

3.60 – 3.52 (m, 1H), 2.75 – 2.66 (m, 1H), 2.44 – 2.38 (m, 1H), 2.23 – 2.15 (m, 2H), 2.11 – 2.04 (m, 1H), 1.13 – 0.96 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  163.4, 158.7, 157.7, 141.4, 134.9, 131.0, 128.9, 128.4, 127.5, 127.4, 114.4, 113.9, 113.2, 107.7, 55.6, 55.3, 49.6, 29.6, 27.8, 25.0; IR (neat): 2950, 1611, 1502, 1442, 1310, 1242, 1002, 847, 755, 612, 514; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 444.1240, found 444.1247.

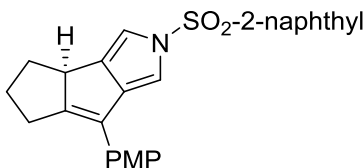
**(R)-2-((4-bromophenyl)sulfonyl)-7-(4-methoxyphenyl)-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2d)**



**2d**

Compound **2d** was prepared in 85% yield (79.7 mg) according to the general procedure. White solid (mp 188-189 °C).  $[\alpha]_{\text{D}}^{20} = -99.2^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 92% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 12.92 min (major), 15.94 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.8$  Hz, 2H), 7.62 – 7.57 (m, 2H), 7.44 (d,  $J = 8.8$  Hz, 2H), 7.03 (d,  $J = 0.8$  Hz, 1H), 6.97 – 6.92 (m, 3H), 3.84 (s, 3H), 3.61 – 3.54 (m, 1H), 2.72 – 2.67 (m, 1H), 2.45 – 2.37 (m, 1H), 2.24 – 2.16 (m, 2H), 2.12 – 2.04 (m, 1H), 1.10 – 0.98 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 158.2, 142.1, 138.3, 135.5, 132.5, 128.6, 128.4, 128.1, 127.3(1), 127.2(7), 113.9, 113.3, 107.7, 55.3, 49.6, 29.6, 27.8, 25.0; IR (neat): 2934, 1616, 1525, 1428, 1361, 1262, 1180, 1057, 757, 704, 574; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{20}\text{BrNNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 492.0239, found 492.0237.

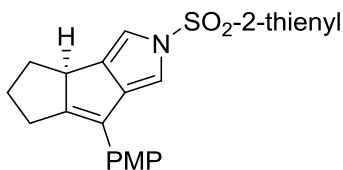
**(R)-7-(4-methoxyphenyl)-2-(naphthalen-2-ylsulfonyl)-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2e)**



**2e**

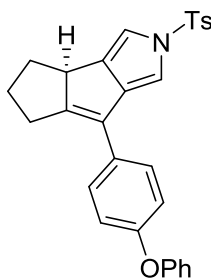
Compound **2e** was prepared in 90% yield (79.4 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -45.0^{\circ}$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 93% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 21.39 min (major), 33.24 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.48 (s, 1H), 7.96 – 7.79 (m, 4H), 7.63 – 7.58 (m, 2H), 7.45 (d,  $J = 8.8$  Hz, 2H), 7.13 (d,  $J = 1.2$  Hz, 1H), 7.06 – 7.02 (m, 1H), 6.97 – 6.91 (m, 2H), 3.83 (s, 3H), 3.59 – 3.51 (m, 1H), 2.69 – 2.65 (m, 1H), 2.40 – 2.35 (m, 1H), 2.23 – 2.12 (m, 2H), 2.10 – 2.03 (m, 1H), 1.09 – 0.94 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.7, 157.9, 141.7, 136.3, 135.1(1), 135.0(7), 132.0, 129.6, 129.4, 129.2, 128.4, 128.2, 127.9, 127.7, 127.5, 127.3, 121.6, 113.9, 113.3, 107.8, 55.3, 49.6, 29.6, 27.8, 25.0; IR (neat): 2935, 1634, 1555, 1312, 1240, 1044, 744, 703, 641, 574; HRESIMS Calcd for  $[\text{C}_{27}\text{H}_{23}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 464.1291, found 464.1294.

**(R)-7-(4-methoxyphenyl)-2-(thiophen-2-ylsulfonyl)-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-*c*]pyrrole (2f)**



Compound **2f** was prepared in 87% yield (69.1 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -2.8^{\circ}$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 89% ee (determined by HPLC: Chiralpak ADH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 19.33 min (major), 31.46 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 – 7.54 (m, 2H), 7.46 (d,  $J = 8.0$  Hz, 2H), 7.08 – 6.92 (m, 5H), 3.84 (s, 3H), 3.63 – 3.55 (m, 1H), 2.75 – 2.68 (m, 1H), 2.46 – 2.35 (m, 1H), 2.31 – 2.05 (m, 3H), 1.16 – 0.99 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.7, 158.2, 142.0, 139.8, 135.4, 133.1, 132.8, 128.4, 127.3, 113.9, 113.3, 107.7, 55.3, 49.6, 29.5, 27.8, 25.0; IR (neat): 2218, 1622, 1420, 1310, 1220, 1141, 1020, 700, 610, 510; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{19}\text{NNaO}_3\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 420.0699, found 420.0702.

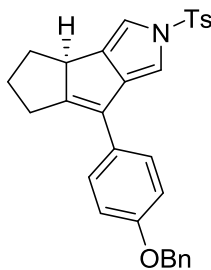
**(R)-7-(4-phenoxyphenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-*c*]pyrrole (2g)**



**2g**

Compound **2g** was prepared in 85% yield (79.4 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -52.3^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 90% ee (determined by HPLC: Chiralpak ASH Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.79 min (major), 19.07 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.48 (d,  $J = 8.8$  Hz, 2H), 7.37 – 7.29 (m, 2H), 7.27 – 7.24 (m, 2H), 7.14 – 6.96 (m, 7H), 3.62 – 3.54 (m, 1H), 2.75 – 2.65 (m, 1H), 2.45 – 2.38 (m, 1H), 2.36 (s, 3H), 2.24 – 2.05 (m, 3H), 1.11 – 0.98 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.9, 157.0, 156.3, 144.4, 141.3, 136.5, 134.8, 129.8(4), 129.8(0), 129.7, 128.6, 127.2, 126.7, 123.4, 119.0, 118.7, 113.3, 107.8, 49.8, 29.6, 27.8, 25.0, 21.5; IR (neat): 2244, 1611, 1410, 1302, 1241, 1141, 1070, 704, 652, 525; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{25}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 490.1447, found 490.1448.

**(R)-7-(4-(benzyloxy)phenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2h)**

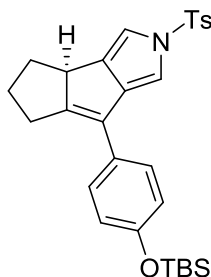


**2h**

Compound **2h** was prepared in 75% yield (72.1 mg) according to the general procedure except at 10 °C for 72 h. Pale yellow oil.  $[\alpha]_D^{20} = -87.6^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 92% ee (determined by HPLC: Chiralpak ASH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.97 min (major), 25.79 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,

$J = 8.4$  Hz, 2H), 7.47 – 7.30 (m, 7H), 7.25 – 7.22 (m, 2H), 7.08 – 6.95 (m, 4H), 5.08 (s, 2H), 3.58 – 3.51 (m, 1H), 2.74 – 2.64 (m, 1H), 2.42 – 2.37 (m, 1H), 2.35 (s, 3H), 2.21 – 2.11 (m, 2H), 2.10 – 2.03 (m, 1H), 1.09 – 0.96 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.9, 157.8, 144.4, 141.5, 136.9, 136.5, 134.9, 129.8, 128.5, 128.4, 127.9, 127.7, 127.4, 127.3, 126.7, 114.8, 113.2, 107.8, 70.0, 49.6, 29.6, 27.8, 25.0, 21.5; IR (neat): 2911, 2221, 1712, 1355, 1212, 1152, 1047, 952, 752; HRESIMS Calcd for  $[\text{C}_{30}\text{H}_{27}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 504.1604, found 504.1601.

**(*R*)-7-(4-((*tert*-butyldimethylsilyl)oxy)phenyl)-2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (2i)**

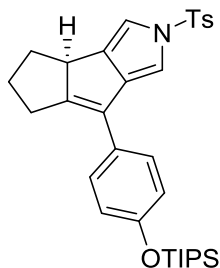


**2i**

Compound **2i** was prepared in 82% yield (82.4 mg) according to the general procedure except at 10 °C for 72 h. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -84.7^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 92% ee (determined by HPLC: Chiralpak ASH Column, 2/98 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.08 min (major), 12.33 min (minor)).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.5$  Hz, 2H), 7.39 (d,  $J = 8.5$  Hz, 2H), 7.26 – 7.22 (m, 2H), 7.07 – 6.95 (m, 2H), 6.90 – 6.85 (m, 2H), 3.59 – 3.52 (m, 1H), 2.73 – 2.65 (m, 1H), 2.43 – 2.37 (m, 1H), 2.36 (s, 3H), 2.21 – 2.06 (m, 3H), 1.12 – 0.98 (m, 10H), 0.22 (s, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.9, 154.8, 144.4, 141.5, 136.5, 134.9, 129.8, 128.3, 127.9, 127.4, 126.6, 120.0, 113.2, 107.8, 49.6, 29.6, 27.8, 25.7, 25.0, 21.5, 18.2, -4.4; IR (neat): 2927, 2240, 1611, 1421, 1370, 611, 645, 575; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{35}\text{NNaO}_3\text{SSi}]^+$  ( $\text{M} + \text{Na}^+$ ) 528.1999, found 528.2007.

**(*R*)-2-tosyl-7-(4-((*triisopropylsilyl*)oxy)phenyl)-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (2j)**

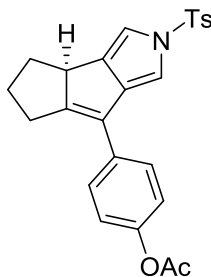




**2j**

Compound **2j** was prepared in 88% yield (96.3 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -75.1^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 94% ee (determined by HPLC: Chiralpak ASH Column, 1/99 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.23 min (minor), 10.87 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.38 (d,  $J = 8.4$  Hz, 2H), 7.27 – 7.22 (m, 2H), 7.05 (d,  $J = 1.2$  Hz, 1H), 6.98 – 6.88 (m, 3H), 3.60 – 3.52 (m, 1H), 2.75 – 2.65 (m, 1H), 2.45 – 2.39 (m, 1H), 2.37 (s, 3H), 2.23 – 2.14 (m, 2H), 2.13 – 2.06 (m, 1H), 1.34 – 1.21 (m, 3H), 1.13 – 1.00 (m, 19H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 155.3, 144.4, 141.5, 136.6, 135.0, 129.8, 128.3, 127.7, 127.5, 126.7, 119.9, 113.2, 107.9, 49.7, 29.6, 27.8, 25.1, 21.5, 17.9, 12.7; IR (neat): 2925, 2214, 1612, 1310, 1242, 1110, 1041, 910, 610; HRESIMS Calcd for  $[\text{C}_{32}\text{H}_{41}\text{NNaO}_3\text{SSi}]^+$  ( $\text{M} + \text{Na}^+$ ) 570.2469, found 570.2462.

**(R)-4-(2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrol-7-yl)phenyl acetate (2k)**

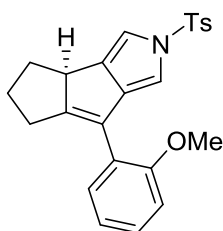


**2k**

Compound **2k** was prepared in 63% yield (54.5 mg) according to the general procedure except at 10 °C for 72 h. White solid (mp 114-115 °C).  $[\alpha]_D^{20} = -8.13^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 84% ee (determined by HPLC: Chiralpak ASH Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 35.58 min (minor), 47.77 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.51 (d,  $J = 8.8$  Hz, 2H),

7.28 – 7.24 (m, 2H), 7.15 – 7.10 (m, 2H), 7.05 – 6.97 (m, 2H), 3.63 – 3.55 (m, 1H), 2.78 – 2.67 (m, 1H), 2.49 – 2.39 (m, 1H), 2.38 (s, 3H), 2.32 (s, 3H), 2.29 – 2.05 (m, 3H), 1.14 – 0.99 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.5, 160.0, 149.5, 144.5, 141.1, 136.4, 134.7, 132.5, 129.8, 128.2, 127.2, 126.7, 121.6, 113.3, 107.8, 49.8, 29.5, 27.8, 25.0, 21.5, 21.1; IR (neat): 2912, 2241, 1698(s), 1642, 1520, 1341, 1120, 1020, 820, 671, 542; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{23}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 456.1240, found 456.1240.

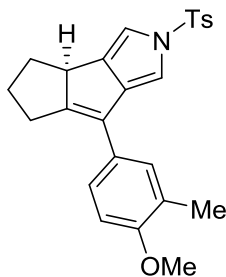
**(R)-7-(2-methoxyphenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2l)**



**2l**

Compound **2l** was prepared in 71% yield (57.5 mg) according to the general procedure except at 10 °C for 72 h. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -21.3^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 80% ee (determined by HPLC: Chiralpak ASH Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.53 min (major), 12.79 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.4$  Hz, 2H), 7.45 – 7.40 (m, 1H), 7.30 – 7.21 (m, 3H), 7.01 – 6.91 (m, 3H), 6.83 (d,  $J = 1.2$  Hz, 1H), 3.81 (s, 3H), 3.65 – 3.57 (m, 1H), 2.57 – 2.50 (m, 1H), 2.37 (s, 3H), 2.22 – 2.05 (m, 4H), 1.19 – 1.08 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.8, 156.7, 144.3, 142.8, 136.6, 134.9, 129.7, 129.6, 128.6, 126.6, 124.2, 123.8, 120.4, 113.1, 111.0, 108.1, 55.1, 49.3, 28.8, 28.3, 25.1, 21.5; IR (neat): 2244, 1642, 1144, 1020, 1042, 777, 620, 542, 572; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 428.1291, found 428.1291.

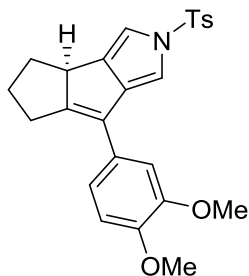
**(R)-7-(4-methoxy-3-methylphenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2m)**



**2m**

Compound **2m** was prepared in 81% yield (67.9 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -7.47^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 92% ee (determined by HPLC: Chiralpak ASH Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.85 min (major), 12.41 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.0$  Hz, 2H), 7.34 – 7.21 (m, 4H), 7.07 – 7.03 (m, 1H), 6.98 – 6.94 (m, 1H), 6.85 (d,  $J = 8.4$  Hz, 1H), 3.84 (s, 3H), 3.58 – 3.51 (m, 1H), 2.75 – 2.65 (m, 1H), 2.41 – 2.38 (m, 1H), 2.36 (s, 3H), 2.26 (s, 3H), 2.23 – 2.14 (m, 2H), 2.12 – 2.03 (m, 1H), 1.09 – 0.96 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.5, 157.0, 144.4, 141.6, 136.5, 135.0, 129.8, 129.5, 127.5, 127.0, 126.7, 126.6, 125.8, 113.2, 109.9, 107.8, 55.3, 49.5, 29.5, 27.8, 25.0, 21.5, 16.3; IR (neat): 2220, 1610, 1320, 1149, 1024, 702, 612, 612, 548, 516; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{25}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 442.1447, found 442.1452.

**(R)-7-(3,4-dimethoxyphenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2n)**

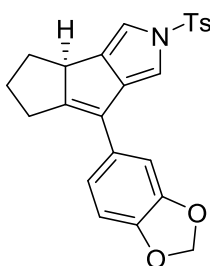


**2n**

Compound **2n** was prepared in 86% yield (74.8 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -8.21^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 90% ee (determined by HPLC: Chiralpak ASH Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.67 min (major), 32.33 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.24

(d,  $J = 8.4$  Hz, 2H), 7.12 – 7.02 (m, 3H), 7.00 – 6.89 (m, 2H), 3.91 (s, 3H), 3.90 (s, 3H), 3.60 – 3.53 (m, 1H), 2.77 – 2.67 (m, 1H), 2.50 – 2.39 (m, 1H), 2.36 (s, 3H), 2.26 – 2.05 (m, 3H), 1.12 – 0.98 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.1, 148.8, 148.3, 144.4, 141.4, 136.4, 134.9, 129.7, 127.7, 127.6, 126.6, 119.8, 113.3, 111.2, 110.6, 107.6, 55.9, 49.6, 29.5, 27.8, 25.0, 21.5; IR (neat): 2278, 1653, 1483, 1325, 1277, 1145, 1022, 784, 670, 577; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{25}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 458.1397, found 458.1393.

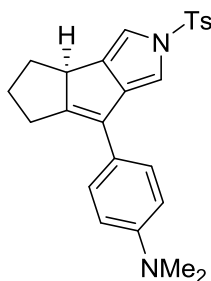
**(*R*)-7-(benzo[*d*][1,3]dioxol-5-yl)-2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (2o)**



**2o**

Compound **2o** was prepared in 85% yield (71.2 mg) according to the general procedure except at 10 °C for 72 h. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -20.3^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 92% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 18.76 min (major), 31.34 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.25 (d,  $J = 8.0$  Hz, 2H), 7.04 – 6.95 (m, 4H), 6.85 (d,  $J = 8.4$  Hz, 1H), 5.98 (s, 2H), 3.60 – 3.52 (m, 1H), 2.74 – 2.64 (m, 1H), 2.43 – 2.39 (m, 1H), 2.37 (s, 3H), 2.23 – 2.04 (m, 3H), 1.11 – 0.97 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.4, 147.7, 146.6, 144.4, 141.4, 136.5, 134.7, 129.8, 129.0, 127.6, 126.7, 121.0, 113.3, 108.3, 107.7, 107.6, 101.0, 49.7, 29.5, 27.8, 25.0, 21.5; IR (neat): 2241, 1622, 1410, 1320, 1241, 1141, 1020, 740, 678, 552; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{21}\text{NNaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 442.1083, found 442.1080.

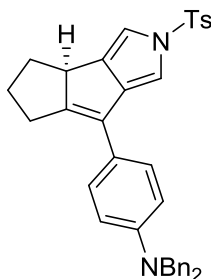
**(*R*)-*N,N*-dimethyl-4-(2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrol-7-yl)aniline (2p)**



**2p**

Compound **2p** was prepared in 86% yield (71.9 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -12.5^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 99% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 16.63 min (major), 21.24 min (minor)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.41 (d,  $J = 8.4$  Hz, 2H), 7.22 (d,  $J = 7.6$  Hz, 2H), 7.08 – 6.94 (m, 2H), 6.75 (d,  $J = 8.4$  Hz, 2H), 3.57 – 3.49 (m, 1H), 2.96 (s, 6H), 2.72 – 2.65 (m, 1H), 2.46 – 2.38 (m, 1H), 2.34 (s, 3H), 2.22 – 2.01 (m, 3H), 1.07 – 0.94 (m, 1H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.9, 149.5, 144.3, 141.8, 136.5, 135.2, 129.7, 128.1, 127.6, 126.6, 123.0, 113.1, 112.2, 107.8, 49.4, 40.4, 29.6, 27.9, 25.0, 21.5; IR (neat): 2944, 1633, 1555, 1342, 1222, 1171, 1077, 774, 574; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{26}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 441.1607, found 441.1601.

**(R)-N,N-dibenzyl-4-(2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrol-7-yl)aniline (2q)**

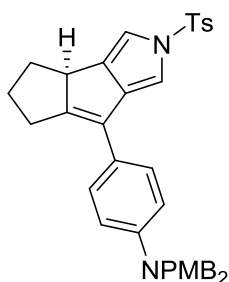


**2q**

Compound **2q** was prepared in 99% yield (112.8 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -17.8^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 96% ee (determined by HPLC: Chiralpak IC Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.23 min (major), 10.45 min (minor)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.4$  Hz, 2H), 7.36 – 7.29 (m, 6H), 7.26 – 7.18 (m, 8H), 7.02 – 6.91 (m, 2H), 6.76 (d,  $J = 8.8$  Hz, 2H), 4.67

(s, 4H), 3.55 – 3.47 (m, 1H), 2.67 – 2.58 (m, 1H), 2.41 – 2.36 (m, 1H), 2.33 (s, 3H), 2.16 – 2.00 (m, 3H), 1.04 – 0.91 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.9, 148.1, 144.2, 141.7, 138.3, 136.5, 135.1, 129.7, 128.6, 128.3, 127.4, 126.9, 126.6(1), 126.5(6), 123.4, 113.1, 112.3, 107.8, 54.3, 49.5, 29.6, 27.9, 25.1, 21.5; IR (neat): 2955, 1635, 1545, 1322, 1247, 1174, 1014, 774, 578; HRESIMS Calcd for  $[\text{C}_{37}\text{H}_{34}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 593.2233, found 593.2238.

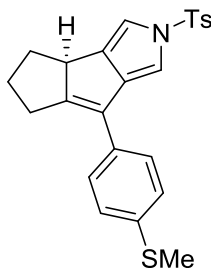
**(R)-N,N-bis(4-methoxybenzyl)-4-(2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrol-7-yl)aniline (2r)**



**2r**

Compound **2r** was prepared in 92% yield (116.2 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -36.8^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 97% ee (determined by HPLC: Chiralpak IC Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.78 min (major), 16.92 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.4$  Hz, 2H), 7.34 (d,  $J = 8.8$  Hz, 2H), 7.23 – 7.12 (m, 6H), 7.03 – 6.82 (m, 6H), 6.77 (d,  $J = 8.8$  Hz, 2H), 4.57 (s, 4H), 3.77 (s, 6H), 3.55 – 3.47 (m, 1H), 2.69 – 2.58 (m, 1H), 2.44 – 2.36 (m, 1H), 2.33 (s, 3H), 2.21 – 1.99 (m, 3H), 1.05 – 0.91 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.6, 155.8, 148.2, 144.2, 141.8, 136.5, 135.1, 130.3, 129.7, 128.2, 127.8, 127.5, 126.6, 123.2, 114.0, 113.0, 112.4, 107.8, 55.2, 53.5, 49.4, 29.6, 27.9, 25.1, 21.5; IR (neat): 2944, 1633, 1555, 1342, 1222, 1171, 1077, 774, 574; HRESIMS Calcd for  $[\text{C}_{39}\text{H}_{38}\text{N}_2\text{NaO}_4\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 653.2444, found 653.2448.

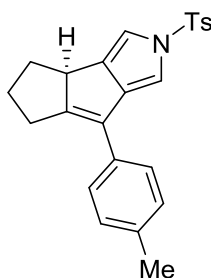
**(R)-7-(4-(methylthio)phenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2s)**



**2s**

Compound **2s** was prepared in 77% yield (64.8 mg) according to the general procedure. White solid (mp 108-109 °C).  $[\alpha]_D^{20} = -5.2^\circ$  (c = 1.0, CHCl<sub>3</sub>). 91% ee (determined by HPLC: Chiralpak ASH Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.70 min (major), 22.01 min (minor)). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.30 – 7.25 (m, 4H), 7.10 – 6.96 (m, 2H), 3.62 – 3.54 (m, 1H), 2.75 – 2.70 (m, 1H), 2.50 (s, 3H), 2.45 – 2.40 (m, 1H), 2.37 (s, 3H), 2.26 – 2.02 (m, 3H), 1.12 – 0.98 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.5, 144.4, 141.1, 137.2, 136.5, 134.8, 131.6, 129.8, 127.6, 127.4, 126.7, 126.6, 113.3, 107.8, 49.8, 29.6, 27.8, 25.1, 21.5, 15.8; IR (neat): 2934, 1700, 1616, 1511, 1452, 1300, 1272, 1171, 712, 610, 577; HRESIMS Calcd for [C<sub>24</sub>H<sub>23</sub>NNaO<sub>2</sub>S<sub>2</sub>]<sup>+</sup> (M + Na<sup>+</sup>) 444.1062, found 444.1060.

**(R)-7-(*p*-tolyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-*c*]pyrrole (2t)**

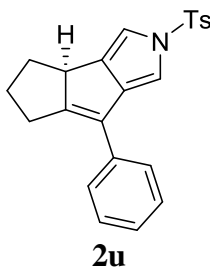


**2t**

Compound **2t** was prepared in 88% yield (68.5 mg) according to the general procedure except at 20 °C for 5 d. Pale yellow oil.  $[\alpha]_D^{20} = -38.1^\circ$  (c = 1.0, CHCl<sub>3</sub>). 73% ee (determined by HPLC: Chiralpak ASH Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.40 min (major), 15.67 min (minor)). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.18 (m, 4H), 7.08 – 6.95 (m, 2H), 3.60 – 3.53 (m, 1H), 2.76 – 2.65 (m, 1H), 2.44 – 2.39 (m, 1H), 2.36 (s, 3H), 2.35 (s, 3H), 2.22

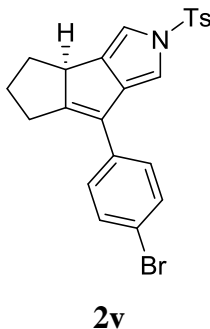
– 2.06 (m, 3H), 1.10 – 0.96 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.9, 144.4, 141.4, 136.8, 136.5, 134.9, 131.8, 129.8, 129.1, 127.7, 127.1, 126.7, 113.2, 107.9, 49.7, 29.5, 27.8, 25.0, 21.5, 21.2; IR (neat): 2922, 1652, 1520, 1371, 1220, 1171, 1020, 671, 622; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{23}\text{NNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 412.1342, found 412.1340.

**(R)-7-phenyl-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2u)**



Compound **2u** was prepared in 73% yield (54.7 mg) according to the general procedure except at 20 °C for 5 d. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -71.1^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 64% ee (determined by HPLC: Chiralpak IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.65 min (minor), 12.81 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 8.4$  Hz, 2H), 7.43 (d,  $J = 7.6$  Hz, 2H), 7.35 – 7.28 (m, 2H), 7.22 – 7.14 (m, 3H), 7.02 – 6.98 (m, 1H), 6.92 – 6.88 (m, 1H), 3.54 – 3.46 (m, 1H), 2.69 – 2.60 (m, 1H), 2.44 – 2.30 (m, 1H), 2.27 (s, 3H), 2.17 – 1.97 (m, 3H), 1.02 – 0.90 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.9, 144.4, 141.2, 136.4, 134.8, 134.6, 129.8, 128.4, 127.9, 127.2, 127.1, 126.7, 113.2, 107.9, 49.8, 29.5, 27.7, 25.0, 21.5; IR (neat): 2912, 1744, 1614, 1520, 1371, 1141, 1020, 920, 620, 510; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{21}\text{NNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 398.1185, found 398.1185.

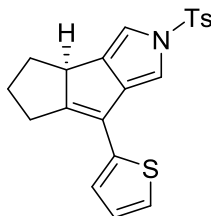
**(R)-7-(4-bromophenyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2v)**





Compound **2v** was prepared in 61% yield (55.3 mg) according to the general procedure except at 20 °C for 5 d. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -87.6^{\circ}$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 56% ee (determined by HPLC: Chiralpak IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.75 min (major), 12.76 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.4$  Hz, 2H), 7.66 – 7.60 (m, 1H), 7.48 – 7.38 (m, 2H), 7.31 – 7.26 (m, 3H), 7.07 – 6.98 (m, 2H), 3.65 – 3.56 (m, 1H), 2.78 – 2.70 (m, 1H), 2.48 – 2.43 (m, 1H), 2.38 (s, 3H), 2.26 – 2.16 (m, 2H), 2.14 – 2.09 (m, 1H), 1.13 – 0.99 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.4, 144.5, 140.7, 136.8, 134.5, 130.1, 130.0(0), 129.9(7), 129.9, 126.8, 125.8, 122.7, 113.5, 107.8, 50.0, 29.5, 27.8, 25.1, 21.5; IR (neat): 2972, 1620, 1541, 1352, 1241, 1142, 1042, 642, 610, 541; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{20}\text{BrNNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 476.0290, found 476.0290.

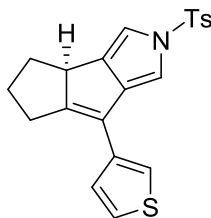
**(*R*)-7-(thiophen-2-yl)-2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (2w)**



**2w**

Compound **2w** was prepared in 82% yield (62.5 mg) according to the general procedure except at 10 °C for 72 h. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -69.0^{\circ}$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 84% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.63 min (major), 18.77 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.29 – 7.22 (m, 3H), 7.16 (d,  $J = 3.2$  Hz, 1H), 7.12 – 7.07 (m, 2H), 6.99 – 6.95 (m, 1H), 3.65 – 3.57 (m, 1H), 2.64 – 2.51 (m, 2H), 2.37 (s, 3H), 2.27 – 2.06 (m, 3H), 1.15 – 1.00 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.6, 144.5, 141.0, 137.9, 136.4, 134.4, 129.8, 127.3, 126.7, 124.4, 124.3, 121.7, 113.3, 107.9, 50.0, 29.7, 28.1, 25.2, 21.5; IR (neat): 2278, 1675, 1485, 1312, 1220, 1148, 1055, 750, 672, 520; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{19}\text{NNaO}_2\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 404.0749, found 404.0744.

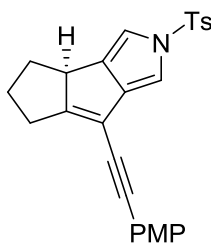
**(*R*)-7-(thiophen-3-yl)-2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (2x)**



**2x**

Compound **2x** was prepared in 92% yield (70.1 mg) according to the general procedure except at 10 °C for 72 h. Pale yellow oil.  $[\alpha]_D^{20} = -104.3^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 84% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 12.51 min (major), 21.14 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.37 – 7.24 (m, 5H), 7.04 (d,  $J = 1.2$  Hz, 1H), 6.99 – 6.95 (m, 1H), 3.62 – 3.53 (m, 1H), 2.66 – 2.62 (m, 1H), 2.51 – 2.42 (m, 1H), 2.37 (s, 3H), 2.25 – 2.08 (m, 3H), 1.13 – 0.99 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.5, 144.4, 141.6, 136.5, 136.0, 134.7, 129.8, 126.7, 125.6, 122.8, 121.4, 113.3, 107.6, 49.7, 29.6, 28.0, 24.9, 21.5; IR (neat): 2928, 1655, 1571, 1374, 1212, 1140, 1044, 641, 610; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{19}\text{NNaO}_2\text{S}_2]^+$  ( $\text{M} + \text{Na}^+$ ) 404.0749, found 404.0753.

**(R)-7-((4-methoxyphenyl)ethynyl)-2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrole (2y)**

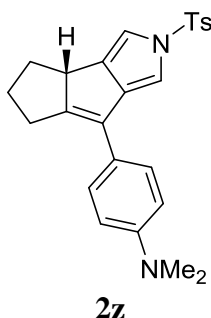


**2y**

Compound **2y** was prepared in 72% yield (61.8 mg) according to the general procedure. White solid (mp 106-108 °C).  $[\alpha]_D^{20} = -19.2^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 90% ee (determined by HPLC: Chiralpak ADH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.72 min (minor), 19.63 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.42 (d,  $J = 8.8$  Hz, 2H), 7.28 – 7.24 (m, 2H), 6.93 – 6.82 (m, 4H), 3.82 (s, 3H), 3.62 – 3.52 (m, 1H), 2.56 – 2.50 (m, 2H), 2.38 (s, 3H), 2.24 – 2.04 (m, 3H), 1.15 – 1.03 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  169.1, 159.6, 144.5, 141.6, 136.4, 133.9, 133.0, 129.8,

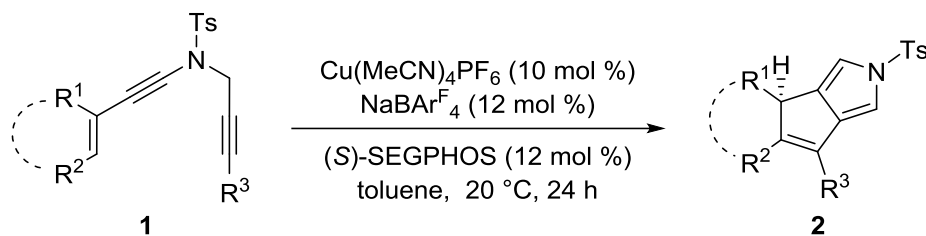
126.7, 115.3, 114.0, 113.4, 110.2, 107.6, 93.4, 81.7, 55.3, 49.2, 28.8, 28.2, 24.0, 21.5; IR (neat): 2933, 2201, 1648, 1571, 1367, 1285, 1172, 1041, 716, 625, 545; HRESIMS Calcd for  $[C_{26}H_{23}NNaO_3S]^+$  ( $M + Na^+$ ) 452.1291, found 452.1297.

**(S)-N,N-dimethyl-4-(2-tosyl-3b,4,5,6-tetrahydro-2H-pentaleno[1,2-c]pyrrol-7-yl)aniline (2z)**



Compound **2z** was prepared in 88% yield (73.6 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = +12.6^\circ$  ( $c = 1.0$ ,  $CHCl_3$ ). 99% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 16.23 min (minor), 20.33 min (major)).

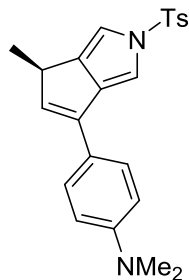
**General procedure for the synthesis of chiral pyrroles 2aa-2al:**



The powdered  $\text{Cu(MeCN)}_4\text{PF}_6$  (0.02 mmol, 7.5 mg), (S)-SEGPHOS (0.024 mmol, 14.6 mg) and  $\text{NaBARF}_4$  (0.024 mmol, 21.3 mg) were introduced into an oven-dried Schlenk tube under argon atmosphere. After toluene (1 mL) was injected into the Schlenk tube, the solution was stirred at rt under the argon atmosphere for 0.5 h. Then the reaction was cooled to 20 °C, *N*-propargyl ynamide **1** (0.2 mmol) in toluene (1 mL) were introduced into the system dropwise. The resulting mixture was stirred at indicating temperature and the progress of the reaction was monitored by TLC. After concentration in vacuo, the

residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate) to give chiral pyrrole **2**.

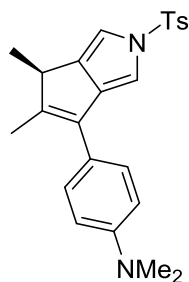
**(R)-N,N-dimethyl-4-(6-methyl-2-tosyl-2,6-dihydrocyclopenta[c]pyrrol-4-yl)aniline (2aa)**



**2aa**

Compound **2aa** was prepared in 70% yield (54.9 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -78.4^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 90% ee (determined by HPLC: Chiralpak ADH Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.18 min (minor), 21.69 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.52 – 7.45 (m, 2H), 7.24 (d,  $J = 8.0$  Hz, 2H), 7.17 (d,  $J = 1.6$  Hz, 1H), 6.98 – 6.94 (m, 1H), 6.74 (d,  $J = 8.8$  Hz, 2H), 6.32 (d,  $J = 2.4$  Hz, 1H), 3.54 – 3.46 (m, 1H), 2.98 (s, 6H), 2.36 (s, 3H), 1.25 (d,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.2, 144.4, 140.4, 137.1, 136.5, 136.4, 135.5, 129.8, 127.1, 126.7, 122.8, 112.3, 111.5, 109.1, 40.5, 38.0, 21.5, 18.1; IR (neat): 2922, 1671, 1572, 1312, 1172, 1072, 1072, 620, 544; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{24}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 415.1451, found 415.1458.

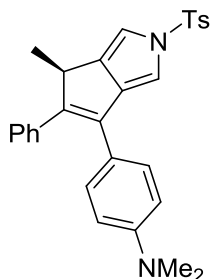
**(R)-4-(5,6-dimethyl-2-tosyl-2,6-dihydrocyclopenta[c]pyrrol-4-yl)-N,N-dimethylaniline (2ab)**



**2ab**

Compound **2ab** was prepared in 88% yield (72.7 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -74.0^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 90% ee (determined by HPLC: Chiralpak ODH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.18 min (minor), 7.55 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.4$  Hz, 2H), 7.37 – 7.31 (m, 2H), 7.21 (d,  $J = 8.0$  Hz, 2H), 6.94 – 6.88 (m, 2H), 6.79 – 6.73 (m, 2H), 3.26 (q,  $J = 7.2$  Hz, 1H), 2.97 (s, 6H), 2.34 (s, 3H), 2.02 (s, 3H), 1.26 (d,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.5, 145.7, 144.2, 139.6, 138.5, 136.5, 130.3, 129.7, 128.8, 126.6, 123.4, 112.3, 112.2, 107.5, 41.9, 40.4, 21.5, 17.2, 13.8; IR (neat): 2198, 1632, 1511, 1321, 1202, 1141, 1040, 1046, 644, 510; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{26}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 429.1607, found 429.1608.

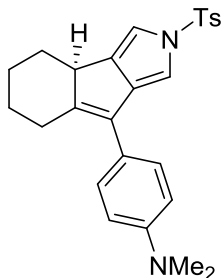
**(*R*)-*N,N*-dimethyl-4-(6-methyl-5-phenyl-2-tosyl-2,6-dihydrocyclopenta[*c*]pyrrol-4-yl)aniline (**2ac**)**



**2ac**

Compound **2ac** was prepared in 82% yield (77.2 mg) according to the general procedure. Pale yellow oil.  $[\alpha]_D^{20} = -101.0^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 93% ee (determined by HPLC: Chiralpak ADH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.21 min (major), 10.65 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.17 (m, 9H), 7.07 – 7.01 (m, 2H), 6.60 (d,  $J = 8.8$  Hz, 2H), 3.92 – 3.84 (m, 1H), 2.93 (s, 6H), 2.35 (s, 3H), 1.14 (d,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.5, 147.7, 144.4, 139.4, 138.2, 136.8, 136.4, 131.6, 129.8, 129.4, 129.1, 128.2, 126.7, 122.9, 112.4, 111.9, 109.1, 40.9, 40.3, 21.5, 17.6; IR (neat): 2278, 1614, 1555, 1320, 1241, 1171, 1002, 671, 602, 571; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{28}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 491.1764, found 491.1765.

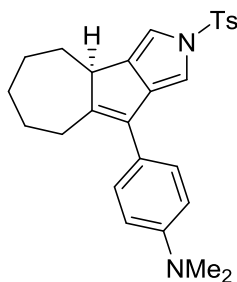
**(R)-N,N-dimethyl-4-(2-tosyl-2,3b,4,5,6,7-hexahydroindeno[1,2-c]pyrrol-8-yl)aniline (2ad)**



**2ad**

Compound **2ad** was prepared in 81% yield (70.2 mg) according to the general procedure except using 2-Me-THF as the solvent. Pale yellow oil.  $[\alpha]_D^{20} = -74.7^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 83% ee (determined by HPLC: Chiralpak ODH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.51 min (minor), 7.98 min (major)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.4$  Hz, 2H), 7.36 – 7.29 (m, 2H), 7.21 (d,  $J = 8.0$  Hz, 2H), 6.94 – 6.90 (m, 2H), 6.76 (d,  $J = 8.8$  Hz, 2H), 3.16 – 3.09 (m, 1H), 3.03 – 2.95 (m, 7H), 2.34 (s, 3H), 2.32 – 2.19 (m, 2H), 1.88 – 1.73 (m, 2H), 1.56 – 1.44 (m, 1H), 1.27 – 1.10 (m, 2H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.5, 148.4, 144.2, 139.9, 137.2, 136.5, 129.7, 128.9, 127.9, 126.6, 123.2, 112.2(9), 112.2(6), 107.6, 44.6, 40.5, 33.1, 27.7, 27.4, 25.5, 21.5; IR (neat): 2947, 1641, 1520, 1372, 1272, 1200, 1071, 913, 776, 516; HRESIMS Calcd for  $[\text{C}_{26}\text{H}_{28}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 455.1764, found 455.1775.

**(R)-N,N-dimethyl-4-(2-tosyl-3b,4,5,6,7,8-hexahydro-2H-azuleno[1,2-c]pyrrol-9-yl)aniline (2ae)**

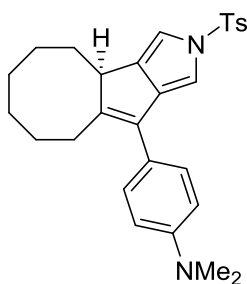


**2ae**

Compound **2ae** was prepared in 91% yield (81.1 mg) according to the general procedure except using 2-Me-THF as the solvent. Pale yellow oil.  $[\alpha]_D^{20} = -24.0^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

95% ee (determined by HPLC: Chiralpak ADH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.01 min (minor), 17.37 min (major)). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.35 (m, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 6.91 – 6.85 (m, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.47 – 3.40 (m, 1H), 2.97 (s, 6H), 2.76 – 2.71 (m, 2H), 2.35 (s, 3H), 2.17 – 2.12 (m, 1H), 1.94 – 1.74 (m, 5H), 1.65 – 1.53 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 151.1, 149.3, 144.2, 139.8, 138.3, 136.6, 129.8, 129.7, 128.7, 126.6, 123.8, 112.1, 107.4, 47.4, 40.4, 34.2, 30.6, 29.4, 27.0, 21.5; IR (neat): 2258, 1620, 1510, 1314, 1255, 1289, 1094, 1046, 676, 523; HRESIMS Calcd for [C<sub>27</sub>H<sub>30</sub>N<sub>2</sub>NaO<sub>2</sub>S]<sup>+</sup> (M + Na<sup>+</sup>) 469.1920, found 469.1928.

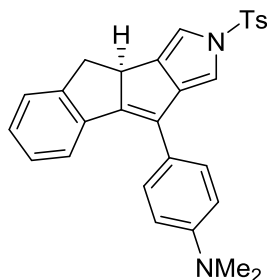
**(*R*)-*N,N*-dimethyl-4-(2-tosyl-2,3b,4,5,6,7,8,9-octahydrocycloocta[3,4]cyclopenta[1,2-*c*]pyrrol-10-yl)aniline (2af)**



**2af**

Compound **2af** was prepared in 93% yield (85.8 mg) according to the general procedure except using 2-Me-THF as the solvent. Pale yellow oil. [ $\alpha$ ]<sub>D</sub><sup>20</sup> = -22.1 °(c = 1.0, CHCl<sub>3</sub>). 93% ee (determined by HPLC: Chiralpak ADH Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.03 min (minor), 26.78 min (major)). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.33 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.90 – 6.85 (m, 2H), 6.79 – 6.72 (m, 2H), 3.46 – 3.41 (m, 1H), 2.97 (s, 6H), 2.94 – 2.85 (m, 1H), 2.35 (s, 3H), 2.25 – 2.16 (m, 1H), 1.85 – 1.76 (m, 1H), 1.73 – 1.56 (m, 3H), 1.52 – 1.34 (m, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 150.3, 149.4, 144.2, 140.4, 137.0, 136.6, 131.6, 129.6, 128.5, 126.6, 124.0, 112.2, 107.7, 46.9, 40.4, 28.6, 28.4, 27.7, 26.7, 25.7, 24.4, 21.5; IR (neat): 2924, 1620, 1530, 1332, 1120, 1074, 920, 721, 527, 504; HRESIMS Calcd for [C<sub>28</sub>H<sub>32</sub>N<sub>2</sub>NaO<sub>2</sub>S]<sup>+</sup> (M + Na<sup>+</sup>) 483.2077, found 483.2084.

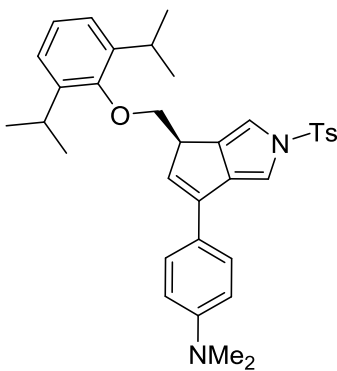
**(R)-N,N-dimethyl-4-(2-tosyl-3b,4-dihydro-2H-benzo[4,5]pentaleno[1,2-c]pyrrol-9-yl)aniline (2ag)**



**2ag**

Compound **2ag** was prepared in 91% yield (85.0 mg) according to the general procedure except at 0 °C for 48 h. Pale yellow oil.  $[\alpha]_D^{20} = -27.5^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 95% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.79 min (major), 16.31 min (minor)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 – 7.67 (m, 3H), 7.55 (d,  $J = 8.0$  Hz, 2H), 7.26 – 7.23 (m, 3H), 7.15 – 6.96 (m, 4H), 6.79 (d,  $J = 8.4$  Hz, 2H), 4.31 (t,  $J = 8.4$  Hz, 1H), 3.23 (dd,  $J = 14.8, 8.4$  Hz, 1H), 3.00 (s, 6H), 2.71 (dd,  $J = 14.4, 9.2$  Hz, 1H), 2.35 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  152.2, 150.1, 150.0, 144.5, 144.0, 137.1, 136.4, 134.0, 129.8, 129.1, 128.6, 127.3, 126.7(2), 126.6(7), 125.5, 122.6, 121.9, 113.3, 112.0, 109.1, 51.2, 40.4, 33.8, 21.5; IR (neat): 2921, 1640, 1574, 1320, 1220, 1141, 1075, 677, 646, 570; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{26}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 489.1607, found 489.1608.

**(R)-4-(6-((2,6-diisopropylphenoxy)methyl)-2-tosyl-2,6-dihydrocyclopenta[*c*]pyrrol-4-yl)-N,N-dimethylaniline (2ah)**

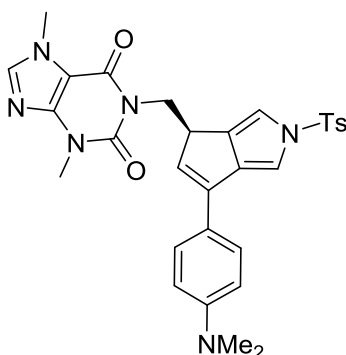


**2ah**



Compound **2ah** was prepared in 64% yield (0.1 mmol scale, 35.4 mg) according to the general procedure except using DCE as the solvent at 0 °C. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -98.7^{\circ}$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 78% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.19 min (minor), 8.05 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H), 7.54 (d,  $J = 8.8$  Hz, 2H), 7.29 – 7.25 (m, 3H), 7.14 – 7.08 (m, 4H), 6.76 (d,  $J = 8.8$  Hz, 2H), 6.48 (d,  $J = 2.4$  Hz, 1H), 4.00 (t,  $J = 7.2$  Hz, 1H), 3.79 – 3.69 (m, 2H), 3.34 – 3.26 (m, 2H), 2.99 (s, 6H), 2.38 (s, 3H), 1.20 (t,  $J = 6.8$  Hz, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.0, 150.4, 144.6, 141.8, 138.9, 137.1, 136.5, 135.7, 129.9, 129.1, 127.3, 126.7, 124.6, 123.9, 122.4, 113.6, 112.3, 109.5, 75.5, 44.7, 40.4, 26.5, 24.1, 23.9, 21.5; IR (neat): 2974, 1707, 1612, 1547, 1312, 1212, 1185, 1074, 644, 651, 528; HRESIMS Calcd for  $[\text{C}_{35}\text{H}_{40}\text{N}_2\text{NaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 591.2652, found 591.2657.

**(R)-1-((6-(4-(dimethylamino)phenyl)-2-tosyl-2,4-dihydrocyclopenta[c]pyrrol-4-yl)methyl)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (2ai)**

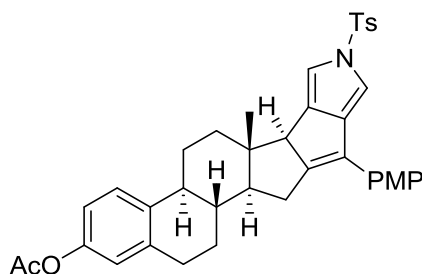


**2ai**

Compound **2ai** was prepared in 70% yield (0.1 mmol scale, 39.9 mg) according to the general procedure except at 60 °C for 4 h. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -71.5^{\circ}$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 76% ee (determined by HPLC: Chiralpak IC Column, 50/50 *i*-PrOH/hexane, 1.5 mL/min, 254 nm; TR = 78.28 min (major), 104.20 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.4$  Hz, 2H), 7.53 (s, 1H), 7.48 (d,  $J = 8.8$  Hz, 2H), 7.25 (d,  $J = 8.0$  Hz, 2H), 7.15 (d,  $J = 1.6$  Hz, 1H), 6.91 (s, 1H), 6.72 (d,  $J = 8.8$  Hz, 2H), 6.32 (d,  $J = 2.4$  Hz, 1H), 4.28 – 4.14 (m, 2H), 4.04 – 3.96 (m, 4H), 3.58 (s, 3H), 2.98 (s, 6H), 2.38 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.2, 151.6, 150.3, 148.9, 144.5, 141.6, 138.0, 137.4,

136.6, 135.7, 130.9, 129.8, 127.3, 126.6, 126.4, 122.7, 113.5, 112.2, 109.3, 43.2, 42.6, 40.4, 33.6, 29.7, 21.5; IR (neat): 2934, 1704(s), 1696(s), 1611, 1530, 1363, 1222, 1132, 1025, 675, 651, 526; HRESIMS Calcd for $[C_{30}H_{30}N_6NaO_4S]^+$  ( $M + Na^+$ ) 593.1941, found 593.1948.

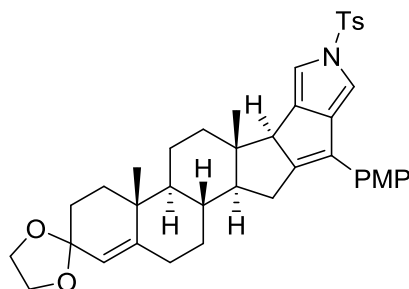
**(6b*S*,8a*S*,8b*R*,13a*S*,13b*S*)-12-(4-methoxyphenyl)-8a-methyl-10-tosyl-2,6b,7,8,8a,8b,10,13,13a,13b-decahydro-1*H*-phenanthro[1',2':5,6]pentaleno[1,2-c]pyrrol-4-yl acetate (2aj)**



**2aj**

Compound **2aj** was prepared in 61% yield (72.2 mg) according to the general procedure except using DCE as the solvent at 40 °C. Pale yellow oil.  $[\alpha]_D^{20} = -47.8^\circ$  ( $c = 1.0$ ,  $CHCl_3$ ).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.74 (d,  $J = 8.0$  Hz, 2H), 7.51 (d,  $J = 8.8$  Hz, 2H), 7.31 – 7.26 (m, 2H), 7.25 – 7.20 (m, 1H), 7.11 (s, 1H), 7.00 – 6.92 (m, 3H), 6.87 – 6.82 (m, 1H), 6.78 (s, 1H), 3.84 (s, 3H), 3.47 – 3.37 (m, 1H), 2.97 – 2.78 (m, 3H), 2.39 – 2.35 (m, 5H), 2.27 (s, 3H), 2.11 – 1.99 (m, 4H), 1.72 – 1.63 (m, 1H), 1.55 – 1.41 (m, 3H), 0.29 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  169.8, 158.7, 154.5, 148.5, 144.4, 142.1, 138.0, 137.8, 136.5, 132.6, 129.8, 129.4, 128.3, 127.5, 126.6, 126.2, 121.5, 118.6, 113.9, 113.1, 108.3, 62.0, 57.5, 55.3, 44.0, 41.0, 38.3, 37.6, 29.5, 28.4, 27.5, 26.2, 21.5, 21.1, 11.9; IR (neat): 2931, 2258, 2105, 1695(s), 1625, 1520, 1364, 1220, 1142, 1040, 678, 655, 521; HRESIMS Calcd for $[C_{39}H_{39}NNaO_5S]^+$  ( $M + Na^+$ ) 656.2441, found 656.2438.

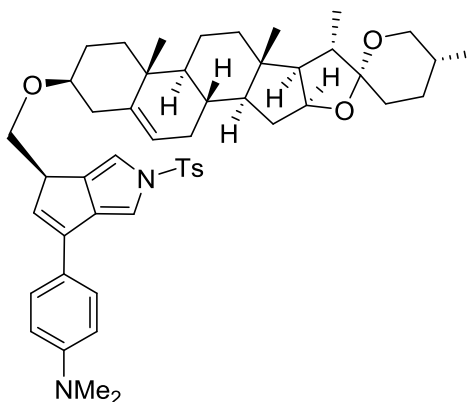
**(6a*R*,6b*S*,8a*S*,8b*R*,13a*S*,13b*S*)-12-(4-methoxyphenyl)-6a,8a-dimethyl-10-tosyl-1,2,5,6,6a,6b,7,8,8a,8b,10,13,13a,13b-tetradecahydrospiro[phenanthro[1',2':5,6]pentaleno[1,2-c]pyrrole-4,2'-[1,3]dioxolane] (2ak)**



**2ak**

Compound **2ak** was prepared in 62% yield (41.0 mg, 0.1 mmol scale) according to the general procedure except using DCE as the solvent at 40 °C. Pale yellow oil.  $[\alpha]_D^{20} = -18.2$  (c = 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 1.6 Hz, 1H), 6.96 – 6.90 (m, 3H), 5.38 – 5.34 (m, 1H), 4.00 – 3.89 (m, 4H), 3.83 (s, 3H), 3.33 (s, 1H), 2.83 (dd, *J* = 17.8, 8.2 Hz, 1H), 2.57 (dd, *J* = 14.2, 2.2 Hz, 1H), 2.37 (s, 3H), 2.16 – 2.04 (m, 2H), 2.02 – 1.93 (m, 2H), 1.84 – 1.68 (m, 5H), 1.57 – 1.31 (m, 5H), 1.01 (s, 3H), 0.93 – 0.80 (m, 1H), 0.28 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.6, 155.0, 144.4, 142.2, 140.3, 136.5, 132.6, 129.8, 129.2, 128.3, 127.5, 126.6, 121.6, 113.9, 113.0, 109.4, 108.2, 64.4, 64.2, 61.9, 58.7, 55.3, 49.8, 41.8, 40.5, 37.6, 36.8, 36.2, 31.9, 31.6, 31.0, 28.7, 21.5, 20.8, 18.8, 11.8; IR (neat): 2943, 2222, 2135, 1711, 1632, 1510, 1323, 1212, 1143, 1020, 671, 635, 524; HRESIMS Calcd for[C<sub>40</sub>H<sub>45</sub>NNaO<sub>5</sub>S]<sup>+</sup> (M + Na<sup>+</sup>) 674.2911, found 674.2917.

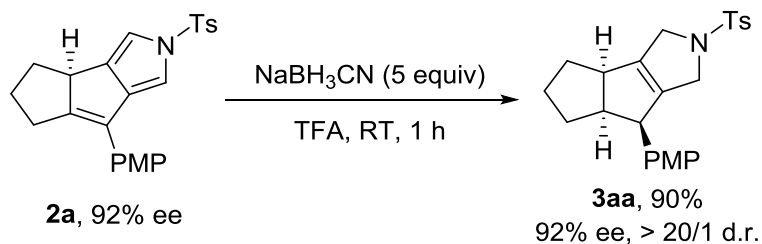
***N,N*-dimethyl-4-((*R*)-6-(((4*S*,5'*R*,6*aR*,6*bS*,8*aS*,8*bR*,9*S*,10*R*,11*aS*,12*aS*,12*bS*)-5',6*a*,8*a*,9-tetramethyl-1,3,3',4,4',5,5',6,6*a*,6*b*,6',7,8,8*a*,8*b*,9,11*a*,12,12*a*,12*b*-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-*b*]furan-10,2'-pyran]-4-yl)oxy)methyl)-2-tosyl-2,6-dihydrocyclopenta[*c*]pyrrol-4-yl)aniline (2al)**



## 2al

Compound **2al** was prepared in 50% yield (40.2 mg, 0.1 mmol scale) according to the general procedure except using DCE as the solvent at 40 °C. Pale yellow oil.  $[\alpha]_D^{20} = -58.2^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.4$  Hz, 2H), 7.51 (d,  $J = 8.8$  Hz, 2H), 7.26 – 7.24 (m, 2H), 7.20 (d,  $J = 1.6$  Hz, 1H), 7.06 (d,  $J = 1.2$  Hz, 1H), 6.75 (d,  $J = 8.8$  Hz, 2H), 6.39 (d,  $J = 2.4$  Hz, 1H), 5.34 (d,  $J = 4.8$  Hz, 1H), 4.42 (dd,  $J = 15.0, 7.4$  Hz, 1H), 3.74 – 3.54 (m, 2H), 3.53 – 3.28 (m, 3H), 3.24 – 3.12 (m, 1H), 3.00 (s, 6H), 2.43 – 2.35 (m, 4H), 2.32 – 2.18 (m, 1H), 2.07 – 1.84 (m, 5H), 1.82 – 1.68 (m, 3H), 1.65 – 1.42 (m, 9H), 1.35 – 1.26 (m, 3H), 1.22 – 1.10 (m, 2H), 1.06 (s, 3H), 1.01 – 0.95 (m, 4H), 0.94 – 0.84 (m, 2H), 0.81 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  150.3, 144.5, 140.9, 138.3, 137.2, 136.5, 136.4, 130.0, 129.8, 127.2, 126.7, 122.5, 121.3, 113.5, 112.2, 109.3, 80.8, 79.4, 69.8, 66.8, 62.1, 56.5, 50.1, 44.7, 41.6, 40.4, 40.2, 39.8, 39.2, 37.2, 37.0, 32.1, 31.8, 31.4(1), 31.3(6), 30.3, 28.8, 28.5, 21.5, 20.8, 19.4, 17.1, 16.3, 14.5; IR (neat): 2928, 2274, 2130, 1666, 1609, 1566, 1364, 1260, 1184, 1042, 677, 612, 561; HRESIMS Calcd for  $[\text{C}_{50}\text{H}_{64}\text{N}_2\text{NaO}_5\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 827.4428, found 827.4438.

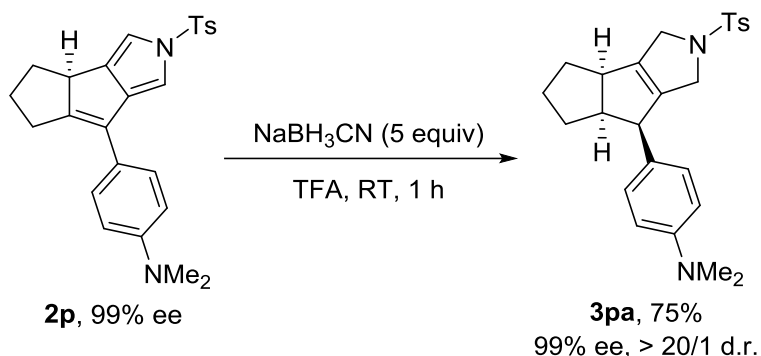
### (3b*R*,6a*S*,7*R*)-7-(4-methoxyphenyl)-2-tosyl-2,3,3b,4,5,6,6a,7-octahydro-1*H*-pentaleno[1,2-*c*]pyrrole (3aa)



Compound **3aa** was prepared in 90% yield (73.5 mg) according to the known procedure (0.2 mmol scale).<sup>7</sup> Pale yellow oil.  $[\alpha]_D^{20} = -27.9^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 92% ee (determined by HPLC: Chiralpak ADH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 18.96 min (minor), 30.51 min (major)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 8.4$  Hz, 2H), 7.34 (d,  $J = 8.0$  Hz, 2H), 6.79 – 6.75 (m, 4H), 4.22 – 4.14 (m, 1H), 4.07 – 3.84 (m, 3H), 3.78 (s, 3H), 3.78 – 3.71 (m, 1H), 3.28 – 3.18 (m, 1H), 3.06 – 2.99 (m, 1H), 2.45 (s, 3H), 1.61 – 1.52 (m, 1H), 1.42 – 1.22 (m, 3H), 1.10 – 1.03 (m, 1H), 0.94 – 0.87 (m, 1H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 144.9, 143.3, 140.8, 134.5, 131.8, 129.6, 129.4,

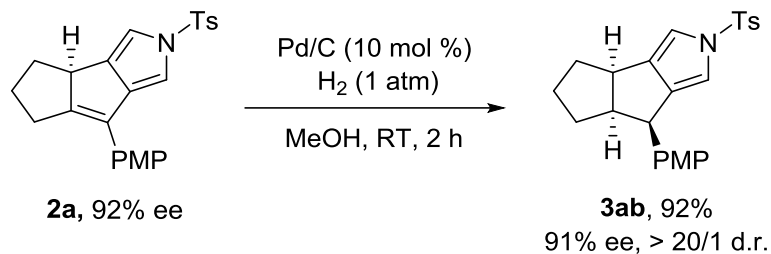
127.4, 113.5, 55.1, 52.5, 51.7, 51.6, 49.0, 45.9, 30.1, 29.0, 26.4, 21.5; IR (neat): 2942, 1672, 1541, 1340, 1251, 1122, 743, 676, 520; HRESIMS Calcd for  $[C_{24}H_{27}NNaO_3S]^+$  ( $M + Na^+$ ) 432.1604, found 432.1600.

***N,N*-dimethyl-4-((3*bR*,6*aS*,7*R*)-2-tosyl-2,3,3*b*,4,5,6,6*a*,7-octahydro-1*H*-pentaleno[1,2-*c*]pyrrol-7-yl)aniline (3*pa*)**



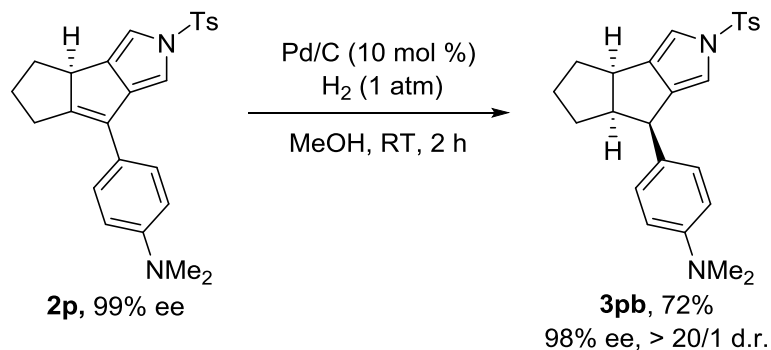
Compound **3pa** was prepared in 75% yield (63.4 mg) according to the known procedure (0.2 mmol scale)<sup>7</sup>. Pale yellow oil.  $[\alpha]_D^{20} = -39.8^\circ$  ( $c = 1.0$ , CHCl<sub>3</sub>). 99% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.31 min (major), 21.04 min (minor)). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.73 (d,  $J = 8.4$  Hz, 2H), 7.34 (d,  $J = 8.0$  Hz, 2H), 6.73 (d,  $J = 8.4$  Hz, 2H), 6.62 (d,  $J = 8.8$  Hz, 2H), 4.22 – 3.71 (m, 5H), 3.27 – 3.18 (m, 1H), 3.08 – 2.97 (m, 1H), 2.92 (s, 6H), 2.45 (s, 3H), 1.59 – 1.51 (m, 1H), 1.44 – 1.28 (m, 3H), 1.13 – 0.92 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  149.2, 144.4, 143.2, 141.3, 134.6, 129.7, 129.2, 127.7, 127.4, 112.4, 52.6, 51.8, 51.6, 49.0, 46.0, 40.6, 30.2, 29.1, 26.5, 21.5; IR (neat): 2917, 1678, 1544, 1311, 1247, 1148, 935, 744, 647, 545; HRESIMS Calcd for  $[C_{25}H_{30}N_2NaO_2S]^+$  ( $M + Na^+$ ) 445.1920, found 445.1928.

**(3*bR*,6*aS*,7*R*)-7-(4-methoxyphenyl)-2-tosyl-3*b*,4,5,6,6*a*,7-hexahydro-2*H*-pentaleno[1,2-*c*]pyrrole (3*ab*)**



Compound **3ab** was prepared in 92% yield (37.0 mg) according to the known procedure (0.1 mmol scale)<sup>8</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -68.1$  (c = 1.0,  $\text{CHCl}_3$ ). 91% ee (determined by HPLC: Chiralpak ASH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.40 min (major), 15.53 min (minor)). <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.4$  Hz, 2H), 7.27 (d,  $J = 8.0$  Hz, 2H), 7.13 (d,  $J = 8.4$  Hz, 2H), 6.86 – 6.75 (m, 4H), 4.39 (d,  $J = 8.0$  Hz, 1H), 3.79 (s, 3H), 3.43 – 3.35 (m, 1H), 3.23 – 3.12 (m, 1H), 2.40 (s, 3H), 2.01 – 1.94 (m, 1H), 1.68 – 1.63 (m, 1H), 1.48 – 1.32 (m, 2H), 1.15 – 0.94 (m, 2H); <sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 144.4, 141.4, 137.2, 136.6, 133.0, 129.8, 129.1, 126.7, 113.5, 112.4, 57.0, 55.2, 45.9, 42.3, 33.1, 28.6, 26.6, 21.5; IR (neat): 2914, 1672, 1540, 1372, 1171, 1027, 810, 671, 610, 572; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{25}\text{NNaO}_3\text{S}]^+$  (M +  $\text{Na}^+$ ) 430.1447, found 430.1447.

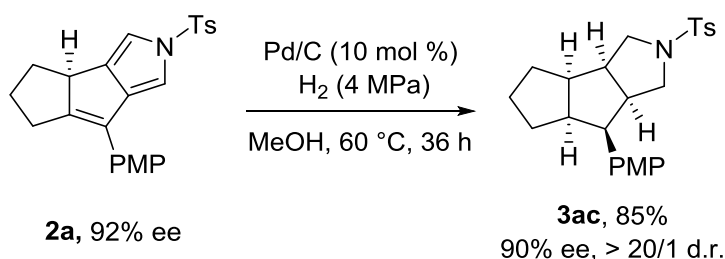
***N,N*-dimethyl-4-((3*bR*,6*aS*,7*R*)-2-tosyl-3*b*,4,5,6,6*a*,7-hexahydro-2*H*-pentaleno[1,2-*c*]pyrrol-7-yl)aniline (3*pb*)**



Compound **3pb** was prepared in 72% yield (30.3 mg) according to the known procedure (0.1 mmol scale)<sup>8</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -77.5$  (c = 1.0,  $\text{CHCl}_3$ ). 98% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.24 min (major), 11.19 min (minor)). <sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.0$  Hz, 2H), 7.27 (d,  $J = 9.2$  Hz, 2H), 7.09 (d,  $J = 8.8$  Hz, 2H), 6.79 (d,  $J = 8.4$  Hz, 2H), 6.69 (d,  $J =$

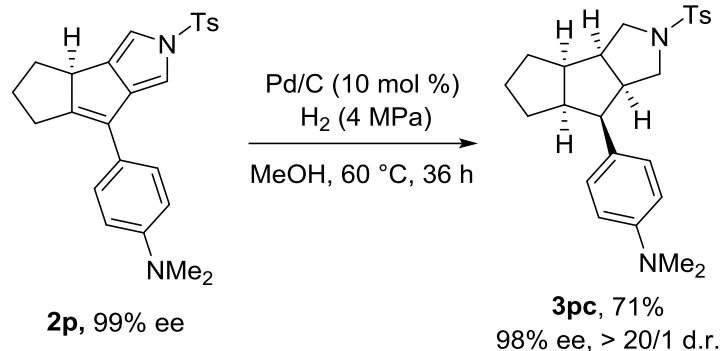
8.8 Hz, 2H), 4.36 (d,  $J = 8.0$  Hz, 1H), 3.43 – 3.33 (m, 1H), 3.22 – 3.12 (m, 1H), 2.93 (s, 6H), 2.40 (s, 3H), 2.03 – 1.94 (m, 1H), 1.70 – 1.65 (m, 1H), 1.46 – 1.33 (m, 2H), 1.17 – 1.00 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.1, 144.4, 141.5, 137.7, 136.6, 129.8, 128.8, 126.7, 113.6, 112.7, 112.3, 57.1, 45.9, 42.3, 40.9, 33.2, 28.6, 26.6, 21.6; IR (neat): 2956, 1633, 1544, 1342, 1174, 1020, 971, 847, 641, 571; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{28}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 443.1764, found 443.1768.

**(3aR,3bR,6aS,7S,7aS)-7-(4-methoxyphenyl)-2-tosyldecahydro-1H-pentaleno[1,2-c]pyrrole (3ac)**



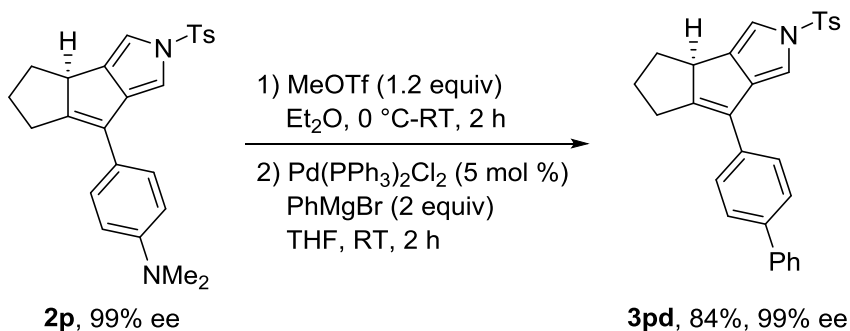
Compound **3ac** was prepared in 85% yield (35.0 mg) according to the known procedure (0.1 mmol scale)<sup>8</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -27.1$  °( $c = 1.0$ ,  $\text{CHCl}_3$ ). 90% ee (determined by HPLC: Chiralpak ADH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.04 min (minor), 16.38 min (major)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 7.6$  Hz, 2H), 7.14 – 7.08 (m, 2H), 6.87 – 6.81 (m, 2H), 3.80 (s, 3H), 3.51 – 3.46 (m, 1H), 3.45 – 3.37 (m, 2H), 3.26 – 3.11 (m, 2H), 3.09 – 2.87 (m, 2H), 2.84 – 2.66 (m, 2H), 2.43 (s, 3H), 1.78 – 1.67 (m, 1H), 1.67 – 1.61 (m, 1H), 1.57 – 1.52 (m, 1H), 1.38 – 1.28 (m, 2H), 1.19 – 1.04 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.6, 143.3, 133.6, 133.3, 129.5, 129.3, 127.6, 113.6, 55.2, 49.9, 49.8, 49.7, 48.5, 47.3, 45.7, 45.0, 30.8, 28.1, 27.8, 21.5; IR (neat): 2925, 1610, 1540, 1341, 1104, 1031, 875, 695, 646, 520; HRESIMS Calcd for  $[\text{C}_{24}\text{H}_{29}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 434.1760, found 434.1755.

***N,N*-dimethyl-4-((3aR,3bR,6aS,7S,7aS)-2-tosyldecahydro-1H-pentaleno[1,2-c]pyrrol-7-yl)aniline (3pc)**



Compound **3pc** was prepared in 71% yield (30.1 mg) according to the known procedure (0.1 mmol scale)<sup>8</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -78.9^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 98% ee (determined by HPLC: Chiralpak IC Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 25.28 min (major), 34.27 min (minor)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.30 (d,  $J = 8.0$  Hz, 2H), 7.07 (d,  $J = 8.4$  Hz, 2H), 6.68 (d,  $J = 8.8$  Hz, 2H), 3.49 – 3.35 (m, 3H), 3.26 – 3.13 (m, 2H), 3.05 – 2.96 (m, 1H), 2.92 (s, 6H), 2.91 – 2.84 (m, 1H), 2.80 – 2.60 (m, 2H), 2.42 (s, 3H), 1.78 – 1.50 (m, 4H), 1.37 – 1.27 (m, 1H), 1.21 – 1.08 (m, 1H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.7, 143.2, 133.6, 129.5, 129.1, 129.0, 127.5, 112.6, 49.9, 49.8, 49.7, 48.6, 47.1, 45.6, 44.9, 40.7, 30.9, 28.1, 27.8, 21.5; IR (neat): 2926, 2874, 1634, 1522, 1345, 1114, 1067, 978, 823, 696, 522; HRESIMS Calcd for  $[\text{C}_{25}\text{H}_{32}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 447.2077, found 447.2078.

**(*R*)-7-([1,1'-biphenyl]-4-yl)-2-tosyl-3b,4,5,6-tetrahydro-2*H*-pentaleno[1,2-*c*]pyrrole (3pd)**

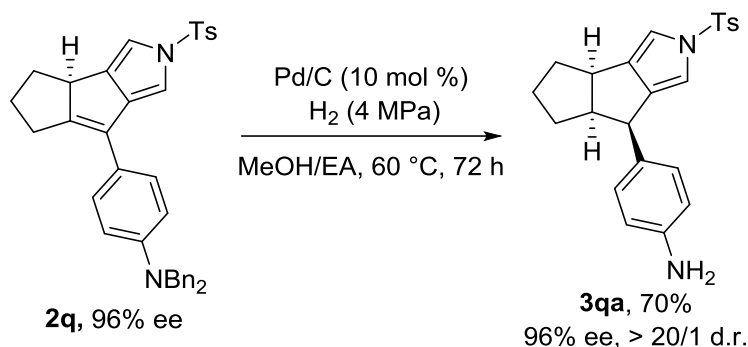


Compound **3pd** was prepared in 84% yield (37.9 mg) according to the known procedure (0.1 mmol scale)<sup>9</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -102.4^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 99% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.61 min (minor), 15.83 min (major)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H),



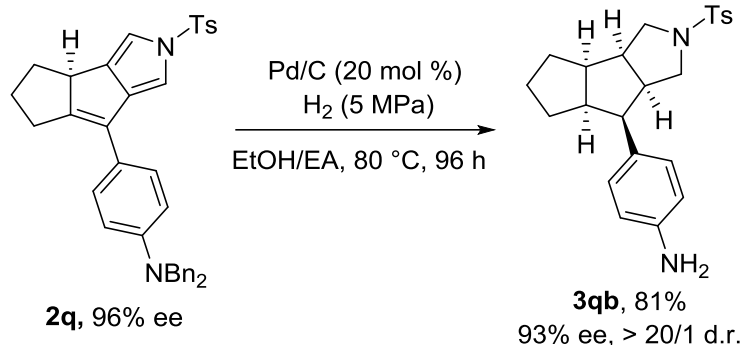
7.67 – 7.56 (m, 6H), 7.49 – 7.42 (m, 2H), 7.38 – 7.34 (m, 1H), 7.26 (d,  $J = 9.2$  Hz, 2H), 7.15 – 6.98 (m, 2H), 3.66 – 3.58 (m, 1H), 2.82 – 2.72 (m, 1H), 2.55 – 2.43 (m, 1H), 2.37 (s, 3H), 2.29 – 2.06 (m, 3H), 1.14 – 1.01 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.1, 144.5, 141.2, 140.7, 139.8, 136.5, 134.8, 133.7, 129.8, 128.8, 127.7, 127.6, 127.3, 127.1, 127.0, 126.7, 113.3, 108.0, 49.9, 29.6, 27.8, 25.2, 21.5; IR (neat): 2934, 1704, 1623, 1525, 1375, 1189, 1013, 934, 835, 676, 511; HRESIMS Calcd for  $[\text{C}_{29}\text{H}_{25}\text{NNaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 474.1498, found 474.1490.

**4-((3bR,6aS,7R)-2-tosyl-3b,4,5,6,6a,7-hexahydro-2H-pentaleno[1,2-c]pyrrol-7-yl)aniline (3qa)**



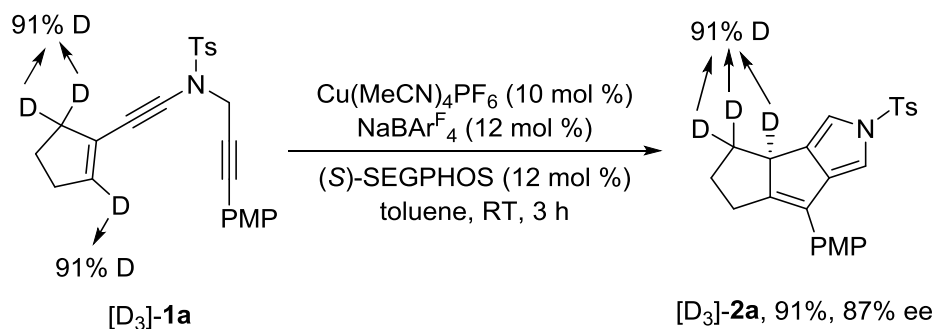
Compound **3qa** was prepared in 70% yield (27.4 mg) according to the known procedure (0.1 mmol scale)<sup>8,10</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -48.2^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 96% ee (determined by HPLC: Chiralpak ASH Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 13.87 min (major), 29.47 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 8.0$  Hz, 2H), 7.27 (d,  $J = 8.4$  Hz, 2H), 7.00 (d,  $J = 8.4$  Hz, 2H), 6.79 (d,  $J = 10.8$  Hz, 2H), 6.62 (d,  $J = 8.0$  Hz, 2H), 4.34 (d,  $J = 7.6$  Hz, 1H), 3.42 – 3.33 (m, 1H), 3.21 – 3.09 (m, 1H), 2.40 (s, 3H), 2.02 – 1.94 (m, 1H), 1.65 – 1.60 (m, 1H), 1.46 – 1.35 (m, 2H), 1.11 – 0.98 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.4, 141.5, 137.5, 136.6, 131.0, 129.8, 129.0, 126.7, 115.0, 113.5, 112.3, 57.0, 46.0, 42.3, 33.2, 28.6, 26.6, 21.6; IR (neat): 3474 (br), 2913, 1635, 1556, 1487, 1367, 1214, 1055, 931, 887, 642, 574; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{24}\text{N}_2\text{NaO}_2\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 415.1451, found 415.1457.

**4-((3aR,3bR,6aS,7S,7aS)-2-tosyldecahydro-1H-pentaleno[1,2-c]pyrrol-7-yl)aniline (3qb)**



Compound **3qb** was prepared in 81% yield (32.0 mg) according to the known procedure (0.1 mmol scale)<sup>8,10</sup>. Pale yellow oil.  $[\alpha]_{\text{D}}^{20} = -79.2^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 93% ee (determined by HPLC: Chiralpak IC Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 32.45 min (major), 44.83 min (minor)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 8.0$  Hz, 2H), 7.31 (d,  $J = 8.0$  Hz, 2H), 6.98 (d,  $J = 8.0$  Hz, 2H), 6.63 (d,  $J = 8.4$  Hz, 2H), 3.60 (s, 2H), 3.49 – 3.34 (m, 3H), 3.23 – 3.06 (m, 2H), 3.06 – 2.83 (m, 2H), 2.79 – 2.63 (m, 2H), 2.42 (s, 3H), 1.75 – 1.65 (m, 3H), 1.41 – 1.30 (m, 2H), 1.17 – 1.06 (m, 1H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.3, 133.7, 131.2, 129.5, 129.2, 127.5, 115.1, 49.9, 49.8, 49.7, 48.5, 47.3, 45.6, 45.0, 30.8, 28.1, 27.8, 21.5; IR (neat): 3470 (br), 2934, 1634, 1551, 1486, 1345, 1274, 1051, 928, 874, 633, 577; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{28}\text{N}_2\text{NaO}_2\text{S}]^+$  (M +  $\text{Na}^+$ ) 419.1764, found 419.1763.

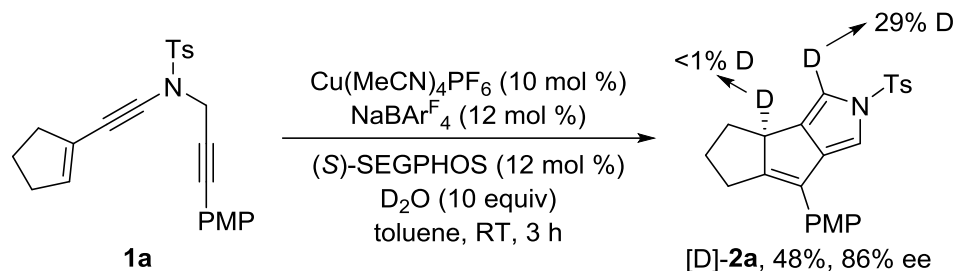
**[D<sub>3</sub>]-2a (91% D)**



$[\alpha]_{\text{D}}^{20} = -69.0^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 87% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.33 min (major), 23.72 min (minor)).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.45 (d,  $J = 8.8$  Hz, 2H), 7.28 – 7.22 (m, 2H), 7.08 – 7.03 (m, 1H), 6.98 – 6.93 (m, 3H), 3.83 (s, 3H), 3.57 – 3.53 (m, 0.09H), 2.77 – 2.64 (m, 1H), 2.46 – 2.40 (m, 1H), 2.37 (s, 3H), 2.23 – 2.13 (m, 2H), 2.06

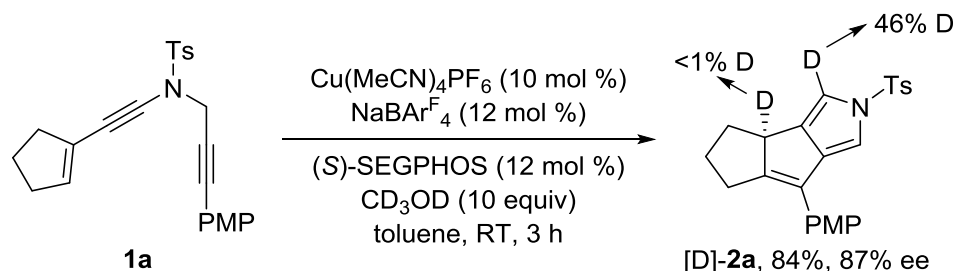
– 2.04 (m, 0.09H), 1.05 – 1.00 (m, 0.09H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.7, 157.8, 144.4, 141.5, 136.5, 134.9, 129.8, 128.4, 127.4, 126.7, 113.9, 113.2, 107.8, 55.3, 29.4, 25.0, 21.5.

[D]-2a (29% D)



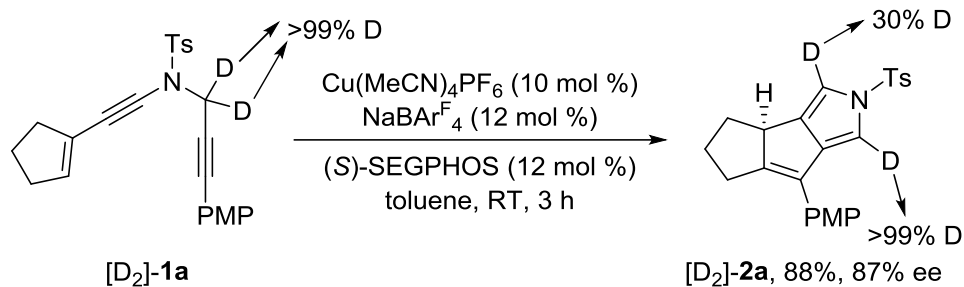
$[\alpha]_{\text{D}}^{20} = -67.5^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 86% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.76 min (major), 24.66 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 – 7.72 (m, 2H), 7.48 – 7.42 (m, 2H), 7.26 – 7.23 (m, 2H), 7.06 – 7.02 (m, 1H), 6.99 – 6.96 (m, 0.71H), 6.96 – 6.92 (m, 2H), 3.84 (s, 3H), 3.61 – 3.53 (m, 1H), 2.76 – 2.66 (m, 1H), 2.46 – 2.39 (m, 1H), 2.37 (s, 3H), 2.25 – 2.04 (m, 3H), 1.09 – 1.01 (m, 1H).

[D]-2a (46% D)



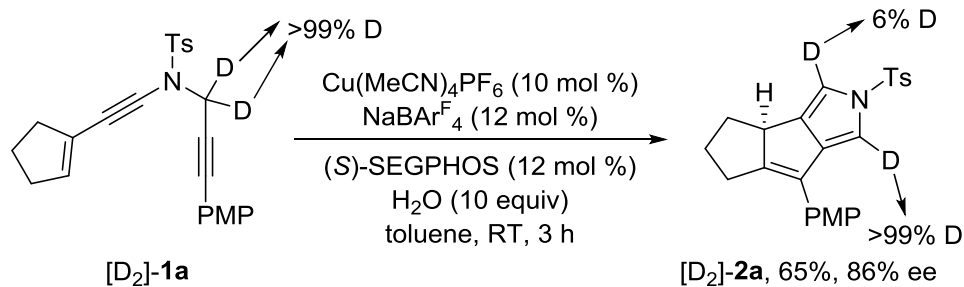
$[\alpha]_{\text{D}}^{20} = -69.5^\circ$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ). 87% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.73 min (major), 24.54 min (minor)).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.45 (d,  $J = 8.8$  Hz, 2H), 7.25 (d,  $J = 6.0$  Hz, 2H), 7.06 – 7.03 (m, 1H), 6.98 – 6.92 (m, 2.54H), 3.84 (s, 3H), 3.60 – 3.52 (m, 1H), 2.76 – 2.66 (m, 1H), 2.46 – 2.39 (m, 1H), 2.37 (s, 3H), 2.25 – 2.03 (m, 3H), 1.11 – 0.97 (m, 1H).

[D<sub>2</sub>]-**2a** (30% D)



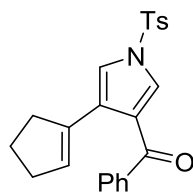
$[\alpha]_{\text{D}}^{20} = -70.2^\circ (c = 1.0, \text{CHCl}_3)$ . 87% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.73 min (major), 24.53 min (minor)).  
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.75 (d,  $J = 8.5$  Hz, 2H), 7.48 – 7.42 (m, 2H), 7.25 (d,  $J = 7.0$  Hz, 2H), 6.97 (d,  $J = 1.5$  Hz, 0.7H), 6.96 – 6.91 (m, 2H), 3.83 (s, 3H), 3.60 – 3.52 (m, 1H), 2.75 – 2.65 (m, 1H), 2.45 – 2.38 (m, 1H), 2.36 (s, 3H), 2.25 – 2.14 (m, 2H), 2.12 – 2.05 (m, 1H), 1.09 – 0.98 (m, 1H).

[D<sub>2</sub>]-**2a** (6% D)



$[\alpha]_{\text{D}}^{20} = -68.2^\circ (c = 1.0, \text{CHCl}_3)$ . 86% ee (determined by HPLC: Chiralpak ASH Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.15 min (major), 23.39 min (minor)).  
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.75 (d,  $J = 8.5$  Hz, 2H), 7.45 (d,  $J = 8.5$  Hz, 2H), 7.25 (d,  $J = 6.0$  Hz, 2H), 6.97 (d,  $J = 1.5$  Hz, 0.94H), 6.96 – 6.91 (m, 2H), 3.84 (s, 3H), 3.61 – 3.54 (m, 1H), 2.76 – 2.66 (m, 1H), 2.46 – 2.40 (m, 1H), 2.38 (s, 3H), 2.27 – 2.16 (m, 2H), 2.13 – 2.05 (m, 1H), 1.09 – 0.99 (m, 1H).

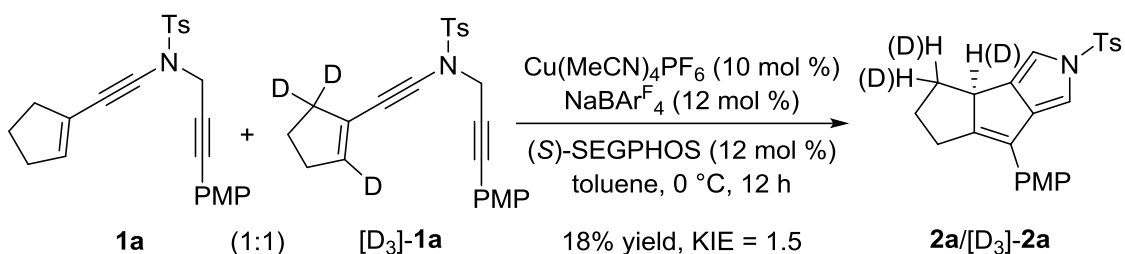
**2u'** (4-(cyclopent-1-en-1-yl)-1-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone



**2u'**

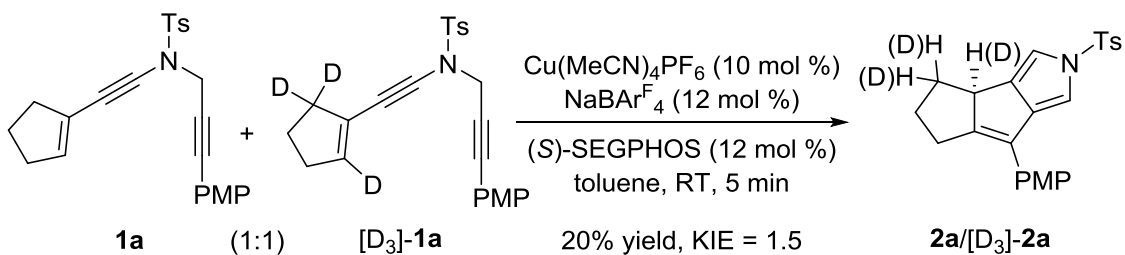
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 – 7.81 (m, 4H), 7.62 – 7.56 (m, 1H), 7.50 – 7.44 (m, 2H), 7.40 (d,  $J = 2.4$  Hz, 1H), 7.33 (d,  $J = 8.0$  Hz, 2H), 7.13 (d,  $J = 2.4$  Hz, 1H), 6.09 – 6.06 (m, 1H), 2.59 – 2.51 (m, 2H), 2.46 – 2.36 (m, 5H), 1.96 – 1.84 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  191.4, 145.8, 138.5, 135.0, 133.4, 132.8, 130.2, 129.9, 129.6, 128.3, 127.1, 126.7, 126.1, 125.9, 118.8, 34.8, 33.4, 22.9, 21.6; IR (neat): 2914, 1701(s), 1654, 1523, 1422, 1317, 1227, 1051, 971, 877; HRESIMS Calcd for  $[\text{C}_{23}\text{H}_{21}\text{NNaO}_3\text{S}]^+$  ( $\text{M} + \text{Na}^+$ ) 414.1134, found 414.1137.

**2a**/ $[\text{D}_3]$ -**2a** (41% D)



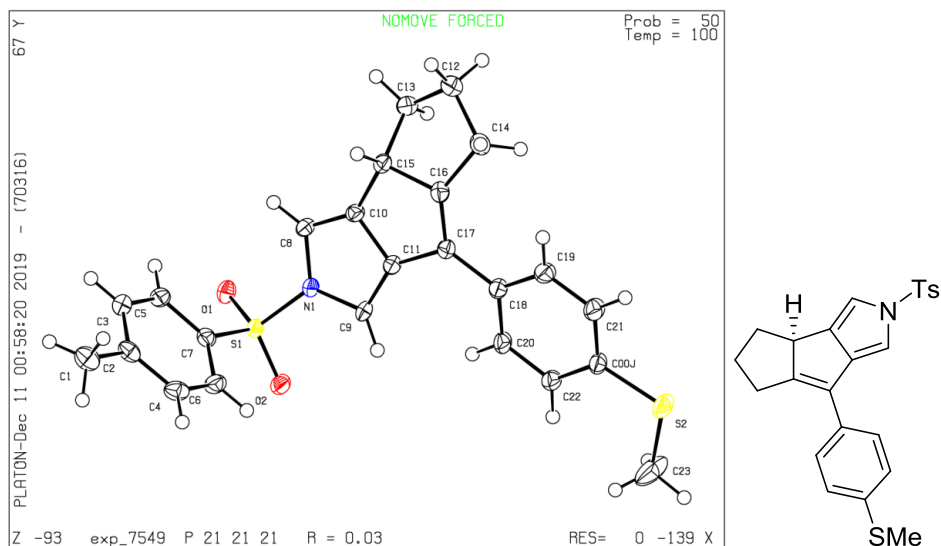
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.5$  Hz, 2H), 7.47 – 7.41 (m, 2H), 7.25 (d,  $J = 6.0$  Hz, 2H), 7.08 – 6.91 (m, 4H), 3.84 (s, 3H), 3.60 – 3.53 (m, 0.59H), 2.76 – 2.67 (m, 1H), 2.47 – 2.40 (m, 1H), 2.38 (s, 3H), 2.25 – 2.16 (m, 2H), 2.11 – 2.08 (m, 0.59H), 1.10 – 1.00 (m, 0.59H).

**2a**/ $[\text{D}_3]$ -**2a** (40% D)



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.5$  Hz, 2H), 7.48 – 7.42 (m, 2H), 7.25 (d,  $J = 6.0$  Hz, 2H), 7.08 – 6.91 (m, 4H), 3.84 (s, 3H), 3.61 – 3.53 (m, 0.6H), 2.75 – 2.66 (m, 1H), 2.46 – 2.39 (m, 1H), 2.38 (s, 3H), 2.25 – 2.15 (m, 2H), 2.11 – 2.05 (m, 0.6H), 1.08 – 1.00 (m, 0.6H).

Crystal data and structure refinement for **2s**. CCDC Number = 2046032.



Bond precision: C-C = 0.0034 Å

Wavelength=1.54184

Cell: a=5.24790 (4) b=18.15502 (12) c=21.35505 (16)

alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2034.62 (3)	2034.62 (3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C24 H23 N O2 S2	C24 H23 N O2 S2
Sum formula	C24 H23 N O2 S2	C24 H23 N O2 S2
Mr	421.55	421.55
Dx, g cm <sup>-3</sup>	1.376	1.376
Z	4	4
Mu (mm <sup>-1</sup> )	2.535	2.535
F000	888.0	888.0
F000'	892.83	
h, k, lmax	6, 22, 26	6, 21, 25
Nref	3905 [ 2290]	3781
Tmin, Tmax	0.859, 0.881	0.534, 1.000
Tmin'	0.776	

Correction method= # Reported T Limits: Tmin=0.534 Tmax=1.000  
AbsCorr = MULTI-SCAN

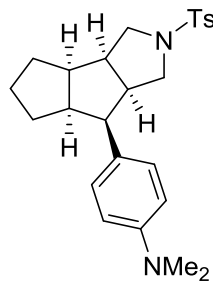
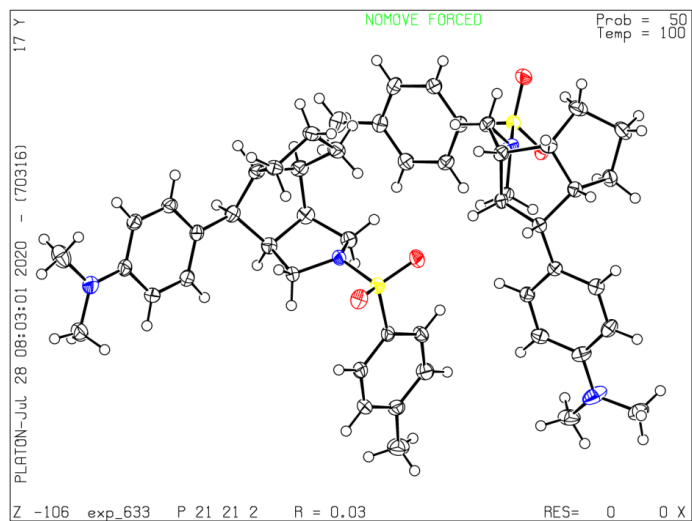
Data completeness= 1.65/0.97 Theta (max)= 70.570

R(reflections)= 0.0281( 3719) wR2(reflections)= 0.0745( 3781)

S = 1.040

Npar= 264

Crystal data and structure refinement for **3pc**. CCDC Number = 2046033.



Bond precision: C-C = 0.0030 Å

Wavelength=1.54184

Cell: a=24.65475 (12)

b=20.81653 (9)

c=8.55464 (4)

alpha=90

beta=90

gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4390.47 (4)	4390.47 (4)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> S	2 (C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> S)
Sum formula	C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> S	C <sub>50</sub> H <sub>65</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub>
Mr	424.59	850.18
Dx, g cm <sup>-3</sup>	1.285	1.286
Z	8	4
Mu (mm <sup>-1</sup> )	1.493	1.493
F000	1824.0	1828.0
F000'	1831.31	
h, k, lmax	29, 25, 10	29, 25, 10
Nref	8257 [ 4638]	7983
Tmin, Tmax	0.861, 0.928	0.477, 1.000
Tmin'	0.861	

Correction method= # Reported T Limits: Tmin=0.477 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.97

Theta(max)= 69.478

R(reflections)= 0.0270 ( 7804)

wR2(reflections)= 0.0707 ( 7983)

S = 0.983

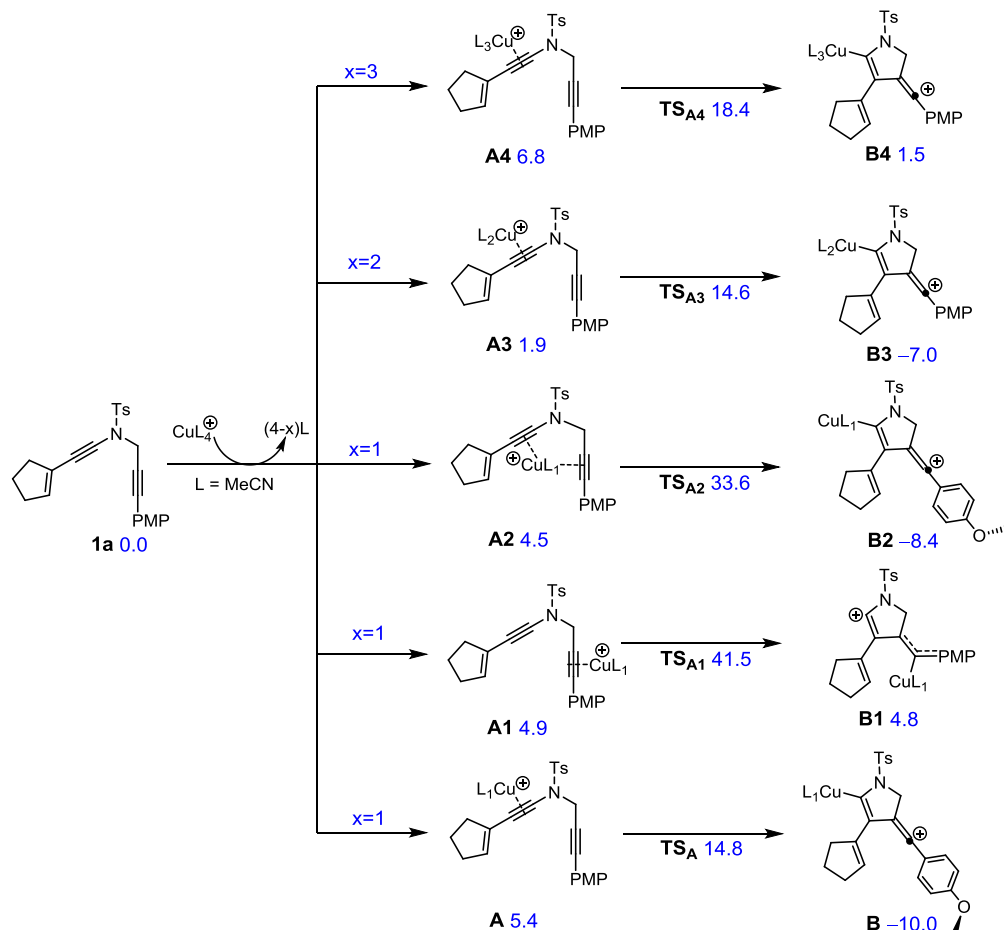
Npar= 547



## Computational Methods.

All calculations were performed using Gaussian 09 package.<sup>11</sup> Geometry optimizations and vibration frequencies were calculated by using M06<sup>12</sup> level of density function theory with the LANL2DZ basis set<sup>13-14</sup> and pseudopotential for the Cu atom, and the 6-31G(d,p)<sup>15-16</sup> for C, H, O, N, P and S atom. All local minimums were confirmed with no imaginary frequency and all transition states had only one imaginary frequency. And every transition state was checked by intrinsic reaction coordinate (IRC). Single-point energies of the transition states [CuL8]-R TS<sub>B</sub> and [CuL8]-S TS<sub>B</sub> that are related to enantioselectivity were further computed at the M06-D3/def2TZVP<sup>17</sup> level of theory. The SMD<sup>18</sup> solvation model with toluene or DCE was used for all calculations. The ball stick models of molecules were drawn by CYLview 2.0.<sup>19</sup>

## S1. Effects of ligand coordination number on the achiral Cu(I) catalysis



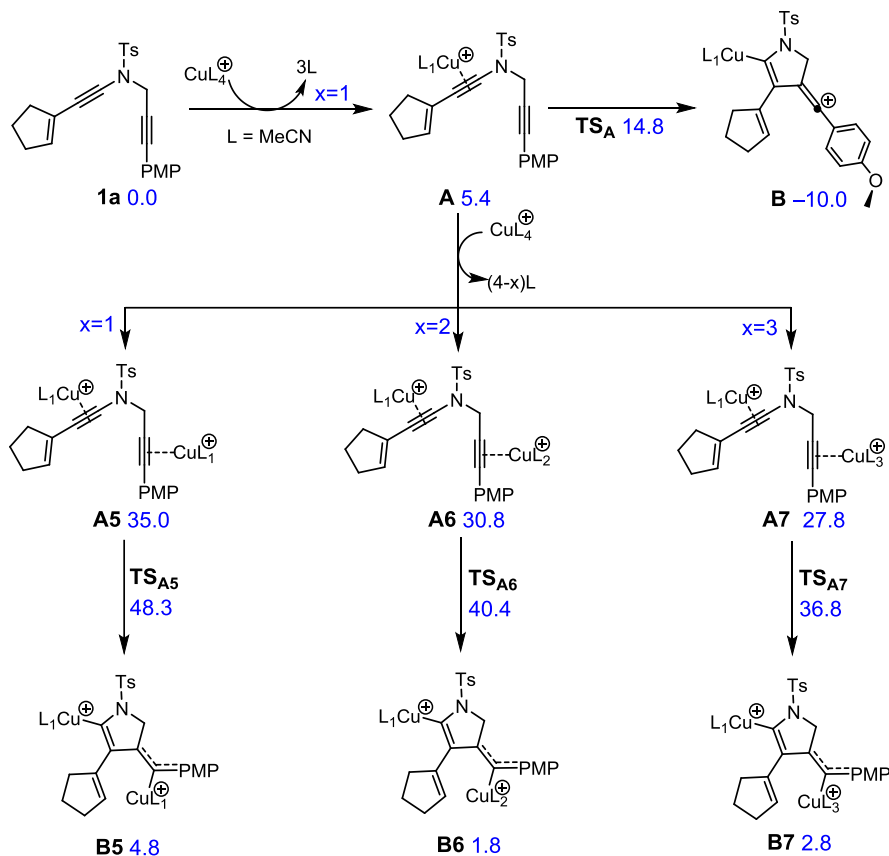
Supplementary Figure 6. Relative free energies (ΔG, in kcal/mol) of the Cu(I)-bound

precursors with different number of L ligands (L= MeCN), the transition states and intermediates of the first cyclization step induced by Cu(I) coordination from SMD(toluene)-M06/6-31G(d,p)&LANL2DZ computations.

The pristine Cu(I) species is  $[\text{Cu}(\text{L})_4]^+$  containing the achiral ligand  $\text{L}=\text{CH}_3\text{CN}$ . Upon coordination of Cu(I) to the ynamide or N-propargyl group (**Supplementary Figure 6**), the most stable Cu(I)-binding precursor is **A3** with the Cu(I) species being preferentially attached to the electron-rich ynamide  $\text{C}\equiv\text{C}$  bond, following which the subsequent cyclization has the lowest activation barrier (14.6 kcal/mol with respect to **1a**) with formation of the vinyl-cation intermediate **B3**. In such intramolecular cyclization step **A3**  $\rightarrow$  **B3** the Cu(I) center has two L ligands attached. In case that only one L ligand is attached onto the Cu(I) center, such intramolecular cyclization, i.e., **A**  $\rightarrow$  **B**, gives similar value of activation barrier (14.8 kcal/mol with respect **1a**), and the formed vinyl-cation **B** is even by 3.0 kcal/mol lower than **B3** in free energy. Accordingly, it is reasonable to assume that the catalytic Cu(I) species has one L ligand attached in the subsequent steps involving Cu(I)-C bonding.

Furthermore, it is noteworthy that the intramolecular cyclization, **A1**  $\rightarrow$  **B1**, initiated by Cu(I)-activated  $\text{C}\equiv\text{C}$  bond of the *N*-propargyl suffers a high activation barrier (41.5 kcal/mol with respect to **1a**) and the formed vinyl-cation intermediate **B1** is quite higher in free energy than **B**.

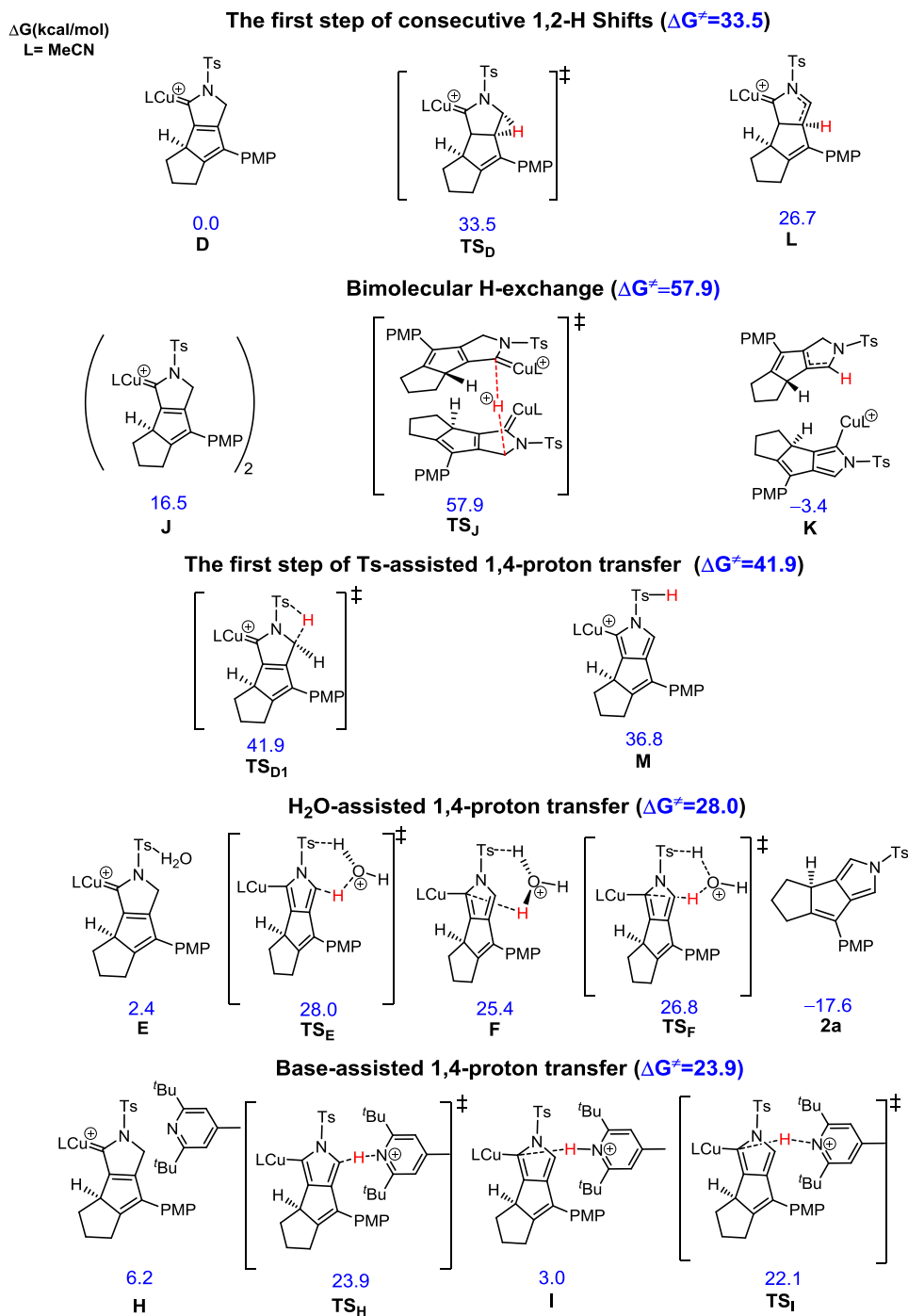
## S2. single-copper catalysis vs. dual-copper catalysis



**Supplementary Figure 7.** Initiation of intramolecular cyclization in single-copper catalysis and dual-copper catalysis. Relative free energies ( $\Delta G$ , in kcal/mol) were computed at the SMD(toluene)-M06/6-31G(d,p)&LANL2DZ level of theory.

As the substrate has two  $\text{C}\equiv\text{C}$  bonds both capable of forming dative bond with Cu(I) species, the possibility of dual-copper catalysis should be considered and compared with single-copper catalysis. However, our DFT computations (**Supplementary Figure 7**) disclosed that that dual-copper catalysis is unlikely to occur. First, formation of the precursors (**A5-A7**) for dual-copper catalysis are predicted to be highly unfavorable in free energy change. Second, the transition states ( $\text{TS}_{A5}$ - $\text{TS}_{A7}$ ) of intramolecular cyclization in the dual-copper catalysis are by at least 36.8 kcal/mole higher than the isolated reactants in free energy. Third, the as-formed intermediates **B5-B7** are by at least 11.8 kcal/mol higher in free energy than the vinyl-cation intermediate **B** in single-copper catalysis.

### S3. Possible mechanisms for [1,4]-H shift within the intermediate D



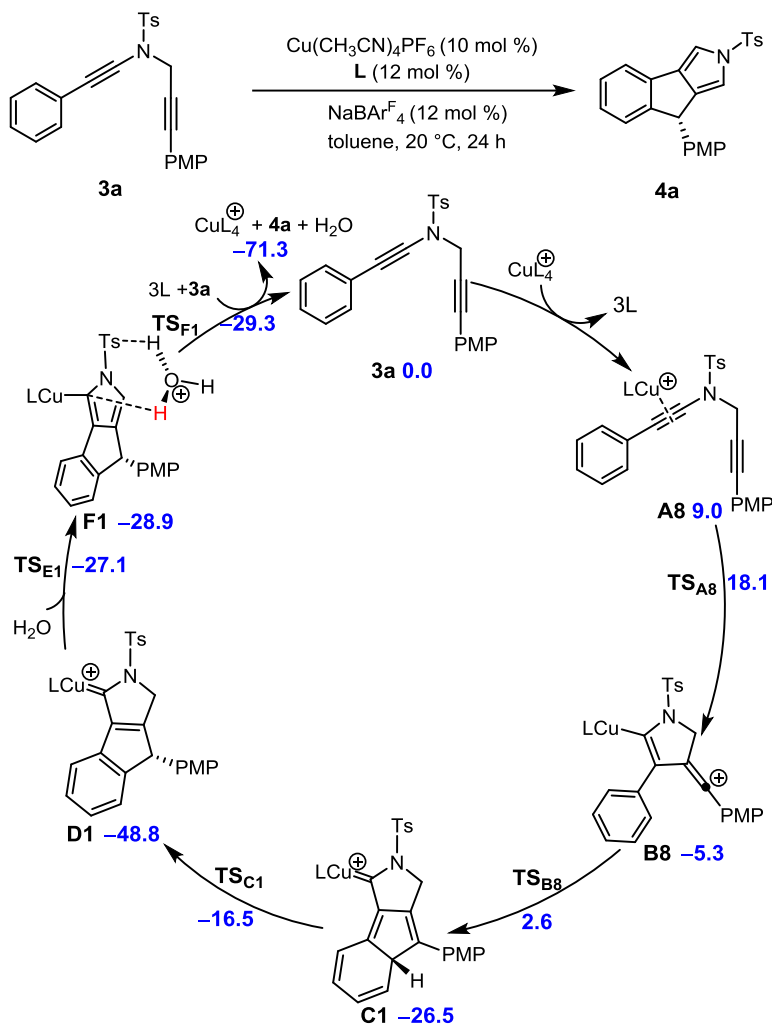
**Supplementary Figure 8.** Possible mechanisms for the [1,4]-H shift within the intermediate **D**. Relative free energies ( $\Delta G$ , in kcal/mol) were computed at the SMD(toluene)-M06/6-31G(d,p)&LANL2DZ level of theory.

Possible mechanisms concerned for the [1,4]-H shift within the intermediate **D** include consecutive [1,2]-H shifts, bimolecular H-exchange, Ts-assisted 1,4-proton transfer, H<sub>2</sub>O-assisted 1,4-proton transfer, and base-assisted 1,4-proton transfer (**Supplementary Figure 8**).

For the consecutive [1,2]-H shifts over the N-heterocycle, the first step (**D**→**L**) is predicted to be highly endothermic with a free energy change of 26.7 kcal/mol and a high activation barrier of 33.5 kcal/mol. The bimolecular H-exchange is even worse, suffering a very high activation barrier of 57.9 kcal/mol in free energy. The Ts group may work as H-bond acceptor and assist the 1,4-proton transfer. However, the Ts-assisted 1,4-proton transfer is stepwise and also suffers a high activation barrier of 41.9 kcal/mol and a highly unstable Ts-protonated intermediate **M**. As the experiments were performed in open air, it is likely that H<sub>2</sub>O may be involved in the reaction and facilitate the proton transfer process. Indeed, the H<sub>2</sub>O-assisted proton transfer is found to be stepwise via an intermediate **F** with a slightly lower activation barrier (28.0 kcal/mol). The use of a hindered base, 2,6-di-*tert*-butyl-4-methylpyridine, lowers the activation barrier by 4.1 kcal/mol and the relative energy of the protonated intermediate (**I**) by over 20.0 kcal/mol. It should be noted that the 1,4-proton transfer assisted by H<sub>2</sub>O or organic base is rate-limiting for the whole process. In accordance with such theoretical prediction, complementary experiments did disclose that the use of the organic base as additive accelerates the catalytic process significantly.

#### S4. Revised mechanism for Cu-catalyzed synthesis of 4a/6a from diyne substrate

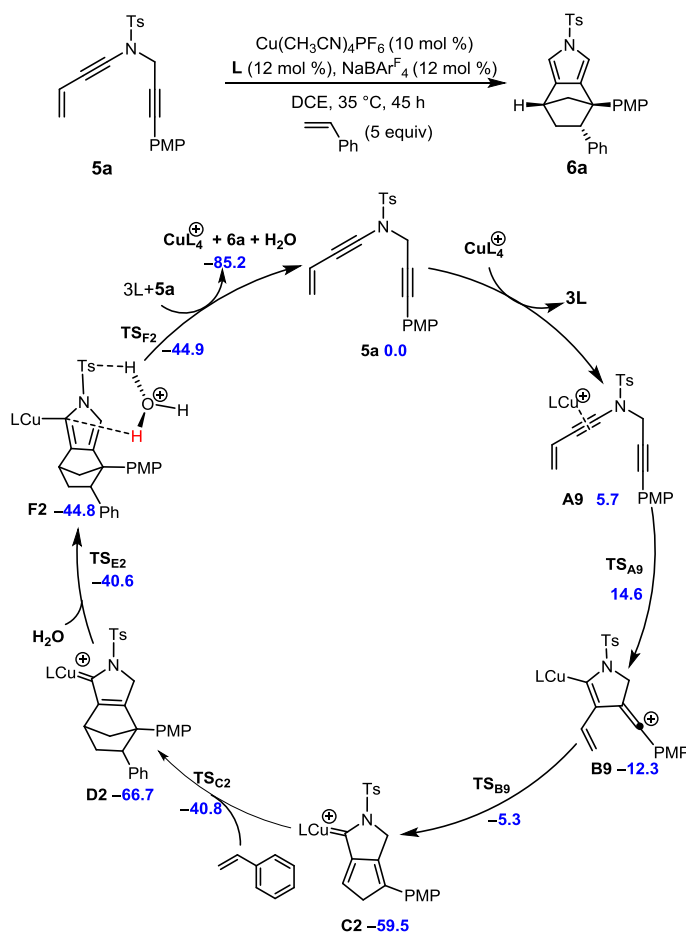
3a/5a<sup>4,20</sup>



**Supplementary Figure 9.** Revised mechanism for the synthesis of **4a** (L = MeCN) from diyne substrate **3a**. Relative free energies ( $\Delta G$ , in kcal/mol) of the key intermediates and transition states are calculated at the SMD(toluene)-M06/6-31G(d,p)&LANL2DZ level of theory at 298 K.

Our DFT computations disclosed that the mechanism for Cu(I)-catalyzed synthesis of tricyclic pyrrole **4a** from *N*-propargyl ynamide **3a**<sup>4</sup> (**Supplementary Figure 9**) is quite similar to that for the synthesis of **2a** from **1a**, i.e., preferential coordination and activation of the electron-rich amide-tethered C $\equiv$ C bonds to Cu(I) catalyst, intramolecular cyclization due to electrophilic attack of the copper-activated C $\equiv$ C bonds

to the *N*-propargyl moiety to give the vinyl-cation intermediate **B8**, intramolecular cyclization due to electrophilic addition of the vinyl-cation to the phenyl group to form the cyclopentadiene intermediate **C1**, a normal suprafacial [1,5]-H shift within the cyclopentadienic ring, H<sub>2</sub>O-assisted 1,4-proton transfer with the N-heterocycle, and a final demetallation to afford **4a**. The computed activation barrier in free energy is 9.1 kcal/mol for the formation of vinyl-cation, 7.8 kcal/mol for the electrophilic addition of vinyl-cation, 10.0 kcal/mol for the suprafacial 1,5-H shift step, and 21.7 kcal/mol for the H<sub>2</sub>O-assisted 1,4-proton transfer. As such, the whole process can occur smoothly with the H<sub>2</sub>O-assisted 1,4-proton transfer being rate determining.



**Supplementary Figure 10.** Revised mechanism for the formation of product **6a** (**L** = MeCN). Relative free energies ( $\Delta G$ , in kcal/mol) of the key intermediates and transition states are calculated at the SMD(DCE)-M06/6-31G(d,p)/LANL2DZ level of theory at 298 K.

The vinyl-cation-based mechanism also well accounts for the Cu(I)-catalyzed synthesis of **6a** from substrate **5a** and styrene.<sup>20</sup> As shown in **Supplementary Figure 10**, following the formation of the vinyl-cation intermediate **B9** occurs readily the intramolecular cyclization with a free energy barrier of only 7.0 kcal/mol to form the cyclopentadiene intermediate **C2**. Further [4 + 2] cycloaddition of **C2** with the dienophile styrene is found to be exergonic ( $\Delta G = -7.2$  kcal/mol) with a free energy barrier of 18.7 kcal/mol. Subsequent H<sub>2</sub>O-assisted 1,4-proton transfer with a free energy barrier of 26.1 kcal/mol turns out to be rate limiting for the whole process.

### Reference:

1. R. B. Dateer, K. Pati and R.-S. Liu, *Chem. Commun.*, 2012, **48**, 7200.
2. S. Hajra and D. Sinha, *J. Org. Chem.*, 2011, **76**, 7334.
3. R. K. Shiroodi, M. Sugawara, M. Ratushnyy, D. C. Yarbrough, D. J. Wink and V. Gevorgyan, *Org. Lett.*, 2015, **17**, 4062.
4. F.-L. Hong, Z.-S. Wang, D.-D. Wei, T.-Y. Zhai, G.-C. Deng, X. Lu, R.-S. Liu and L.-W. Ye, *J. Am. Chem. Soc.*, 2019, **141**, 16961.
5. R. Sharma, K. Kumar, M. Chouhan, V. Groverb and V. A. Nair, *RSC Adv.*, 2013, **3**, 14521.
6. J. Zheng, J.-H. Lin, L.-Y. Yu, Y. Wei, X. Zheng and J.-C. Xiao, *Org. Lett.*, 2015, **17**, 6150.
7. H. T. You, A. C. Grosse, J. K. Howard, C. J. T. Hyland, J. Just, P. P. Molesworth and J. A. Smith, *Org. Biomol. Chem.*, 2011, **9**, 3948.
8. F. K. Signaigo and H. Adkins, *J. Am. Chem. Soc.*, 1936, **58**, 709.
9. J. T. Reeves, D. R. Fandrick, Z. Tan, J. J. Song, H. Lee, N. K. Yee and C. H. Senanayake, *Org. Lett.*, 2010, **12**, 4388.
10. G. Kumaraswamy, A. N. Murthy and A. Pitchaiah, *J. Org. Chem.*, 2010, **75**, 3916.
11. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. Izmaylov, F. Bloino, J. G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro,



- M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision E.01*, Gaussian, Inc., Wallingford CT, 2013.
12. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.
  13. W. R. Wadt and P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284.
  14. P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270.
  15. R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724.
  16. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257.
  17. F. Weigend and R. Ahlrichs, *Phys Chem Chem Phys.*, 2005, **7**, 3297.
  18. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.
  19. CYLview, b. L., C. Y., Universit de Sherbrooke, 2009, (<http://www.cylview.org>).
  20. F.-L. Hong, Y.-B. Chen, S.-H. Ye, G.-Y. Zhu, X.-Q. Zhu, X. Lu, R.-S. Liu and L.-W. Ye, *J. Am. Chem. Soc.*, 2020, **142**, 7618.

## XYZ Coordinates

1a

C	-1.19241500	2.16063300	0.05411800
C	-1.07325300	0.95436300	-0.04549400
N	-0.92766200	-0.37611000	-0.10345300
C	-0.18735500	-1.08933200	0.95924100
C	1.25106800	-1.03484300	0.76126900
C	2.45135200	-0.98316300	0.60138400
C	3.86042700	-0.92691900	0.39453500
C	4.46002900	-1.65412600	-0.64934800
C	4.67703500	-0.14491300	1.21841600
C	5.82334400	-1.59380500	-0.85692800
H	3.83460700	-2.26443600	-1.29674500
C	6.05031900	-0.08044200	1.01832600
H	4.22326500	0.42260100	2.02788100
C	6.62907200	-0.80568200	-0.02604400
H	6.29904400	-2.14772300	-1.66240900
H	6.65750000	0.53634800	1.67434600
S	-1.82087600	-1.27192100	-1.25329400
O	-1.11442600	-2.53477400	-1.39146500
O	-2.04441500	-0.37783100	-2.37274000
C	-3.36377800	-1.57014900	-0.43997500
C	-3.57641400	-2.78558100	0.20247700
C	-4.32408800	-0.55894800	-0.42024300
C	-4.77593900	-2.98794100	0.87427700
H	-2.81939500	-3.56463700	0.15670400
C	-5.51223100	-0.78135400	0.25772600
H	-4.14273400	0.38081600	-0.93636500
C	-5.75647100	-1.99471800	0.91252700
H	-4.95800000	-3.93768000	1.37433800
H	-6.27316200	-0.00263600	0.27957800

C	-7.05802300	-2.22106600	1.61546400
H	-7.32716300	-1.36415900	2.24378800
H	-7.87356600	-2.35502400	0.89334900
H	-7.02703100	-3.11350500	2.24853600
H	-0.46742900	-0.64158300	1.92134500
H	-0.53603100	-2.12911300	0.97235300
C	-1.31043200	3.57023200	0.08075200
C	-1.34107600	4.36082100	1.16874700
C	-1.31545100	4.39720400	-1.18803400
C	-1.35725400	5.81213100	0.79836300
H	-1.29588100	3.99834600	2.19268300
C	-1.74192600	5.78384300	-0.68987800
H	-1.98333600	3.98746200	-1.95514800
H	-0.30545200	4.40233300	-1.62461300
H	-2.05198700	6.40554500	1.40680300
H	-0.36063200	6.25741700	0.95263900
H	-1.29432000	6.60116800	-1.26466800
H	-2.83140800	5.88027900	-0.78016000
O	7.94890700	-0.80959200	-0.31247100
C	8.80101900	-0.01788600	0.48417800
H	9.80772300	-0.14177400	0.07855800
H	8.52840300	1.04579200	0.43891400
H	8.79876800	-0.34491400	1.53344400

**Cu(MeCN)<sub>4</sub><sup>⊕</sup>**

N	-1.41633300	0.72258900	-0.92420500
N	-1.50798800	0.40612600	2.38904000
N	-3.95749900	-0.91934900	0.58719500
C	-0.68762800	0.77037700	-1.82247300
C	-0.85409000	0.20709300	3.32338600
C	-4.69686200	-1.80537300	0.49486400

C	-0.03744000	-0.04698600	4.48784200
C	0.22237000	0.83071900	-2.94294300
C	-5.61941000	-2.91108900	0.37878600
H	0.72742900	0.72881500	4.58720500
H	-0.65904600	-0.04986000	5.38802000
H	0.45373100	-1.01991600	4.39301200
H	0.46552600	1.87256900	-3.17160800
H	1.14555900	0.29420700	-2.70452500
H	-0.23733400	0.37187700	-3.82314200
H	-5.17679600	-3.81469400	0.80788700
H	-6.54679800	-2.68217100	0.91220800
H	-5.85178500	-3.09539800	-0.67428400
Cu	-2.66642300	0.67391200	0.70143200
C	-5.04182300	4.65079700	1.06436300
H	-5.88125000	4.66060800	0.36285100
H	-4.38587200	5.49789300	0.84348300
H	-5.42849000	4.75687900	2.08216300
C	-4.30888700	3.41208000	0.94051400
N	-3.72179300	2.41927700	0.84144700

## A

C	0.18105600	1.72337800	-1.15415800
C	0.72421300	0.70041600	-0.69978300
N	1.04836600	-0.60429600	-0.58567000
C	0.23780800	-1.62133900	-1.30597100
C	-1.14579600	-1.66959600	-0.87805000
C	-2.31091200	-1.69967200	-0.54287400
C	-3.67509700	-1.75945000	-0.13997500
C	-4.09624000	-2.70168600	0.81630300
C	-4.62582300	-0.89242500	-0.69076400
C	-5.41983700	-2.77163700	1.19812500

H	-3.36576400	-3.37979200	1.25124100
C	-5.95953100	-0.95427000	-0.31021300
H	-4.30962600	-0.16028800	-1.43090100
C	-6.36307700	-1.90020800	0.63716200
H	-5.76045400	-3.49663700	1.93286600
H	-6.67643400	-0.26976100	-0.75372800
S	1.87722800	-1.10255500	0.83187300
O	1.01039400	-1.94888400	1.62724300
O	2.39068500	0.16229700	1.38600500
C	3.21035100	-2.04663600	0.18585900
C	3.25733200	-3.41255500	0.44290300
C	4.19784100	-1.40006100	-0.56044500
C	4.32431800	-4.14493100	-0.06322100
H	2.47587300	-3.88624400	1.03174000
C	5.24962800	-2.15057200	-1.05278100
H	4.14020400	-0.32971100	-0.74788400
C	5.33029500	-3.53037100	-0.81105400
H	4.37952500	-5.21426700	0.12938800
H	6.03270100	-1.66655200	-1.63384800
C	6.48327100	-4.31520100	-1.34788600
H	6.54789000	-4.22438500	-2.43875500
H	7.43204400	-3.94301700	-0.94261200
H	6.40248500	-5.37717200	-1.09873700
H	0.31911000	-1.37866700	-2.37272300
H	0.74102000	-2.58814100	-1.16597500
C	-0.47716600	2.89610700	-1.59278300
C	-0.41697100	3.39997700	-2.84135600
C	-1.44543600	3.67803800	-0.72959600
C	-1.33288000	4.56818900	-3.00063400
H	0.17744600	2.97697700	-3.64734500
C	-1.66658400	4.95602600	-1.55039700

H	-1.04394000	3.87143500	0.27403400
H	-2.37129200	3.10032100	-0.59311800
H	-0.88186000	5.38490600	-3.57684300
H	-2.22887100	4.25925900	-3.56196600
H	-2.67515900	5.36427700	-1.43948600
H	-0.96335200	5.72832000	-1.21505700
O	-7.62920800	-2.04867200	1.07134200
C	-8.62159100	-1.20096400	0.53207400
H	-9.56230800	-1.48593500	1.00767200
H	-8.41634800	-0.14465600	0.75414300
H	-8.71847800	-1.33065100	-0.55457700
Cu	1.52820100	2.02566900	0.56732600
N	2.11573900	3.49648000	1.62712000
C	2.48632100	4.32795600	2.34092100
C	2.94865500	5.36180300	3.23155200
H	2.83038600	6.34164800	2.75932200
H	2.36810900	5.33845100	4.15860700
H	4.00503700	5.20166400	3.46751000

### TSA

Number of imaginary frequencies: 1

Lowest frequency ( $\text{cm}^{-1}$ ): -482.0

C	0.38341200	0.74012300	-0.25745500
C	-0.86507200	0.65210300	-0.61868900
N	-1.31844800	-0.36223000	-1.42941800
C	-0.35134900	-1.43877700	-1.74951100
C	0.96179700	-1.00671900	-1.28150600
C	2.18150900	-1.09683000	-1.10579900
C	3.53363000	-1.01198700	-0.75597700
C	3.95035200	-1.35627200	0.54561700
C	4.49474800	-0.53376600	-1.67793400

C	5.27401500	-1.22951900	0.92522200
H	3.21318300	-1.72773000	1.25430400
C	5.81189900	-0.41242700	-1.30898000
H	4.17818600	-0.26586000	-2.68335500
C	6.21425800	-0.75876500	-0.00430300
H	5.57616700	-1.50155400	1.93189100
H	6.56784700	-0.05222800	-2.00131700
S	-2.96564200	-0.70108700	-1.57026700
O	-3.11233800	-1.38418000	-2.84284100
O	-3.64347400	0.56195900	-1.28672400
C	-3.31617400	-1.84196700	-0.26798700
C	-3.33395400	-3.20606600	-0.54369800
C	-3.52489200	-1.35882800	1.02470100
C	-3.56378700	-4.09723000	0.49761900
H	-3.19263900	-3.55886700	-1.56245000
C	-3.75189900	-2.26482900	2.04738300
H	-3.53112600	-0.28847300	1.21894900
C	-3.77367200	-3.64410800	1.80135800
H	-3.58900700	-5.16600000	0.29399200
H	-3.92588100	-1.90287100	3.05960300
C	-4.02934400	-4.60255200	2.92076400
H	-3.29324600	-4.47811900	3.72418900
H	-5.01718800	-4.43283700	3.36622000
H	-3.98822800	-5.64181300	2.58129700
H	-0.64394400	-2.37207600	-1.24179500
H	-0.35081900	-1.62390800	-2.82949800
Cu	-2.05467300	2.06819000	-0.05813300
N	-3.12325600	3.50800700	0.54420400
C	-3.83235400	4.37032500	0.84791000
C	-4.71568000	5.44499700	1.22497100
H	-5.61559300	5.42000400	0.60328200

H	-5.00299700	5.33979800	2.27537900
H	-4.21235700	6.40650100	1.08595000
C	1.49802000	1.45115300	0.25375200
C	1.91065900	1.43412700	1.53834500
C	2.39043800	2.33728700	-0.58957900
C	3.09146900	2.32450700	1.74635100
H	1.41188600	0.88151500	2.33188600
C	3.60937000	2.55515400	0.31659400
H	1.86366000	3.27567600	-0.82017800
H	2.64227200	1.87439300	-1.55226600
H	2.76675100	3.26258600	2.22464400
H	3.84108800	1.88847700	2.41873100
H	4.36629500	1.79332700	0.08371700
H	4.07651500	3.53535700	0.18357500
O	7.51400000	-0.60497200	0.25452700
C	7.99963700	-0.94219000	1.54488800
H	9.07244900	-0.74490900	1.52621200
H	7.53414500	-0.32179200	2.32109500
H	7.83257300	-2.00325900	1.76851900

## **B**

C	-0.30970100	-1.06588700	-0.05156500
C	0.93916900	-0.71769800	-0.51919900
N	0.81853600	0.40758300	-1.32110600
C	-0.53405000	0.97840400	-1.29505600
C	-1.29467900	-0.09642900	-0.54438100
C	-2.59511300	-0.06123000	-0.42854600
C	-3.95001600	0.02541700	-0.38916400
C	-4.76077400	-0.57949300	-1.40770900
C	-4.60350100	0.73313500	0.66955500
C	-6.11819800	-0.46818500	-1.36987800



H	-4.26643700	-1.12374600	-2.20815700
C	-5.96607100	0.85167000	0.70729800
H	-3.98833900	1.18034400	1.44637500
C	-6.73633700	0.25153900	-0.31676100
H	-6.75824900	-0.91129500	-2.12726700
H	-6.44699900	1.39580200	1.51341200
S	2.12007200	1.40251200	-1.73069200
O	1.61544500	2.25910100	-2.79107900
O	3.25967900	0.51739200	-1.92875700
C	2.42304400	2.39509700	-0.29827100
C	1.84426800	3.65856400	-0.21092400
C	3.20854800	1.88559400	0.73581700
C	2.05510300	4.41691300	0.93338900
H	1.25894800	4.04631900	-1.04117000
C	3.40594900	2.65866600	1.86925100
H	3.67174500	0.90492600	0.64138500
C	2.83554000	3.93201500	1.98597900
H	1.61533400	5.40981200	1.01009100
H	4.02279800	2.27646700	2.68105000
C	3.09216400	4.76666400	3.20062000
H	3.10164600	4.15903500	4.11211400
H	4.07095100	5.25864000	3.13249100
H	2.33951300	5.55282300	3.31839100
H	-0.55477100	1.92811600	-0.74091100
H	-0.91430300	1.14977400	-2.30601400
C	-0.63580400	-2.21733300	0.76044500
C	-1.84934000	-2.61299000	1.18359700
C	0.41791700	-3.19942600	1.21505700
C	-1.79322800	-3.88960800	1.96892600
H	-2.78716300	-2.11098400	0.95061800
C	-0.29782700	-4.02056700	2.29555100

H	1.32620600	-2.70056600	1.58585800
H	0.73569900	-3.82323600	0.36309200
H	-2.42168000	-3.87614400	2.86899300
H	-2.15124400	-4.73554800	1.35969200
H	0.04497900	-5.05922500	2.34264900
H	-0.10458100	-3.56887700	3.27688600
O	-8.04973200	0.30836100	-0.37352100
C	-8.77848900	1.01963800	0.63017300
H	-9.82850800	0.93359600	0.35061300
H	-8.62351400	0.56800700	1.61612200
H	-8.48828500	2.07586800	0.64415800
Cu	2.63835000	-1.58122000	-0.34095100
N	4.33754600	-2.39389900	-0.22101700
C	5.40299600	-2.84518000	-0.23096400
C	6.73131500	-3.40576900	-0.24609800
H	7.13400800	-3.43919900	0.77048200
H	6.70094500	-4.42113300	-0.65219900
H	7.38497400	-2.79015400	-0.87123500

### TS<sub>B</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -241.9

C	0.19886400	-1.31793200	-0.20081700
C	-1.05046000	-0.82554700	0.20416600
N	-0.80729200	0.36220900	0.82060500
C	0.61397600	0.75276300	0.86291700
C	1.25632200	-0.47608000	0.27919900
C	2.54074400	-0.86939200	0.30720600
C	3.82699400	-0.31868600	0.17805100
C	4.07650800	0.81038000	-0.64847700
C	4.91737000	-0.88475700	0.87733900

C	5.33433500	1.34837700	-0.74605800
H	3.25042600	1.24515500	-1.20857000
C	6.18368700	-0.34445000	0.79746400
H	4.73348700	-1.76008500	1.49602900
C	6.39996100	0.77820800	-0.02024300
H	5.54505200	2.21315500	-1.36955800
H	7.00059800	-0.78868300	1.35740600
S	-2.00420900	1.33082800	1.57044500
O	-1.36178700	1.90624500	2.73790900
O	-3.18891200	0.49076900	1.67393200
C	-2.28911100	2.59427100	0.37399100
C	-1.66485600	3.82927600	0.52287100
C	-3.11856500	2.31859200	-0.71211900
C	-1.88395200	4.80579100	-0.43984300
H	-1.03342900	4.02286300	1.38672900
C	-3.32068900	3.30717100	-1.66154300
H	-3.60344400	1.34867900	-0.80331600
C	-2.71245500	4.56269500	-1.53905600
H	-1.41011200	5.77992900	-0.33381000
H	-3.96767300	3.10953600	-2.51435400
C	-2.97239900	5.63156400	-2.55219600
H	-3.89014900	6.18137400	-2.30650700
H	-2.15760300	6.36138600	-2.58863200
H	-3.10718800	5.21217300	-3.55485700
H	0.91516800	0.99623400	1.88657400
H	0.79196800	1.62989100	0.22394400
Cu	-2.79195900	-1.61365900	0.16145800
N	-4.47880200	-2.46158100	0.11855200
C	-5.52321800	-2.95850900	0.14954700
C	-6.82446600	-3.57741700	0.18865900
H	-7.01356400	-4.10704600	-0.74999400

H	-6.87054200	-4.29015400	1.01765100
H	-7.59459200	-2.81336700	0.33048900
C	0.60554700	-2.52588300	-0.80689100
C	1.91643000	-2.67931800	-1.19323500
C	-0.12670400	-3.83539100	-0.85940800
C	2.23893500	-4.12836400	-1.42440500
H	2.51290700	-1.86789900	-1.60401800
C	0.84333400	-4.75210000	-1.62370100
H	-1.11106900	-3.74925800	-1.33852900
H	-0.31088000	-4.19239100	0.16605900
H	2.90387200	-4.29645900	-2.27849700
H	2.74132900	-4.55645800	-0.54423500
H	0.79106700	-5.79486700	-1.29605300
H	0.59437400	-4.73235600	-2.69186400
O	7.58065300	1.37374500	-0.17719500
C	8.70906800	0.86178500	0.51857800
H	8.92564700	-0.17070600	0.21845600
H	9.55007200	1.49962000	0.24259100
H	8.56025700	0.90985300	1.60424000

**C**

C	0.07536200	-1.40555900	-0.31581700
C	-1.20595000	-0.92514900	0.10269700
N	-0.95162100	0.25694500	0.66768100
C	0.48466600	0.68792700	0.73223900
C	1.13409800	-0.48075300	0.07410000
C	2.35784600	-0.98562500	-0.22564100
C	3.67870200	-0.41088900	-0.02619700
C	3.86048900	0.76525100	0.72562600
C	4.82107400	-1.00610800	-0.57360500
C	5.11298800	1.30907400	0.92024600

H	3.00261400	1.25784400	1.18018000
C	6.08977400	-0.46837100	-0.39050600
H	4.72535400	-1.91141500	-1.17074200
C	6.24354300	0.69708500	0.36227600
H	5.25220900	2.21447100	1.50569800
H	6.94719700	-0.96163400	-0.83864400
S	-2.18319700	1.26162900	1.38702200
O	-1.64484700	1.66141100	2.67232500
O	-3.41424700	0.49230200	1.27158400
C	-2.21732600	2.63473500	0.29103700
C	-1.61531300	3.82860800	0.68224400
C	-2.83555000	2.49165600	-0.95025800
C	-1.64397500	4.90168000	-0.19649300
H	-1.14713400	3.91055800	1.66028300
C	-2.84711200	3.57673900	-1.81196600
H	-3.30641600	1.55131300	-1.23060800
C	-2.25776500	4.79413200	-1.44884500
H	-1.18365500	5.84451600	0.09283700
H	-3.32481300	3.48599700	-2.78554300
C	-2.30494100	5.97014700	-2.37029100
H	-1.38296700	6.55882000	-2.31891500
H	-2.46378400	5.66477100	-3.40920500
H	-3.12986600	6.64017500	-2.09621500
H	0.75684900	0.83763200	1.78502200
H	0.60505800	1.64397900	0.20168900
Cu	-2.95789900	-1.68873200	0.06584700
N	-4.64572500	-2.53473000	0.04626600
C	-5.70289300	-3.00220800	0.09564400
C	-7.02015000	-3.58320600	0.15938200
H	-7.07660800	-4.27924500	1.00179200
H	-7.76685700	-2.79521400	0.29549400

H	-7.23461900	-4.12432200	-0.76716800
C	0.61909500	-2.50542200	-0.90057400
C	2.10256800	-2.30507500	-0.92458600
C	0.25148200	-3.92079900	-1.16937900
C	2.55520500	-3.66739800	-0.36916600
H	2.43842000	-2.24133200	-1.97681300
C	1.62074100	-4.64206100	-1.10477500
H	-0.25202900	-4.05658200	-2.13568600
H	-0.44685300	-4.28440100	-0.40432500
H	3.61683500	-3.87698200	-0.53476800
H	2.37296700	-3.69222500	0.71418000
H	1.55814100	-5.62061700	-0.62005400
H	1.99897900	-4.80897900	-2.12134700
O	7.42244000	1.30394300	0.60490300
C	8.59143100	0.71587300	0.07464900
H	8.56313800	0.67509300	-1.02299500
H	9.42521500	1.34970300	0.38375400
H	8.74895700	-0.29719300	0.46979900

### TSc

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -1052.7

C	-0.05439100	-1.47016200	0.06787600
C	1.20706900	-0.92221300	-0.24234800
N	0.93425800	0.27390800	-0.80795400
C	-0.50925500	0.62197300	-0.90193300
C	-1.11580000	-0.59638600	-0.30240900
C	-2.35615500	-1.09848800	0.06628500
C	-3.67630700	-0.49340800	-0.10292900
C	-3.90391200	0.46079800	-1.10849900
C	-4.75331600	-0.83414500	0.71937000

C	-5.14505900	1.04163100	-1.28062600
H	-3.09795000	0.73366600	-1.78749000
C	-6.00975900	-0.26081500	0.55730000
H	-4.61021800	-1.55096500	1.52587500
C	-6.21335600	0.68531200	-0.44896400
H	-5.32214500	1.77462200	-2.06387000
H	-6.81715600	-0.55299000	1.22234000
S	2.12870300	1.33360200	-1.45395100
O	1.56088300	1.84807300	-2.68595200
O	3.36990600	0.57157200	-1.43419000
C	2.19637000	2.61618600	-0.24976900
C	1.52891500	3.81202000	-0.49383000
C	2.89434000	2.39307100	0.93807500
C	1.56728100	4.80472200	0.47738400
H	1.00421200	3.96378600	-1.43383300
C	2.91505200	3.39510900	1.89248500
H	3.42074200	1.45470100	1.10105000
C	2.25377000	4.61279100	1.67825700
H	1.05817800	5.74992900	0.29963100
H	3.45655700	3.24178600	2.82456700
C	2.30008900	5.68271600	2.72173900
H	1.70156300	6.55305800	2.43682100
H	1.92710100	5.31216200	3.68408400
H	3.32973400	6.02136100	2.88968200
H	-0.76738200	0.78457000	-1.95566100
H	-0.71452000	1.55020100	-0.34915600
Cu	2.98443500	-1.61989300	-0.13566200
N	4.69264100	-2.41946600	-0.07136600
C	5.76500600	-2.85249600	-0.10673600
C	7.10229700	-3.38818400	-0.15340600
H	7.76004900	-2.79744900	0.49124500

H	7.10178700	-4.42683400	0.18946100
H	7.47969700	-3.34899100	-1.17957700
C	-0.62354400	-2.60130900	0.69819200
C	-2.06399000	-2.36406500	0.69640900
C	-0.33506900	-4.03101600	1.02833500
C	-2.76925800	-3.65244300	1.01362100
H	-1.31105800	-2.12132000	1.73365800
C	-1.65967700	-4.50588500	1.65868600
H	0.53541800	-4.18803500	1.67266900
H	-0.14343900	-4.55685700	0.08212200
H	-3.65406600	-3.55814000	1.64926600
H	-3.09983300	-4.08654000	0.05923200
H	-1.82564100	-5.57818600	1.52907000
H	-1.63654900	-4.30864100	2.73900300
O	-7.38604900	1.30496100	-0.69528400
C	-8.49538600	0.96575000	0.10835500
H	-8.31700100	1.20267700	1.16649500
H	-9.33421000	1.56552700	-0.25115200
H	-8.75366300	-0.09814000	0.01501000

## **D**

C	-0.09766400	-1.39201700	0.22251800
C	1.16574700	-0.91357300	-0.18817100
N	0.91054800	0.26187100	-0.81342700
C	-0.51694900	0.63463600	-0.83838100
C	-1.10628500	-0.51324000	-0.11407700
C	-2.39994900	-0.98208200	0.32447300
C	-3.69733100	-0.36144600	0.06037300
C	-3.87363300	0.54926100	-0.99440200
C	-4.81176100	-0.66176800	0.85008100
C	-5.10291700	1.12376000	-1.24937400



H	-3.03834200	0.79847300	-1.64556200
C	-6.05620300	-0.09384900	0.60582600
H	-4.70433200	-1.33792500	1.69583700
C	-6.20896700	0.80600500	-0.45174200
H	-5.24118700	1.82478000	-2.06867600
H	-6.89480000	-0.35043600	1.24631800
S	2.10045100	1.28191900	-1.52589900
O	1.45542600	1.84971200	-2.69465500
O	3.30239100	0.46742700	-1.61869100
C	2.32445400	2.53190300	-0.30473100
C	1.67418700	3.75397800	-0.45299100
C	3.12818700	2.25742700	0.80093700
C	1.83820200	4.71749800	0.53291800
H	1.06547400	3.94887600	-1.33251200
C	3.27381200	3.23303000	1.77392700
H	3.63799300	1.30018200	0.88898900
C	2.63506800	4.47373500	1.65558400
H	1.34318300	5.68120300	0.42894500
H	3.89834200	3.03582300	2.64328100
C	2.82947600	5.52794500	2.69799500
H	1.97178100	6.20563800	2.75264300
H	2.98881500	5.09044800	3.68906900
H	3.71183300	6.13885500	2.46768900
H	-0.84705300	0.72804400	-1.88094400
H	-0.68245400	1.60051500	-0.33949700
Cu	2.91442400	-1.68037700	-0.12122200
N	4.60455000	-2.52117700	-0.07269900
C	5.65148400	-3.01278200	-0.10258500
C	6.95584000	-3.62466600	-0.14012500
H	7.00657000	-4.33708600	-0.96913400
H	7.72199300	-2.85642000	-0.28098900

H	7.14649500	-4.15331800	0.79878400
C	-0.68752800	-2.51779500	0.98697700
C	-2.14706000	-2.17652800	0.95785100
C	-0.72810900	-3.97101900	0.49750900
C	-2.96776000	-3.37396900	1.29801200
C	-1.93589500	-4.52796500	1.26747300
H	0.19980700	-4.52009900	0.68811700
H	-0.91676100	-3.98376400	-0.58476600
H	-3.46901600	-3.29541400	2.27234700
H	-3.76782500	-3.49848400	0.55435500
H	-2.33990800	-5.44195600	0.82256400
H	-1.62994800	-4.77712900	2.29165500
O	-7.36394800	1.41768900	-0.77701000
C	-8.51149500	1.12656900	-0.00673900
H	-8.37850700	1.41843300	1.04400300
H	-9.32766400	1.71128600	-0.43602500
H	-8.77330000	0.06094400	-0.05650500
H	-0.32503300	-2.51302600	2.03074400

## **E**

C	-0.05789000	-1.49681700	-0.44585300
C	-1.31881900	-0.94836900	-0.14201800
N	-1.06063600	0.31587000	0.28843800
C	0.38079500	0.64783700	0.34835900
C	0.95983000	-0.60415000	-0.17937000
C	2.25509700	-1.16490100	-0.47717800
C	3.56134500	-0.56556600	-0.20588300
C	3.74114600	0.34918900	0.84448900
C	4.67752300	-0.90435900	-0.97532100
C	4.98064900	0.89768400	1.10893600
H	2.90269700	0.60596200	1.49008300

C	5.93160700	-0.36114100	-0.72129000
H	4.56207100	-1.59389500	-1.80996600
C	6.08866500	0.54856300	0.32685600
H	5.12714200	1.59974300	1.92604300
H	6.77356300	-0.64486900	-1.34587100
S	-2.22946400	1.31494400	1.04930500
O	-1.77800600	1.52518200	2.42050300
O	-3.51628600	0.69074200	0.77830700
C	-2.07229000	2.82192200	0.15841000
C	-1.40241400	3.89359800	0.74405200
C	-2.60985600	2.90060200	-1.12487200
C	-1.27685000	5.06987500	0.01986400
H	-0.99787500	3.80191700	1.74901300
C	-2.47125700	4.08659800	-1.82878400
H	-3.13027800	2.04937300	-1.55894700
C	-1.80917400	5.18552000	-1.26872900
H	-0.76003800	5.91973800	0.46194800
H	-2.88627000	4.17005000	-2.83129300
C	-1.69050600	6.47182400	-2.02103400
H	-0.69843400	6.91937300	-1.89571600
H	-1.87566700	6.33420900	-3.09071400
H	-2.41996700	7.20352900	-1.65095100
H	0.61257100	1.53429300	-0.25705300
H	0.65550200	0.82525000	1.39772800
Cu	-3.07155400	-1.70105600	-0.14150200
N	-4.76716700	-2.53024300	-0.14420500
C	-5.83171200	-2.98154700	-0.10407600
C	-7.15887900	-3.54133000	-0.05103100
H	-7.28378800	-4.28323700	-0.84525600
H	-7.31792200	-4.02402100	0.91808000
H	-7.90104500	-2.74781300	-0.18003700

C	0.53130200	-2.73271300	-1.01795600
C	1.99733800	-2.42421700	-0.96188300
C	0.50882500	-4.09594300	-0.31435100
C	2.80142000	-3.67310400	-1.08106800
C	1.73975600	-4.78902500	-0.92235500
H	-0.42318800	-4.64899000	-0.47058500
H	0.63922200	-3.94459800	0.76601300
H	3.34130500	-3.75312800	-2.03431200
H	3.56877100	-3.69591800	-0.29456300
H	2.09713300	-5.62729000	-0.31716200
H	1.47809300	-5.19364400	-1.90864000
O	7.25354200	1.13901900	0.66023600
C	8.40345800	0.80854100	-0.08942200
H	8.29278700	1.08838300	-1.14607900
H	9.22867500	1.37807000	0.34306200
H	8.63757800	-0.26261700	-0.02138900
H	0.21322000	-2.87333300	-2.06646100
O	0.26777100	-0.40625800	3.14078800
H	0.64612700	-0.48141800	4.02164200
H	-0.51170900	0.15610400	3.24679300

### TS<sub>E</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -147.5

C	-0.38298600	-1.58173500	-0.36731600
C	-1.55577100	-0.87450800	-0.24624700
N	-1.11469700	0.46038700	-0.09701900
C	0.31049300	0.55551000	-0.00069300
C	0.75870600	-0.72772100	-0.26146700
C	1.98530300	-1.51300900	-0.40473000
C	3.34825800	-1.01491700	-0.22327100

C	3.61459200	0.12240000	0.55688600
C	4.43777000	-1.66298000	-0.81313000
C	4.90499000	0.57909200	0.74613700
H	2.79626100	0.64986800	1.04500800
C	5.74176000	-1.21606700	-0.63409200
H	4.26068100	-2.52474500	-1.45359700
C	5.98275200	-0.08614500	0.15035600
H	5.11369300	1.45535000	1.35514200
H	6.55755900	-1.74425300	-1.11871900
S	-2.12964000	1.59421300	0.64420400
O	-1.93159600	1.46947700	2.11635600
O	-3.47197500	1.39835700	0.13138600
C	-1.46609500	3.13364200	0.13345500
C	-0.68730100	3.88712700	1.01065500
C	-1.72553500	3.55261100	-1.17043000
C	-0.15946900	5.08625400	0.55937700
H	-0.50737500	3.54174500	2.02532000
C	-1.18608600	4.75604600	-1.59729900
H	-2.33890100	2.94705800	-1.83379000
C	-0.39898500	5.53726300	-0.74431900
H	0.44964300	5.69191400	1.22799900
H	-1.37743400	5.10057000	-2.61137500
C	0.16887400	6.84171600	-1.20169400
H	1.23459400	6.91782800	-0.95800700
H	0.05193700	6.97978100	-2.28045500
H	-0.33278800	7.67929700	-0.70102600
H	0.80468500	1.51842700	-0.07973900
H	0.33943300	-0.02310500	1.70385600
Cu	-3.38157300	-1.41317100	-0.24301500
N	-5.16009800	-2.04022400	-0.25494800
C	-6.26392100	-2.38635700	-0.28131800

C	-7.63971400	-2.81642500	-0.31650400
H	-7.76629900	-3.59587700	-1.07386100
H	-7.93133000	-3.21496700	0.65967100
H	-8.28530300	-1.96867700	-0.56453300
C	0.09068700	-2.96485200	-0.66272700
C	1.58883800	-2.79767500	-0.62811200
C	-0.07881800	-4.13058100	0.31607000
C	2.24909200	-4.13039900	-0.48053500
C	1.07614600	-5.06370500	-0.08191100
H	-1.06236900	-4.61096600	0.26640200
H	0.06451700	-3.75904400	1.34310200
H	2.73857600	-4.47597400	-1.40108400
H	3.03560900	-4.08512500	0.28556200
H	1.34865800	-5.76494100	0.71280900
H	0.77197500	-5.66545000	-0.94789900
O	7.20335800	0.43911700	0.38363800
C	8.31908800	-0.19540500	-0.20374500
H	8.25036000	-0.20389800	-1.30034400
H	9.19636000	0.38450300	0.09105300
H	8.43578800	-1.22639800	0.15800700
H	-0.23716300	-3.29689900	-1.66291400
O	-0.10296000	-0.16640900	2.63339900
H	-0.39128600	-1.09446400	2.69420100
H	-0.92731400	0.46242300	2.58452400

## F

C	-0.30612600	-1.60677100	-0.34126000
C	-1.49860600	-0.93513200	-0.25245300
N	-1.06869000	0.43813800	-0.17349800
C	0.34919000	0.55401800	-0.14177800
C	0.82368500	-0.71248900	-0.28621700

C	2.06249300	-1.48588700	-0.40165400
C	3.41546100	-0.95492600	-0.24280100
C	3.65931600	0.20414500	0.51191200
C	4.51453300	-1.59127000	-0.82668900
C	4.94054800	0.69331100	0.68231600
H	2.82810700	0.71326300	0.99725900
C	5.80955400	-1.11091900	-0.66667800
H	4.35149500	-2.47116300	-1.44618900
C	6.02913000	0.03954900	0.09327700
H	5.13435400	1.58492100	1.27395100
H	6.63405000	-1.63027400	-1.14623500
S	-2.03422200	1.53427300	0.62454200
O	-1.75111200	1.38288500	2.11560800
O	-3.41395200	1.34127600	0.22434500
C	-1.43350000	3.11632200	0.19188900
C	-0.60787100	3.83416600	1.05408400
C	-1.81816800	3.61228000	-1.05617000
C	-0.16387700	5.08403400	0.64668400
H	-0.32676200	3.42924500	2.02188000
C	-1.35691400	4.85927700	-1.43721500
H	-2.46928200	3.03461300	-1.70810300
C	-0.52778100	5.61277400	-0.59492900
H	0.47470500	5.66690100	1.30691900
H	-1.64738700	5.26698200	-2.40348100
C	-0.04491900	6.95765500	-1.03075300
H	0.62410700	6.86975600	-1.89560000
H	-0.88190600	7.59405400	-1.34052900
H	0.49986400	7.47197300	-0.23387500
H	0.82271200	1.52730800	-0.11110700
H	-1.08605400	-1.31695700	1.77115800
Cu	-3.32725100	-1.45772500	-0.31054900

N	-5.13058700	-2.00448800	-0.39866600
C	-6.24600900	-2.29967300	-0.48781000
C	-7.63563600	-2.66700700	-0.59882200
H	-7.75688300	-3.43348100	-1.37027100
H	-7.99525700	-3.06071800	0.35641800
H	-8.22979300	-1.78922500	-0.87057800
C	0.20072800	-2.99093500	-0.58524200
C	1.69668900	-2.78484600	-0.56775000
C	0.06196000	-4.11733700	0.44342200
C	2.38811900	-4.09494800	-0.36346100
C	1.23883800	-5.03761500	0.07988300
H	-0.90790800	-4.62779100	0.41588700
H	0.20206900	-3.70040600	1.45313100
H	2.88169600	-4.47168600	-1.26964800
H	3.17528900	-3.99878700	0.39712100
H	1.52966400	-5.69759600	0.90310100
H	0.94583000	-5.68242400	-0.75869400
O	7.24068900	0.59561500	0.30975500
C	8.36644400	-0.03390100	-0.26168300
H	8.30203000	-0.06501200	-1.35831600
H	9.23519800	0.56312900	0.02445000
H	8.49652800	-1.05642500	0.11954400
H	-0.13136100	-3.36910300	-1.56727200
O	-1.14149100	-0.87510100	2.65762700
H	-1.77493600	-1.36752500	3.20030000
H	-1.47416400	0.28587600	2.43790700

### TS<sub>F</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -79.7

C	-0.19744400	-1.65609700	-0.29188600
---	-------------	-------------	-------------



C	-1.42327300	-1.04536000	-0.14179900
N	-1.06058500	0.34509300	-0.04245800
C	0.33626900	0.52630000	-0.05077700
C	0.88152800	-0.70888600	-0.24153900
C	2.15868000	-1.41342900	-0.39381900
C	3.48425600	-0.81389400	-0.25026200
C	3.67707300	0.35622100	0.50244700
C	4.60873600	-1.39293000	-0.84641800
C	4.93289400	0.91137600	0.65852000
H	2.82799300	0.82277700	0.99932300
C	5.87885800	-0.84625100	-0.70004900
H	4.48616600	-2.28069800	-1.46402100
C	6.04728300	0.31427200	0.05763400
H	5.08569800	1.81207400	1.24823200
H	6.72404500	-1.32280300	-1.18806700
S	-2.07543100	1.39596300	0.79869400
O	-1.73999800	1.27602400	2.24617000
O	-3.44279800	1.08200300	0.41024700
C	-1.58329600	2.98547500	0.25466000
C	-0.96737000	3.86793700	1.13596500
C	-1.84593900	3.32265900	-1.07488600
C	-0.60715200	5.12388000	0.66460400
H	-0.78073200	3.57590000	2.16588700
C	-1.47228200	4.57774900	-1.51955500
H	-2.32740700	2.61193700	-1.74328300
C	-0.84952900	5.49449600	-0.66034200
H	-0.12898900	5.83185000	1.33813700
H	-1.66414600	4.86170400	-2.55263600
C	-0.44503100	6.83932700	-1.17125500
H	0.34618300	6.74631300	-1.92561900
H	-1.28648400	7.34729900	-1.65661400

H	-0.07171800	7.48363800	-0.37001700
H	0.76419000	1.51887300	0.02512500
H	-1.27576100	-1.43381100	1.58848400
Cu	-3.26212700	-1.52274000	-0.32449700
N	-5.08250900	-1.98937800	-0.52797700
C	-6.20761500	-2.21701800	-0.67463500
C	-7.60961900	-2.50073800	-0.85500200
H	-7.73934600	-3.24942500	-1.64229500
H	-8.03472200	-2.88486100	0.07704200
H	-8.13988600	-1.58676200	-1.13921600
C	0.37419700	-3.00958800	-0.55669800
C	1.85851400	-2.72697900	-0.57225100
C	0.31876400	-4.14144100	0.47462100
C	2.61989800	-4.00110900	-0.39249100
C	1.53230300	-5.00028300	0.08280700
H	-0.62369900	-4.70156400	0.47098900
H	0.46249800	-3.71542500	1.47964000
H	3.10354200	-4.35317400	-1.31386400
H	3.42399600	-3.86722200	0.34436000
H	1.87720000	-5.64078600	0.90054500
H	1.25152000	-5.66305300	-0.74583400
O	7.23102300	0.93149900	0.26167000
C	8.38264100	0.35468500	-0.31370700
H	8.31673300	0.32162200	-1.41018700
H	9.22429100	0.99014000	-0.02955200
H	8.56008000	-0.66108000	0.06640900
H	0.03443500	-3.40099300	-1.53047300
O	-1.24160700	-1.18668500	2.60257900
H	-1.91956700	-1.68155400	3.09403800
H	-1.43890600	-0.17185800	2.62915800

**G**

C	0.13245900	1.12781300	-1.35024500
C	-1.02070700	0.54752000	-1.89062900
N	-0.82233000	-0.84393700	-1.77080100
C	0.35061800	-1.11398000	-1.08856800
C	0.96595400	0.08502200	-0.82961200
C	2.21955700	0.66445600	-0.33156900
C	3.37276300	-0.09416100	0.14695700
C	3.60032400	-1.41768600	-0.26662200
C	4.29936700	0.48353000	1.02030900
C	4.70635300	-2.12191800	0.16653900
H	2.91529100	-1.89112200	-0.96745400
C	5.41679400	-0.21264100	1.46620800
H	4.13036100	1.49747200	1.37898800
C	5.62607700	-1.52578300	1.03810800
H	4.89168200	-3.14213700	-0.16016300
H	6.11029900	0.26786600	2.15046300
S	-2.10895800	-1.98114200	-1.93945600
O	-1.46682500	-3.27623900	-1.85534400
O	-2.85449900	-1.53454700	-3.09802600
C	-3.06367700	-1.67663800	-0.48129000
C	-2.64291400	-2.21677800	0.73325200
C	-4.19558900	-0.86778800	-0.57163400
C	-3.37191500	-1.92513000	1.87780200
H	-1.77168700	-2.86668100	0.77867100
C	-4.91124400	-0.59474700	0.58627700
H	-4.51488700	-0.47781900	-1.53582300
C	-4.51263800	-1.11646100	1.82174700
H	-3.05982200	-2.34371700	2.83285200
H	-5.80340800	0.02682100	0.53293100
C	-5.30939200	-0.83808400	3.05669700

H	-5.84284900	0.11651500	2.98979700
H	-6.06988100	-1.61514200	3.20726400
H	-4.68079200	-0.83363900	3.95383200
H	0.62079300	-2.13974400	-0.86979500
H	-1.72199200	0.92449600	-2.63099100
Cu	-1.77952500	1.14673800	-0.07538800
N	-2.58754100	1.79040500	1.52491900
C	-2.99712000	2.25096900	2.50437700
C	-3.51053500	2.81742900	3.72620700
H	-2.79590500	3.54242500	4.12757100
H	-4.46100400	3.32388000	3.53197000
H	-3.66843600	2.02610100	4.46534300
C	0.83896000	2.43617200	-1.18054600
C	2.13313700	2.00625700	-0.52431500
C	1.38916900	3.22849900	-2.37411800
C	3.14874000	3.09612500	-0.65387600
C	2.52313500	4.03307900	-1.71909800
H	0.64305500	3.85950300	-2.86800000
H	1.78881600	2.52455200	-3.11684900
H	3.34417400	3.63235800	0.28450000
H	4.11157500	2.67689000	-0.97596500
H	3.25622700	4.39056300	-2.44818300
H	2.09967800	4.92071700	-1.23107100
O	6.66986400	-2.29519500	1.40724600
C	7.63482800	-1.73371400	2.27069900
H	7.19943200	-1.46012900	3.24193100
H	8.39475900	-2.50220900	2.42745500
H	8.11041700	-0.84836000	1.82616800
H	0.26940800	3.12783500	-0.53610200

**H**

C	0.44732900	-2.09813400	-0.15963600
C	1.54706300	-1.21665500	-0.10965400
N	1.06790700	-0.08167800	0.45478300
C	-0.36619500	-0.14029700	0.80546400
C	-0.68254900	-1.52010100	0.38412600
C	-1.81439600	-2.41547200	0.33820500
C	-3.19078500	-2.10935900	0.72907900
C	-3.70534300	-0.80829900	0.60853900
C	-4.03471500	-3.10285800	1.23206900
C	-5.00178000	-0.51456700	0.98267400
H	-3.09308900	-0.01754400	0.17526100
C	-5.34466100	-2.82397300	1.60638700
H	-3.65438000	-4.11444600	1.36510100
C	-5.83494200	-1.52156600	1.48602800
H	-5.39976300	0.49373600	0.88631900
H	-5.96904700	-3.61952700	2.00239000
S	1.99096300	1.36019000	0.63506400
O	1.02817700	2.33114300	1.12165800
O	2.73326400	1.54581500	-0.60064900
C	3.11554400	0.92810900	1.92401600
C	2.65450800	0.93455900	3.23962900
C	4.41750400	0.55106800	1.60798800
C	3.52027000	0.55123200	4.25072100
H	1.63756900	1.24912700	3.46482900
C	5.26899700	0.17133800	2.63861000
H	4.75970200	0.58046400	0.57568200
C	4.83612000	0.16338100	3.96703900
H	3.17805100	0.55655200	5.28406000
H	6.29497600	-0.11390300	2.41285600
C	5.75996900	-0.22632500	5.07640500
H	6.68928800	-0.66115900	4.69597300

H	6.02579100	0.64649300	5.68588400
H	5.29085400	-0.95268100	5.74982000
H	-0.91118300	0.64073400	0.24764600
Cu	3.33925200	-1.42394500	-0.73979400
N	5.09824000	-1.67768600	-1.39210200
C	6.15695700	-1.81090800	-1.83982900
C	7.47440600	-1.97434400	-2.40081000
H	7.63727300	-1.22696100	-3.18315200
H	8.23096400	-1.84754900	-1.62066200
H	7.57223300	-2.97400700	-2.83467900
C	0.11630500	-3.47809000	-0.59196100
C	-1.34259900	-3.56241800	-0.25160100
C	0.06699900	-3.89284200	-2.06941200
C	-1.99318700	-4.67941900	-0.99451700
C	-0.91957300	-5.07153100	-2.04007200
H	1.04729200	-4.15403300	-2.48196500
H	-0.33996700	-3.05737600	-2.65814300
H	-2.27170600	-5.52720800	-0.35456500
H	-2.92575500	-4.32334500	-1.45396400
H	-1.34943700	-5.28952100	-3.02210900
H	-0.39346200	-5.97689700	-1.71105000
O	-7.08184600	-1.13950400	1.82616300
C	-7.96367400	-2.12248300	2.32532400
H	-7.59200400	-2.56259100	3.26108600
H	-8.91080500	-1.61656600	2.52420200
H	-8.13472400	-2.92267800	1.59201400
H	0.69028000	-4.23455200	-0.02892500
H	-0.52382300	0.04642900	1.87690400
C	-0.99117200	2.11584100	-2.22386800
C	0.04621400	3.03152300	-2.42042300
C	0.11952700	4.17020400	-1.63044400

C	-0.88497600	4.36620100	-0.68215200
C	-1.88067900	3.40988500	-0.51882800
N	-1.91090800	2.29061000	-1.26835300
H	0.79470800	2.86749100	-3.19386000
H	-0.86399200	5.26609700	-0.07196100
C	1.24103200	5.14829900	-1.76840900
H	1.97731000	4.99826100	-0.96776900
H	1.76474400	5.03476700	-2.72325900
H	0.88588700	6.18192200	-1.68794500
C	-1.14398900	0.92959000	-3.17601300
C	-2.98410600	3.55860500	0.52720500
C	0.18903000	0.19591900	-3.34846200
H	0.05585300	-0.67483400	-4.00509600
H	0.96251700	0.82847600	-3.79991800
H	0.57513900	-0.15833500	-2.38201700
C	-2.19414500	-0.06407900	-2.69231400
H	-1.89461400	-0.54801200	-1.75347800
H	-3.16363400	0.41768900	-2.52387300
H	-2.32755400	-0.85336000	-3.44445900
C	-1.59580000	1.48348700	-4.53401300
H	-1.71697300	0.66761300	-5.25920000
H	-2.55944700	2.00058700	-4.44189900
H	-0.86996900	2.19549800	-4.94559500
C	-2.65886600	2.65567200	1.72160300
H	-2.65548900	1.59694000	1.43744100
H	-1.67547400	2.90245500	2.14518100
H	-3.41429800	2.78120500	2.50951200
C	-4.33071300	3.15059500	-0.07405800
H	-5.11870500	3.22171800	0.68777600
H	-4.60782000	3.81119900	-0.90597700
H	-4.30816300	2.12573700	-0.46075400

C	-3.10268900	4.99460200	1.03566400
H	-3.25975900	5.70633200	0.21508800
H	-3.96222900	5.07329800	1.71286100
H	-2.21775400	5.31093400	1.60193200

### **TS<sub>H</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -1175.9

C	0.28417700	-1.96697700	-0.34339800
C	1.40578500	-1.15228900	-0.23635100
N	0.92513000	0.00298600	0.33855700
C	-0.50544600	-0.01223100	0.58092900
C	-0.84955800	-1.34059800	0.19773700
C	-2.00302400	-2.23106600	0.09408800
C	-3.39060100	-1.91215300	0.43253700
C	-3.88226500	-0.60498000	0.30223500
C	-4.27655900	-2.89674400	0.87759100
C	-5.19344700	-0.29274200	0.60591700
H	-3.21821800	0.17480500	-0.06740900
C	-5.60159400	-2.60213700	1.18279800
H	-3.91775600	-3.91497500	1.01802100
C	-6.06704300	-1.29223000	1.05064200
H	-5.57569300	0.72094900	0.50359200
H	-6.25721300	-3.39305800	1.53544700
S	1.95389400	1.26502000	0.82777800
O	1.06849400	2.29821800	1.34349000
O	2.87310000	1.53235400	-0.26931000
C	2.85839300	0.54639400	2.16457800
C	2.25262200	0.46966800	3.41699300
C	4.13268100	0.03327500	1.94085100
C	2.94251000	-0.13317300	4.45692800



H	1.25915700	0.88578000	3.57324700
C	4.80673100	-0.56697400	2.99703800
H	4.59160200	0.12116900	0.95776600
C	4.22546300	-0.65983500	4.26434600
H	2.48352400	-0.19756900	5.44202700
H	5.80704700	-0.96731500	2.84096300
C	4.96185200	-1.28368400	5.40694800
H	5.82216900	-1.86752800	5.06540400
H	5.33633400	-0.51515100	6.09512700
H	4.30952000	-1.94245800	5.99100200
H	-1.06277200	1.07241800	-0.27962200
Cu	3.20426600	-1.39046200	-0.82718000
N	4.97194000	-1.67291300	-1.44812000
C	6.04229800	-1.82080700	-1.86262700
C	7.37463600	-2.00172200	-2.38307700
H	7.56917600	-1.26176700	-3.16508200
H	8.10920700	-1.87692600	-1.58196500
H	7.47563000	-3.00526800	-2.80705000
C	-0.07965100	-3.33358900	-0.80002100
C	-1.54740700	-3.38154800	-0.48263900
C	-0.11427200	-3.73463900	-2.27993200
C	-2.20454800	-4.49591000	-1.22881300
C	-1.13433500	-4.88589400	-2.28227400
H	0.86485700	-4.02272500	-2.67922000
H	-0.48362000	-2.88317700	-2.87084500
H	-2.47096200	-5.35010600	-0.59172000
H	-3.14269100	-4.14767400	-1.68227000
H	-1.56640700	-5.06870500	-3.27108700
H	-0.63392400	-5.81355400	-1.97571300
O	-7.32667200	-0.89433400	1.32785800
C	-8.24304000	-1.86843400	1.77786300

H	-7.91872200	-2.32474800	2.72348700
H	-9.19083100	-1.35107500	1.94179500
H	-8.39457000	-2.65897900	1.02970300
H	0.46599700	-4.11145900	-0.23760100
H	-0.81404000	0.41262100	1.53482900
C	-0.40153100	2.22180300	-2.04320900
C	0.42768600	3.30541600	-2.30594700
C	0.44642500	4.40432700	-1.45933500
C	-0.48591500	4.42758000	-0.42099000
C	-1.27875200	3.32714000	-0.14914800
N	-1.14580200	2.19501400	-0.90753800
H	1.05831700	3.29843300	-3.19173400
H	-0.56778800	5.32264400	0.18656600
C	1.39469500	5.53572400	-1.66380300
H	2.22651600	5.45313800	-0.95214600
H	1.81913100	5.53558600	-2.67222300
H	0.91319500	6.50303900	-1.48359400
C	-0.55719900	1.13303600	-3.10423600
C	-2.42502600	3.40959000	0.86217500
C	0.75751000	0.38180000	-3.32519900
H	0.64657500	-0.31862900	-4.16366200
H	1.58154000	1.06426300	-3.56687700
H	1.04798800	-0.19475800	-2.43872000
C	-1.67927300	0.14869300	-2.78638600
H	-1.46255500	-0.46829600	-1.91127100
H	-2.63473100	0.66362900	-2.62283400
H	-1.81280700	-0.52919000	-3.63873600
C	-0.94817200	1.84031500	-4.41513200
H	-1.14430000	1.08374700	-5.18517300
H	-1.86067700	2.43657200	-4.29043200
H	-0.15999600	2.49854600	-4.79641000

C	-2.37686200	2.34420100	1.95811100
H	-2.57497600	1.33834400	1.57888300
H	-1.41232500	2.35441000	2.48130500
H	-3.16193400	2.55559700	2.69436100
C	-3.72993400	3.26451200	0.06379100
H	-4.58982000	3.32975500	0.74305600
H	-3.82774900	4.06462600	-0.68112900
H	-3.78238200	2.30668200	-0.46814500
C	-2.45203400	4.77034200	1.56004300
H	-2.57261500	5.60022300	0.85385400
H	-3.30833600	4.80125600	2.24339300
H	-1.54719100	4.94364900	2.15629700

## I

C	0.52195200	-2.04145800	-0.17660500
C	1.56869600	-1.15602400	-0.22564100
N	0.99216000	0.03201500	0.28339900
C	-0.34397500	-0.14068400	0.69588400
C	-0.65066300	-1.43770300	0.39021300
C	-1.75079300	-2.41226300	0.37987500
C	-3.14101100	-2.12872400	0.73250700
C	-3.62540100	-0.81070700	0.77437800
C	-4.04516500	-3.14987100	1.04339900
C	-4.94018300	-0.52956500	1.09732400
H	-2.94524500	0.00663200	0.53267100
C	-5.37361500	-2.88694300	1.36041600
H	-3.69617200	-4.18010100	1.06550000
C	-5.83180600	-1.56869000	1.38638000
H	-5.30959800	0.49393200	1.14195600
H	-6.03636200	-3.71323400	1.60112900
S	1.88952800	1.41435800	0.60889600

O	0.94263200	2.38556700	1.15006800
O	2.66940400	1.75019200	-0.57834800
C	3.00930600	0.91204300	1.88319000
C	2.50615600	0.67329500	3.15896200
C	4.35745000	0.73029500	1.58728900
C	3.37503100	0.24519000	4.15173300
H	1.44846000	0.81926700	3.36901300
C	5.21105900	0.30354900	2.59592800
H	4.72517100	0.93274800	0.58382400
C	4.73563800	0.05496700	3.88731100
H	2.99500200	0.05391000	5.15367900
H	6.26961500	0.16139100	2.38281100
C	5.67129200	-0.37881600	4.97145000
H	6.45792200	-1.03609200	4.58541200
H	6.16916200	0.48705200	5.42695300
H	5.14426900	-0.90828000	5.77176000
H	-2.69053900	1.74432700	-1.20879400
Cu	3.36934800	-1.31981100	-0.80094800
N	5.14976100	-1.55875700	-1.39932400
C	6.22777900	-1.71267500	-1.79183700
C	7.56964900	-1.90227800	-2.28612500
H	7.78675300	-1.16361300	-3.06331000
H	8.28967700	-1.78573900	-1.47072100
H	7.67159900	-2.90588800	-2.70974600
C	0.21706900	-3.46861200	-0.48720200
C	-1.24651000	-3.57057700	-0.12415200
C	0.18156300	-4.01955500	-1.91537100
C	-1.84675600	-4.78479100	-0.76311900
C	-0.75795800	-5.22629500	-1.77480200
H	1.16777400	-4.28177200	-2.31628300
H	-0.26225400	-3.25932800	-2.57665700

H	-2.07912800	-5.58942600	-0.05122700
H	-2.79522000	-4.53019500	-1.25781100
H	-1.17844700	-5.55847800	-2.72978500
H	-0.19466000	-6.07378000	-1.36192700
O	-7.09716100	-1.19740400	1.68216300
C	-8.03440600	-2.21477000	1.95829000
H	-7.75742600	-2.79189100	2.85153900
H	-8.98895800	-1.71656600	2.14212900
H	-8.14963600	-2.90238200	1.10871300
H	0.81620200	-4.16006800	0.13246700
H	-0.88112500	0.68180300	1.14936900
C	-0.93429700	2.06138900	-2.17736600
C	0.16740300	2.89394900	-2.23884900
C	0.26181800	4.01473200	-1.41453500
C	-0.79243700	4.29876600	-0.54090700
C	-1.88124800	3.45895900	-0.45407000
N	-1.89136700	2.37140100	-1.26952500
H	0.97118000	2.67124700	-2.93401600
H	-0.73480600	5.17389700	0.09894400
C	1.48366700	4.86139400	-1.42493800
H	2.18382200	4.46382700	-0.67789100
H	1.99186600	4.83346800	-2.39329500
H	1.26503200	5.90038900	-1.16029200
C	-1.17471400	0.91157400	-3.13880000
C	-3.03337600	3.63127000	0.51873000
C	0.10906600	0.10049800	-3.32646600
H	-0.07554100	-0.69187900	-4.06244400
H	0.93978400	0.70592700	-3.70681700
H	0.43107400	-0.37307600	-2.38949400
C	-2.27916100	-0.02975000	-2.66123900
H	-2.03216300	-0.48238500	-1.69250100

H	-3.26847900	0.44976000	-2.60205400
H	-2.38592600	-0.84536000	-3.38478100
C	-1.59509300	1.54038100	-4.47659300
H	-1.79509900	0.74659600	-5.20651700
H	-2.50899600	2.13883900	-4.36953400
H	-0.80978800	2.18674100	-4.88633000
C	-2.70550600	2.83725800	1.79106500
H	-2.68083100	1.75621100	1.60470400
H	-1.73401600	3.13402300	2.20580200
H	-3.47797700	3.02075700	2.54813600
C	-4.34866600	3.12881400	-0.08420600
H	-5.16007300	3.30653000	0.63079000
H	-4.59964100	3.65583400	-1.01311000
H	-4.35644600	2.04735000	-0.28449200
C	-3.20345100	5.10580300	0.88523800
H	-3.33761400	5.73552100	-0.00259900
H	-4.09376700	5.21675700	1.51405600
H	-2.35526900	5.48987600	1.46290100

### TS<sub>i</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -863.2

C	-0.66020400	-0.55935200	1.19101300
C	0.52357700	-0.18040400	0.56497200
N	0.04244600	0.53674800	-0.58657300
C	-1.34269700	0.60115800	-0.61784900
C	-1.79897200	-0.09433600	0.47164100
C	-3.02825100	-0.57249300	1.11096400
C	-4.37401300	-0.46938700	0.55065200
C	-4.57890900	-0.40492700	-0.83789700
C	-5.50208800	-0.46444100	1.37509400

C	-5.85242000	-0.34428300	-1.37089700
H	-3.72036800	-0.43713400	-1.50867200
C	-6.78995900	-0.40339900	0.85399900
H	-5.36925900	-0.48397100	2.45535000
C	-6.97097700	-0.34289400	-0.52887300
H	-6.01642900	-0.30443400	-2.44506600
H	-7.64001300	-0.39434400	1.52984300
S	0.99781000	1.59764300	-1.52066200
O	0.59904900	1.42816700	-2.90735000
O	2.37381100	1.34417600	-1.10238700
C	0.48793000	3.20377500	-0.97952300
C	-0.31247900	3.97449900	-1.81929700
C	0.87683100	3.66420500	0.27602500
C	-0.72680500	5.22515400	-1.38590500
H	-0.59539700	3.59823900	-2.79885400
C	0.44730300	4.91605000	0.69156100
H	1.50976900	3.05422700	0.92001900
C	-0.35891200	5.71255900	-0.12766200
H	-1.34781100	5.84024900	-2.03498500
H	0.74490000	5.29004000	1.66966700
C	-0.83445700	7.05458300	0.33020200
H	-0.69613500	7.81340800	-0.44819300
H	-1.90649500	7.02935600	0.56286500
H	-0.30758500	7.38641600	1.23018200
H	1.29325900	-1.32631800	0.05576500
Cu	2.13924800	0.56111900	1.35846400
N	3.52511800	1.50055900	2.25844900
C	4.31781100	2.14868600	2.79900100
C	5.30873900	2.94880400	3.47508400
H	4.82376100	3.78154200	3.99320800
H	5.84350000	2.33678700	4.20754400

H	6.02419000	3.34709200	2.74947500
C	-1.14398500	-1.27894000	2.41078600
C	-2.64743800	-1.22402400	2.23860200
C	-0.95561900	-2.78156100	2.65979800
C	-3.30754200	-2.22475700	3.13071200
C	-2.12617400	-3.10909500	3.60078900
H	0.01624900	-3.04067100	3.09380100
H	-1.06223100	-3.32195500	1.70752700
H	-3.83013300	-1.77172100	3.98446900
H	-4.06610600	-2.79216700	2.57340700
H	-2.37288000	-4.17544300	3.60782900
H	-1.84814700	-2.83966800	4.62828900
O	-8.17185600	-0.27913600	-1.14387800
C	-9.32794500	-0.29252500	-0.33631100
H	-9.36543900	0.57739300	0.33445400
H	-10.18209400	-0.25208800	-1.01583100
H	-9.39334900	-1.21125100	0.26335400
H	-0.82755200	-0.73681600	3.31995400
C	3.37785200	-1.89685900	-0.30692500
C	4.34042100	-1.47656000	-1.20674100
C	3.99165300	-1.19781100	-2.53240900
C	2.70176500	-1.52294700	-2.94225500
C	1.75756600	-1.95487400	-2.01924700
N	2.07985400	-2.00043800	-0.70254300
H	5.37807600	-1.38223600	-0.89463600
H	2.43448200	-1.44378000	-3.99382200
C	4.97736200	-0.60542100	-3.47933100
H	4.77674400	-0.89848900	-4.51451000
H	4.90937100	0.48981700	-3.43259200
H	6.00614600	-0.88030400	-3.22507000
C	3.75198800	-2.47876200	1.05511900



C	0.43601600	-2.56783800	-2.47708800
C	2.58777800	-2.55357500	2.04160700
H	2.89855500	-3.14427500	2.91251300
H	2.26526200	-1.57201300	2.41715500
H	1.71695200	-3.05043000	1.59829900
C	4.17023600	-3.92883800	0.74216200
H	3.34364500	-4.48587700	0.28170700
H	5.02718900	-3.96408300	0.05913100
H	4.45259700	-4.44262300	1.67010700
C	4.93067200	-1.75557600	1.70287700
H	5.14155100	-2.20803100	2.67965900
H	5.84899500	-1.83382300	1.11004800
H	4.71857200	-0.69151400	1.86183300
C	-0.46092400	-2.98876300	-1.31680400
H	0.06720400	-3.65005200	-0.61724900
H	-0.85715400	-2.13395600	-0.76014100
H	-1.32001600	-3.54224800	-1.71478600
C	0.84426000	-3.84978400	-3.22938900
H	-0.05768900	-4.39278200	-3.53899000
H	1.43170600	-3.63336900	-4.12910500
H	1.43648100	-4.51502600	-2.58686000
C	-0.34969300	-1.66454600	-3.42625800
H	0.23770700	-1.35848400	-4.29955400
H	-1.22893200	-2.20846000	-3.79377500
H	-0.69384700	-0.75387500	-2.92547000
H	-1.86071600	1.12767500	-1.41255300

## 2a

C	-2.89584700	-2.59628800	-0.57211300
C	-3.28315100	-2.01712600	-1.91602500
C	-4.26784700	-3.08919500	-2.39678300

C	-5.08223600	-3.37704300	-1.12619500
C	-4.07629900	-3.27349100	0.04983300
H	-4.88934800	-2.77552600	-3.24287600
H	-5.86120200	-2.61094500	-1.01388500
H	-4.50811300	-2.71737200	0.89394500
C	-1.95199000	-1.79150300	-2.55121500
C	-1.35663900	-1.31910100	-3.67882600
N	0.02224300	-1.43195500	-3.47752200
C	0.28878600	-1.90961400	-2.18943400
C	-0.92615000	-2.15712200	-1.61526300
C	-1.55210800	-2.69611900	-0.40148800
C	-0.84418200	-3.31909800	0.71630300
C	0.42220100	-3.90087100	0.53995500
C	-1.40794600	-3.37498700	1.99450700
C	1.08215000	-4.51688200	1.58663200
H	0.88154500	-3.89400600	-0.44658300
C	-0.75678200	-3.99155600	3.05822100
H	-2.37203500	-2.90115800	2.17091000
C	0.49739100	-4.56943400	2.85664500
H	2.05861000	-4.97525200	1.44801900
H	-1.22923100	-4.00517100	4.03634700
S	1.17269000	-0.62680900	-4.42931200
O	2.44242200	-1.26887000	-4.13891200
O	0.61224600	-0.58704700	-5.76864200
C	1.19002800	1.01239200	-3.76536200
C	2.08020500	1.32660600	-2.74243100
C	0.28460200	1.94867100	-4.25566100
C	2.05586400	2.60616800	-2.20654700
H	2.79070400	0.58417600	-2.38729300
C	0.27655900	3.22263600	-3.70578200
H	-0.38747600	1.68332300	-5.06838800

C	1.15436800	3.56788200	-2.67381000
H	2.75193200	2.86957000	-1.41192900
H	-0.41950800	3.96822600	-4.08641500
C	1.11870100	4.93489900	-2.06584500
H	2.11665800	5.26455800	-1.75719900
H	0.48412300	4.94652600	-1.17005900
H	0.71232100	5.67566500	-2.76231800
H	-1.73469200	-0.95163400	-4.62362300
H	1.31224100	-2.03385800	-1.86180000
H	-3.78956300	-4.25796100	0.44549500
H	-5.59170600	-4.34570900	-1.16049600
H	-3.70205600	-3.97998200	-2.70390800
O	1.22061600	-5.19137100	3.81713700
C	0.66028200	-5.28554100	5.10562200
H	-0.28871200	-5.84058300	5.09893200
H	1.38173300	-5.82981900	5.71965700
H	0.49255600	-4.29509700	5.55265000
H	-3.83509600	-1.06960000	-1.78928800

## **A1**

C	3.03307400	2.25510800	0.27444600
C	2.20307400	1.37170700	0.18998200
N	1.28063700	0.39331800	0.08185600
C	0.40537200	0.35331000	-1.11023100
C	-1.02169300	0.31418400	-0.77203700
C	-2.25456500	0.42802700	-0.79694100
C	-3.65250500	0.69884800	-0.86616600
C	-4.59488600	-0.34584900	-0.92962000
C	-4.10488400	2.02515100	-0.88443100
C	-5.94087400	-0.06576400	-1.00899200
H	-4.25222500	-1.37914600	-0.92049500

C	-5.45799800	2.31282500	-0.96864400
H	-3.38216300	2.83618500	-0.83359200
C	-6.38544400	1.26589500	-1.02956500
H	-6.68389600	-0.85696700	-1.06310400
H	-5.78166400	3.34858200	-0.98555500
S	1.66225400	-1.10011700	0.83180100
O	0.39998500	-1.85892900	0.77696100
O	2.27216500	-0.77462600	2.10149100
C	2.81628500	-1.89692300	-0.22870600
C	2.36988200	-2.81981800	-1.17377200
C	4.16148100	-1.53427600	-0.13332500
C	3.29820500	-3.39158800	-2.03235700
H	1.32084800	-3.10144500	-1.21628600
C	5.06657900	-2.11751000	-1.00444000
H	4.48949100	-0.81764400	0.61542100
C	4.65232100	-3.05213500	-1.96202900
H	2.96887100	-4.12136700	-2.76936900
H	6.11999600	-1.85064700	-0.94194000
C	5.65105800	-3.69018500	-2.87296400
H	6.35557600	-2.95317600	-3.27401900
H	6.24539500	-4.43789100	-2.33260800
H	5.16645300	-4.19758200	-3.71260100
H	0.62053300	1.25912000	-1.68646500
H	0.67292500	-0.50149900	-1.74953700
C	3.98423000	3.28982000	0.44462400
C	4.65240300	3.92243300	-0.53653900
C	4.30298400	3.89255100	1.79698200
C	5.50142700	5.03125900	0.00025800
H	4.55035200	3.69585500	-1.59506100
C	5.55689100	4.72851900	1.50669100
H	4.45886200	3.13244400	2.57154700

H	3.45744800	4.51213100	2.13154800
H	6.49372700	5.07609200	-0.46546300
H	5.02463400	6.00325300	-0.20511700
H	5.61957000	5.63076600	2.12274900
H	6.44898800	4.12645000	1.71927100
O	-7.71273100	1.43314300	-1.10822600
C	-8.22702300	2.75243200	-1.15138600
H	-9.31125400	2.65489900	-1.22771000
H	-7.98085000	3.31020000	-0.23835700
H	-7.85453400	3.29904100	-2.02729000
Cu	-1.60074400	-1.00925800	0.63522600
N	-2.55013100	-2.13217500	1.88830700
C	-3.05016900	-2.80899600	2.68193600
C	-3.67153500	-3.65391200	3.67089600
H	-3.52396400	-3.22665200	4.66735700
H	-4.74423200	-3.73421400	3.47144100
H	-3.22440200	-4.65182500	3.63991200

### TS<sub>A1</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -468.6

C	-0.31016200	0.25946100	0.96929900
C	-1.51532600	0.74624700	0.89249800
N	-2.01176300	1.14286900	-0.31505100
C	-1.20226200	0.58512700	-1.43738800
C	0.11823900	0.31472700	-0.82475600
C	1.33109400	0.06923600	-1.18143800
C	2.53890600	-0.63852600	-1.15163600
C	2.53036100	-2.00004900	-0.76812000
C	3.77948400	-0.02190300	-1.45159500
C	3.70473500	-2.71915700	-0.67839700

H	1.57982500	-2.47525900	-0.53601600
C	4.94841400	-0.73348800	-1.36555700
H	3.79518900	1.02071300	-1.76394500
C	4.92528600	-2.08921700	-0.97784500
H	3.67287000	-3.76253900	-0.38143200
H	5.91011000	-0.28256300	-1.59409600
S	-3.69726900	1.27506100	-0.54544000
O	-3.83328500	1.59963600	-1.95751700
O	-4.17384300	2.15831400	0.50015600
C	-4.32019100	-0.35507500	-0.26669200
C	-4.60006100	-1.17232100	-1.35782400
C	-4.49398200	-0.80352600	1.04311700
C	-5.06429700	-2.46183200	-1.12796300
H	-4.47739100	-0.78916500	-2.36798700
C	-4.95263900	-2.09479200	1.24870200
H	-4.28244500	-0.14538300	1.88193800
C	-5.24749000	-2.93970000	0.17142600
H	-5.30009800	-3.10742500	-1.97211100
H	-5.09770600	-2.45886600	2.26464300
C	-5.77836300	-4.31642600	0.41773200
H	-5.74076700	-4.93346400	-0.48544200
H	-5.21736100	-4.82749900	1.20845400
H	-6.82460300	-4.27589900	0.74639600
H	-1.63571300	-0.37093100	-1.77759800
H	-1.15770700	1.26652900	-2.29181500
C	0.74941200	-0.24903700	1.80266700
C	0.81524800	-1.49513300	2.30112800
C	1.94395300	0.56625300	2.24152400
C	2.03545200	-1.69689900	3.14196700
H	0.04698700	-2.25116100	2.15315500
C	2.92005500	-0.49662100	2.76204300

H	1.63668500	1.28146900	3.02005600
H	2.37598400	1.17029800	1.42552100
H	1.76708600	-1.68975100	4.20959600
H	2.52271800	-2.66315700	2.95663200
H	3.59149800	-0.79557400	1.94481000
H	3.54495400	-0.14334100	3.58751700
O	6.11175000	-2.68858300	-0.92524600
C	6.17844700	-4.05796500	-0.54859200
H	7.23509200	-4.32676200	-0.57293500
H	5.79096700	-4.20889100	0.46645000
H	5.62797000	-4.68985000	-1.25605900
Cu	1.21305900	2.05024400	-0.50860500
N	1.57807300	3.83341900	0.01684700
C	1.68761300	4.92032700	0.39809100
C	1.82046000	6.27234300	0.87515900
H	2.63175300	6.77767500	0.34278000
H	0.88550600	6.81477800	0.70418400
H	2.04074700	6.26667400	1.94687500

## **B1**

C	-0.21619200	-1.25470000	-0.17461900
C	-1.56189000	-1.49935700	0.35552400
N	-1.82820200	-0.37042300	0.99493900
C	-0.80386400	0.68823700	0.97913300
C	0.29760800	-0.02339800	0.25069400
C	1.64636700	0.37650600	0.15243100
C	2.08128500	1.71412400	-0.03244300
C	1.24601300	2.75144200	-0.53576800
C	3.43005300	2.04963300	0.24624600
C	1.72137000	4.02152900	-0.72352200
H	0.21967200	2.52265900	-0.81174000

C	3.91876100	3.32710400	0.08647900
H	4.08495000	1.26446500	0.62275700
C	3.06120500	4.32852600	-0.40368600
H	1.09569900	4.81619800	-1.12058700
H	4.95214300	3.55094000	0.33195300
S	-3.30245300	-0.15300400	1.91818400
O	-3.06032000	1.07012200	2.66725300
O	-3.57961000	-1.41475800	2.57088300
C	-4.48812700	0.14724200	0.65136100
C	-4.77072300	1.46273300	0.29371300
C	-5.09492100	-0.93485200	0.01663900
C	-5.68909400	1.69309600	-0.72115300
H	-4.28975800	2.28654200	0.81616500
C	-6.00599600	-0.67967000	-0.99605800
H	-4.85457300	-1.95170400	0.31642000
C	-6.31767000	0.63111700	-1.37750400
H	-5.92957500	2.71537300	-1.00754000
H	-6.49351200	-1.51083900	-1.50264200
C	-7.32681500	0.88373600	-2.45208900
H	-7.24342600	0.14987100	-3.26103500
H	-8.34601500	0.80568700	-2.05236800
H	-7.21885400	1.88482100	-2.88136900
H	-1.17538100	1.57273800	0.44306300
H	-0.54892200	1.00025300	1.99836300
C	0.50224300	-2.18298100	-0.98466600
C	1.54663100	-1.86957200	-1.81361000
C	0.27876500	-3.67282300	-0.96796500
C	2.13889400	-3.09816400	-2.44186500
H	1.76652300	-0.85982700	-2.15566500
C	1.06002500	-4.16774800	-2.19169800
H	-0.78548300	-3.93021200	-0.98101000



H	0.68154900	-4.08332000	-0.02783500
H	2.36727300	-2.95659800	-3.50441700
H	3.09114800	-3.35982700	-1.95357700
H	1.47513700	-5.17140900	-2.05960900
H	0.38852600	-4.20550100	-3.05809400
O	3.42194700	5.58916900	-0.60783800
C	4.75659100	5.98600700	-0.31273300
H	4.81399200	7.04830400	-0.55297200
H	4.98465100	5.84096600	0.75003600
H	5.47726800	5.43535500	-0.92907800
Cu	2.83480800	-1.14542400	0.21066900
N	4.04300000	-2.58475700	0.59166800
C	4.75115300	-3.45941300	0.86271700
C	5.63405100	-4.54844700	1.19753300
H	6.25802500	-4.80063300	0.33491300
H	6.27697700	-4.26130500	2.03486100
H	5.04772800	-5.42705000	1.48349300

## A2

C	1.21966100	1.71487800	0.34059200
C	1.21388500	0.57411700	0.83087300
N	1.63070100	-0.56774000	1.40839000
C	0.79253000	-1.78253900	1.36662900
C	-0.57598200	-1.44622500	0.97569800
C	-1.78047000	-1.48584500	0.73566600
C	-3.17745700	-1.47384300	0.47333800
C	-4.07245200	-0.99135400	1.44775700
C	-3.67755100	-1.87245000	-0.77330500
C	-5.42112400	-0.91200600	1.17574100
H	-3.68862300	-0.67666100	2.41593400
C	-5.03398600	-1.79839100	-1.05282200

H	-2.98964300	-2.24465800	-1.52943800
C	-5.91403400	-1.31287200	-0.07760600
H	-6.12989200	-0.54862600	1.91559000
H	-5.39740000	-2.12231700	-2.02315800
S	3.31956100	-0.75593300	1.73369100
O	3.36489300	-1.83191900	2.70635000
O	3.79789000	0.58307700	2.00966700
C	3.97837200	-1.32363600	0.20011500
C	4.14217100	-2.69141000	-0.00378500
C	4.29123600	-0.39309900	-0.79275600
C	4.62292400	-3.13032200	-1.23060100
H	3.92012400	-3.39400700	0.79551900
C	4.76415900	-0.85571600	-2.00999500
H	4.19027200	0.67306000	-0.60299300
C	4.93342900	-2.22600300	-2.24896200
H	4.77016500	-4.19532800	-1.39970900
H	5.02263400	-0.14403300	-2.79228300
C	5.43881100	-2.70058400	-3.57409600
H	4.69234100	-2.53255400	-4.36068400
H	6.34218500	-2.15615600	-3.87198800
H	5.67323500	-3.76926400	-3.56004700
H	1.20870300	-2.50321400	0.64442100
H	0.80422300	-2.25285200	2.35616900
C	1.33736700	3.04905300	-0.11562000
C	0.75206700	3.59853800	-1.19572100
C	2.14577600	4.07314300	0.65584200
C	1.07094000	5.05581300	-1.30393000
H	0.09005100	3.06574100	-1.87578900
C	2.27041900	5.21937100	-0.35678900
H	3.11103900	3.67669400	0.99239500
H	1.59484600	4.37044800	1.56036800

H	1.28842200	5.36898300	-2.33228300
H	0.20604800	5.65587300	-0.97790700
H	2.31002000	6.20357700	0.11911000
H	3.19812600	5.09489100	-0.92851100
O	-7.23713300	-1.17914100	-0.24743200
C	-7.80818500	-1.59136300	-1.47690800
H	-8.88109600	-1.41079000	-1.39164600
H	-7.41216800	-1.00779800	-2.31891700
H	-7.63798000	-2.65999900	-1.66023400
Cu	-0.75342800	0.63819500	0.31425900
N	-2.36905000	1.53871900	-0.29386800
C	-3.44381900	1.87547600	-0.56043600
C	-4.79469100	2.26668200	-0.87897400
H	-4.92330600	3.34277300	-0.72949000
H	-5.01812600	2.01908900	-1.92135900
H	-5.48851200	1.72492300	-0.22565800

**TS<sub>A2</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -330.5

C	0.13262300	-1.84255600	-1.08458200
C	-1.16842700	-2.01202300	-1.02026800
N	-2.00585400	-0.93484200	-1.04740100
C	-1.24842900	0.30429600	-1.41314600
C	0.18263000	0.07028000	-1.04902800
C	1.22300600	0.75330400	-0.83149600
C	2.42679200	1.44457100	-0.69201600
C	3.18091200	1.79387900	-1.84160800
C	2.91184200	1.81910300	0.57966400
C	4.35904600	2.48527700	-1.71416800
H	2.81371000	1.50528600	-2.82376300

C	4.09241700	2.52116100	0.70945000
H	2.33992000	1.54519200	1.46493300
C	4.82600700	2.86028500	-0.43996100
H	4.95372400	2.76150000	-2.58050300
H	4.44607000	2.80125300	1.69679800
S	-2.90269600	-0.81048800	0.43529200
O	-1.93918000	-0.32353500	1.43734200
O	-3.56982800	-2.08091800	0.63049600
C	-4.05693700	0.46730800	0.07535700
C	-4.02014900	1.65908400	0.79624500
C	-5.01955200	0.22572400	-0.90216600
C	-4.97417500	2.62701500	0.52107500
H	-3.26058600	1.81123800	1.55935200
C	-5.95931200	1.21149300	-1.16317300
H	-5.03043500	-0.71553600	-1.44753800
C	-5.95294500	2.41976200	-0.45819500
H	-4.96696900	3.56294700	1.07727200
H	-6.71801500	1.04305100	-1.92472600
C	-6.96912400	3.48091200	-0.73662900
H	-7.53202200	3.73369700	0.16982600
H	-6.48842400	4.40526300	-1.07941200
H	-7.68424400	3.16775300	-1.50290000
H	-1.32665100	0.43097900	-2.49868600
H	-1.67653400	1.19018900	-0.93253800
C	1.31034500	-2.60149400	-1.39051300
C	2.56808800	-2.17076300	-1.59618200
C	1.20978400	-4.09967800	-1.58090800
C	3.48511800	-3.30369100	-1.94082500
H	2.87933000	-1.12906400	-1.59974300
C	2.67678700	-4.54500300	-1.53415900
H	0.73635600	-4.30862000	-2.55181500

H	0.58043400	-4.57380600	-0.81870200
H	3.70339100	-3.29352000	-3.02067500
H	4.45667200	-3.23868500	-1.43522900
H	2.93544500	-4.82116700	-0.50418500
H	2.87883100	-5.41567600	-2.16511300
O	5.97627000	3.53284900	-0.42604500
C	6.51407300	3.95361100	0.81917900
H	7.42860600	4.50001000	0.58402800
H	5.82208300	4.62194500	1.34609800
H	6.76218200	3.09513700	1.45542700
Cu	0.40230700	-0.85921400	0.83394000
N	0.97030100	-1.19495200	2.63607300
C	1.16711500	-1.49183000	3.73687700
C	1.40763500	-1.86650000	5.10836300
H	0.49778800	-2.29884800	5.53552900
H	2.21108600	-2.60780300	5.15592600
H	1.69424200	-0.98746400	5.69324500

## **B2**

C	0.38982700	-1.14248100	-0.30061600
C	-0.93239900	-0.86700400	-0.02196700
N	-1.04727100	0.47513200	0.30046600
C	0.24431100	1.17323300	0.31593100
C	1.20200700	0.04901700	-0.03119200
C	2.49716800	0.21502800	-0.05443300
C	3.83737300	0.44350500	-0.02642400
C	4.53163300	0.94964100	-1.17497000
C	4.59300000	0.16921200	1.15671800
C	5.87745300	1.16316700	-1.13394100
H	3.96188700	1.15364000	-2.07809800
C	5.94146800	0.39931900	1.20688700

H	4.06793400	-0.22621100	2.02263700
C	6.59761800	0.89637500	0.05747000
H	6.43005900	1.53963900	-1.99005500
H	6.49645300	0.19090400	2.11542600
S	-2.33064600	1.10282500	1.21041000
O	-1.83190500	1.47780900	2.52660400
O	-3.42345000	0.14540500	1.07723100
C	-2.71272800	2.57397000	0.31067700
C	-2.51387100	3.81351100	0.91134000
C	-3.22098500	2.46026400	-0.98127700
C	-2.83417700	4.95897300	0.19631600
H	-2.12390200	3.86969200	1.92455300
C	-3.53291600	3.61770900	-1.67851100
H	-3.36890300	1.47907900	-1.42942900
C	-3.34683000	4.87925500	-1.10214200
H	-2.69185100	5.93695000	0.65360200
H	-3.93443700	3.54702500	-2.68774200
C	-3.68031200	6.12734500	-1.85639200
H	-4.30971500	6.79523600	-1.25701500
H	-2.77232900	6.68891900	-2.10976600
H	-4.20845100	5.90842500	-2.78947300
H	0.26830000	1.96101000	-0.44699000
H	0.44192400	1.62003500	1.29778600
C	0.93615200	-2.40178400	-0.75000700
C	2.18729000	-2.64447400	-1.18218600
C	0.10618300	-3.66182800	-0.82877400
C	2.38699400	-4.07661000	-1.57877600
H	2.95677500	-1.88656600	-1.32061100
C	1.15648700	-4.77079900	-0.97527100
H	-0.56523100	-3.61281300	-1.70161400
H	-0.54155800	-3.79560100	0.05012800

H	2.41157700	-4.17375200	-2.67648300
H	3.33220100	-4.50178500	-1.21618700
H	1.41291800	-5.15541800	0.02000500
H	0.80514100	-5.61983800	-1.57051000
O	7.89046000	1.14317300	-0.00046700
C	8.71469800	0.90203700	1.14207400
H	9.72471100	1.18304700	0.84362200
H	8.39830000	1.52080300	1.98897800
H	8.69656700	-0.15810800	1.41722200
Cu	-2.45508900	-2.02554700	0.08068500
N	-3.90267000	-3.23099000	0.21693200
C	-4.81687300	-3.92642200	0.35620000
C	-5.95569300	-4.79320800	0.53197400
H	-6.32250400	-5.12930000	-0.44238200
H	-5.67066400	-5.66638300	1.12646800
H	-6.75580600	-4.25475500	1.04853200

### A3

C	-1.50735000	1.29013200	-0.76502400
C	-1.36303600	0.07682600	-0.88941800
N	-1.07030000	-1.20875600	-1.15156000
C	-0.03266900	-1.50190800	-2.17498300
C	1.25734900	-0.91029400	-1.86664800
C	2.30895100	-0.37753200	-1.58125400
C	3.55005800	0.23554800	-1.24603300
C	3.79223200	1.58761600	-1.54863400
C	4.55624600	-0.49700600	-0.60557500
C	4.99483500	2.17782700	-1.21828800
H	3.01939400	2.16596200	-2.05020800
C	5.77077800	0.08762200	-0.27196100
H	4.37563500	-1.54513200	-0.37228100

C	5.99554900	1.43298200	-0.57935100
H	5.19670600	3.22097200	-1.44809400
H	6.53540900	-0.50682300	0.22027400
S	-1.23368000	-2.32528500	0.15456200
O	-1.47660200	-3.61716400	-0.46347300
O	-2.22146100	-1.69961500	1.03225300
C	0.34064800	-2.32810600	0.93777200
C	1.20639500	-3.39575000	0.71951100
C	0.72111400	-1.21104700	1.68150000
C	2.47849400	-3.34105400	1.27205100
H	0.88439000	-4.25111200	0.13081600
C	1.99790500	-1.17639200	2.21733300
H	0.02935200	-0.38509200	1.83162300
C	2.89123600	-2.23752900	2.02456300
H	3.16854400	-4.16844100	1.11600400
H	2.31688700	-0.31026800	2.79428700
C	4.25951000	-2.19356700	2.62720000
H	4.62964000	-1.16580600	2.70695100
H	4.25027600	-2.61520400	3.64069200
H	4.97785000	-2.77827700	2.04166000
H	0.02333600	-2.59399800	-2.26484600
H	-0.42408700	-1.12871100	-3.12898100
C	-1.62176600	2.69573500	-0.60289900
C	-0.64689200	3.49498000	-0.13104500
C	-2.83247100	3.50036800	-1.02234600
C	-1.05942100	4.93161200	-0.15332700
H	0.33421300	3.14418400	0.18098300
C	-2.58334000	4.85339300	-0.34348100
H	-3.77753600	3.03105800	-0.71928600
H	-2.85907300	3.58701300	-2.11887300
H	-0.76232400	5.47917800	0.74917800



H	-0.56739900	5.44337700	-0.99580200
H	-2.99011900	5.69889900	-0.90592000
H	-3.06645800	4.85463800	0.64316000
O	7.13398800	2.09768200	-0.30452300
C	8.18382500	1.39181700	0.32372100
H	9.00152200	2.10424600	0.44988100
H	7.88454200	1.01485900	1.31155800
H	8.53352500	0.55323600	-0.29347000
Cu	-3.43158700	0.19347500	0.02962200
N	-4.10183400	1.30057900	1.51511300
C	-4.45547300	1.92560100	2.42267400
C	-4.89444400	2.70727600	3.55344800
H	-4.68005500	2.16943000	4.48187100
H	-4.36983600	3.66735700	3.56889500
H	-5.97109600	2.88918700	3.48724500
N	-4.39133100	-1.11723200	-1.14099100
C	-4.80018600	-2.05421800	-1.68375300
C	-5.29502300	-3.23567400	-2.34781800
H	-4.54344800	-4.02894400	-2.28320900
H	-6.21575400	-3.57665200	-1.86535100
H	-5.50060500	-3.02025200	-3.40037800

### TS<sub>A3</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -536.7

C	0.57393800	0.36404600	0.04343000
C	-0.64308200	0.36427500	-0.42525000
N	-1.01604500	-0.43800700	-1.47738000
C	0.00065700	-1.41916600	-1.93413500
C	1.27177100	-1.04612700	-1.31835800
C	2.50174200	-1.07993600	-1.19889300

C	3.85126300	-0.92829800	-0.86246700
C	4.61120100	0.12895000	-1.41663700
C	4.46200700	-1.78557300	0.07478200
C	5.91751300	0.32111400	-1.03593100
H	4.14608000	0.79022700	-2.14405600
C	5.77926500	-1.60604700	0.45197600
H	3.87945900	-2.59851600	0.50270100
C	6.51512300	-0.54659400	-0.10211800
H	6.51926900	1.12792600	-1.44537100
H	6.23166800	-2.28115600	1.17155600
S	-2.64509800	-0.81745700	-1.72166800
O	-2.72406000	-1.31412000	-3.08486100
O	-3.38990600	0.36242300	-1.28940300
C	-2.99121700	-2.14795700	-0.60965900
C	-2.97221800	-3.45687600	-1.08884600
C	-3.23141700	-1.87063100	0.73480500
C	-3.19993900	-4.49824000	-0.20145800
H	-2.79876000	-3.64600000	-2.14534800
C	-3.45594500	-2.92816300	1.60493300
H	-3.25087300	-0.84159500	1.08874600
C	-3.44417500	-4.25147900	1.15355500
H	-3.19550500	-5.52498900	-0.56361000
H	-3.64958700	-2.72767600	2.65730000
C	-3.70727300	-5.38752100	2.09054700
H	-3.69148800	-5.06321500	3.13555100
H	-4.69006400	-5.83525900	1.89610600
H	-2.96538800	-6.18502100	1.96811600
H	-0.28332700	-2.43810800	-1.62499100
H	0.06379300	-1.39971400	-3.02703400
C	1.57635400	1.10207800	0.73044300
C	2.46450700	0.60382100	1.61519100

C	1.88959500	2.55179400	0.41847700
C	3.47587800	1.62453000	2.02129200
H	2.47704100	-0.43200900	1.94815500
C	2.84568400	2.94683300	1.55140500
H	0.98347500	3.17048600	0.37210800
H	2.36695200	2.61910200	-0.57227300
H	3.70325800	1.60743800	3.09397800
H	4.42947100	1.42083100	1.50293500
H	3.58911800	3.68981100	1.24741700
H	2.26830200	3.38099100	2.37708600
O	7.78902200	-0.28125300	0.19524900
C	8.46562400	-1.12171500	1.11686900
H	9.47521200	-0.71859600	1.21083700
H	7.97973300	-1.10772000	2.10058300
H	8.52245600	-2.15320900	0.74746800
Cu	-1.94304800	1.67112000	0.28469500
N	-2.23787300	3.43276300	-0.78402000
C	-2.48402100	4.27599800	-1.53837700
C	-2.79141100	5.32641600	-2.48095800
H	-2.93096200	4.89961300	-3.47863300
H	-3.70933900	5.84194300	-2.18378400
H	-1.97202900	6.05051900	-2.51542800
N	-3.15187400	1.94576100	1.86800200
C	-3.88050500	2.15929600	2.74202400
C	-4.78784900	2.43003400	3.83216000
H	-5.45929100	3.25078100	3.56378900
H	-5.38442000	1.54023800	4.05372900
H	-4.22259800	2.71048600	4.72601400

**B3**

C	-0.44812900	-1.03867200	-0.01348200
---	-------------	-------------	-------------

C	0.78550900	-0.60074500	-0.45912800
N	0.57786800	0.40635400	-1.38151700
C	-0.83537900	0.78225300	-1.52936100
C	-1.50464500	-0.21033900	-0.59981600
C	-2.80005000	-0.22713900	-0.42490000
C	-4.16004400	-0.21766400	-0.35434900
C	-4.95671900	-0.97712200	-1.27348300
C	-4.83021800	0.56261000	0.63816900
C	-6.31830400	-0.94400800	-1.20389300
H	-4.45061100	-1.57930000	-2.02368600
C	-6.19785100	0.61605900	0.69722700
H	-4.22508800	1.12352800	1.34596600
C	-6.95438400	-0.13869300	-0.22757300
H	-6.94676800	-1.51082200	-1.88486200
H	-6.69060300	1.22202700	1.45068400
S	1.77202300	1.49023100	-1.87315400
O	1.27602400	2.06579100	-3.11363600
O	3.03309400	0.76440400	-1.81365400
C	1.78035200	2.75543400	-0.63522500
C	1.11001000	3.95094700	-0.87742400
C	2.42592900	2.51903800	0.57882700
C	1.08900700	4.92271500	0.11550100
H	0.63100800	4.11782500	-1.83926100
C	2.38992400	3.50052100	1.55635000
H	2.95273100	1.58115600	0.74609300
C	1.72538000	4.71446800	1.34115200
H	0.57580600	5.86585100	-0.06487800
H	2.89061800	3.33209600	2.50888500
C	1.72619600	5.77376600	2.39804700
H	1.58323900	5.34504000	3.39634800
H	2.68476200	6.30814000	2.41364300

H	0.94067000	6.51687800	2.22775300
H	-1.00706000	1.82257700	-1.21965000
H	-1.16774200	0.66579400	-2.56565400
C	-0.69293400	-2.15524000	0.86902400
C	-1.87857400	-2.68792200	1.21773600
C	0.43376400	-2.94242400	1.49734200
C	-1.72854300	-3.86690600	2.13319600
H	-2.84298000	-2.36913300	0.82502000
C	-0.26785900	-3.75233700	2.59566200
H	1.23846500	-2.29771700	1.88130400
H	0.89778500	-3.59377200	0.73788400
H	-2.43704600	-3.86264200	2.97221200
H	-1.90930300	-4.80821800	1.58819100
H	0.20352100	-4.72310400	2.78200600
H	-0.23309000	-3.18710200	3.53598200
O	-8.27255800	-0.15737800	-0.25840300
C	-9.01882900	0.63874100	0.66242800
H	-10.06832300	0.44699600	0.43724600
H	-8.80875400	0.34341000	1.69628900
H	-8.80354400	1.70338100	0.51879200
Cu	2.58021200	-1.22834900	-0.04689100
N	3.71018500	-2.54397500	-1.17798800
C	4.31275400	-3.11815800	-1.98293800
C	5.06492700	-3.83207800	-2.98904400
H	4.38667400	-4.23647200	-3.74601700
H	5.77259700	-3.15292600	-3.47342600
H	5.61910000	-4.65603800	-2.53028200
N	3.90457100	-0.98681600	1.48626400
C	4.65212900	-0.89501500	2.36600700
C	5.58344800	-0.78126600	3.46458400
H	6.50733700	-1.31825800	3.23013600

H	5.82132800	0.27096900	3.64677700
H	5.14469500	-1.20814500	4.37123900

#### A4

C	-0.44843200	0.28380100	-0.21803400
C	0.57154000	-0.12601300	0.37610300
N	1.08526100	-1.09799000	1.17432800
C	0.33988100	-2.39329500	1.31497700
C	-1.08776600	-2.21079400	1.19165800
C	-2.27334700	-2.02047800	1.02029100
C	-3.65308400	-1.77131700	0.77274200
C	-4.41774500	-0.98735100	1.65621500
C	-4.26524800	-2.26234200	-0.38686600
C	-5.73993300	-0.70228800	1.37972900
H	-3.95479300	-0.60451700	2.56350800
C	-5.59851600	-1.99144700	-0.66712500
H	-3.68140500	-2.86730800	-1.07758600
C	-6.34334400	-1.20419000	0.21760900
H	-6.34282800	-0.09782600	2.05264400
H	-6.04511200	-2.39712200	-1.56970200
S	2.77100600	-1.20413300	1.43430600
O	2.91599100	-2.11742100	2.55574700
O	3.25095300	0.16564600	1.50662000
C	3.40068200	-1.97615900	-0.02386700
C	3.68109900	-3.34161800	-0.00465100
C	3.56651000	-1.21374700	-1.17853300
C	4.14111100	-3.94419100	-1.16591200
H	3.55368600	-3.91112400	0.91262900
C	4.02252100	-1.83981400	-2.33030400
H	3.35027500	-0.14695300	-1.16907600
C	4.31615100	-3.20675700	-2.34229200

H	4.37386900	-5.00784800	-1.16473400
H	4.16006700	-1.25934100	-3.24087700
C	4.81704900	-3.87768700	-3.58180400
H	5.83022500	-4.27112700	-3.43381700
H	4.18401700	-4.73073400	-3.85376000
H	4.84431200	-3.19023400	-4.43264200
H	0.69253600	-3.09775500	0.54424600
H	0.61394100	-2.80248100	2.29329500
C	-1.65674700	0.84265700	-0.69137400
C	-2.32268100	0.45764900	-1.79776800
C	-2.46440900	1.83873200	0.11189200
C	-3.65150100	1.13444300	-1.89249800
H	-1.96809800	-0.29824400	-2.49469700
C	-3.52514000	2.29784400	-0.89481100
H	-1.84764200	2.65350300	0.51192900
H	-2.91711700	1.31937900	0.97149300
H	-3.90654000	1.45231200	-2.91070700
H	-4.43674800	0.42307900	-1.58262600
H	-4.47784400	2.56039700	-0.42434700
H	-3.15986600	3.19029500	-1.42388600
O	-7.63747300	-0.87681700	0.04370400
C	-8.30237900	-1.35446300	-1.10801500
H	-9.32680300	-0.98142200	-1.04880200
H	-7.83876700	-0.97576400	-2.02943200
H	-8.32532600	-2.45208000	-1.13776300
Cu	1.21370700	1.77003100	-0.11778800
N	1.08401500	2.58486000	2.02111300
C	1.42137100	2.09548500	3.01859700
C	1.84510400	1.46980100	4.25076700
H	1.30786000	0.52676100	4.39406300
H	2.91763400	1.25829500	4.20706200

H	1.64087600	2.12553700	5.10223000
N	3.16053400	2.34725300	-0.45306400
C	4.24761500	2.74320600	-0.46894100
C	5.60713800	3.23117300	-0.48025300
H	6.00161800	3.22251000	-1.50036600
H	5.63933200	4.25490300	-0.09626900
H	6.23489800	2.59471200	0.15036600
N	0.29251900	3.34280700	-1.10374800
C	-0.29187600	4.22049900	-1.58071500
C	-1.03131000	5.31498800	-2.16590900
H	-1.58089000	4.96863500	-3.04643600
H	-1.74083600	5.71647100	-1.43584000
H	-0.34609000	6.11259400	-2.46755100

#### TS<sub>A4</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -519.9

C	-0.59661700	-0.13768700	-0.18301300
C	0.64410300	-0.07692800	-0.57311400
N	1.07673400	0.91291800	-1.42885200
C	0.07958400	1.99126600	-1.68261700
C	-1.21932400	1.50508400	-1.22288500
C	-2.45245900	1.55914000	-1.13632300
C	-3.81395500	1.39854400	-0.85375400
C	-4.65366600	0.66420900	-1.72424300
C	-4.35932500	1.91540800	0.33789100
C	-5.97382200	0.45353900	-1.40643100
H	-4.24038900	0.26851100	-2.64924300
C	-5.68716700	1.70828300	0.66289500
H	-3.71732900	2.48467300	1.00652300
C	-6.50399000	0.97381200	-0.21064000



H	-6.63633500	-0.10697600	-2.06026000
H	-6.08495100	2.11865300	1.58558700
S	2.70231500	1.36957000	-1.52556400
O	2.75137900	2.29544200	-2.64752400
O	3.48433100	0.14391400	-1.52344900
C	3.03064400	2.26902300	-0.03658900
C	3.08953100	3.66082500	-0.07757700
C	3.19671900	1.57165900	1.15859600
C	3.32380800	4.35691200	1.09946600
H	2.97134200	4.18086800	-1.02495800
C	3.42465200	2.28866800	2.32510600
H	3.15408700	0.48412100	1.16944400
C	3.49394900	3.68486000	2.31435700
H	3.38204300	5.44407600	1.07909900
H	3.55806700	1.75817400	3.26647800
C	3.76082400	4.45518000	3.56890000
H	4.73878500	4.95035500	3.52344300
H	3.01350700	5.24335800	3.71809500
H	3.75476800	3.80813200	4.45149700
H	0.35404400	2.90312700	-1.12794600
H	0.06519900	2.23575400	-2.74932300
C	-1.67799200	-0.94213200	0.28892200
C	-2.42118800	-0.70004300	1.38431000
C	-2.24022500	-2.09987200	-0.50553100
C	-3.56330200	-1.65571100	1.50937100
H	-2.23934200	0.12241800	2.07338100
C	-3.23819500	-2.74380400	0.46799000
H	-1.45170500	-2.78651300	-0.84203700
H	-2.73256800	-1.71386400	-1.41268100
H	-3.68427700	-2.05315600	2.52556600
H	-4.50691100	-1.13213900	1.27821600

H	-4.13223700	-3.13171000	-0.03001700
H	-2.75727900	-3.59515200	0.96838400
O	-7.79754200	0.71851400	0.00455100
C	-8.40755200	1.22331800	1.18178800
H	-9.45121100	0.90750100	1.14305800
H	-7.93992900	0.80746200	2.08338000
H	-8.36474900	2.31924100	1.21620400
Cu	1.55420200	-1.72057500	0.11561300
N	1.80315900	-2.86635400	-1.80591200
C	2.27307000	-2.49204100	-2.79987000
C	2.85470400	-1.99936100	-4.02786400
H	2.36711600	-1.06159900	-4.31304500
H	3.92087800	-1.80455300	-3.88094200
H	2.72843100	-2.73003000	-4.83205000
N	3.46963200	-2.05295100	0.81055000
C	4.58111600	-2.29823200	1.02205400
C	5.96989400	-2.60242200	1.28137500
H	6.20748400	-2.41085600	2.33189400
H	6.17054700	-3.65464300	1.05894300
H	6.61117600	-1.97780300	0.65250300
N	0.54819600	-3.12985000	1.30601400
C	0.00448500	-3.85996700	2.02148900
C	-0.68152700	-4.76929600	2.91188500
H	-1.47903000	-4.24220500	3.44508900
H	-1.11880700	-5.59434700	2.34166700
H	0.02062400	-5.18003900	3.64342400

**B4**

C	0.80179100	-0.74606000	0.16135100
C	-0.48935900	-0.35612400	0.47305300
N	-0.41218500	0.90970400	1.03542200

C	0.92678100	1.51041100	0.95375600
C	1.73993600	0.33373200	0.46861800
C	3.04395400	0.36082000	0.36969600
C	4.40114900	0.43707800	0.29413700
C	5.22220200	0.04487800	1.40168500
C	5.04563900	0.91629800	-0.88861600
C	6.58071800	0.14895900	1.33358500
H	4.73570400	-0.32990300	2.29837800
C	6.41040200	1.00404800	-0.96861300
H	4.42426200	1.20615700	-1.73295900
C	7.18991100	0.62757800	0.14909200
H	7.22499000	-0.13145100	2.16198800
H	6.88508600	1.36383100	-1.87586800
S	-1.69024900	1.87650000	1.53643100
O	-1.12002500	2.77845700	2.52833700
O	-2.79642400	0.99528600	1.87343700
C	-2.11172800	2.83428400	0.10536400
C	-1.79904800	4.19098700	0.07997600
C	-2.72024600	2.20980400	-0.98078400
C	-2.11406600	4.93076900	-1.05161800
H	-1.32526300	4.65366500	0.94193100
C	-3.02208400	2.96715800	-2.10404800
H	-2.95128800	1.14621500	-0.94410200
C	-2.72999200	4.33383100	-2.15562400
H	-1.88132000	5.99424000	-1.08134100
H	-3.49777500	2.49208300	-2.96061400
C	-3.08397200	5.15319700	-3.35670700
H	-3.94241700	5.80358000	-3.14592300
H	-2.25554600	5.80651800	-3.65335400
H	-3.34785700	4.52482000	-4.21316700
H	0.94347800	2.32600300	0.21665500

H	1.25319900	1.90279200	1.92114300
C	1.24724000	-2.04413400	-0.31829900
C	2.34459400	-2.30871700	-1.04996000
C	0.60359000	-3.33624500	0.13107100
C	2.56958400	-3.78338300	-1.22143900
H	3.01422600	-1.55579300	-1.46351200
C	1.21192300	-4.37572200	-0.81335000
H	-0.49131100	-3.31136600	0.11352300
H	0.88807700	-3.52105600	1.18065400
H	2.86756200	-4.06433400	-2.24000700
H	3.37676000	-4.13699500	-0.55802400
H	1.28726100	-5.37546500	-0.37254800
H	0.57723800	-4.45457800	-1.70825900
O	8.50719900	0.68859100	0.17825700
C	9.22083900	1.15780400	-0.96624000
H	10.27629600	1.11353100	-0.69714700
H	9.03702600	0.51238300	-1.83214600
H	8.94721300	2.19295800	-1.19908400
Cu	-2.14972100	-1.32715400	0.05892000
N	-2.74784600	-2.57683300	1.90352100
C	-2.76237400	-2.03061700	2.92916600
C	-2.75886000	-1.32598200	4.19169300
H	-1.79244500	-0.83063800	4.33083000
H	-3.54118800	-0.56156300	4.19213800
H	-2.92720000	-2.02111600	5.01925600
N	-4.17005900	-0.93218200	-0.27589700
C	-5.31576800	-0.76596800	-0.25794800
C	-6.74583400	-0.55687500	-0.23087200
H	-7.13475200	-0.47391300	-1.24988800
H	-7.23733200	-1.39776200	0.26728600
H	-6.97935300	0.36263800	0.31414800

N	-2.26915700	-2.90467200	-1.48806900
C	-2.27257900	-3.76670500	-2.26192300
C	-2.26594600	-4.85358500	-3.21630300
H	-1.53834000	-4.65492100	-4.00872600
H	-1.99413700	-5.78613900	-2.71217600
H	-3.25660900	-4.97087800	-3.66513500

## A5

C	0.52601000	2.04528900	-1.29829100
C	1.03469700	1.02763200	-0.79315200
N	1.35959200	-0.27628600	-0.65662000
C	0.64148900	-1.28974400	-1.44050400
C	-0.77409900	-1.40281400	-1.03296200
C	-1.82193800	-0.90190000	-0.58584400
C	-3.02678600	-0.38885600	-0.05737900
C	-3.24965500	-0.42148100	1.33848300
C	-4.00982800	0.16465600	-0.89779400
C	-4.41517500	0.08010300	1.86496800
H	-2.48778100	-0.84533400	1.99028500
C	-5.18210000	0.67398600	-0.37169500
H	-3.84055400	0.18890900	-1.97182900
C	-5.39361300	0.63138600	1.01623200
H	-4.61019500	0.06518900	2.93374900
H	-5.93014300	1.09685500	-1.03514100
S	2.05848800	-0.79029800	0.83939800
O	1.18983700	-1.80172300	1.41516600
O	2.30242400	0.47475200	1.54761900
C	3.58023900	-1.50835500	0.34504700
C	3.80953800	-2.85733800	0.60209600
C	4.53593800	-0.70096100	-0.27582100
C	5.02877000	-3.40398900	0.22483800

H	3.05173300	-3.46027700	1.09555900
C	5.74136400	-1.27048700	-0.64329400
H	4.33840500	0.35105300	-0.47309100
C	6.00920300	-2.62471300	-0.39552600
H	5.22817900	-4.45562800	0.42018900
H	6.49866100	-0.65928500	-1.13014900
C	7.33156800	-3.21116900	-0.76770700
H	7.71741500	-2.77801000	-1.69648500
H	8.07409200	-3.00747000	0.01449000
H	7.27364900	-4.29714100	-0.88764800
H	0.70380500	-1.00295200	-2.49668400
H	1.18090800	-2.23719500	-1.33882200
C	-0.06770900	3.21068700	-1.83369200
C	0.16578700	3.69428800	-3.07114000
C	-1.14475500	4.00361000	-1.12410900
C	-0.72063000	4.85419500	-3.37652400
H	0.87068700	3.26333900	-3.77791900
C	-1.26104300	5.26318600	-1.99589500
H	-0.88060700	4.22485600	-0.08145900
H	-2.07974400	3.42470600	-1.09685800
H	-0.19498100	5.66340300	-3.89683900
H	-1.52381400	4.52958300	-4.05678000
H	-2.27957900	5.65860400	-2.03751100
H	-0.62231100	6.05188000	-1.58077100
O	-6.48789600	1.08841100	1.62257200
C	-7.52137100	1.66447900	0.83584500
H	-8.30013400	1.96980800	1.53577000
H	-7.16046500	2.54588600	0.29149100
H	-7.93677000	0.93519200	0.12955300
Cu	1.61291300	2.35519300	0.59447100
N	2.10935700	3.88467900	1.61673900

C	2.43857300	4.77884900	2.27315200
C	2.84635400	5.89200000	3.09121000
H	3.91129300	6.09322100	2.93963200
H	2.27183900	6.78330700	2.82093800
H	2.67326600	5.65935800	4.14645100
Cu	-1.73903100	-3.08105900	-0.59482100
N	-2.46127700	-4.78426900	-0.20048100
C	-2.90211700	-5.82246400	0.05814700
C	-3.45328000	-7.11235000	0.38190600
H	-3.32050100	-7.31472400	1.44922800
H	-4.52095700	-7.12913600	0.14298200
H	-2.94500500	-7.88986600	-0.19645000

### TS<sub>A5</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -460.2

C	-0.23251500	1.23022800	-0.77419100
C	1.06247200	1.08181000	-0.84227300
N	1.65436300	-0.18100400	-1.00653200
C	0.65020900	-1.18682400	-1.40842100
C	-0.65706700	-0.83026600	-0.81025500
C	-1.86321600	-1.14367000	-0.60561600
C	-3.25248700	-1.24856200	-0.59416800
C	-3.96893000	-0.89721300	-1.76350600
C	-3.97165700	-1.65103700	0.56015400
C	-5.34577800	-0.94338800	-1.78819200
H	-3.41827900	-0.59145500	-2.65045100
C	-5.33974100	-1.69645700	0.53900000
H	-3.42506800	-1.92097700	1.46191800
C	-6.04453200	-1.34253200	-0.63343800
H	-5.87743300	-0.67436200	-2.69513500

H	-5.91486600	-2.00154300	1.40892100
S	2.54200000	-0.60202800	0.40654600
O	1.55583900	-1.05253000	1.41273200
O	3.37417500	0.55313000	0.711107500
C	3.49516600	-1.97290400	-0.12413800
C	3.27432100	-3.22970200	0.43322800
C	4.47120700	-1.75286000	-1.09787000
C	4.05397900	-4.29061400	-0.00590700
H	2.51196300	-3.36756000	1.19598000
C	5.23190200	-2.82858800	-1.52035800
H	4.62156900	-0.76075300	-1.51823400
C	5.03761400	-4.10897500	-0.98320400
H	3.89912300	-5.28127000	0.41658500
H	5.99405800	-2.68190300	-2.28331800
C	5.88445600	-5.25198100	-1.43938100
H	6.08830500	-5.19582300	-2.51391100
H	6.85555500	-5.23791500	-0.92829800
H	5.41445200	-6.21639200	-1.22438500
H	0.55991600	-1.14079600	-2.49995800
H	0.97558900	-2.19805400	-1.14023800
Cu	2.15642600	2.63309200	-0.50429700
N	3.20704700	4.17737800	-0.21614900
C	3.91007600	5.06931300	0.00603100
C	4.78740000	6.17694300	0.28658200
H	4.76501900	6.89114900	-0.54218700
H	4.46748200	6.68174900	1.20331600
H	5.81062900	5.81216400	0.41759000
C	-1.42065500	1.99392200	-0.77046900
C	-1.85976900	2.77017800	-1.78811400
C	-2.36325400	2.06744400	0.41257700
C	-3.12636400	3.46741400	-1.43160300



H	-1.33182700	2.90204300	-2.73003600
C	-3.62188200	2.70466700	-0.19019200
H	-1.91256300	2.69160700	1.19937400
H	-2.55334700	1.08284500	0.86512800
H	-2.90526600	4.52295800	-1.20452200
H	-3.84652300	3.48659500	-2.25811100
H	-4.31499700	1.91184400	-0.50429900
H	-4.15698700	3.34444700	0.51641600
O	-7.36434200	-1.41609600	-0.54794200
C	-8.15876800	-1.07072900	-1.68025900
H	-9.19471000	-1.22890400	-1.37970100
H	-8.01456100	-0.01827000	-1.95151900
H	-7.92560800	-1.71490700	-2.53582400
Cu	-0.65399400	-0.59035900	1.21533200
N	-1.13244900	-0.39232400	3.07840500
C	-1.31115400	-0.36796100	4.22166600
C	-1.53352200	-0.34525200	5.64495000
H	-2.59878200	-0.21107900	5.85582000
H	-1.19673900	-1.28896100	6.08506100
H	-0.97182500	0.47789900	6.09647000

## **B5**

C	0.15256800	-0.80159400	-0.27177600
C	-1.18960800	-0.60629200	0.22905400
N	-1.15408300	0.49632700	0.96741400
C	0.15660400	1.14346100	1.03081800
C	0.99700200	0.18616800	0.24049500
C	2.40998800	0.17494600	0.18883600
C	3.23569100	1.30179800	0.03545300
C	4.62737900	1.19534300	0.34202600
C	2.77630900	2.54862800	-0.47977800

C	5.47883400	2.25078800	0.18589200
H	4.99426800	0.24723500	0.73351200
C	3.62198100	3.61362100	-0.65965600
H	1.73613400	2.64705600	-0.78261000
C	4.98711400	3.47736300	-0.31750100
H	6.53388400	2.18776700	0.43633600
H	3.24699000	4.54506400	-1.07202200
S	-2.52722800	1.09124500	1.90395300
O	-1.89559400	1.90747900	2.92004000
O	-3.30512900	-0.09553700	2.21001500
C	-3.39101300	2.08819100	0.74715400
C	-3.02451800	3.42513400	0.60156200
C	-4.42466400	1.52229600	-0.00017700
C	-3.70839000	4.20165500	-0.32191700
H	-2.23841900	3.85343900	1.21879800
C	-5.09269400	2.31939900	-0.91554300
H	-4.71542300	0.48560200	0.15780500
C	-4.74850500	3.66586900	-1.08921900
H	-3.44469000	5.25048300	-0.44260300
H	-5.90900000	1.89963300	-1.50017600
C	-5.50863300	4.52148600	-2.04871500
H	-5.79040600	3.96618600	-2.94942300
H	-6.43853000	4.87842900	-1.58780200
H	-4.93398100	5.40304300	-2.34804100
H	0.10893500	2.14272300	0.57327600
H	0.47652600	1.26920600	2.07144200
C	0.57435300	-1.88645300	-1.10503700
C	1.69947600	-1.88938500	-1.87800200
C	-0.10152200	-3.23446200	-1.15934500
C	1.92986400	-3.22603500	-2.51636100
H	2.26038200	-0.99510400	-2.14445100

C	0.57112000	-3.92873600	-2.35158000
H	-1.19269700	-3.14944300	-1.26800900
H	0.07174700	-3.76970400	-0.21210600
H	2.24743100	-3.14393400	-3.56166800
H	2.73495100	-3.76591700	-1.99311700
H	0.66182200	-5.01033300	-2.21923200
H	-0.02780900	-3.76041800	-3.25443000
O	5.88188500	4.43698600	-0.44172500
C	5.48840200	5.72274400	-0.92432300
H	6.39316400	6.33071800	-0.92287800
H	5.09747100	5.65235500	-1.94520400
H	4.74381800	6.17520700	-0.26011700
Cu	-2.76048300	-1.67668800	0.00209700
N	-4.31975600	-2.70932200	-0.26280800
C	-5.28616200	-3.33625700	-0.37527500
C	-6.48848000	-4.11682200	-0.51449100
H	-7.32765500	-3.46512600	-0.77582800
H	-6.35775500	-4.86551700	-1.30186100
H	-6.71069000	-4.62387800	0.42964500
Cu	3.15527200	-1.60458600	0.27939200
N	3.95669400	-3.29249900	0.69246000
C	4.47512600	-4.27876300	1.00696500
C	5.12498900	-5.50229500	1.40229700
H	5.64655900	-5.94133700	0.54652000
H	5.85070500	-5.29483800	2.19452400
H	4.38406600	-6.21533400	1.77602100

## A6

C	-1.07040800	2.03293700	1.44694500
C	-1.43339600	1.01362300	0.83271000
N	-1.55597900	-0.30028200	0.54283600

C	-0.57936600	-1.25916400	1.09678700
C	0.78477600	-0.98662100	0.63633300
C	1.73883200	-0.35861100	0.18077200
C	2.87449100	0.26574100	-0.39635700
C	3.09851400	0.16762400	-1.78626400
C	3.77866000	0.99475600	0.39103200
C	4.18419500	0.78895300	-2.36032400
H	2.39739100	-0.39989600	-2.39543900
C	4.87268600	1.62228100	-0.18146900
H	3.60994700	1.07034700	1.46318000
C	5.07823200	1.52620600	-1.56512700
H	4.37373900	0.73205500	-3.42888100
H	5.55839300	2.18460000	0.44480900
S	-2.31145600	-0.72552100	-0.94821600
O	-1.33589900	-1.41157700	-1.77508900
O	-2.91131800	0.54116100	-1.39469500
C	-3.56965000	-1.83888900	-0.44417300
C	-3.50010900	-3.16913300	-0.84681200
C	-4.61546400	-1.35979300	0.34837400
C	-4.50544100	-4.03653800	-0.43959900
H	-2.67963400	-3.51210600	-1.47172200
C	-5.60244200	-2.24418500	0.74240700
H	-4.65181400	-0.31476900	0.64909200
C	-5.56443100	-3.59229000	0.35536100
H	-4.47168900	-5.07961700	-0.74687200
H	-6.42595800	-1.89195100	1.36073000
C	-6.65284600	-4.52274800	0.78065100
H	-6.86871700	-4.41953900	1.85003100
H	-7.58406600	-4.29719300	0.24584900
H	-6.39806600	-5.56733800	0.57897600
H	-0.64012300	-1.19597100	2.18947300

H	-0.91293000	-2.26741200	0.81946000
C	-0.62671300	3.21001100	2.09288000
C	-0.93038200	3.55408300	3.36112300
C	0.34667100	4.18942800	1.47221800
C	-0.20532600	4.78831000	3.77921800
H	-1.58080400	2.97810700	4.01492900
C	0.30377500	5.37296000	2.45039800
H	0.05952400	4.46621400	0.44894000
H	1.34541600	3.73308300	1.40455900
H	-0.84055600	5.48016400	4.34487500
H	0.61988200	4.51573500	4.45584000
H	1.26931000	5.87618800	2.55118600
H	-0.41403800	6.11793500	2.08693900
O	6.09251700	2.10163600	-2.21934000
C	7.01814300	2.88733600	-1.48638500
H	7.73375500	3.27415400	-2.21358500
H	6.52031800	3.72976800	-0.98939900
H	7.55358400	2.28533600	-0.74134700
Cu	-2.21077800	2.39294400	-0.39740000
N	-2.80274800	3.92002700	-1.37268300
C	-3.22107200	4.79397000	-2.00508700
C	-3.74571500	5.88158800	-2.79059100
H	-4.81134500	6.01068700	-2.57775700
H	-3.21601400	6.80740700	-2.54633300
H	-3.61766000	5.66489500	-3.85561400
Cu	2.26907100	-2.64012600	0.48948200
N	2.31554400	-3.53932400	-1.27123200
C	2.37185200	-4.09317300	-2.28633700
C	2.44654600	-4.78815700	-3.54807500
H	1.71912300	-4.37127200	-4.25084400
H	3.45085300	-4.68450800	-3.96979400

H	2.23264500	-5.85099100	-3.39933000
N	3.10694500	-3.13235500	2.21077600
C	3.64668900	-3.45679600	3.18236900
C	4.32190600	-3.86306800	4.39038900
H	4.13756500	-4.92477500	4.58047600
H	5.39913400	-3.70362800	4.28273400
H	3.95764600	-3.27915600	5.24081400

### TS<sub>A6</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -501.5

C	-0.12259200	-0.07499400	0.92588000
C	1.12045900	-0.20692200	0.54522600
N	1.48965200	0.07792000	-0.74498900
C	0.48635000	0.76946900	-1.56714100
C	-0.82697000	0.47785000	-0.96361900
C	-2.08672100	0.64400500	-0.95746400
C	-3.32784400	1.16864300	-0.58371500
C	-3.35601100	2.42940800	0.06023500
C	-4.54921500	0.48579800	-0.80731700
C	-4.54759800	2.99473200	0.46086700
H	-2.41889900	2.95578300	0.22962200
C	-5.73594000	1.04341300	-0.41006800
H	-4.53025600	-0.48453600	-1.29903200
C	-5.75075700	2.30589600	0.22306100
H	-4.54891600	3.96592000	0.94505500
H	-6.68759300	0.54553100	-0.57357900
S	3.04637500	-0.19356900	-1.34033800
O	2.86024400	-0.52715400	-2.74541800
O	3.65208700	-1.14430000	-0.41309600
C	3.87074100	1.35677800	-1.21924000

C	3.88742000	2.20465200	-2.32364500
C	4.45006700	1.72557300	-0.00402500
C	4.50021300	3.44480400	-2.20192300
H	3.44567900	1.88756200	-3.26526400
C	5.05408100	2.96791800	0.09339700
H	4.44637500	1.04054400	0.84157200
C	5.08973700	3.84431100	-0.99984700
H	4.52958500	4.11518000	-3.05861500
H	5.52112000	3.26860900	1.02981400
C	5.77037200	5.16974600	-0.87901700
H	5.56163200	5.81162400	-1.73992900
H	5.45818800	5.69832200	0.02888000
H	6.85817000	5.04247600	-0.81458500
H	0.65133800	1.85813400	-1.54255400
H	0.55002500	0.42467900	-2.60502800
Cu	2.30655700	-1.04083500	1.81949700
N	3.41646000	-1.82203700	3.13700200
C	4.13024900	-2.29679800	3.91439700
C	5.01791300	-2.88799700	4.88313700
H	6.05538700	-2.76627200	4.55751200
H	4.88726800	-2.40097800	5.85422700
H	4.79862500	-3.95515300	4.98517000
C	-1.17764100	-0.05110000	1.86835200
C	-1.40476900	0.94335400	2.75679500
C	-2.23469100	-1.12778500	1.98388900
C	-2.60251800	0.67062100	3.59883600
H	-0.76542300	1.81662300	2.86776800
C	-3.31719700	-0.47049100	2.85227600
H	-1.80218100	-2.02238400	2.45558100
H	-2.61013300	-1.44600100	0.99788900
H	-2.28299900	0.37166300	4.60960400

H	-3.22805800	1.56176200	3.73527000
H	-4.09652800	-0.04563300	2.20565500
H	-3.80791800	-1.17583300	3.52832600
O	-6.95069800	2.75957600	0.55807100
C	-7.06544900	4.04514100	1.16185200
H	-8.13133000	4.20557800	1.32669700
H	-6.53987000	4.07782900	2.12361400
H	-6.67985200	4.82599700	0.49569300
Cu	-1.64723000	-1.37359900	-1.35991100
N	-3.15625000	-2.68576700	-1.50838600
C	-3.89789900	-3.56200300	-1.65855700
N	-0.07086800	-2.47921700	-1.97426400
C	0.88960200	-3.02194300	-2.32661800
C	-4.82254600	-4.65243100	-1.84666300
H	-5.00473000	-5.15508400	-0.89189300
H	-5.77163300	-4.27432800	-2.23790200
H	-4.40677400	-5.37382000	-2.55642600
C	2.09608900	-3.68288600	-2.75899700
H	1.87523100	-4.37227700	-3.57899800
H	2.81291400	-2.92550600	-3.09563600
H	2.53146000	-4.24217300	-1.92516800

## **B6**

C	0.15340000	-0.78323400	0.26496700
C	1.53896100	-0.75643900	-0.12201900
N	1.69227100	0.32864500	-0.88102800
C	0.47655400	1.12545300	-1.05265800
C	-0.53038500	0.28926900	-0.32007700
C	-1.92544100	0.45670400	-0.37474700
C	-2.60342300	1.68531900	-0.24712100
C	-3.94064100	1.80722000	-0.72747100



C	-2.03601600	2.82042500	0.39798800
C	-4.63406700	2.98064500	-0.61994400
H	-4.39583300	0.94366600	-1.20918200
C	-2.73213800	3.99600700	0.54330000
H	-1.03955600	2.74208600	0.82887000
C	-4.03932300	4.09164200	0.01940300
H	-5.64187700	3.09419100	-1.00935000
H	-2.27905100	4.83518300	1.06159600
S	3.18101100	0.77220000	-1.69358100
O	2.73984900	1.30300500	-2.96755200
O	4.02876200	-0.40188600	-1.58227900
C	3.78564700	2.06339700	-0.67003900
C	3.50419800	3.38337100	-1.01461700
C	4.50688300	1.73572000	0.47821000
C	3.96464700	4.39499200	-0.18370100
H	2.95502900	3.60684300	-1.92660800
C	4.95367900	2.76343000	1.29173300
H	4.72392500	0.69618700	0.71489900
C	4.69358600	4.10326300	0.97359000
H	3.76698600	5.43400700	-0.43993800
H	5.52604900	2.53054000	2.18779600
C	5.21762200	5.19892700	1.84368200
H	5.14770000	4.93885500	2.90528200
H	6.27795900	5.38462200	1.62965100
H	4.68231600	6.13896000	1.67922800
H	0.60511900	2.11742200	-0.59393200
H	0.25423800	1.27087700	-2.11618200
C	-0.48287200	-1.79481000	1.05051400
C	-1.67731200	-1.64312000	1.69549000
C	-0.00740900	-3.22139200	1.15129800
C	-2.15883300	-2.93952100	2.27890000

H	-2.12738800	-0.67912800	1.93011600
C	-0.90049500	-3.82546500	2.24472500
H	1.06617000	-3.28990100	1.38008500
H	-0.14093600	-3.71944100	0.17749900
H	-2.57094400	-2.81990400	3.28736200
H	-2.96921400	-3.36045700	1.66310600
H	-1.12599400	-4.88204400	2.07384200
H	-0.38743700	-3.75544500	3.21135900
O	-4.79081200	5.17645500	0.08781500
C	-4.28352100	6.35598200	0.71050100
H	-5.07669800	7.09993400	0.63142400
H	-4.05877200	6.17470000	1.76748600
H	-3.39098800	6.72078600	0.18989000
Cu	2.94615500	-2.00110300	0.25507900
N	4.31084600	-3.24233000	0.66839100
C	5.19171500	-3.97159300	0.84609900
C	6.28818700	-4.87923800	1.06803800
H	7.18234000	-4.31653800	1.35356000
H	6.03540100	-5.58178700	1.86739400
H	6.49735800	-5.43763700	0.15030500
Cu	-2.89200400	-1.25509200	-0.44598200
N	-2.97177600	-3.05172000	-1.35651200
C	-3.07880200	-4.03736000	-1.95471400
C	-3.21639800	-5.26334800	-2.70357500
H	-4.23990300	-5.35655800	-3.07867800
H	-2.52564000	-5.26241700	-3.55207900
H	-2.99272200	-6.12198800	-2.06363700
N	-4.85763500	-1.34359600	0.46245600
C	-5.90767700	-1.38639400	0.95020400
C	-7.21820700	-1.44232500	1.55541500
H	-7.98890300	-1.31170200	0.78988700

H	-7.36469500	-2.41144500	2.04173200
H	-7.32164600	-0.65075900	2.30343800

### A7

C	0.96582600	-2.67200000	1.31941000
C	1.45407400	-1.62079100	0.86451200
N	1.67895700	-0.28608300	0.77510400
C	0.75135000	0.64380900	1.44919500
C	-0.61955300	0.57389800	0.93421200
C	-1.69617000	0.13795000	0.53246100
C	-2.96540700	-0.33349900	0.09656400
C	-3.31124000	-0.30716200	-1.26807900
C	-3.90633400	-0.79163100	1.02793900
C	-4.55828200	-0.72615800	-1.67810000
H	-2.58466700	0.05579900	-1.99237400
C	-5.16339100	-1.21647100	0.62165900
H	-3.64646700	-0.80861800	2.08421700
C	-5.49629200	-1.18343100	-0.73812100
H	-4.84526900	-0.71680900	-2.72637100
H	-5.87267000	-1.57501200	1.36157700
S	2.37208100	0.25507700	-0.70933400
O	1.32556100	0.74815300	-1.58713800
O	3.19628900	-0.88998200	-1.12663700
C	3.39073900	1.58139800	-0.18166600
C	3.00689700	2.88369500	-0.48984800
C	4.55613800	1.30159200	0.53416200
C	3.82266300	3.92787300	-0.07315600
H	2.08893700	3.06886000	-1.04480500
C	5.34974600	2.35962500	0.93954900
H	4.83421300	0.27454600	0.75981800
C	5.00002300	3.68446400	0.63945500

H	3.55110000	4.95369100	-0.31557800
H	6.26557900	2.16333000	1.49396300
C	5.88910600	4.80661500	1.06731500
H	6.15206600	4.72319700	2.12804300
H	6.83172200	4.78825800	0.50650300
H	5.42333600	5.78283300	0.90209000
H	0.76544100	0.38996600	2.51589300
H	1.17743600	1.65178100	1.35764600
C	0.35921400	-3.87416000	1.74514500
C	0.57395200	-4.46763900	2.93775100
C	-0.71377800	-4.59407500	0.95515400
C	-0.31893500	-5.64703400	3.12583500
H	1.27053800	-4.10238500	3.68849600
C	-0.84495000	-5.92636000	1.70761900
H	-0.44057400	-4.71990600	-0.10037900
H	-1.64425700	-4.00762200	0.97202700
H	0.19784700	-6.50212600	3.57724800
H	-1.12877000	-5.38156100	3.82368400
H	-1.86547100	-6.31890100	1.70230000
H	-0.20474500	-6.67780500	1.23005700
O	-6.68128800	-1.56227500	-1.23849600
C	-7.67724300	-2.02211300	-0.34286800
H	-8.54199600	-2.28601600	-0.95435500
H	-7.34401600	-2.91115500	0.20778300
H	-7.96852200	-1.23836500	0.36935900
Cu	2.42226200	-2.85566200	-0.37152100
N	3.16596800	-4.28320200	-1.40166100
C	3.66004800	-5.09522100	-2.06118500
C	4.27689600	-6.10411600	-2.88435200
H	5.33827400	-6.18881700	-2.63224000
H	3.79072100	-7.07019400	-2.71840000

H	4.18109900	-5.83043700	-3.93939800
Cu	-1.42795700	2.44505300	0.15312500
N	-1.22545400	2.75239700	-1.92108500
C	-1.05371700	2.92838700	-3.05262400
C	-0.83981900	3.14191300	-4.46566800
H	-0.11257600	2.41853600	-4.84634400
H	-1.78127200	3.02040200	-5.00931300
H	-0.45992400	4.15303300	-4.63877800
N	-3.42253100	2.91113100	0.46339100
C	-4.57823500	2.90412700	0.53754400
C	-6.01922800	2.87855900	0.63366600
H	-6.41072400	3.89383600	0.74499600
H	-6.44251500	2.43041500	-0.27047100
H	-6.32093300	2.28173200	1.49995000
N	-0.26955000	3.89086200	1.02886500
C	0.13753500	4.82627100	1.57791300
C	0.64085300	5.99438100	2.26101300
H	0.41470300	6.89317200	1.67931100
H	0.16913800	6.08339100	3.24428400
H	1.72394800	5.91632900	2.39385000

### TS<sub>A7</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -477.4

C	0.14204200	-1.01765000	-0.55174200
C	1.30856300	-0.44147400	-0.47566900
N	1.51513700	0.64145700	0.34609100
C	0.46308000	0.89309000	1.34545600
C	-0.77597100	0.31201200	0.80533500
C	-2.00729100	0.05399800	0.89114500

C	-3.19774100	-0.65905500	1.08187900
C	-3.14045900	-1.90124200	1.75462700
C	-4.44579300	-0.19652000	0.60064900
C	-4.27980100	-2.65742200	1.94606800
H	-2.18084100	-2.25708900	2.12410400
C	-5.58093400	-0.94049300	0.79545800
H	-4.49173500	0.75817800	0.08007400
C	-5.51198500	-2.17706000	1.47181600
H	-4.21876200	-3.60813300	2.46676100
H	-6.55207900	-0.60309500	0.44444700
S	2.99125000	1.45549300	0.40422900
O	2.67076900	2.77002000	0.93812900
O	3.57380900	1.30581100	-0.92575100
C	3.97758400	0.57054500	1.56617400
C	4.00907600	0.99699500	2.89144500
C	4.67211600	-0.56555900	1.14828700
C	4.75280400	0.26804700	3.80938200
H	3.47554700	1.89644200	3.18986500
C	5.40416600	-1.28001100	2.08377500
H	4.65489700	-0.87268300	0.10217800
C	5.45856300	-0.87521100	3.42328900
H	4.79404300	0.59465500	4.84664800
H	5.95791600	-2.16498200	1.77477800
C	6.28387400	-1.63362100	4.41259800
H	5.90808900	-1.50776900	5.43288000
H	6.30846400	-2.70378200	4.18241600
H	7.32187300	-1.27739900	4.40287500
H	0.70708500	0.39204200	2.29602800
H	0.35605400	1.96879300	1.52605600
Cu	2.68582400	-1.18471800	-1.60071700
N	4.08309400	-1.88017800	-2.67430900

C	4.96854900	-2.22411000	-3.33547500
C	6.07280400	-2.64843400	-4.15781500
H	6.26851400	-3.71341600	-4.00012700
H	5.83622200	-2.48036600	-5.21295500
H	6.96900100	-2.07672700	-3.89753900
C	-0.78459000	-1.99452400	-0.98069700
C	-0.80034700	-3.28092400	-0.56273100
C	-1.89927700	-1.73552500	-1.97163400
C	-1.88336800	-4.06197100	-1.22468000
H	-0.08059900	-3.70173700	0.13675600
C	-2.79382800	-2.97359600	-1.81988300
H	-1.47732100	-1.63941800	-2.98298900
H	-2.43085500	-0.79662500	-1.76252400
H	-1.44902700	-4.71168800	-2.00094600
H	-2.40129500	-4.73405700	-0.52840100
H	-3.59941600	-2.75114500	-1.10662000
H	-3.26420700	-3.28087300	-2.75812000
O	-6.66900800	-2.81472400	1.61385700
C	-6.69293700	-4.06080300	2.30046000
H	-7.73748500	-4.37378400	2.32097100
H	-6.10022600	-4.81550500	1.76972700
H	-6.32715700	-3.95329800	3.32864400
Cu	-1.77724800	1.69434000	-0.51024300
N	-3.20396000	1.87915500	-1.96123100
C	-3.91250200	2.09763500	-2.85038800
N	-0.21469800	2.79783000	-1.22703700
C	0.70654700	3.43935600	-1.51028800
C	-4.79446400	2.37521400	-3.95867700
H	-4.50073700	1.78059400	-4.82885800
H	-5.82609900	2.12853700	-3.69074200
H	-4.73975700	3.43633400	-4.21959600

C	1.85998600	4.23256600	-1.86224900
H	1.65124800	4.82029700	-2.76097600
H	2.10991600	4.90526200	-1.03673800
H	2.71418100	3.57248900	-2.04598400
N	-2.57664200	3.20153300	0.96211700
C	-3.03562800	3.99711300	1.66855500
C	-3.61093600	4.98831400	2.54867800
H	-2.85443900	5.35382400	3.24918200
H	-3.98850000	5.83291400	1.96487300
H	-4.43772600	4.55079000	3.11583800

### **B7**

C	-0.32319800	-0.52728700	-0.46616600
C	-1.64646900	-0.49972500	0.08009900
N	-1.67083800	0.47991600	0.99157000
C	-0.40342400	1.19555500	1.12359500
C	0.47034200	0.42640200	0.17912900
C	1.86624800	0.59360500	0.11192800
C	2.52233000	1.80472400	-0.16644200
C	3.91821500	1.93400500	0.10264800
C	1.86364900	2.91733700	-0.76476300
C	4.58805200	3.09541000	-0.16227200
H	4.43155200	1.08307700	0.54832300
C	2.52777900	4.08328300	-1.05471200
H	0.81186500	2.82409900	-1.03022600
C	3.90101000	4.18684100	-0.74092800
H	5.64552900	3.21652300	0.05532900
H	2.00363300	4.90764400	-1.52781400
S	-3.04047400	0.85677700	2.00145300
O	-2.46296400	1.66675100	3.05632600
O	-3.70550600	-0.40798700	2.25668800



C	-4.04352100	1.84449200	0.94664300
C	-3.80760200	3.21739200	0.87914700
C	-5.04156700	1.23362000	0.19062600
C	-4.59223300	3.98317300	0.03211700
H	-3.04143400	3.67678800	1.49954500
C	-5.81518500	2.02225400	-0.64973900
H	-5.22116800	0.16348800	0.27981700
C	-5.60506100	3.40150200	-0.74124000
H	-4.43156100	5.05823100	-0.02582700
H	-6.60778500	1.56431500	-1.23828300
C	-6.45601300	4.25516800	-1.62501200
H	-7.10059200	3.65400100	-2.27314100
H	-7.10111900	4.90964700	-1.02584200
H	-5.84312100	4.90718200	-2.25795200
H	-0.51109600	2.24465900	0.80913100
H	-0.06135000	1.19297800	2.16413900
C	0.15690600	-1.44346600	-1.46589400
C	1.31374000	-1.30855900	-2.15233100
C	-0.48828500	-2.77583500	-1.75776000
C	1.65786900	-2.54459800	-2.92067800
H	1.91719300	-0.40292700	-2.17567900
C	0.33388200	-3.32919100	-2.93459400
H	-1.55760400	-2.67919800	-2.00268900
H	-0.43721000	-3.41945300	-0.86326400
H	2.04070800	-2.33873600	-3.92735000
H	2.45541300	-3.09166600	-2.39097200
H	0.47925000	-4.41284100	-2.87913300
H	-0.19439400	-3.12650900	-3.87369500
O	4.63236800	5.26488000	-0.96071900
C	4.02937900	6.42828100	-1.52535800
H	4.82155200	7.17481400	-1.58765500

H	3.64486400	6.22218500	-2.53062700
H	3.22594400	6.80258900	-0.88129700
Cu	-3.12812700	-1.66367000	-0.26638900
N	-4.63395700	-2.76501900	-0.56588000
C	-5.56512300	-3.43878600	-0.70238600
C	-6.72153100	-4.28057800	-0.87391700
H	-6.77106800	-4.64020900	-1.90594300
H	-6.65876500	-5.13781800	-0.19672300
H	-7.63041600	-3.71518000	-0.64623000
Cu	2.90765500	-1.05895700	0.43424100
N	2.31139300	-3.04680200	0.66363300
C	1.96396300	-4.14747600	0.75852700
C	1.51995900	-5.51914200	0.86408600
H	1.35099600	-5.93495200	-0.13422300
H	2.27724500	-6.12249100	1.37322200
H	0.58717400	-5.56798000	1.43383100
N	4.58575400	-1.42911400	-0.88383300
C	5.50430100	-1.62820900	-1.56108900
C	6.65079700	-1.88069600	-2.40410600
H	7.57241800	-1.65707500	-1.85846600
H	6.66760300	-2.93090500	-2.70945200
H	6.60815900	-1.25203900	-3.29820400
N	4.08537500	-1.00328200	2.28346900
C	4.60996500	-1.02093200	3.31634300
C	5.26347100	-1.04592900	4.60535600
H	6.00703700	-0.24571400	4.66639800
H	4.52578800	-0.90652800	5.40113400
H	5.76488500	-2.00708900	4.75262400

**J**

C	-1.81938300	-0.31029700	-2.08230300
---	-------------	-------------	-------------

C	-2.66842200	0.42478400	-1.22327200
N	-1.85025700	1.30994800	-0.60341000
C	-0.43471700	1.21092800	-1.00501200
C	-0.51342300	0.12095400	-2.00023200
C	0.37090400	-0.66465800	-2.83391800
C	1.83014300	-0.56032900	-2.88505000
C	2.53351400	0.31949100	-2.04412800
C	2.58440200	-1.33857300	-3.77237500
C	3.91687400	0.39593500	-2.07601700
H	2.01354900	0.97672600	-1.34931200
C	3.97177100	-1.27615900	-3.81200100
H	2.08330800	-2.00122000	-4.47292600
C	4.65123400	-0.40628100	-2.95757800
H	4.45454400	1.09724400	-1.43992900
H	4.50973500	-1.89403600	-4.52474500
S	-2.36958100	2.52231600	0.50598900
O	-1.29252700	2.59032200	1.48143700
O	-3.72256600	2.13995600	0.88266000
C	-2.39039500	3.99324500	-0.45133500
C	-1.26921700	4.82237800	-0.43472400
C	-3.51751500	4.28683100	-1.21698500
C	-1.29250200	5.97508700	-1.20447400
H	-0.40923600	4.56954700	0.18193900
C	-3.51467600	5.44550100	-1.97779100
H	-4.38330600	3.62827000	-1.20383600
C	-2.40965500	6.30500100	-1.98034100
H	-0.43157300	6.64100500	-1.19948900
H	-4.38729000	5.69949000	-2.57633300
C	-2.42943700	7.57122900	-2.77377200
H	-3.16908500	7.53305600	-3.57920100
H	-2.68754900	8.42331900	-2.13194300

H	-1.44887100	7.78608800	-3.21159400
H	0.17981500	0.95704700	-0.12894000
H	-0.05470300	2.16637800	-1.39352300
Cu	-4.49662900	0.20147400	-0.70275900
N	-6.33021200	-0.02326700	-0.28658200
C	-7.41834100	-0.15179000	0.08561200
C	-8.77013200	-0.30692500	0.56071600
H	-8.79647700	-0.13317400	1.64078800
H	-9.42696600	0.41341400	0.06388300
H	-9.12632000	-1.31949300	0.34721500
C	-1.89453800	-1.39534300	-3.08695500
C	-0.45076200	-1.58407200	-3.44759100
C	-2.32804000	-2.83226700	-2.78934800
C	-0.26134800	-2.90806000	-4.10955200
C	-1.62671600	-3.60912300	-3.91561200
H	-3.41448300	-2.96552300	-2.77919700
H	-1.94200800	-3.12931500	-1.80201100
H	0.02007500	-2.82963500	-5.16878400
H	0.55800100	-3.45558100	-3.61801600
H	-1.52198000	-4.67718600	-3.69720400
H	-2.21925100	-3.52766400	-4.83528700
O	5.99587700	-0.26371600	-2.92455800
C	6.74731800	-0.94767900	-3.91179800
H	6.41406800	-0.68075200	-4.92285000
H	7.78561500	-0.63020200	-3.79423900
H	6.68474300	-2.03761300	-3.78611500
C	1.08345400	-1.86794700	1.22729800
C	2.07204600	-0.86548700	1.34875500
N	1.47503300	0.13382900	2.04466700
C	0.06259800	-0.14130600	2.39800200
C	-0.11514100	-1.47404500	1.78615100

C	-1.13653300	-2.48911700	1.62406600
C	-2.56779400	-2.35777000	1.90369800
C	-3.17490700	-1.10305200	2.08429400
C	-3.39308600	-3.48655000	1.96356200
C	-4.53798000	-0.98440000	2.29133700
H	-2.58399900	-0.18961000	2.05852500
C	-4.76452100	-3.38478800	2.16793800
H	-2.95514700	-4.47775800	1.87176000
C	-5.34672900	-2.12624500	2.32829900
H	-4.99866600	-0.00994000	2.43792800
H	-5.36464000	-4.28896100	2.21200300
S	2.06183600	1.75987700	2.13634800
O	1.30330400	2.33994300	3.22700000
O	1.99419800	2.32268900	0.79182200
C	3.75252900	1.52564900	2.57186500
C	4.06479200	0.89582200	3.77775000
C	4.74153600	2.00512100	1.71870600
C	5.39743000	0.72839200	4.11206900
H	3.27690000	0.53718700	4.43719100
C	6.07262900	1.83953900	2.08285600
H	4.46850800	2.51221700	0.79605000
C	6.41974900	1.19588900	3.27270500
H	5.66039100	0.23301600	5.04515400
H	6.85859900	2.21760600	1.43088200
C	7.85125800	1.01162000	3.66182600
H	8.06143500	-0.03225900	3.92316500
H	8.53176400	1.31169100	2.85886500
H	8.09632000	1.61231000	4.54638200
H	-0.57911500	0.66645600	2.02058200
H	-0.06190800	-0.15681300	3.48968900
Cu	3.86125300	-0.88483200	0.66159100

N	5.69922700	-1.08513100	0.19809200
C	6.79510000	-1.08107900	-0.17380200
C	8.16832000	-1.05809700	-0.61308400
H	8.33202300	-0.18608000	-1.25444000
H	8.83522200	-1.00067100	0.25289900
H	8.39897900	-1.96845200	-1.17513100
C	0.95242000	-3.26526300	0.74940200
C	-0.49661100	-3.54315300	1.01426500
C	1.05442300	-3.67710400	-0.72200900
C	-0.93836500	-4.74278000	0.24918400
C	0.21204900	-4.96390900	-0.76638300
H	2.08519500	-3.81543300	-1.06884800
H	0.59338400	-2.88826400	-1.33538500
H	-1.08934000	-5.62104800	0.89230400
H	-1.90835900	-4.55610500	-0.23374100
H	-0.16054900	-5.18686700	-1.77333500
H	0.82545900	-5.81909700	-0.45757300
O	-6.66715200	-1.91413000	2.52848100
C	-7.49880900	-3.04862100	2.68488700
H	-7.17382200	-3.67207300	3.52801200
H	-8.50285400	-2.67454100	2.89736600
H	-7.52723800	-3.66141100	1.77277800
H	1.58298300	-3.93905300	1.35686700
H	-2.44247400	-1.04888400	-3.98273800

### TS<sub>j</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -590.8

C	-0.62170800	-2.55492700	0.68697900
C	-1.48283400	-1.80652400	-0.09922600
N	-0.65385100	-1.30991700	-1.12166000

C	0.68786400	-1.69826300	-0.97307400
C	0.70023100	-2.49752800	0.18564000
C	1.63310900	-3.11098100	1.11439700
C	3.08611200	-2.95320500	1.01692000
C	3.69294700	-2.73720000	-0.23427000
C	3.91189900	-2.94932500	2.14521000
C	5.05229200	-2.50787300	-0.34659700
H	3.09390300	-2.78927300	-1.14078700
C	5.27938000	-2.70895600	2.04965700
H	3.48224600	-3.12474200	3.12914900
C	5.85356000	-2.47294100	0.79965900
H	5.51968800	-2.35362400	-1.31682200
H	5.88604900	-2.70920100	2.95074000
S	-1.29618500	-0.80736900	-2.63331400
O	-0.12474700	-0.59720500	-3.46277900
O	-2.24675800	0.26119400	-2.34446800
C	-2.19902600	-2.21240600	-3.20188800
C	-1.49186300	-3.30063700	-3.71162700
C	-3.58912600	-2.21262200	-3.13241400
C	-2.20028800	-4.40757400	-4.15000400
H	-0.40650200	-3.27377300	-3.77920800
C	-4.27858500	-3.33121500	-3.58279100
H	-4.11837000	-1.34122900	-2.75308300
C	-3.59984500	-4.44040100	-4.09394500
H	-1.66485200	-5.26400300	-4.55620200
H	-5.36634900	-3.34303800	-3.54801100
C	-4.34335600	-5.63563400	-4.59734300
H	-5.41012800	-5.58058600	-4.36078100
H	-4.24703100	-5.72251200	-5.68671700
H	-3.94378700	-6.56226300	-4.16956100
H	1.53799000	-0.32365700	-0.32203500

H	1.34929900	-1.65503700	-1.83403000
Cu	-3.28087600	-1.20922500	0.09115900
N	-5.01959300	-0.48839200	0.24340200
C	-6.08385700	-0.03400700	0.28233100
C	-7.41031000	0.52886200	0.33171000
H	-7.35086500	1.61791400	0.44857200
H	-7.94697700	0.29743200	-0.59371200
H	-7.96138600	0.10156200	1.17549100
C	-0.61334100	-3.50845600	1.83385700
C	0.86064100	-3.65918900	2.10565000
C	-1.24615600	-3.40062800	3.22004000
C	1.06056200	-4.19573600	3.48422000
C	-0.37498300	-4.38312300	4.02220500
H	-2.30614200	-3.67433800	3.22810100
H	-1.16624100	-2.38150800	3.62148000
H	1.66869500	-5.10858000	3.52753000
H	1.59594500	-3.44521700	4.08875400
H	-0.44072900	-4.23254500	5.10435700
H	-0.71169200	-5.40806900	3.81979900
O	7.16116400	-2.18860000	0.59942200
C	8.01427800	-2.17629400	1.72779900
H	8.03959300	-3.15430500	2.22593900
H	9.01601500	-1.94578300	1.35790300
H	7.71099100	-1.40917300	2.45534000
C	0.56795300	1.03322100	1.13853200
C	1.31168600	0.83640000	-0.03024700
N	0.64178700	1.51886800	-1.04740200
C	-0.58351600	2.16310000	-0.55715800
C	-0.59672100	1.74836000	0.86203000
C	-1.48256700	1.78242000	1.99396700
C	-2.86907000	2.24710900	1.97994700



C	-3.39182100	2.92880500	0.86507500
C	-3.73854300	2.00371600	3.05122500
C	-4.71069300	3.33356200	0.82128500
H	-2.75875500	3.17047500	0.01578200
C	-5.06916600	2.40128100	3.02148900
H	-3.38014700	1.49320800	3.94074000
C	-5.56381100	3.07043000	1.89893400
H	-5.10719400	3.87025900	-0.03708400
H	-5.70386000	2.19456900	3.87835500
S	1.47116400	2.11306600	-2.42337400
O	0.47975000	2.24947200	-3.46507500
O	2.62691400	1.22133800	-2.51518500
C	2.01171000	3.73131200	-1.95575000
C	1.23117500	4.82820500	-2.32605800
C	3.19539400	3.89782600	-1.23972700
C	1.64033200	6.09827700	-1.95126300
H	0.33101600	4.68368400	-2.91829500
C	3.58535900	5.17823000	-0.87311000
H	3.82572500	3.04442100	-0.99873100
C	2.81579400	6.29385600	-1.21697700
H	1.04601200	6.96241500	-2.24317600
H	4.51475000	5.32297000	-0.32547000
C	3.23460500	7.67274200	-0.82137700
H	2.52601300	8.10675300	-0.10517100
H	4.22631700	7.67908200	-0.35949300
H	3.25705100	8.34211000	-1.68896400
H	-1.44458400	1.79887700	-1.14191200
H	-0.53487100	3.25846200	-0.66677000
Cu	3.31512500	0.64368200	-0.13420200
N	5.21248500	0.80336100	-0.03351700
C	6.36645800	0.81675500	-0.12644100

C	7.80088100	0.81416300	-0.26146900
H	8.11720600	-0.16165700	-0.64544800
H	8.11138800	1.60051800	-0.95592200
H	8.27096800	0.98912500	0.71140800
C	0.61281100	0.77852700	2.59524400
C	-0.77807500	1.15467500	3.00828900
C	0.88408200	-0.51558400	3.34891800
C	-1.08089700	0.54597200	4.32946600
C	0.20789000	-0.21906400	4.69581900
H	1.95108400	-0.75309700	3.43576800
H	0.39224100	-1.34787200	2.83445600
H	-1.40575700	1.26360000	5.09443300
H	-1.92378600	-0.15409500	4.19319900
H	0.00421100	-1.12122500	5.28255600
H	0.85974800	0.42119000	5.30397700
O	-6.83861500	3.48762000	1.75218200
C	-7.72679700	3.33050200	2.84491200
H	-7.37417500	3.87775900	3.72836100
H	-8.68304400	3.74868600	2.52532000
H	-7.86709800	2.27199800	3.10640600
H	-0.94781900	-4.48393300	1.42710900
H	1.28532700	1.55074600	3.02119200

## **K**

C	0.86115800	-1.75518300	1.65807800
C	1.77335100	-0.74670700	1.48806300
N	0.94068600	0.39431800	1.36377000
C	-0.43196500	0.09400900	1.51227900
C	-0.48629500	-1.26260300	1.67481100
C	-1.41529800	-2.39824400	1.79145400
C	-2.87037100	-2.32665700	1.66366700

C	-3.50187100	-1.17576700	1.16067600
C	-3.69343500	-3.40493300	2.00932600
C	-4.87383100	-1.11523300	0.98847900
H	-2.89995900	-0.30677000	0.89988100
C	-5.07314900	-3.36306000	1.83915800
H	-3.24931900	-4.29636200	2.44716700
C	-5.67370100	-2.21451100	1.31970400
H	-5.35321400	-0.21496000	0.60676800
H	-5.67039600	-4.22253200	2.12959100
S	1.49902500	1.97753300	1.27279000
O	0.59023000	2.67676900	0.36357800
O	2.92206200	1.92013000	0.95596700
C	1.28931900	2.64008500	2.89391500
C	0.14110200	3.36727900	3.19780000
C	2.26936500	2.38583300	3.84907900
C	-0.01176200	3.85735800	4.48626800
H	-0.61266400	3.54371200	2.43313700
C	2.09497800	2.88626700	5.13126200
H	3.15459800	1.81052800	3.58694600
C	0.95954200	3.62900500	5.46740500
H	-0.90182100	4.43050300	4.74128300
H	2.85386300	2.70123400	5.88940700
C	0.78749300	4.19006900	6.84367400
H	1.47648000	3.72875000	7.55808600
H	0.97850300	5.27085800	6.85130500
H	-0.23485600	4.04423600	7.21013400
H	-1.17482600	0.88298900	1.50165400
Cu	3.63999100	-0.66588200	1.14771100
N	5.49266900	-0.57528600	0.77699700
C	6.59441900	-0.42014400	0.45875800
C	7.96515900	-0.21744800	0.05626500

H	8.01457900	0.60046200	-0.66908800
H	8.57704000	0.03943700	0.92621600
H	8.36088100	-1.13031900	-0.39922400
C	0.83128600	-3.22949400	1.86488900
C	-0.65096500	-3.52127000	1.89739800
C	1.28532000	-4.21837900	0.79077300
C	-0.88113700	-4.98348700	1.66374200
C	0.49849000	-5.48491600	1.15955900
H	2.37050100	-4.37105400	0.75710500
H	0.96734100	-3.82849800	-0.19019500
H	-1.19718500	-5.52803700	2.56498500
H	-1.67766300	-5.14106000	0.91984400
H	0.41188700	-6.19724200	0.33018400
H	1.01992000	-6.00894400	1.97149400
O	-7.00141600	-2.06819800	1.11196000
C	-7.84558600	-3.14058600	1.46644900
H	-7.79337900	-3.36112600	2.54177600
H	-8.86330300	-2.83020400	1.21948800
H	-7.60598100	-4.05285100	0.90155200
C	-1.94427600	-1.18484600	-2.23123600
C	-2.92115200	-0.25830200	-1.90056200
N	-2.35426100	0.93942000	-1.66660500
C	-0.89164700	0.85583300	-1.79612600
C	-0.70829100	-0.55092900	-2.20889500
C	0.35490700	-1.44528400	-2.58085400
C	1.78777100	-1.15359600	-2.60398200
C	2.32721600	-0.05525800	-1.91546600
C	2.67247800	-1.96970200	-3.31688100
C	3.68491300	0.20519700	-1.92627000
H	1.68465400	0.60132700	-1.33205800
C	4.03962800	-1.72242600	-3.33828600

H	2.28783500	-2.80642100	-3.89618600
C	4.55435800	-0.62928800	-2.63762800
H	4.09118300	1.04937900	-1.37345200
H	4.68782200	-2.37687300	-3.91318400
S	-3.18867400	2.26128700	-0.88897600
O	-2.57787100	2.40894100	0.41762700
O	-4.58731800	1.90907700	-1.04583800
C	-2.74548600	3.61057800	-1.91811900
C	-1.56600900	4.30999100	-1.65230300
C	-3.58736000	3.94715600	-2.97540900
C	-1.23529700	5.36881600	-2.48301500
H	-0.92389100	4.02559700	-0.81904300
C	-3.23324900	5.01520900	-3.78635400
H	-4.50766700	3.39441200	-3.14626400
C	-2.05937300	5.73839100	-3.55403900
H	-0.32170600	5.93005500	-2.29462900
H	-3.88047700	5.30115600	-4.61282900
C	-1.68435300	6.89789900	-4.41983600
H	-0.67600800	6.77372100	-4.83210400
H	-2.38145900	7.02519700	-5.25337600
H	-1.67719300	7.82943100	-3.84080500
H	-0.43059600	1.09094700	-0.82285900
H	-0.52053800	1.58912500	-2.52605400
C	-1.75824000	-2.58930600	-2.65736500
C	-0.26954700	-2.65153400	-2.82822300
C	-1.95670300	-3.76768000	-1.69535800
C	0.17832600	-4.07065900	-2.87134300
C	-1.04603700	-4.84145300	-2.31132200
H	-3.00154600	-4.07805400	-1.59037800
H	-1.58731300	-3.46446500	-0.70448200
H	0.43880500	-4.39542400	-3.88876200

H	1.08518400	-4.20644600	-2.26665700
H	-0.75587300	-5.60731300	-1.58372800
H	-1.57164300	-5.35429200	-3.12632000
O	5.86644400	-0.29886900	-2.59844000
C	6.75920200	-1.06604500	-3.38027900
H	6.47934000	-1.05383200	-4.44219000
H	7.74431700	-0.60457700	-3.27781500
H	6.81179800	-2.10820500	-3.03459200
H	-2.26688200	-2.80419900	-3.61197300
H	1.30090500	-3.52006000	2.82194200
H	-3.99647800	-0.37972500	-1.80703800

### TS<sub>b</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -920.1

C	0.29016200	1.03529300	0.20991700
C	-0.87788500	0.57896600	-0.33236000
N	-0.52688000	-0.68791600	-0.85777800
C	0.78035300	-1.02302400	-0.68022900
C	1.36095300	0.07582300	0.03762500
C	2.65763300	0.70190100	0.37766700
C	3.97507700	0.10257000	0.18210800
C	4.20707500	-0.86128300	-0.81340800
C	5.05598800	0.48154000	0.98445600
C	5.45948800	-1.41392400	-0.99650400
H	3.40082300	-1.16301600	-1.47983100
C	6.32209500	-0.06375300	0.81105300
H	4.90057200	1.20375400	1.78378200
C	6.53078600	-1.02147100	-0.18424500
H	5.64279300	-2.15504300	-1.77044600
H	7.13203700	0.25378200	1.46104200

S	-1.68550900	-1.81270000	-1.53832500
O	-0.88762000	-2.99353800	-1.81186200
O	-2.38001200	-1.08642100	-2.58169600
C	-2.76954700	-2.08359800	-0.17978200
C	-2.32119100	-2.84233600	0.90101400
C	-4.04249900	-1.52217100	-0.20659800
C	-3.17205200	-3.02869100	1.97704200
H	-1.32939200	-3.28997000	0.89030100
C	-4.87948500	-1.72494700	0.88369200
H	-4.37206300	-0.96128800	-1.07797200
C	-4.45933700	-2.47264300	1.98668900
H	-2.84434100	-3.62281700	2.82837700
H	-5.88387100	-1.30572400	0.87539100
C	-5.35910800	-2.69474600	3.15970400
H	-4.89917700	-2.32613900	4.08440400
H	-6.32275300	-2.19198200	3.03496100
H	-5.55256800	-3.76411200	3.30729800
H	1.05831600	-0.92147300	0.72225600
Cu	-2.61985900	1.34353600	-0.40691600
N	-4.31969200	2.16609600	-0.46008300
C	-5.34202800	2.69996200	-0.55645400
C	-6.61396500	3.36656900	-0.68208800
H	-7.32694000	2.95251700	0.03701900
H	-6.49205900	4.43664200	-0.48851100
H	-7.00566300	3.22989500	-1.69461700
C	0.86838900	2.24763200	0.85125900
C	2.34551400	1.93848700	0.84595100
C	0.86310200	3.61390000	0.15723300
C	3.12786500	3.19760400	1.03061200
C	2.07218500	4.31009700	0.80355800
H	-0.07425900	4.16559400	0.28693200

H	1.02540100	3.46879300	-0.92004900
H	3.58741900	3.27788500	2.02482700
H	3.95300000	3.23706400	0.30673500
H	2.45710000	5.13451000	0.19612600
H	1.77204100	4.73679400	1.76915600
O	7.71010500	-1.62291000	-0.43336000
C	8.82177700	-1.25948800	0.35856100
H	8.65383800	-1.48811300	1.42001000
H	9.66528900	-1.85210900	-0.00142400
H	9.06428000	-0.19351300	0.25082300
H	0.50660000	2.37873700	1.88634500
H	1.20576300	-1.95395600	-1.03765600

## L

C	-0.20516000	-0.79471500	0.97585300
C	0.87096800	-0.62442600	0.17783900
N	0.58538900	0.64960100	-0.46773600
C	-0.58970000	1.15585100	-0.20381600
C	-1.21189200	0.30809900	0.83241000
C	-2.53653800	-0.46277400	0.77769800
C	-3.80477100	0.10380400	0.32181700
C	-3.87074400	1.08169500	-0.68462400
C	-5.01525300	-0.33787700	0.86923700
C	-5.08054500	1.58041300	-1.12841100
H	-2.95852500	1.43854800	-1.16004900
C	-6.24026700	0.15086800	0.43308400
H	-5.00101600	-1.06756300	1.67573500
C	-6.27979000	1.11744100	-0.57424200
H	-5.13012400	2.33015800	-1.91409400
H	-7.15416900	-0.21676200	0.89011700
S	1.77282600	1.49334300	-1.51400100



O	0.98520100	2.53325700	-2.14315600
O	2.42002200	0.43505100	-2.26012200
C	2.86069200	2.16380500	-0.31606400
C	2.58052400	3.42365200	0.21106000
C	3.97494600	1.42516200	0.08257600
C	3.44708000	3.95077000	1.15544200
H	1.71154700	3.98516300	-0.12373800
C	4.82470000	1.97500900	1.02855000
H	4.17251500	0.44742500	-0.35207000
C	4.57872400	3.24136500	1.57328400
H	3.25253700	4.93606800	1.57376700
H	5.70381800	1.41886000	1.34837500
C	5.53004000	3.83501800	2.56065100
H	5.06215700	4.63382800	3.14402000
H	5.91640100	3.07937800	3.25274100
H	6.39525900	4.27002100	2.04401300
Cu	2.31169700	-1.76013500	-0.32226300
N	3.72344300	-2.92471600	-0.78056400
C	4.56737500	-3.65171800	-1.09445500
C	5.61853600	-4.55792400	-1.48320100
H	5.28151800	-5.18159500	-2.31660500
H	6.50087400	-3.99144700	-1.79610800
H	5.88662200	-5.20035500	-0.63919700
C	-0.85800500	-1.96849400	1.61752700
C	-2.30658900	-1.69233900	1.28473500
C	-0.68039400	-3.38234700	1.06355400
C	-3.09191500	-2.96539200	1.34845700
C	-2.00003700	-4.05822500	1.46644300
H	0.20243300	-3.90513900	1.44851000
H	-0.59300900	-3.32413900	-0.03140900
H	-3.78347500	-3.00280200	2.20067400

H	-3.70887700	-3.07732200	0.44647200
H	-2.22422000	-4.94113000	0.86002800
H	-1.93074100	-4.39596600	2.50862200
O	-7.40966800	1.66147300	-1.06851800
C	-8.64272200	1.20914000	-0.54963800
H	-8.73331400	1.42155200	0.52466700
H	-9.42313900	1.75440300	-1.08430900
H	-8.78190000	0.13216400	-0.71766300
H	-0.70561500	-1.98346100	2.71169700
H	-0.89742300	2.12405400	-0.59187300
H	-1.22642000	0.99889500	1.70518700

### TS<sub>D1</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -823.9

C	0.27185700	-1.51270600	-0.32687900
C	-1.02127900	-1.08865900	-0.13753100
N	-0.87845500	0.30313200	0.09028200
C	0.52268000	0.70960300	0.22268600
C	1.20414600	-0.45545000	-0.13613500
C	2.55680800	-0.92335600	-0.37492100
C	3.77792500	-0.14320500	-0.17798600
C	3.80018100	0.95892500	0.69222100
C	4.96224200	-0.46896800	-0.84499800
C	4.95411000	1.69085600	0.89243100
H	2.89826300	1.22811500	1.23972400
C	6.13139400	0.25987400	-0.65725400
H	4.96747600	-1.29777700	-1.55059300
C	6.13202000	1.34897200	0.21688600
H	4.97724100	2.53905400	1.57235800
H	7.02811200	-0.01916800	-1.20300200

S	-1.90627800	1.08093700	1.16556600
O	-0.84379900	1.63075900	2.15164800
O	-2.93022900	0.21752500	1.70710400
C	-2.60441400	2.47270400	0.37413800
C	-1.87559900	3.65691900	0.25768300
C	-3.86778900	2.31511800	-0.19417600
C	-2.44711000	4.70763600	-0.43984200
H	-0.89702600	3.76392700	0.71787700
C	-4.41280700	3.38384900	-0.88793200
H	-4.41333300	1.38077900	-0.08561400
C	-3.71662900	4.58993700	-1.02010200
H	-1.90345400	5.64537700	-0.53512300
H	-5.39979900	3.28509300	-1.33464600
C	-4.32113900	5.74755300	-1.74527300
H	-5.15461700	5.43661000	-2.38207100
H	-4.70744600	6.48744900	-1.03267200
H	-3.57980900	6.25984300	-2.36776300
H	0.78626400	1.69979700	-0.15422000
Cu	-2.68642700	-2.00648600	-0.09039100
N	-4.34088100	-2.91031600	-0.07282700
C	-5.34012000	-3.49270800	-0.03463500
C	-6.58251000	-4.22242800	0.01149300
H	-7.14138400	-3.94977800	0.91179800
H	-7.18548300	-3.98661700	-0.87046100
H	-6.37923500	-5.29736300	0.02882500
C	1.02041300	-2.73252700	-0.74202400
C	2.44418300	-2.24622200	-0.70252300
C	1.13409100	-3.99442100	0.11993000
C	3.38360600	-3.40487500	-0.67826800
C	2.45319400	-4.60747900	-0.37801300
H	0.27893300	-4.67181700	0.02071400

H	1.21450800	-3.70208900	1.17637200
H	3.92510400	-3.53986000	-1.62451600
H	4.15097500	-3.25389000	0.09375400
H	2.89196700	-5.30899200	0.33791100
H	2.26562500	-5.16826500	-1.30271500
O	7.20322700	2.12829000	0.47077500
C	8.41272400	1.82995800	-0.19263300
H	8.30829500	1.91352200	-1.28332900
H	9.14299000	2.56590100	0.15039600
H	8.77690100	0.82438500	0.05931700
H	0.75052200	-3.03234500	-1.76974400
H	0.07390100	1.25549200	1.70324600

## M

C	-0.50654300	-1.53415500	-0.31934900
C	-1.64151400	-0.78423500	-0.27448900
N	-1.11418100	0.56945100	-0.27379000
C	0.33062100	0.57899000	-0.20204500
C	0.69162800	-0.73012900	-0.28057900
C	1.86645900	-1.59978500	-0.32876300
C	3.25320700	-1.16425100	-0.17245500
C	3.56580100	0.06129100	0.43869800
C	4.31842000	-1.95616300	-0.61352700
C	4.87542500	0.46619700	0.61073500
H	2.76309600	0.69617000	0.80999600
C	5.64165100	-1.56475400	-0.44558600
H	4.11053500	-2.89394800	-1.12534900
C	5.92792100	-0.34546700	0.17196300
H	5.11883200	1.41124900	1.09041000
H	6.43893500	-2.20729600	-0.80790000
S	-1.92326600	1.68192300	0.59758600

O	-1.58570000	1.43112500	2.14084700
O	-3.35386400	1.63265600	0.43137100
C	-1.20044400	3.22145400	0.20572000
C	-0.77593800	4.08764700	1.21131900
C	-1.15216300	3.56549800	-1.14941000
C	-0.27323900	5.32471800	0.83634400
H	-0.83319900	3.80680500	2.25891600
C	-0.64432200	4.80551800	-1.49029700
H	-1.48984700	2.86893300	-1.91416800
C	-0.19986800	5.70180400	-0.50781400
H	0.07216900	6.01484000	1.60285500
H	-0.58749300	5.09141100	-2.53853400
C	0.33067200	7.04063000	-0.90217800
H	0.80425200	7.55405400	-0.06058000
H	1.06401800	6.95349200	-1.71178100
H	-0.47888700	7.68105700	-1.27392300
Cu	-3.46601200	-1.30903700	-0.22223600
N	-5.21426300	-2.02033000	-0.18468400
C	-6.29077100	-2.44376600	-0.15559100
C	-7.63220100	-2.97095600	-0.11657800
H	-7.76744100	-3.70500000	-0.91643600
H	-7.81212800	-3.45590200	0.84774200
H	-8.35444400	-2.15986700	-0.24853700
C	-0.10832700	-2.96227700	-0.47933700
C	1.39701400	-2.87465000	-0.42613000
C	-0.36918900	-4.03210600	0.58562100
C	1.97318200	-4.22415400	-0.14305800
C	0.73814000	-5.05558700	0.28957600
H	-1.37678100	-4.46064300	0.54100600
H	-0.23274100	-3.58877100	1.58251800
H	2.47263800	-4.67359000	-1.01228600

H	2.73554200	-4.15522000	0.64566500
H	0.95119100	-5.70975100	1.14067000
H	0.42131400	-5.70185800	-0.53923500
O	7.17156600	0.13457100	0.38316200
C	8.26484600	-0.66302900	-0.01704600
H	8.26697600	-0.83616200	-1.10214500
H	9.16694900	-0.11013800	0.25391500
H	8.27171800	-1.63133900	0.50247100
H	-0.43597700	-3.35731300	-1.45690900
H	-0.71552600	0.98875300	2.22502800
H	0.87319600	1.51097700	-0.29815300

**[CuL8]-R TS<sub>B</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -223.2

C	2.46300400	-0.96305000	-0.00858200
C	1.61643200	0.05066500	0.49105400
N	2.44458400	0.93948300	1.09798400
C	3.88009200	0.59033500	1.06226800
C	3.81916500	-0.75497800	0.38955600
C	4.76439700	-1.71188600	0.27498200
C	6.14459100	-1.76524500	-0.00380300
C	6.79070500	-0.78920200	-0.80962700
C	6.93273100	-2.81244100	0.52387000
C	8.14177000	-0.84537900	-1.04205300
H	6.19448300	0.00964500	-1.24724400
C	8.29479300	-2.87189400	0.31058600
H	6.43932400	-3.57579500	1.12128900
C	8.90944200	-1.88166000	-0.47424800
H	8.65219500	-0.10447500	-1.65183400
H	8.87629900	-3.67943400	0.74440200

S	1.89252400	2.26679200	2.02337000
O	2.48150800	2.14350800	3.34678200
O	0.44534500	2.30001000	1.84436700
C	2.64489000	3.62002400	1.17690000
C	3.60656900	4.38631600	1.83096100
C	2.26625000	3.88441000	-0.13726700
C	4.19342500	5.44040400	1.14607800
H	3.88003600	4.15579800	2.85754700
C	2.86680400	4.94373200	-0.80223600
H	1.51053900	3.27652600	-0.63443400
C	3.83480000	5.73413400	-0.17422300
H	4.94530400	6.05180400	1.64248500
H	2.57171500	5.16605900	-1.82666500
C	4.48248000	6.87684900	-0.89019300
H	5.57191200	6.75605200	-0.92260100
H	4.12103400	6.96833500	-1.91889700
H	4.28452600	7.82569900	-0.37683800
H	4.30101400	0.58168800	2.07372900
H	4.43411700	1.32069700	0.45568100
Cu	-0.33825100	0.25185000	0.47290000
C	2.18902900	-2.17508600	-0.67465600
C	3.21926300	-2.90974700	-1.21386500
C	0.91946300	-2.97343000	-0.63550100
C	2.77865200	-4.31913000	-1.49248700
H	4.09742000	-2.45950900	-1.67115200
C	1.24061000	-4.19481400	-1.51140700
H	0.04166100	-2.40719300	-0.98194100
H	0.70496300	-3.25783700	0.40775800
H	3.18325400	-4.72606600	-2.42612500
H	3.10931500	-4.99202200	-0.68720000
H	0.73412300	-5.10510400	-1.17445100

H	0.90537400	-4.00053000	-2.53905600
O	10.21478700	-1.83863900	-0.74217200
C	11.06317900	-2.83846400	-0.19727300
H	10.80382400	-3.83288000	-0.58067300
H	12.07501500	-2.58460000	-0.51673400
H	11.02172100	-2.84164300	0.89888800
P	-1.95112700	-0.81767200	1.77706000
P	-1.58587400	1.02598600	-1.34233200
O	-3.52048400	-4.41339100	-2.64995500
O	-4.28645400	-2.25645200	-2.72224300
O	-6.18428900	-1.12537700	-0.00682900
O	-7.38063700	0.83514500	-0.13213600
C	-2.63052400	-2.01197000	0.56257100
C	-2.21008500	-3.34186500	0.60716900
H	-1.65393500	-3.69195100	1.47409200
C	-2.45852400	-4.25104500	-0.43062300
H	-2.13674700	-5.28657800	-0.37307400
C	-3.12641500	-3.76019100	-1.52600200
C	-3.98958000	-3.39226100	-3.52176100
H	-4.89414900	-3.73091400	-4.03458800
H	-3.19426300	-3.13340800	-4.24273900
C	-3.57864500	-2.44362600	-1.57362400
C	-3.36032500	-1.52784500	-0.56431800
C	-1.33620000	-1.83063900	3.17232000
C	0.02926700	-1.77692000	3.46428800
H	0.68181200	-1.14940500	2.85571500
C	0.55216900	-2.50702800	4.52832200
H	1.61533600	-2.45413000	4.75066900
C	-0.28745800	-3.29463100	5.30701200
H	0.11810900	-3.86318700	6.14073900
C	-1.65127400	-3.35257100	5.02465800



H	-2.30832400	-3.96664200	5.63620900
C	-2.17478700	-2.62294800	3.96528200
H	-3.24207100	-2.67041500	3.75389900
C	-3.37270400	0.09518900	2.46800100
C	-4.61948100	-0.49106900	2.70834900
H	-4.79768800	-1.53065900	2.43466900
C	-5.64295800	0.26165000	3.27334400
H	-6.60876000	-0.19942800	3.47114400
C	-5.43152300	1.60140700	3.59408800
H	-6.23553800	2.18687000	4.03400500
C	-4.19537400	2.19036900	3.35042800
H	-4.02939500	3.23602700	3.59888400
C	-3.16680900	1.43932200	2.78941000
H	-2.19120500	1.89118700	2.60214800
C	-3.39514400	1.02195000	-1.07733200
C	-4.01384400	-0.19287700	-0.67087000
C	-5.36602300	-0.11597900	-0.40817700
C	-7.47910100	-0.55639100	0.14506600
H	-8.17476500	-1.02493900	-0.56494200
H	-7.82853000	-0.70293300	1.17630200
C	-6.09230600	1.06703200	-0.48457900
C	-5.50561200	2.24878700	-0.86511700
H	-6.07190600	3.17248200	-0.93101800
C	-4.13938700	2.19737600	-1.17168500
H	-3.65166900	3.11577800	-1.48754500
C	-1.18590600	2.75956700	-1.76452400
C	-1.18960100	3.69616800	-0.72195700
H	-1.43371300	3.37464000	0.29060000
C	-0.88248700	5.02761200	-0.97140500
H	-0.89252800	5.74633200	-0.15518000
C	-0.54166800	5.43348800	-2.26052900

H	-0.29493800	6.47486400	-2.45573400
C	-0.51270100	4.50451100	-3.29569900
H	-0.24680300	4.81711400	-4.30307900
C	-0.83931000	3.17189200	-3.05284400
H	-0.82763100	2.45436300	-3.87173300
C	-1.31853300	0.10201500	-2.89479300
C	-0.06893700	-0.49497400	-3.08982300
H	0.69367800	-0.40716500	-2.31419100
C	0.20215700	-1.19311000	-4.26173900
H	1.17919200	-1.65130400	-4.40375500
C	-0.77798900	-1.30261200	-5.24488500
H	-0.56961100	-1.84987000	-6.16158000
C	-2.02340500	-0.70639600	-5.05818000
H	-2.78622900	-0.78520300	-5.83025300
C	-2.29647200	-0.00557200	-3.88715900
H	-3.27351000	0.45375500	-3.74201400

**[CuL8]-S TS<sub>B</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -173.4

C	2.50378700	-0.64244500	-0.13463800
C	1.63047300	0.16608100	0.61506300
N	2.42504000	0.86473300	1.47673900
C	3.87201700	0.62174500	1.32285600
C	3.87583700	-0.31891300	0.14742900
C	4.90085400	-0.70780000	-0.62519600
C	6.24104800	-1.11496500	-0.52107600
C	7.14776100	-0.87546200	-1.58633100
C	6.72393500	-1.79859900	0.62143500
C	8.46056800	-1.26324100	-1.49799600
H	6.77845200	-0.36926700	-2.47512900

C	8.03767300	-2.20855800	0.71453000
H	6.03330700	-2.00580300	1.43743800
C	8.91721900	-1.93702900	-0.34804900
H	9.17131300	-1.07692600	-2.29854400
H	8.38252000	-2.73251100	1.60064900
S	1.87739100	2.21454200	2.36926100
O	2.74345000	2.28029600	3.53397800
O	0.43548100	2.04262600	2.49300300
C	2.22462500	3.58640000	1.31332100
C	3.33183600	4.38872400	1.56910500
C	1.38935300	3.82291500	0.22175100
C	3.59871800	5.44830900	0.70986300
H	3.96090300	4.19174500	2.43398400
C	1.67231900	4.88461100	-0.62095000
H	0.51827700	3.19524600	0.04823300
C	2.77956000	5.71219800	-0.39044200
H	4.45781700	6.08890200	0.90005400
H	1.01435000	5.08285300	-1.46759800
C	3.05951000	6.86416100	-1.30228800
H	3.04708400	6.55182800	-2.35297500
H	2.29422300	7.64293300	-1.19348100
H	4.03161600	7.32092700	-1.09281700
H	4.27723800	0.14261200	2.22309000
H	4.41465500	1.56098700	1.15744900
Cu	-0.33087000	0.33647900	0.60758200
C	2.28469800	-1.56301000	-1.18272800
C	3.31673600	-2.34659100	-1.64061800
C	1.08041800	-1.71028200	-2.06726800
C	2.95889000	-2.99681500	-2.94444000
C	1.69560300	-2.23300300	-3.37552200
H	0.51613500	-0.77919800	-2.19572800

H	0.39141600	-2.44938800	-1.63189100
H	3.76223900	-2.95428300	-3.69023800
H	2.74959600	-4.06650700	-2.78076700
H	1.00026900	-2.84671400	-3.95965000
H	1.97973200	-1.37549400	-4.00014900
O	10.20387600	-2.28416700	-0.35994400
C	10.74198500	-2.97547100	0.75752900
H	10.24138700	-3.93996300	0.90733100
H	11.79396500	-3.15070300	0.52700500
H	10.66950900	-2.37301700	1.67139100
P	-1.75854400	-1.10333100	1.78511000
P	-1.80411400	1.28028900	-0.93716400
O	-2.06898400	-4.45498600	-3.09497500
O	-3.33538200	-2.55294800	-3.04609500
O	-5.58920700	-2.38795400	-0.63623300
O	-7.31854300	-0.88295300	-0.59331700
C	-2.00790700	-2.26601100	0.38325100
C	-1.26309600	-3.44709900	0.34437900
H	-0.69115700	-3.74034200	1.22236900
C	-1.21941800	-4.27901100	-0.78338700
H	-0.65027900	-5.20369400	-0.79005000
C	-1.92244700	-3.85235800	-1.88443400
C	-2.67633000	-3.46395100	-3.91263400
H	-3.40167300	-3.92882200	-4.58467500
H	-1.89158600	-2.92644700	-4.47579000
C	-2.67811100	-2.68296900	-1.85767700
C	-2.76230000	-1.85394100	-0.75645000
C	-1.02929000	-2.11025600	3.12656800
C	0.27594900	-1.81278100	3.52598000
H	0.81006900	-0.99795000	3.03753600
C	0.88104800	-2.53825700	4.54870600

H	1.89463800	-2.29456100	4.85872800
C	0.18409700	-3.56382100	5.17702500
H	0.65406400	-4.12871200	5.97887400
C	-1.12030000	-3.86346800	4.78766300
H	-1.66647600	-4.66250200	5.28366700
C	-1.72695700	-3.13890300	3.76997800
H	-2.74895500	-3.37405500	3.47579000
C	-3.42089500	-0.66749300	2.40497200
C	-4.51108600	-1.54200400	2.36159800
H	-4.40218800	-2.52685600	1.90793800
C	-5.74238000	-1.14748800	2.87298200
H	-6.58849600	-1.83048700	2.83385900
C	-5.89250400	0.11787400	3.43541900
H	-6.85733000	0.42524200	3.83205900
C	-4.81046300	0.99103300	3.48588600
H	-4.92612200	1.97981300	3.92367800
C	-3.57844200	0.60027100	2.97106400
H	-2.72767800	1.28298700	3.00726100
C	-3.52193500	0.64927700	-0.86691800
C	-3.76309500	-0.75042700	-0.78395100
C	-5.09244100	-1.12383500	-0.74131600
C	-6.99665900	-2.25561700	-0.78260700
H	-7.29376700	-2.56784700	-1.79650300
H	-7.50661600	-2.86216500	-0.02751600
C	-6.14393400	-0.21525900	-0.71386700
C	-5.92452100	1.13990500	-0.76190200
H	-6.74173000	1.85392100	-0.73375700
C	-4.58927800	1.54990900	-0.85246000
H	-4.38735500	2.61624500	-0.91126100
C	-1.99040500	3.08379100	-0.70845300
C	-2.05375700	3.55902100	0.60682000

H	-1.95257800	2.85801600	1.43663100
C	-2.22084300	4.91599600	0.85558400
H	-2.26714300	5.27671800	1.88023200
C	-2.31592200	5.81069900	-0.20770300
H	-2.44165300	6.87346700	-0.01405800
C	-2.24781000	5.34604800	-1.51812100
H	-2.32698800	6.04384900	-2.34872000
C	-2.08897100	3.98603800	-1.77130500
H	-2.05132000	3.62501200	-2.79791400
C	-1.27824800	1.08878200	-2.67925100
C	-0.01527800	1.57845700	-3.04039800
H	0.59222100	2.11165200	-2.30657400
C	0.47775700	1.37648500	-4.32286500
H	1.45508700	1.76823000	-4.59558300
C	-0.27379000	0.65854100	-5.25279300
H	0.11707700	0.48932700	-6.25346600
C	-1.52229100	0.16097600	-4.89691600
H	-2.11760400	-0.39134400	-5.62168400
C	-2.03031300	0.38220200	-3.61789900
H	-3.01032800	-0.00921400	-3.35140300
H	4.09874400	-2.73501500	-0.99254500

### **3a**

C	2.75867400	1.26693600	-0.42691600
C	2.60416700	0.14025900	-0.85119300
N	2.40559300	-1.08416700	-1.37336600
C	1.36737500	-1.21165700	-2.42409500
C	0.05022700	-0.76209300	-1.99638900
C	-1.02143800	-0.34436200	-1.61178400
C	-2.28289600	0.14269700	-1.16085800
C	-3.20947500	-0.71698600	-0.54476600

C	-2.62698600	1.48997000	-1.31641300
C	-4.42813000	-0.24242600	-0.10116500
H	-2.94858300	-1.76602000	-0.41654500
C	-3.85021200	1.97730800	-0.87352100
H	-1.91991400	2.16507100	-1.79328600
C	-4.75843000	1.10954100	-0.26202500
H	-5.15217000	-0.89975300	0.37519600
H	-4.08673800	3.02855700	-1.00881200
S	2.63629900	-2.43810400	-0.33286000
O	3.72302800	-2.06173100	0.55063500
O	2.72425000	-3.58553700	-1.22167900
C	1.12618300	-2.54188800	0.57791400
C	0.87956900	-1.61228500	1.58883400
C	0.17579400	-3.48733000	0.20912700
C	-0.34930100	-1.63582700	2.22777300
H	1.63914200	-0.88400900	1.86250700
C	-1.04514400	-3.50131900	0.87193400
H	0.39577100	-4.19963200	-0.58196500
C	-1.32835400	-2.57409600	1.87693600
H	-0.56249100	-0.91275800	3.01344300
H	-1.79808700	-4.23960500	0.59991500
C	-2.65668700	-2.56216700	2.56603700
H	-3.12206600	-1.57078600	2.49700500
H	-3.34697500	-3.29207900	2.12939000
H	-2.55365600	-2.79383100	3.63349300
H	1.71686000	-0.62449100	-3.28214300
H	1.36015200	-2.26075700	-2.74309400
O	-5.97073700	1.47862900	0.20279400
C	-6.34743600	2.83120700	0.06609300
H	-7.34648000	2.92055500	0.49845800
H	-5.66448800	3.49961700	0.60864600

H	-6.38816400	3.13715200	-0.98848400
C	2.92747800	2.59059800	0.07035800
C	1.93781700	3.55863700	-0.16138800
C	4.07343700	2.94595300	0.79762800
C	2.09744300	4.85109800	0.31762500
H	1.04767600	3.27819000	-0.72057500
C	4.21725500	4.23773200	1.28520400
H	4.84144000	2.19626700	0.97378000
C	3.23401800	5.19443000	1.04521800
H	1.32619600	5.59472000	0.12915500
H	5.10700500	4.50165200	1.85258700
H	3.35362700	6.20629900	1.42563600

#### **A8**

C	1.92948000	1.33574200	-0.93852800
C	1.70885600	0.13877000	-1.18622900
N	1.26863300	-0.97166500	-1.81046200
C	0.12660400	-0.85222200	-2.75606500
C	-1.09239200	-0.39269300	-2.11528500
C	-2.09115500	0.00027400	-1.54933400
C	-3.26989000	0.43933000	-0.88067500
C	-4.14960500	-0.49392200	-0.30208400
C	-3.57985800	1.80090900	-0.78068600
C	-5.28770400	-0.07606200	0.35578600
H	-3.91950500	-1.55516000	-0.38124400
C	-4.72207900	2.23109300	-0.11844100
H	-2.91433300	2.53200200	-1.23511300
C	-5.58254200	1.29093800	0.45644700
H	-5.97995500	-0.78687400	0.80095200
H	-4.93896800	3.29343500	-0.05859300
S	1.50286200	-2.48003800	-1.01643100



O	2.63347500	-2.21052900	-0.11477500
O	1.59977100	-3.47127200	-2.06671600
C	0.05354800	-2.75116000	-0.06252100
C	-0.12357000	-2.03251200	1.12111100
C	-0.92119500	-3.61789800	-0.54893000
C	-1.30523900	-2.19422500	1.82340300
H	0.65124000	-1.36338100	1.48912100
C	-2.09393900	-3.76969500	0.17745000
H	-0.75688500	-4.16536100	-1.47389500
C	-2.30368200	-3.06457200	1.36635000
H	-1.46388800	-1.64152600	2.74750000
H	-2.86450800	-4.44756400	-0.18490400
C	-3.56809600	-3.23600700	2.14476400
H	-3.89970000	-2.28759300	2.58166100
H	-4.37576200	-3.63409200	1.52133300
H	-3.42051700	-3.93912700	2.97461500
H	0.45136900	-0.16698300	-3.54802100
H	0.00409300	-1.83716600	-3.22507900
O	-6.71067900	1.59756000	1.12278300
C	-7.06443000	2.96030900	1.24447500
H	-7.99188600	2.98762300	1.81993700
H	-6.29435100	3.53069300	1.78148600
H	-7.23940600	3.42187900	0.26315800
C	2.02055500	2.71830800	-0.59641200
C	0.87965000	3.38401500	-0.11855000
C	3.22545900	3.42148000	-0.75404900
C	0.94703000	4.73518600	0.18501900
H	-0.04840500	2.82910100	0.00092500
C	3.28475800	4.76936700	-0.43413800
H	4.10217100	2.89883900	-1.13192700
C	2.14736800	5.42612100	0.03150900

H	0.06275900	5.25299000	0.54745100
H	4.21779100	5.31334400	-0.55519000
H	2.19627400	6.48448900	0.27537700
Cu	3.16924100	-0.06642200	0.17846200
N	4.56364200	-0.07525600	1.48020300
C	5.44627300	-0.18498500	2.21982800
C	6.54722700	-0.32416800	3.13868100
H	7.49106600	-0.14805600	2.61363600
H	6.44874900	0.40220600	3.95100500
H	6.55371400	-1.33482400	3.55743200

### TS<sub>A8</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -431.4

C	0.37013100	-0.57925600	-0.23895500
C	-0.85849100	-0.56815200	-0.66279400
N	-1.35691400	0.39710500	-1.50215300
C	-0.46254100	1.54449900	-1.80386800
C	0.85315800	1.25092800	-1.24938200
C	2.05772900	1.39909100	-1.02874000
C	3.40168500	1.35550200	-0.64015400
C	3.84949800	2.05537700	0.50493900
C	4.31321100	0.54398800	-1.34273900
C	5.15076400	1.93647700	0.92758800
H	3.14885100	2.68484700	1.04880600
C	5.62050100	0.41182900	-0.91589800
H	3.96892800	0.00377800	-2.22175000
C	6.04629700	1.10770200	0.22591400
H	5.51754500	2.46457200	1.80353700
H	6.30480500	-0.22547800	-1.46681400
S	-3.02873700	0.63637800	-1.63266900

O	-3.62220500	-0.67835200	-1.40052400
O	-3.21743600	1.35585500	-2.87897700
C	-3.45364400	1.69762100	-0.28544600
C	-3.61148300	1.15356300	0.98876700
C	-3.59339900	3.06493800	-0.51376600
C	-3.90906500	2.00090800	2.04492700
H	-3.52523200	0.07983900	1.14426700
C	-3.89351900	3.89451500	0.55797000
H	-3.49165000	3.46182600	-1.52098700
C	-4.05070500	3.37967000	1.84796800
H	-4.04620100	1.58885300	3.04314000
H	-4.01865300	4.96292100	0.39146000
C	-4.34898100	4.28727700	2.99887800
H	-4.88596400	3.76485400	3.79725600
H	-3.42076700	4.67960500	3.43444100
H	-4.94783600	5.14937000	2.68745000
H	-0.41363600	1.69188600	-2.88848800
H	-0.86310000	2.46565200	-1.35216300
O	7.28301200	1.04574600	0.72541000
C	8.24745500	0.23939000	0.06731700
H	9.16998100	0.33981900	0.64114700
H	7.94538300	-0.81556500	0.05446500
H	8.42382600	0.58634800	-0.95844300
C	1.50714700	-1.26221000	0.28807500
C	2.17146300	-0.76972200	1.42473300
C	2.00509200	-2.40947500	-0.35703500
C	3.29774800	-1.41646000	1.91114500
H	1.78581100	0.12272000	1.91411700
C	3.12129200	-3.06187600	0.14545800
H	1.49502100	-2.77592200	-1.24582100
C	3.77055400	-2.56193200	1.27350800

H	3.80867900	-1.02982700	2.78957300
H	3.49382600	-3.95698500	-0.34636500
H	4.65134800	-3.07008600	1.65931400
Cu	-1.96075700	-2.04539000	-0.08038300
N	-2.98432400	-3.52376300	0.50349700
C	-3.67515700	-4.41586100	0.75926500
C	-4.53674700	-5.52756400	1.07370100
H	-5.57431300	-5.26900300	0.84149900
H	-4.24576600	-6.40104200	0.48232200
H	-4.45738800	-5.77272900	2.13692800

### **B8**

C	0.32980000	-0.91090900	-0.22038900
C	-0.95050700	-0.61671000	-0.63001300
N	-0.92532300	0.55945500	-1.35814900
C	0.39729400	1.19521500	-1.37147700
C	1.23420700	0.15784800	-0.65090100
C	2.52602100	0.28338000	-0.48605500
C	3.85499600	0.46039300	-0.27356200
C	4.33719100	1.10894700	0.91285400
C	4.81366400	-0.02106700	-1.22156000
C	5.67447200	1.26367000	1.12352200
H	3.61240300	1.47204500	1.63667200
C	6.15749700	0.11863400	-1.00609700
H	4.44701700	-0.51305700	-2.11972100
C	6.59994800	0.76443900	0.17316600
H	6.06901700	1.75134000	2.01034900
H	6.86943900	-0.26151300	-1.73130900
S	-2.29451000	1.46495600	-1.74344600
O	-3.36619700	0.50494600	-1.96598100
O	-1.85354500	2.38335700	-2.78027900

C	-2.65740000	2.39338600	-0.28228300
C	-3.41267300	1.80834500	0.73360200
C	-2.14006500	3.67919900	-0.15034100
C	-3.64355200	2.52868700	1.89577100
H	-3.82804600	0.81067000	0.60302900
C	-2.38259600	4.38291000	1.02217800
H	-1.57721200	4.12593300	-0.96640000
C	-3.13374200	3.82220200	2.05838900
H	-4.23734700	2.08640200	2.69411600
H	-1.98966700	5.39191900	1.13478300
C	-3.42256400	4.59952000	3.30352500
H	-3.42711400	3.95496500	4.18927500
H	-2.68955100	5.39713700	3.46104400
H	-4.41153600	5.07191000	3.24439400
H	0.73781700	1.37750600	-2.39509600
H	0.38888100	2.15004000	-0.82704300
O	7.86684900	0.94755700	0.47804200
C	8.89294500	0.47094200	-0.39653700
H	9.83545000	0.73452400	0.08348500
H	8.83208900	-0.61681500	-0.51008700
H	8.83010900	0.96146300	-1.37373000
C	0.76401100	-2.10832100	0.50413400
C	2.03795800	-2.65412100	0.30640700
C	-0.09091600	-2.74948800	1.41366000
C	2.44345200	-3.79846900	0.98475900
H	2.70997800	-2.19850300	-0.42066700
C	0.31010700	-3.89651500	2.08443600
H	-1.07505900	-2.32121500	1.60387200
C	1.58127700	-4.42742500	1.87589100
H	3.43614100	-4.20686100	0.80759400
H	-0.36909100	-4.37087100	2.78969600

H	1.89642300	-5.32174800	2.40798900
Cu	-2.56223900	-1.62356800	-0.41028900
N	-4.15722200	-2.61382200	-0.19640300
C	-5.15137900	-3.20397300	-0.15044900
C	-6.38914400	-3.94111200	-0.09522200
H	-6.69426500	-4.08089300	0.94603800
H	-7.17216100	-3.39309000	-0.62774000
H	-6.25746400	-4.92107600	-0.56384600

### TS<sub>B8</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -320.3

C	0.18676900	-1.24055900	0.16838800
C	-1.07814100	-0.79932300	-0.22921700
N	-0.88262400	0.38446800	-0.87797700
C	0.52379400	0.81911200	-0.94536100
C	1.20799000	-0.35571900	-0.30707000
C	2.51243100	-0.68769300	-0.27806900
C	3.79007500	-0.10888900	-0.16530900
C	4.00699400	1.10728800	0.53485800
C	4.90178600	-0.74136400	-0.76466200
C	5.25609300	1.67156000	0.59223300
H	3.16575200	1.59250800	1.02650000
C	6.16299600	-0.18584900	-0.71022500
H	4.74071700	-1.68659100	-1.27918300
C	6.34528000	1.03310600	-0.03451600
H	5.44153100	2.60725100	1.11301200
H	6.99954100	-0.68679300	-1.18746300
S	-2.12048600	1.32862500	-1.57838300
O	-3.28476100	0.45792300	-1.66741800
O	-1.52167100	1.94146000	-2.75001700

C	-2.41473200	2.56692400	-0.35680300
C	-3.23596800	2.26331300	0.72778500
C	-1.79912300	3.80925000	-0.48209500
C	-3.43845300	3.22983300	1.69999700
H	-3.71739100	1.29017200	0.79966700
C	-2.01851200	4.76337400	0.50272200
H	-1.17532600	4.02575300	-1.34614900
C	-2.83813000	4.49107700	1.60185900
H	-4.07930800	3.00977200	2.55197600
H	-1.55200300	5.74282500	0.41434900
C	-3.09679800	5.53659300	2.63944300
H	-3.23577500	5.09453800	3.63172400
H	-2.27913700	6.26211800	2.69505800
H	-4.01151800	6.09595000	2.40422200
H	0.81545300	1.02090100	-1.98117000
H	0.67348600	1.73375500	-0.35372600
O	7.51440300	1.66079300	0.07284500
C	8.66329300	1.08247700	-0.53128500
H	9.48877100	1.76565100	-0.32680300
H	8.88855400	0.10197800	-0.09441300
H	8.53371800	0.98595900	-1.61598800
C	0.66821500	-2.45415800	0.74940100
C	2.03899200	-2.42024100	1.11486600
C	-0.01184000	-3.68359200	0.77741400
C	2.73946100	-3.61337200	1.37442600
C	0.68221800	-4.84066800	1.06821300
H	-1.06417200	-3.72085200	0.49743800
C	2.06441600	-4.81442300	1.34077200
H	3.79184400	-3.57284000	1.64652200
H	0.16115200	-5.79528700	1.05463300
H	2.58769700	-5.74328400	1.55321500

Cu	-2.81166600	-1.60575100	-0.14983400
N	-4.49971200	-2.44905500	-0.09103100
C	-5.54976300	-2.93409000	-0.11944100
C	-6.85802700	-3.53814300	-0.15575900
H	-6.91352100	-4.25091800	-0.98414500
H	-7.05156900	-4.06485300	0.78362600
H	-7.61971400	-2.76559100	-0.29708400
H	2.42200700	-1.49758300	1.55788000

### C1

C	-0.00164600	-1.40294500	0.07090800
C	-1.23178500	-0.80464600	-0.30232600
N	-0.88485300	0.37577600	-0.84450400
C	0.57896500	0.67961200	-0.89187800
C	1.12086300	-0.55594700	-0.26025200
C	2.29860300	-1.10970800	0.13208700
C	3.64749100	-0.56971500	0.04840100
C	4.65785600	-0.95964900	0.94646400
C	3.98196300	0.37772500	-0.92768500
C	5.93109000	-0.43057400	0.86855600
H	4.43779900	-1.67068500	1.74092200
C	5.25988900	0.91318200	-1.02237100
H	3.23444200	0.68728400	-1.65636300
C	6.24759900	0.50761100	-0.12088900
H	6.70923300	-0.72590300	1.56779500
H	5.47910200	1.63675400	-1.80194500
S	-2.02258900	1.51342000	-1.48316300
O	-3.29040000	0.80029600	-1.53987500
O	-1.38860700	2.05663100	-2.66894900
C	-2.07398600	2.73241800	-0.21534200
C	-2.81784000	2.47512900	0.93491900



C	-1.34206100	3.90820400	-0.36938700
C	-2.82202000	3.42153700	1.94747100
H	-3.38938800	1.55383900	1.02797400
C	-1.36484400	4.84188700	0.65618700
H	-0.77960600	4.08821000	-1.28227700
C	-2.10014100	4.61453300	1.82450100
H	-3.39848200	3.23845800	2.85213000
H	-0.80487200	5.76940800	0.55150000
C	-2.13225700	5.64262600	2.90910200
H	-1.14512600	6.09147800	3.06479800
H	-2.81678500	6.45952800	2.64746900
H	-2.47353200	5.21944800	3.85894100
H	0.86954100	0.83367500	-1.93798700
H	0.79081800	1.60313900	-0.33388000
O	7.51806600	0.95670600	-0.12249900
C	7.89918200	1.87222800	-1.12766000
H	8.95902500	2.08153900	-0.96848100
H	7.76674600	1.44782500	-2.13230700
H	7.33750500	2.81367400	-1.05530000
C	0.44617300	-2.56763500	0.66404700
C	1.92471400	-2.39650000	0.84861600
C	-0.17391700	-3.78493300	1.02036300
C	2.69562100	-3.66643600	0.85906900
C	0.61803500	-4.87584800	1.24989900
H	-1.25868600	-3.86955000	1.00980600
C	2.05009400	-4.82581100	1.11397100
H	3.77785300	-3.63463100	0.75818300
H	0.15507700	-5.83196800	1.48346900
H	2.61134100	-5.75237400	1.20242400
Cu	-3.03151500	-1.44701700	-0.24645800
N	-4.76035000	-2.20013400	-0.20726400

C	-5.84002400	-2.61183800	-0.26675200
C	-7.18544300	-3.12236500	-0.34490800
H	-7.72718300	-2.60994200	-1.14567400
H	-7.16505900	-4.19545800	-0.55673400
H	-7.70366800	-2.95342000	0.60375100
H	1.98017200	-2.08295600	1.92193700

### TSc1

Number of imaginary frequencies: 1

Lowest frequency ( $\text{cm}^{-1}$ ): -1024.6

C	0.01759400	-1.41897500	0.05704200
C	-1.22803400	-0.83023600	-0.28672500
N	-0.91991000	0.40005300	-0.73409500
C	0.53084600	0.72970000	-0.74887800
C	1.08492300	-0.53244900	-0.19842300
C	2.30464700	-1.08101000	0.19135500
C	3.66191100	-0.54067600	0.06805400
C	4.64474700	-0.75703400	1.04691600
C	4.00456800	0.22422700	-1.04836200
C	5.91588900	-0.23511800	0.90671300
H	4.40511300	-1.32282000	1.94724800
C	5.27982200	0.75777800	-1.20000500
H	3.26877800	0.38739400	-1.83456300
C	6.24707900	0.52753700	-0.21955100
H	6.67729500	-0.39303200	1.66625900
H	5.51192700	1.33854900	-2.08771400
S	-2.07865500	1.50906700	-1.38489500
O	-3.33927800	0.78076900	-1.38783500
O	-1.48045300	2.02069500	-2.60344300
C	-2.11559400	2.77270900	-0.16187900
C	-2.80099200	2.53955900	1.03145100

C	-1.44733300	3.96879900	-0.40315800
C	-2.81020400	3.53385400	1.99383500
H	-3.32583300	1.60001100	1.19307000
C	-1.47467900	4.95356000	0.57616900
H	-0.93128300	4.12663000	-1.34694800
C	-2.15103700	4.75327800	1.78154000
H	-3.34179100	3.37359900	2.93037100
H	-0.96607300	5.89947100	0.40097700
C	-2.18974700	5.81694200	2.83143400
H	-3.21810500	6.15646800	3.00540800
H	-1.81378700	5.44018400	3.79012300
H	-1.59105600	6.68782100	2.54855800
H	0.83041700	0.95685000	-1.77943000
H	0.72808400	1.61554800	-0.12948200
O	7.51041300	0.99432400	-0.26563900
C	7.88290300	1.78910900	-1.37216500
H	8.92461900	2.07370400	-1.21087400
H	7.80889600	1.23156300	-2.31592200
H	7.27084100	2.69915000	-1.44023300
C	0.50411700	-2.61656300	0.62308200
C	1.93783600	-2.45151600	0.74928100
C	-0.09365300	-3.82534400	1.01032500
C	2.74907700	-3.56264600	1.13653800
C	0.70993000	-4.85938300	1.43494900
H	-1.17310100	-3.94520500	0.94033000
C	2.12193000	-4.73065600	1.47875700
H	3.83171600	-3.47176300	1.16650000
H	0.26005300	-5.80470800	1.72806200
H	2.71882300	-5.58657600	1.78348900
Cu	-3.00118200	-1.53968100	-0.31792900
N	-4.70350500	-2.35353800	-0.34075200

C	-5.76966700	-2.79647800	-0.41622200
C	-7.09909000	-3.34448400	-0.51256400
H	-7.04635300	-4.41673300	-0.72304100
H	-7.63390100	-3.18922000	0.42916600
H	-7.64439000	-2.84725500	-1.32041100
H	2.07358300	-1.50278000	1.51953700

**D1**

C	0.41693700	-0.88698000	0.65020500
C	-0.79040200	-0.73090600	-0.11393900
N	-0.75109800	0.52877200	-0.56255700
C	0.44283000	1.29217500	-0.14214600
C	1.13470200	0.27036200	0.65917800
C	2.41404000	0.12943800	1.41996900
C	3.64963900	0.51575000	0.63601700
C	4.50430300	1.52190500	1.09136800
C	3.95884500	-0.12997500	-0.55992400
C	5.63438200	1.87526400	0.37253100
H	4.28212400	2.03484300	2.02641000
C	5.08725300	0.21427000	-1.29547100
H	3.31166300	-0.92880500	-0.92372600
C	5.93404100	1.22418800	-0.82845300
H	6.30763300	2.65399200	0.72219300
H	5.30055100	-0.31116400	-2.22140200
S	-1.99806400	1.27666700	-1.52532600
O	-2.79041600	0.17151100	-2.03769300
O	-1.27778400	2.18958700	-2.38996200
C	-2.91735600	2.17620100	-0.32644000
C	-3.89632900	1.51452500	0.41342800
C	-2.63118000	3.52573900	-0.12691300
C	-4.59619800	2.22866500	1.37327200

H	-4.11350300	0.46422200	0.23049400
C	-3.34556700	4.21860500	0.83882500
H	-1.87605700	4.02287900	-0.73089200
C	-4.33448400	3.58518600	1.59939700
H	-5.36829900	1.73085700	1.95671400
H	-3.14014700	5.27444600	1.00469400
C	-5.11872500	4.35385700	2.61337600
H	-4.50754100	5.12333600	3.09624500
H	-5.96398200	4.86673600	2.13663500
H	-5.52954800	3.69946800	3.38848900
H	1.00884400	1.61686700	-1.02604100
H	0.14612000	2.19032900	0.41710500
O	7.05329400	1.63337400	-1.46155200
C	7.40592900	0.99149900	-2.66806300
H	8.33201400	1.45966000	-3.00846500
H	7.58454400	-0.08239900	-2.51889700
H	6.63567100	1.12610700	-3.44029600
C	1.13097900	-1.92155500	1.39024800
C	2.33033400	-1.33422800	1.83820800
C	0.83803200	-3.25066000	1.66507300
C	3.25194600	-2.08114400	2.55082200
C	1.76672600	-3.99460600	2.38999300
H	-0.09125700	-3.70038300	1.31847800
C	2.95994700	-3.41827900	2.82436100
H	4.18886200	-1.63703200	2.88322400
H	1.56208400	-5.03849000	2.61566800
H	3.67404800	-4.02045300	3.38086800
Cu	-2.17166500	-1.97277100	-0.56294400
N	-3.50515900	-3.22893100	-1.01777900
C	-4.31715300	-3.98289600	-1.35059400
C	-5.32817800	-4.92186800	-1.76495500

H	-5.78392400	-4.58572300	-2.70121500
H	-4.87816800	-5.90738700	-1.91865500
H	-6.10291800	-4.99747000	-0.99587300
H	2.36978500	0.76740300	2.31859700

### **TS<sub>E1</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -221.3

C	0.40513000	1.29534000	-0.95948800
C	-0.78660900	1.15824400	-0.26509200
N	-0.93435500	-0.23518800	-0.16548000
C	0.17600800	-0.94722500	-0.69770100
C	0.98264200	0.02911000	-1.23709300
C	2.35924600	0.16472800	-1.83074800
C	3.34161200	-0.49601900	-0.87924900
C	3.57607600	-1.87479300	-0.98063000
C	3.86936700	0.18211400	0.21516000
C	4.30579900	-2.55109900	-0.02016500
H	3.16758700	-2.42460600	-1.82875600
C	4.60333300	-0.48489900	1.20116400
H	3.69622700	1.25259600	0.31914100
C	4.83158300	-1.86001700	1.08139200
H	4.50279800	-3.61729700	-0.10213200
H	5.01936100	0.08036100	2.03077800
S	-1.94822200	-0.98198700	0.97735200
O	-2.93432300	-0.00120500	1.39209300
O	-1.06001900	-1.58442200	1.99474400
C	-2.69866500	-2.28149100	0.06574100
C	-3.60664600	-1.92837100	-0.93385600
C	-2.40026600	-3.60855800	0.35497700
C	-4.22182200	-2.93719100	-1.65359200

H	-3.81933200	-0.88151300	-1.14173000
C	-3.03302300	-4.60315900	-0.38040000
H	-1.69489700	-3.85576600	1.14343900
C	-3.94856000	-4.28605900	-1.38638100
H	-4.93049200	-2.68339100	-2.43965400
H	-2.81522100	-5.64789500	-0.16761100
C	-4.64436400	-5.35929700	-2.15979200
H	-4.17989100	-6.33774400	-2.00505700
H	-5.69500500	-5.43736700	-1.85305400
H	-4.64206100	-5.14197600	-3.23376600
H	1.17120800	-0.73686900	0.67975200
H	0.13525600	-2.02304600	-0.84030200
O	5.54274300	-2.59829900	1.95544200
C	6.16462300	-1.93354600	3.03608700
H	6.71858000	-2.69476400	3.58866500
H	6.86552600	-1.16386600	2.68644000
H	5.42766200	-1.47308200	3.70932800
C	1.32132800	2.32509100	-1.44246500
C	2.46636900	1.67756800	-1.95230400
C	1.23537500	3.71284300	-1.45882000
C	3.52373200	2.41262800	-2.46289800
C	2.29924100	4.44556300	-1.98104900
H	0.35159300	4.21751700	-1.07187100
C	3.43383000	3.80517000	-2.47721900
H	4.41266800	1.91080900	-2.84314700
H	2.24388600	5.53162600	-2.00197400
H	4.25413800	4.39516800	-2.87891000
Cu	-2.03415100	2.39077100	0.47392700
N	-3.26808700	3.64411200	1.15547600
C	-4.05292300	4.36863700	1.60035700
C	-5.03119500	5.26910900	2.15773500

H	-5.99317500	5.13040700	1.65528800
H	-5.15445800	5.06711600	3.22601100
H	-4.70384000	6.30445400	2.02477900
H	2.43304600	-0.31879900	-2.81579800
O	1.35273800	-0.68050300	1.71482800
H	2.22264200	-1.06478600	1.94450600
H	0.54877700	-1.12140500	2.12526300

**F1**

C	-0.27843300	-1.42251200	-0.99102100
C	0.94165700	-1.18295300	-0.38236300
N	1.04926700	0.23949200	-0.47168300
C	-0.10906000	0.82912300	-1.02251700
C	-0.92421700	-0.19678900	-1.36788500
C	-2.33795000	-0.45068800	-1.82358400
C	-3.27595600	0.20564400	-0.82460600
C	-3.65829000	1.54010400	-1.00117000
C	-3.65893500	-0.43374700	0.35660600
C	-4.38663200	2.21103400	-0.03501200
H	-3.37481700	2.06134500	-1.91527900
C	-4.38710400	0.23364500	1.34798900
H	-3.43202100	-1.49274700	0.49549100
C	-4.75272200	1.56762400	1.15388100
H	-4.69243900	3.24519500	-0.17509200
H	-4.68613700	-0.30524100	2.24279300
S	1.89893900	1.06382300	0.74090500
O	3.10684800	0.31126900	1.02733100
O	0.93114600	1.28250900	1.84976900
C	2.26626000	2.61847000	0.02172100
C	3.26706700	2.66200300	-0.95008000
C	1.57888500	3.75896700	0.42753700



C	3.57516700	3.88358500	-1.52342300
H	3.79482900	1.75663100	-1.24238200
C	1.90827800	4.97145400	-0.16224900
H	0.81282300	3.69611600	1.19593700
C	2.90265000	5.05229400	-1.14151300
H	4.35558900	3.94135200	-2.27977100
H	1.38766300	5.87596700	0.14567300
C	3.23611900	6.35821100	-1.78726900
H	4.31263600	6.45345000	-1.96487700
H	2.74164200	6.44469500	-2.76339100
H	2.91009300	7.20636400	-1.17743300
H	-0.51019300	-1.03397600	1.03186400
H	-0.20382700	1.90608400	-1.10294000
O	-5.45401700	2.30807200	2.03495400
C	-5.88559600	1.68932100	3.22921300
H	-6.43888600	2.44754100	3.78679500
H	-6.55156800	0.83928100	3.02712200
H	-5.03725100	1.34902700	3.83942200
C	-1.17111500	-2.52678600	-1.33505000
C	-2.37150200	-1.97257000	-1.82386200
C	-1.01690300	-3.90613600	-1.23591700
C	-3.42208100	-2.79657300	-2.19626400
C	-2.07301400	-4.72673900	-1.62202700
H	-0.08594600	-4.33468800	-0.86804900
C	-3.26511000	-4.17905900	-2.09598400
H	-4.35634700	-2.37052500	-2.55949400
H	-1.96770600	-5.80704400	-1.55485700
H	-4.07935100	-4.83622600	-2.39189800
Cu	2.35120600	-2.25510900	0.32062600
N	3.73980000	-3.34313800	0.98959400
C	4.62136200	-3.96838400	1.40296300

C	5.71968000	-4.74635200	1.91941500
H	6.64074200	-4.15706100	1.88341600
H	5.51847800	-5.02979400	2.95689200
H	5.85024400	-5.65189100	1.31961900
H	-2.54195800	-0.04750800	-2.82549100
O	-0.91668800	-0.47963400	1.77655300
H	-1.79838100	-0.15961800	1.46108800
H	-0.25274300	0.29493500	1.92280200

### TS<sub>F1</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -366.9

C	-0.29930300	-1.37794500	-0.98713500
C	0.88442600	-1.16040200	-0.28908700
N	1.02700000	0.26938300	-0.38527000
C	-0.09835000	0.86287300	-0.95886700
C	-0.91761900	-0.14788600	-1.35712700
C	-2.32857300	-0.37664500	-1.83434700
C	-3.28202600	0.24182200	-0.82511400
C	-3.73855100	1.55177100	-0.99815100
C	-3.62453300	-0.42155300	0.35472500
C	-4.50778400	2.17582100	-0.03046900
H	-3.48563900	2.09155100	-1.91052200
C	-4.39581500	0.19449800	1.34183500
H	-3.32972000	-1.46368400	0.49405700
C	-4.84176500	1.50405300	1.15116900
H	-4.87414500	3.19055500	-0.16713700
H	-4.66293100	-0.36339500	2.23462000
S	1.95581100	1.08404500	0.79037800
O	3.17103800	0.30747700	0.96921300
O	1.07244300	1.29072700	1.95658500

C	2.28875200	2.63665900	0.05150000
C	3.26378700	2.69171200	-0.94559400
C	1.58703500	3.76598600	0.46436700
C	3.53094100	3.91379500	-1.53770000
H	3.80054500	1.79393200	-1.24395300
C	1.87437000	4.97926200	-0.14559300
H	0.83800500	3.69082600	1.24873900
C	2.84502700	5.07202000	-1.14742100
H	4.28780300	3.98052800	-2.31706800
H	1.33865400	5.87489500	0.16228100
C	3.16848600	6.38592700	-1.78161700
H	4.10877600	6.78599000	-1.38129800
H	3.30078400	6.28554800	-2.86443100
H	2.38760200	7.12945800	-1.59589000
H	0.00550900	-1.16746500	1.00431900
H	-0.19255400	1.94127000	-1.02646500
O	-5.59479000	2.19384500	2.03328200
C	-5.99939200	1.53555200	3.21488200
H	-6.60902300	2.24841100	3.77377300
H	-6.60414200	0.64486300	2.99489700
H	-5.13852200	1.24370700	3.83268800
C	-1.19627800	-2.46846800	-1.34229000
C	-2.37466600	-1.89672100	-1.86292900
C	-1.05895100	-3.85001100	-1.23761500
C	-3.42385600	-2.70753900	-2.26600000
C	-2.11373400	-4.65644100	-1.65272200
H	-0.14315300	-4.28870400	-0.84474200
C	-3.28395800	-4.09123900	-2.16193000
H	-4.34406400	-2.27108300	-2.65120500
H	-2.02616600	-5.73793000	-1.58260700
H	-4.09711100	-4.73868800	-2.48151800

Cu	2.33095200	-2.24909400	0.32667300
N	3.75146300	-3.33916200	0.91758300
C	4.65340400	-3.97157800	1.27164700
C	5.77847900	-4.75996600	1.70836700
H	6.67873000	-4.13868500	1.73245900
H	5.59058000	-5.15623500	2.71069700
H	5.93758700	-5.59334700	1.01766500
H	-2.52516400	0.05082800	-2.82727900
O	-0.57120400	-0.78397000	1.90210900
H	-1.46958600	-0.52467900	1.60980200
H	-0.06970500	0.04224000	2.16213000

#### 4a

C	0.06507700	-1.33221100	0.77060100
C	1.11548700	-0.88772700	1.52289800
N	1.30637900	0.44705800	1.16871700
C	0.41432900	0.82058600	0.16028800
C	-0.36559400	-0.26763900	-0.08401600
C	-1.53912500	-0.69291400	-0.92551500
C	-2.78094000	0.16291600	-0.82057000
C	-3.51865200	0.49259700	-1.96004700
C	-3.25261000	0.59810900	0.41627100
C	-4.68598000	1.23483700	-1.87036300
H	-3.16729700	0.16129600	-2.93752500
C	-4.42029100	1.34583700	0.52624800
H	-2.69390200	0.34876000	1.31819300
C	-5.14428100	1.66772900	-0.62404400
H	-5.26165700	1.49826300	-2.75463900
H	-4.75690200	1.67263600	1.50609000
S	2.70124800	1.33911400	1.56526200
O	3.15865100	0.79643000	2.83189200

O	2.33101900	2.73351300	1.40492400
C	3.84741500	0.89887400	0.29373800
C	4.62017500	-0.25072800	0.44318800
C	3.92534700	1.68633300	-0.85019500
C	5.48495000	-0.60907100	-0.57912400
H	4.54969700	-0.84532500	1.35089900
C	4.79883300	1.30960500	-1.86159600
H	3.31882000	2.58473400	-0.93540000
C	5.58664600	0.16198400	-1.74291800
H	6.09777900	-1.50337200	-0.47809900
H	4.87319100	1.91719000	-2.76172000
C	6.54083100	-0.23059000	-2.82662800
H	6.32228500	0.28843700	-3.76532500
H	7.57343800	0.01451200	-2.54661700
H	6.50882400	-1.30943300	-3.01607900
H	0.42481900	1.83035800	-0.22803800
O	-6.29046100	2.39049700	-0.63058500
C	-6.77811100	2.85656400	0.60523900
H	-7.69356800	3.41259700	0.38887700
H	-7.01960100	2.02986700	1.28863500
H	-6.06322300	3.53034600	1.09891200
C	-0.80226400	-2.48099200	0.55775400
C	-1.74806500	-2.12116000	-0.42325700
C	-0.83205900	-3.74732900	1.13448400
C	-2.72285800	-3.02126000	-0.82121200
C	-1.81127900	-4.64851900	0.72470600
H	-0.10542800	-4.02664900	1.89516000
C	-2.74947000	-4.29077300	-0.24304500
H	-3.46361000	-2.73356300	-1.56672500
H	-1.84809400	-5.64132800	1.16804400
H	-3.51086800	-5.00619700	-0.54593400

H	-1.24921500	-0.73308300	-1.98778800
H	1.72116400	-1.33915900	2.29669800

**5a**

C	-0.74062200	2.23259200	-0.48885500
C	-0.87348600	1.04206800	-0.69399800
N	-1.01418700	-0.27510700	-0.93370100
C	-0.39221100	-1.22600800	0.02925900
C	1.03117700	-0.98066800	0.15026800
C	2.21952800	-0.76412000	0.25739400
C	3.61799600	-0.51763000	0.38211000
C	4.52441800	-1.05466800	-0.54053700
C	4.11705900	0.27144000	1.43462900
C	5.88864500	-0.82016100	-0.42789200
H	4.14988700	-1.66483900	-1.35959800
C	5.47186600	0.50835000	1.55491100
H	3.42322700	0.69576000	2.15700700
C	6.36848500	-0.03573500	0.62526400
H	6.56852000	-1.24768800	-1.15883200
H	5.86912100	1.11620400	2.36430900
S	-2.51111100	-0.75534800	-1.63665900
O	-2.33818300	-2.16269600	-1.96162100
O	-2.79087300	0.23188100	-2.66424000
C	-3.69221500	-0.59747800	-0.33519400
C	-3.95943900	-1.69919100	0.47491100
C	-4.30159800	0.63775600	-0.11270200
C	-4.86089100	-1.55636700	1.52091500
H	-3.47794500	-2.65446200	0.27949300
C	-5.19649100	0.75716400	0.93989100
H	-4.08718900	1.48497900	-0.75953500
C	-5.49091300	-0.33276700	1.76759100

H	-5.08600400	-2.41003000	2.15765600
H	-5.68288700	1.71357000	1.12468400
C	-6.48320900	-0.19163900	2.87752600
H	-6.40339900	0.78751200	3.36221700
H	-7.50779800	-0.27749100	2.49292500
H	-6.35133300	-0.96876300	3.63712900
H	-0.88603600	-1.13432300	1.00876900
H	-0.57964500	-2.23498500	-0.35495500
O	7.67036900	0.25148600	0.82743100
C	8.61524000	-0.27135300	-0.08740100
H	8.43787000	0.09936700	-1.10572700
H	9.59448800	0.07306000	0.25165700
H	8.60435300	-1.36932400	-0.09555500
C	-0.56448100	3.61644400	-0.23591800
H	0.30779700	3.88025600	0.36443000
C	-1.38224800	4.57911400	-0.67959900
H	-2.26009200	4.35140800	-1.28099300
H	-1.18602900	5.62287500	-0.45063000

## A9

C	-0.44383500	1.79895700	1.67843600
C	-0.71217300	0.79448800	1.00097600
N	-0.73026400	-0.49317700	0.60553500
C	0.16912400	-1.48260600	1.24619600
C	1.56688600	-1.26317200	0.92186400
C	2.73680800	-1.06254800	0.67105800
C	4.11272900	-0.83414100	0.37909700
C	4.67503300	-1.28083200	-0.82323500
C	4.93653500	-0.15846100	1.29801100
C	6.01659100	-1.06808900	-1.11125600
H	4.04726100	-1.80335400	-1.54173300

C	6.27169300	0.05554400	1.02007800
H	4.51217000	0.19521400	2.23524800
C	6.82353000	-0.39869200	-0.18612000
H	6.42224600	-1.42720900	-2.05201700
H	6.91889600	0.57414800	1.72330500
S	-1.46150000	-0.89926500	-0.88392100
O	-0.51950700	-1.70297700	-1.63966800
O	-1.93469400	0.38847700	-1.41069100
C	-2.84612100	-1.87564100	-0.41721300
C	-2.81131500	-3.25160500	-0.61857500
C	-3.94150900	-1.24075800	0.17128800
C	-3.90880100	-4.00574200	-0.22166600
H	-1.94611200	-3.71837900	-1.08288600
C	-5.02226400	-2.01404500	0.55821500
H	-3.94828700	-0.16209400	0.31884100
C	-5.02333400	-3.40321200	0.36665200
H	-3.90177800	-5.08331400	-0.37236400
H	-5.88695900	-1.53907300	1.01823200
C	-6.21202200	-4.21548100	0.76835600
H	-6.61249200	-3.88513100	1.73313700
H	-7.01895500	-4.10560700	0.03242800
H	-5.96794700	-5.28000800	0.83572900
H	-0.00325700	-1.41365500	2.32669300
H	-0.16719000	-2.48100400	0.93664700
O	8.13493800	-0.14484000	-0.36405700
C	8.74216300	-0.58518100	-1.56533800
H	8.28540100	-0.11094900	-2.44415300
H	9.79172300	-0.29014100	-1.50592700
H	8.68137400	-1.67641200	-1.67052400
C	-0.13810700	2.93698300	2.47661000
H	-0.93566700	3.34402700	3.09819800



C	1.09298300	3.46392400	2.51294600
H	1.90055000	3.06482600	1.90263500
H	1.32217800	4.29808100	3.17077200
Cu	-1.77782000	2.16489500	-0.03479600
N	-2.78025100	3.61905500	-0.79514100
C	-3.37847200	4.47180000	-1.29942600
C	-4.12146700	5.53308900	-1.92743600
H	-5.18855900	5.40858100	-1.72079400
H	-3.78703000	6.49814600	-1.53558600
H	-3.95700700	5.50570000	-3.00861000

### TS<sub>A9</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -466.6

C	0.56403900	-0.80642600	0.38147300
C	-0.61361500	-0.60906500	0.89740600
N	-0.92541700	0.46408200	1.69519500
C	0.13142700	1.51342700	1.80573300
C	1.35546400	0.99425900	1.20808700
C	2.55212200	0.98106100	0.90628900
C	3.84445200	0.76685700	0.41511800
C	4.73337100	-0.09270500	1.09187500
C	4.25296000	1.34817100	-0.80911400
C	5.98496800	-0.36899000	0.57602000
H	4.41575500	-0.55034500	2.02607800
C	5.50085900	1.08539600	-1.32093100
H	3.56662900	2.00501200	-1.33862700
C	6.37756400	0.22557800	-0.63361900
H	6.65184900	-1.04084100	1.10732800
H	5.83651000	1.52287800	-2.25750200
S	-2.53830500	0.96358800	1.85067700

O	-2.49518200	2.03683200	2.83231600
O	-3.32152500	-0.24096000	2.08711900
C	-2.98570300	1.63757600	0.27849600
C	-2.90595800	3.01572100	0.08628200
C	-3.37290100	0.78257000	-0.75456600
C	-3.22151300	3.53937500	-1.16015100
H	-2.61670000	3.66566400	0.90827100
C	-3.68004900	1.32735700	-1.99296000
H	-3.44194800	-0.29287100	-0.59122500
C	-3.61239100	2.70778000	-2.21406800
H	-3.16869400	4.61480600	-1.32030300
H	-3.98634500	0.67286300	-2.80720200
C	-3.98357500	3.28508600	-3.54266600
H	-3.85487700	2.55437200	-4.34778100
H	-5.03673700	3.59477700	-3.54776900
H	-3.38624800	4.17268400	-3.77683900
H	-0.17753000	2.42630100	1.27472800
H	0.27836800	1.76653300	2.86068600
O	7.56427600	0.03071300	-1.21480700
C	8.50532300	-0.82043600	-0.57388800
H	8.11528700	-1.84091900	-0.47788500
H	9.38980200	-0.83055900	-1.21276400
H	8.77706000	-0.43452200	0.41599500
C	1.54375100	-1.69687400	-0.15355600
H	1.75938000	-2.60689200	0.41053900
C	2.25183000	-1.41175700	-1.25706300
H	2.06817200	-0.50088700	-1.82478600
H	3.03431400	-2.07673300	-1.61542200
Cu	-1.77801300	-2.00161000	0.23385500
N	-2.88800300	-3.37201100	-0.47301900
C	-3.60036900	-4.19345500	-0.87044100

C	-4.48731900	-5.21423000	-1.36409700
H	-4.01747000	-6.19604000	-1.25304400
H	-5.42104100	-5.19595700	-0.79424900
H	-4.70532900	-5.03487900	-2.42106500

**B9**

C	0.33197100	-1.32765700	-0.17598300
C	-0.88081200	-1.05975700	0.42055400
N	-0.68916700	-0.08786200	1.39605000
C	0.66987300	0.48250000	1.36218700
C	1.36097800	-0.44283500	0.38191400
C	2.64440100	-0.37481700	0.15439400
C	3.97501700	-0.22200800	-0.05017300
C	4.92312400	-0.93089800	0.75703100
C	4.46718000	0.65617100	-1.07520000
C	6.26809800	-0.77054800	0.57158900
H	4.54735300	-1.60141800	1.52568400
C	5.80616200	0.81900900	-1.25976000
H	3.74829200	1.18622000	-1.69437400
C	6.72166200	0.11184900	-0.43833300
H	6.97593300	-1.31003600	1.19219700
H	6.20865900	1.47928900	-2.02263100
S	-1.94773500	0.87402800	1.97462600
O	-1.35335400	1.66729400	3.04145800
O	-3.06744700	-0.01836600	2.24003700
C	-2.37784300	1.94507600	0.63416100
C	-1.81750800	3.21780200	0.57411300
C	-3.23094200	1.47937600	-0.36918900
C	-2.11957500	4.03445200	-0.50948300
H	-1.16929800	3.56962600	1.37293100
C	-3.51667900	2.30933200	-1.44153700

H	-3.66890400	0.48367500	-0.30087100
C	-2.96528100	3.59458500	-1.52998800
H	-1.69526600	5.03538400	-0.56336600
H	-4.18627200	1.96256400	-2.22731000
C	-3.28714400	4.46958000	-2.69963200
H	-2.91993800	4.02638100	-3.63367700
H	-4.37085100	4.59342500	-2.81271500
H	-2.83825600	5.46222300	-2.59615000
H	0.66165300	1.51370900	0.98306100
H	1.12849800	0.47541600	2.35427000
O	7.99132300	0.34096000	-0.69149200
C	9.00317100	-0.32928200	0.06982000
H	8.93730200	-1.41244100	-0.07535700
H	9.95395600	0.03809600	-0.31633400
H	8.91338900	-0.08107100	1.13230200
C	0.54905100	-2.33048300	-1.19358400
H	-0.35691700	-2.87295300	-1.47561000
C	1.70213800	-2.64007900	-1.79910400
H	2.64458700	-2.14712100	-1.56353000
H	1.74353000	-3.41171800	-2.56360700
Cu	-2.58344700	-1.83011000	-0.00479600
N	-4.24727500	-2.58776100	-0.51288500
C	-5.27255300	-3.04533200	-0.79586500
C	-6.54768600	-3.61441300	-1.14782900
H	-6.52816100	-3.94912700	-2.18904300
H	-6.76248300	-4.46826400	-0.49851100
H	-7.33299900	-2.86260700	-1.02508700

**TS<sub>B9</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -347.6

C	0.35205700	-1.50229400	-0.22564400
C	-0.81162700	-1.05670000	0.42176400
N	-0.43997900	0.00195800	1.18860600
C	0.97811600	0.39439700	1.04332500
C	1.44178500	-0.59785800	0.01555800
C	2.57287600	-0.61439000	-0.70343500
C	3.95034100	-0.37856800	-0.60451300
C	4.64344500	-0.52500000	0.62298500
C	4.69006000	0.01436200	-1.75058400
C	5.99435200	-0.26929300	0.71744000
H	4.08821200	-0.84140000	1.50419800
C	6.03433600	0.27066600	-1.66786100
H	4.16670500	0.10985500	-2.69919000
C	6.69949700	0.13151600	-0.43247000
H	6.50199700	-0.38056800	1.67030400
H	6.61558600	0.57667600	-2.53368400
S	-1.56390800	1.04761500	1.94885600
O	-0.73524700	1.95412000	2.72741200
O	-2.55279900	0.18889900	2.58026400
C	-2.31973400	1.92033700	0.61726400
C	-1.71385200	3.07792100	0.13537300
C	-3.47926700	1.40493200	0.03716800
C	-2.28676600	3.72675200	-0.95032700
H	-0.81823900	3.47166700	0.61004200
C	-4.03289000	2.06868300	-1.04718700
H	-3.93735300	0.50342600	0.44211300
C	-3.44754300	3.23482000	-1.55566800
H	-1.82898700	4.63540300	-1.33676700
H	-4.94010500	1.68192600	-1.50871100
C	-4.07487100	3.95166500	-2.70815700
H	-3.36376000	4.62189000	-3.20115000

H	-4.46519100	3.24747200	-3.45110400
H	-4.92219400	4.56139300	-2.36865800
H	1.06453800	1.44414700	0.74095700
H	1.51170800	0.26100900	1.99212800
O	8.00344800	0.39820200	-0.45152000
C	8.75132200	0.28370300	0.75510100
H	8.72226500	-0.74169900	1.14169500
H	9.77892000	0.54453100	0.49798000
H	8.37882200	0.97935000	1.51610800
C	0.56803800	-2.51845300	-1.18312600
H	-0.28490200	-2.96476100	-1.69603300
C	1.85438600	-2.78844300	-1.55080300
H	2.65637700	-2.70874100	-0.81710000
H	2.10105000	-3.34736900	-2.45076900
Cu	-2.59118200	-1.70649400	0.13937100
N	-4.32221500	-2.39456900	-0.23545700
C	-5.37598100	-2.83394600	-0.42755900
C	-6.68552300	-3.38383700	-0.66331000
H	-6.61971500	-4.18858700	-1.40168700
H	-7.08927200	-3.78384900	0.27156600
H	-7.35286200	-2.60261500	-1.03898100

## **C2**

C	0.49141400	-1.43689800	-0.20619500
C	-0.70516000	-0.80558900	0.28919900
N	-0.28477500	0.35334900	0.78654300
C	1.18935800	0.64545600	0.70031500
C	1.65331600	-0.59688200	0.02805400
C	2.77106400	-1.21572300	-0.42570400
C	4.15803300	-0.77742300	-0.39712300
C	4.52055000	0.46705900	0.13512900

C	5.18924600	-1.59430300	-0.89460700
C	5.84324200	0.88874800	0.18128700
H	3.75471000	1.13434900	0.52733100
C	6.50972300	-1.18788800	-0.85714800
H	4.95316400	-2.56900100	-1.31769000
C	6.85088300	0.05740400	-0.31574400
H	6.07848900	1.86017300	0.60600700
H	7.30513500	-1.82279200	-1.24077500
S	-1.35713600	1.48974300	1.57783500
O	-0.50435300	2.64030700	1.82028900
O	-1.99280000	0.77797800	2.67292400
C	-2.53569200	1.83606500	0.31937600
C	-2.13698700	2.61628000	-0.76518000
C	-3.82285200	1.31273900	0.41829400
C	-3.05528200	2.86948000	-1.77146600
H	-1.12794600	3.02130300	-0.81626100
C	-4.72529800	1.57953000	-0.60309400
H	-4.10852100	0.71208300	1.27877600
C	-4.35692700	2.35367100	-1.70814200
H	-2.76568400	3.48174200	-2.62341800
H	-5.73751600	1.18375800	-0.53966000
C	-5.32716900	2.61203200	-2.81536100
H	-5.19160000	1.88219400	-3.62410700
H	-6.36219700	2.52917900	-2.46921000
H	-5.18166800	3.60600300	-3.25146200
H	1.33978600	1.57110900	0.12946700
H	1.58839200	0.79884400	1.71090700
O	8.16534300	0.36490000	-0.31749700
C	8.55461600	1.60799200	0.23435900
H	8.27591900	1.68256200	1.29412000
H	9.64198100	1.65798200	0.14696900

H	8.11218500	2.45005600	-0.31473200
C	0.84713500	-2.59471200	-0.81280000
H	0.20948100	-3.42006100	-1.11118400
C	2.32547600	-2.54495600	-0.99915600
H	2.81118900	-3.39627600	-0.49608900
H	2.59544100	-2.65230200	-2.06167900
Cu	-2.47468300	-1.51887900	0.24655100
N	-4.20235300	-2.30838900	0.21382500
C	-5.27195800	-2.75143500	0.20485700
C	-6.60285800	-3.30030900	0.19360000
H	-6.98602000	-3.31587400	-0.83091400
H	-6.58415500	-4.32065000	0.58747200
H	-7.25943400	-2.68500500	0.81597100

### TSc<sub>2</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -455.5

C	0.16531500	-1.86422200	0.13128500
C	-1.05382700	-1.33793600	0.61800800
N	-0.68860300	-0.26737000	1.36241300
C	0.75992800	0.10062800	1.29516400
C	1.28306500	-1.06264500	0.53046600
C	2.45300900	-1.62660400	0.10560100
C	3.81172600	-1.13350100	0.23384400
C	4.07443400	0.19894800	0.58540600
C	4.91604000	-1.96982500	-0.01586800
C	5.37175300	0.68431800	0.69797500
H	3.24949500	0.88719400	0.76269400
C	6.21072600	-1.50117100	0.09684000
H	4.75451500	-3.01104600	-0.28921800
C	6.45173100	-0.16887000	0.45669500



H	5.53038500	1.72398800	0.96856100
H	7.06345400	-2.15040200	-0.08808700
S	-1.79543700	0.66214800	2.28399900
O	-0.96570400	1.36037400	3.25180400
O	-2.84145500	-0.25624400	2.70601600
C	-2.47340700	1.82616600	1.14632800
C	-2.00509700	3.13627000	1.16706100
C	-3.48605200	1.42206000	0.27370700
C	-2.57329700	4.06174900	0.30067500
H	-1.22077600	3.42781700	1.86088800
C	-4.03134100	2.36027000	-0.58865000
H	-3.84716700	0.39345800	0.27971000
C	-3.58770800	3.69039900	-0.58632500
H	-2.22667200	5.09339800	0.31344500
H	-4.82670900	2.06643000	-1.27143100
C	-4.16981700	4.68018400	-1.54361100
H	-5.25005900	4.53932400	-1.65804800
H	-3.98316700	5.70951900	-1.22209100
H	-3.72260400	4.55854100	-2.53913500
H	0.85382200	1.06241400	0.76307400
H	1.17473600	0.21526600	2.30235600
O	7.74890100	0.19523400	0.54215500
C	8.04017500	1.52763800	0.91778900
H	7.64866700	1.75938500	1.91736700
H	9.12867300	1.61308600	0.93366700
H	7.63547500	2.24948600	0.19556200
C	0.60372100	-2.91347000	-0.67993100
H	0.00811600	-3.78435200	-0.94310300
C	2.09336700	-2.98153100	-0.46676000
H	2.26723700	-3.75232000	0.30598100
H	2.67397700	-3.28673400	-1.34281700

Cu	-2.82534600	-1.96753000	0.28316000
N	-4.52321500	-2.67071700	-0.18171700
C	-5.55421100	-3.11724600	-0.46132400
C	-6.83454000	-3.67463200	-0.81093100
H	-6.85562600	-4.73762300	-0.55328500
H	-7.62582800	-3.15482800	-0.26274300
H	-7.00492500	-3.56020700	-1.88563800
C	0.59803800	-2.09936100	-2.65372700
H	0.94607500	-3.03732200	-3.08151600
C	1.46072600	-1.03335800	-2.60399300
H	2.52460800	-1.21379300	-2.76960900
H	-0.47913700	-1.94385700	-2.69473800
C	1.09809600	0.33796500	-2.32845300
C	2.11442500	1.31156600	-2.26694100
C	-0.23098700	0.74722700	-2.10781700
C	1.81776400	2.63988400	-2.00112300
H	3.14623100	1.00498800	-2.43658100
C	-0.52288600	2.08017100	-1.84678400
H	-1.04225800	0.02133600	-2.16177100
C	0.49477100	3.03087000	-1.79225000
H	2.61783800	3.37574900	-1.96044300
H	-1.55675700	2.38191800	-1.68697700
H	0.25538900	4.07322900	-1.59052600

## D2

C	0.07030500	-1.67967400	-0.28628300
C	-1.13089900	-1.24170400	0.35203400
N	-0.72323100	-0.34568900	1.27080500
C	0.73315000	-0.09119400	1.26815200
C	1.15384200	-1.01782900	0.20608800
C	2.33844600	-1.34986200	-0.64292200

C	3.71849800	-1.08083800	-0.12926900
C	3.99352300	0.01166600	0.69299800
C	4.79733800	-1.87788100	-0.53383900
C	5.28828900	0.30937600	1.11289600
H	3.18791200	0.67130600	1.01253900
C	6.09073200	-1.59858600	-0.12650200
H	4.62429700	-2.73539900	-1.18201000
C	6.34749900	-0.50016400	0.70186600
H	5.45753300	1.16983200	1.75388200
H	6.92664300	-2.22122500	-0.43758300
S	-1.78430400	0.46422700	2.37405200
O	-0.90040600	1.36221700	3.09800800
O	-2.55540200	-0.55438100	3.06627500
C	-2.83774700	1.36417600	1.28796800
C	-2.31702900	2.46014800	0.59840900
C	-4.15513700	0.94979100	1.11925100
C	-3.14432900	3.14484800	-0.27648300
H	-1.28433200	2.77402300	0.74772500
C	-4.96556400	1.64924500	0.23257800
H	-4.53808000	0.10194800	1.68158500
C	-4.47566500	2.74937600	-0.47488300
H	-2.76270200	4.01002600	-0.81653600
H	-5.99949500	1.33883400	0.09130200
C	-5.34366300	3.50454000	-1.42898500
H	-4.95029000	3.43791500	-2.45080400
H	-6.36859000	3.12186700	-1.43247800
H	-5.37455300	4.56970900	-1.17082200
H	0.92910300	0.96428100	1.02602900
H	1.17251200	-0.30084600	2.25247100
O	7.64042500	-0.30635500	1.04716000
C	7.94238500	0.80239600	1.87040200

H	7.44007600	0.73184900	2.84480000
H	9.02322400	0.78726400	2.02638100
H	7.66406100	1.75039000	1.39014400
C	0.51348700	-2.46151400	-1.48627300
H	-0.11948800	-3.29370900	-1.80250900
C	1.94924000	-2.79511500	-1.04957400
H	2.00052200	-3.49074000	-0.20360900
H	2.56443200	-3.17299400	-1.87520300
Cu	-2.93601100	-1.74907100	-0.01775900
N	-4.73507000	-2.20598600	-0.41558800
C	-5.83849200	-2.47216300	-0.64351600
C	-7.21056000	-2.80439700	-0.92705700
H	-7.42524600	-2.61473400	-1.98299400
H	-7.38562400	-3.86196300	-0.70783700
H	-7.87340200	-2.19301300	-0.30747400
C	0.79369000	-1.40104200	-2.58440000
H	1.03555000	-1.89449700	-3.53210700
C	2.02534300	-0.63193700	-2.05315200
H	2.90409200	-0.88828800	-2.66099600
H	-0.07397400	-0.75606700	-2.76252200
C	1.94691300	0.86460500	-1.95995500
C	3.12065700	1.61254200	-2.10978700
C	0.76440900	1.54858800	-1.65378900
C	3.12153700	2.99372900	-1.94629200
H	4.04820900	1.09447500	-2.35426300
C	0.76240800	2.93144500	-1.48844600
H	-0.17170500	1.00015900	-1.53808300
C	1.94067500	3.65945200	-1.63017700
H	4.04780400	3.55098800	-2.06857400
H	-0.16999700	3.44221600	-1.25194700
H	1.93616600	4.73955600	-1.50273100

**TS<sub>E2</sub>**

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -251.0

C	-0.37029800	-1.90272900	-0.34501100
C	-1.53237700	-1.40656500	0.21575100
N	-1.05439700	-0.38573500	1.05428200
C	0.36741600	-0.23138100	1.00283400
C	0.76766300	-1.18098900	0.08662800
C	1.94702500	-1.67337300	-0.69753900
C	3.32014800	-1.38561400	-0.17100200
C	3.65108400	-0.12088300	0.32000500
C	4.32818300	-2.35719600	-0.19354500
C	4.92985800	0.17608400	0.78682500
H	2.90003200	0.66858700	0.32743400
C	5.60533300	-2.08085900	0.26735900
H	4.11171600	-3.35414900	-0.57369700
C	5.91634700	-0.81117100	0.76449800
H	5.14252900	1.17349300	1.16094300
H	6.38506500	-2.83935100	0.25543800
S	-2.00414100	0.60329800	2.02812500
O	-1.21673600	0.80452900	3.26325000
O	-3.32768400	0.01527700	2.12454400
C	-2.07604700	2.13911500	1.17361800
C	-1.28524900	3.20954300	1.58389000
C	-2.91482400	2.22346300	0.06267800
C	-1.35369500	4.39479500	0.86558400
H	-0.63737900	3.11834100	2.45162200
C	-2.96282300	3.41779000	-0.64090300
H	-3.52089000	1.37170400	-0.24136200
C	-2.18996500	4.51786000	-0.24981500
H	-0.74622800	5.24434100	1.17257800

H	-3.61115300	3.50305900	-1.51070200
C	-2.25308400	5.80530300	-1.00731300
H	-1.25379000	6.23394600	-1.14469300
H	-2.71313400	5.67093200	-1.99126500
H	-2.84702100	6.54886500	-0.46051800
H	0.81481400	0.71850900	1.29010000
H	0.79116400	-0.90280500	2.53985200
O	7.18680700	-0.63892900	1.19853700
C	7.54394800	0.63124600	1.70367000
H	6.95111200	0.89728100	2.59002100
H	8.59667600	0.56763200	1.98785600
H	7.42662100	1.41713800	0.94501400
C	0.10317900	-2.84699700	-1.41314400
H	-0.53576200	-3.70586200	-1.63669200
C	1.51811400	-3.15112400	-0.89020100
H	1.52671000	-3.71287700	0.05238700
H	2.14045000	-3.67094800	-1.63027000
Cu	-3.36413800	-1.85990300	-0.05778100
N	-5.16370500	-2.31190500	-0.43550500
C	-6.26777700	-2.57382200	-0.66614700
C	-7.64133300	-2.89847100	-0.95397000
H	-7.75511500	-3.10809000	-2.02177100
H	-7.93995000	-3.78044700	-0.37954100
H	-8.28361100	-2.05586900	-0.68133200
C	0.44800800	-1.96831200	-2.64052500
H	0.69595700	-2.59451900	-3.50580900
C	1.69783200	-1.16337300	-2.19101700
H	2.57604300	-1.52355100	-2.74554300
H	-0.39025400	-1.32441000	-2.92942700
C	1.64951800	0.33198300	-2.32854700
C	2.79635200	1.02110000	-2.73691800

C	0.51556100	1.08290800	-1.99111700
C	2.82154000	2.41144900	-2.79655700
H	3.68691100	0.45102000	-3.00251700
C	0.53925500	2.47291100	-2.04209500
H	-0.39845300	0.57861600	-1.67421600
C	1.69234100	3.14394200	-2.44282100
H	3.72652400	2.92257000	-3.11867600
H	-0.35334500	3.03465800	-1.76813800
H	1.70714100	4.23104800	-2.48484300
O	0.69186100	-0.91103500	3.58373700
H	-0.11092900	-0.31538500	3.72738300
H	0.52910500	-1.81411900	3.92315100

## **F2**

C	0.92165200	-1.71293500	-0.34969500
C	1.98140000	-0.83161500	-0.31802100
N	1.30773200	0.43942800	-0.33311300
C	-0.08829700	0.30066100	-0.44346100
C	-0.33525700	-1.03509300	-0.41490400
C	-1.41305000	-2.07901900	-0.32680000
C	-2.79893100	-1.70750000	-0.75676200
C	-3.35695200	-0.48193300	-0.38842500
C	-3.60547800	-2.59758600	-1.47641000
C	-4.66435300	-0.13775500	-0.72454000
H	-2.76633400	0.22432000	0.19444000
C	-4.90781100	-2.27217600	-1.82150300
H	-3.20870500	-3.56606500	-1.77746600
C	-5.44885500	-1.03804400	-1.44713400
H	-5.05677900	0.82647700	-0.41501100
H	-5.53103100	-2.96261700	-2.38576000
S	2.12891000	1.82377600	-0.83983800

O	2.22627000	1.77539100	-2.32249500
O	3.37486000	1.89948200	-0.09444900
C	1.04368900	3.12766500	-0.40189300
C	0.31883700	3.79118100	-1.38684700
C	0.91450200	3.43929100	0.95305200
C	-0.54906100	4.80263100	-0.99738900
H	0.43121000	3.51994900	-2.43303200
C	0.03712500	4.44689100	1.31557600
H	1.48632100	2.89935000	1.70506400
C	-0.70155600	5.14427500	0.34938800
H	-1.12201200	5.33718300	-1.75231200
H	-0.08237900	4.70439200	2.36637900
C	-1.62204500	6.24682200	0.76201900
H	-2.21100500	5.96461400	1.64186400
H	-1.04992500	7.14266300	1.03552200
H	-2.30797000	6.52344700	-0.04432300
H	1.49995900	-0.97505800	-3.57878000
O	-6.72823600	-0.81000900	-1.82740800
C	-7.31642700	0.42115100	-1.46069600
H	-6.78425600	1.27370600	-1.90494000
H	-8.33879700	0.40289100	-1.84498900
H	-7.34833600	0.54706500	-0.36980800
C	0.60955300	-3.17398100	-0.23233500
H	1.40669900	-3.87309300	-0.50021500
C	-0.68821800	-3.23627500	-1.06104400
H	-0.53889300	-3.02400200	-2.12795600
H	-1.20917200	-4.19606100	-0.95010400
Cu	3.86536900	-1.05488000	-0.09135300
N	5.71709000	-1.36889700	0.15340000
C	6.84935800	-1.54180800	0.32328900
C	8.25773100	-1.75565700	0.53582800



H	8.44432000	-2.81491500	0.73633300
H	8.81629600	-1.45348500	-0.35508900
H	8.59444800	-1.16244100	1.39130700
C	0.03750000	-3.37369900	1.19293600
H	-0.08797800	-4.44220400	1.40329100
C	-1.34593700	-2.67048800	1.15150700
H	-2.13506000	-3.43599800	1.17287600
H	0.70414700	-2.96410700	1.95994000
C	-1.65206700	-1.67294700	2.23227800
C	-2.95169800	-1.60084200	2.74571800
C	-0.70577900	-0.75584200	2.70604400
C	-3.30162700	-0.64552300	3.69481600
H	-3.70089000	-2.30605200	2.38522900
C	-1.05253600	0.20421400	3.65240600
H	0.31784400	-0.78760100	2.33411800
C	-2.35177700	0.26429200	4.15038500
H	-4.31893200	-0.61298600	4.07955600
H	-0.30077200	0.90822600	4.00479200
H	-2.62014300	1.01250100	4.89313300
O	2.28121100	-0.67454400	-3.07158100
H	2.26307500	0.34123500	-2.95303300
H	2.24083900	-1.03793300	-2.10429200
H	-0.73242200	1.17130600	-0.47893600

## TS<sub>F2</sub>

Number of imaginary frequencies: 1

Lowest frequency (cm<sup>-1</sup>): -77.9

C	0.92006500	-1.70616400	-0.39363800
C	1.98026700	-0.82320400	-0.37960400
N	1.30364400	0.44771500	-0.37237700
C	-0.09082500	0.30630500	-0.45788600

C	-0.33690300	-1.03087200	-0.43460700
C	-1.41244700	-2.07747000	-0.34354900
C	-2.80310600	-1.70506300	-0.75688800
C	-3.36025500	-0.48318900	-0.37508300
C	-3.61324300	-2.59057600	-1.47815300
C	-4.66982800	-0.13775700	-0.70128700
H	-2.76706700	0.21886500	0.21033500
C	-4.91782000	-2.26395400	-1.81321900
H	-3.21726400	-3.55620300	-1.78920700
C	-5.45742800	-1.03288400	-1.42694600
H	-5.06152600	0.82368200	-0.38228400
H	-5.54353900	-2.95060000	-2.37932800
S	2.12059600	1.84423700	-0.85917500
O	2.22035900	1.82008100	-2.33970500
O	3.36393400	1.90823400	-0.10750700
C	1.02912000	3.13521100	-0.39905600
C	0.29772900	3.80628400	-1.37401900
C	0.90042900	3.42833200	0.95996300
C	-0.57668600	4.80627000	-0.96990000
H	0.41035300	3.54904300	-2.42375700
C	0.01647300	4.42483200	1.33731900
H	1.47819700	2.88281800	1.70332700
C	-0.72911200	5.12916300	0.38161200
H	-1.15517100	5.34648600	-1.71655200
H	-0.10289900	4.66782600	2.39160800
C	-1.65672300	6.21979300	0.80978000
H	-2.23300800	5.92764700	1.69468700
H	-1.09110200	7.12055600	1.08071500
H	-2.35425900	6.49282700	0.01220400
H	1.58439700	-0.98978900	-3.57693000
O	-6.73864700	-0.80233500	-1.79940500

C	-7.32439500	0.42711900	-1.42319500
H	-6.79233600	1.28184700	-1.86338300
H	-8.34780900	0.41254600	-1.80486600
H	-7.35329700	0.54611200	-0.33145200
C	0.61354600	-3.16832100	-0.28588900
H	1.40915400	-3.86294100	-0.56932700
C	-0.69465900	-3.22648500	-1.09761500
H	-0.56033600	-3.00476000	-2.16445100
H	-1.21179800	-4.18843700	-0.98781700
Cu	3.85884700	-1.04758400	-0.09601500
N	5.70639500	-1.36145700	0.17868900
C	6.83625900	-1.53218900	0.36585000
C	8.24169700	-1.74308700	0.59973600
H	8.42728800	-2.80173300	0.80437700
H	8.81282400	-1.44099900	-0.28319800
H	8.56439300	-1.14818100	1.45944700
C	0.06053300	-3.38060100	1.14591600
H	-0.05746900	-4.45123600	1.34938200
C	-1.32638200	-2.68300300	1.12741300
H	-2.11163700	-3.45241600	1.15029200
H	0.73571800	-2.97427700	1.90721400
C	-1.62564200	-1.69722200	2.22090100
C	-2.92086800	-1.63588900	2.74689600
C	-0.67910900	-0.78037000	2.69481100
C	-3.26636000	-0.69165300	3.70854100
H	-3.67016300	-2.34091700	2.38634000
C	-1.02147100	0.16828000	3.65426000
H	0.34127900	-0.80311000	2.31329000
C	-2.31629200	0.21763200	4.16467700
H	-4.28029000	-0.66746400	4.10268800
H	-0.26965900	0.87179900	4.00739400

H	-2.58090100	0.95691600	4.91762900
O	2.35764600	-0.65455600	-3.07991800
H	2.31087000	0.35614400	-3.00352100
H	2.31266000	-0.97630200	-2.07759200
H	-0.73770200	1.17558000	-0.48081900

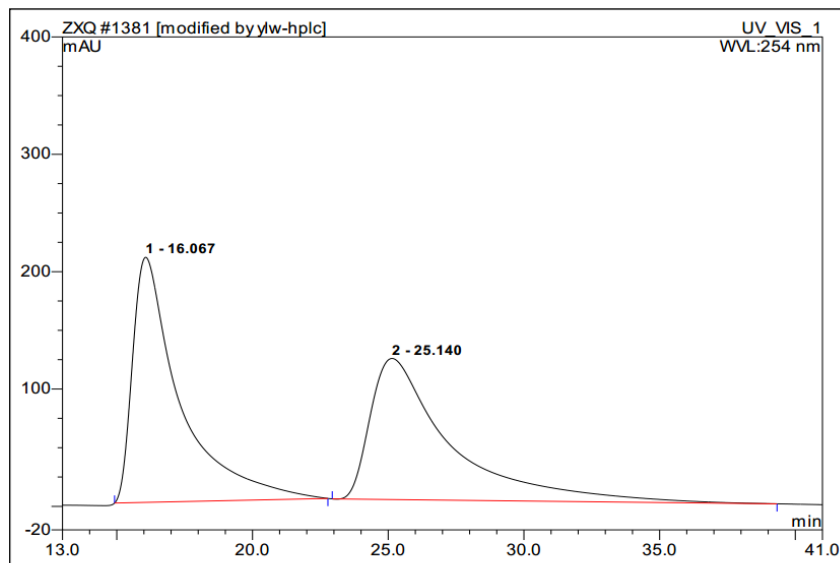
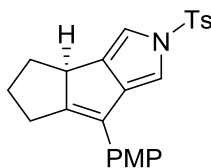
**6a**

S	2.75001900	-1.77354800	-1.63736400
O	-6.11926400	0.89540100	-1.97847200
O	3.65266700	-2.86741300	-1.31648100
O	2.23869000	-1.58173200	-2.98492900
N	1.39409100	-2.00548200	-0.65316300
C	0.21002700	-1.27073100	-0.79296300
H	0.02871300	-0.70124500	-1.69612400
C	-0.51488300	-1.50753200	0.33334000
C	-2.70182900	0.36612200	-0.71892700
H	-1.69131000	0.74609700	-0.86701900
C	-0.79009100	1.04639800	1.94209000
C	-5.04040700	0.44802000	-1.29168600
C	0.23709000	-2.37263400	1.18972000
C	-2.92820600	-0.63650200	0.22613600
C	-3.73644500	0.91050700	-1.47700600
H	-3.51634200	1.68643800	-2.20510800
C	3.19612500	0.91897300	-1.78116400
H	2.58036200	0.89401200	-2.67680000
C	1.07774200	2.40837600	1.19809300
H	2.12701000	2.47799300	0.91416800
C	3.44925400	-0.25232100	-1.07044100
C	3.76277800	2.10406100	-1.33541200
H	3.58337000	3.02670000	-1.88531300
C	4.23551400	-0.25439100	0.07902200

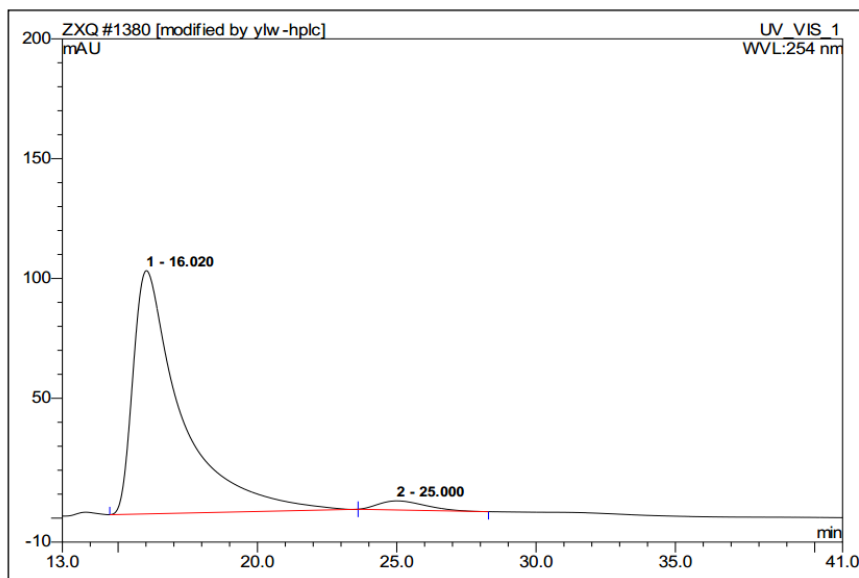
H	4.43008200	-1.18033500	0.61617300
C	-4.24542300	-1.07590000	0.40386200
H	-4.46219200	-1.85495900	1.13300400
C	0.55554700	1.17458900	1.57435600
H	1.21033900	0.30240100	1.57592000
C	4.55918200	2.13611100	-0.18454900
C	-1.41070800	-0.27490600	2.29295300
H	-2.36976200	-0.06928100	2.79035300
C	-1.58700700	2.19622000	1.92672900
H	-2.63667600	2.11352300	2.21011400
C	-1.06840500	3.43183300	1.55074900
H	-1.71098200	4.31005200	1.54830500
C	4.78151500	0.94564800	0.51537500
H	5.40186300	0.96059100	1.40962700
C	0.26916800	3.54195700	1.18207500
H	0.68106600	4.50533300	0.88828700
C	-5.28761900	-0.54727400	-0.34165800
H	-6.30908700	-0.89802200	-0.21053400
C	-0.59322900	-2.57921400	2.42128600
H	-0.36258000	-3.45172000	3.03690900
C	1.42800100	-2.64820700	0.59313500
H	2.27727900	-3.26260400	0.86136100
C	-5.90579200	1.88209200	-2.96576300
H	-6.88069500	2.08999300	-3.41285100
H	-5.22201400	1.52937500	-3.75027400
H	-5.50627000	2.81048500	-2.53443800
C	-2.00363300	-2.52167700	1.79948700
H	-2.79302800	-2.46078000	2.56084700
H	-2.21649000	-3.35461100	1.11828300
C	-1.79887400	-1.18336200	1.04524200
C	-0.57663600	-1.23365900	3.18643100

H	0.44290300	-0.87203400	3.35970400
H	-1.05450300	-1.34960900	4.16649700
C	5.13015300	3.43175900	0.29767500
H	5.61424500	3.98099200	-0.51806300
H	5.86403800	3.27849200	1.09481600
H	4.33753000	4.08167700	0.69201400

2a: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

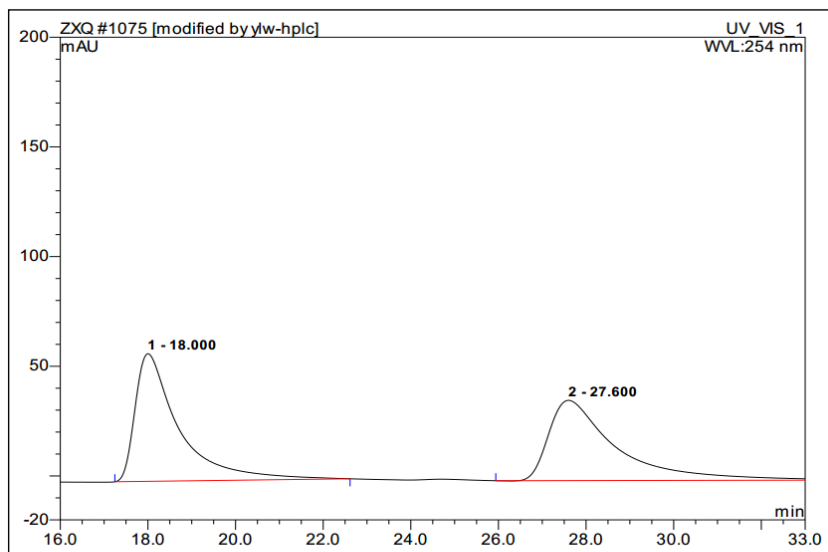
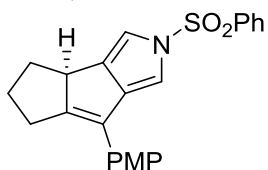


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.07	n.a.	208.818	422.123	50.90	n.a.	BMB*
2	25.14	n.a.	120.205	407.222	49.10	n.a.	BMB*
<b>Total:</b>			329.023	829.345	100.00	0.000	

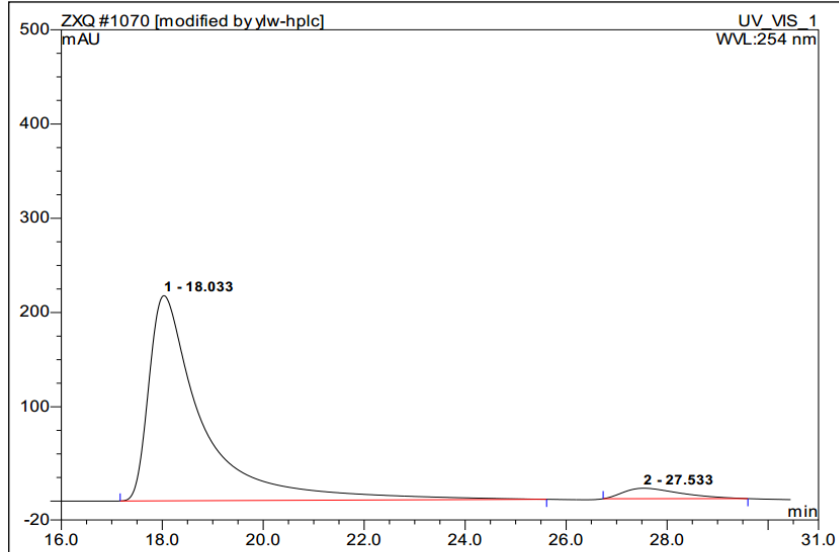


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.02	n.a.	101.471	203.430	96.51	n.a.	BMB*
2	25.00	n.a.	3.791	7.346	3.49	n.a.	bMB*
<b>Total:</b>			105.262	210.776	100.00	0.000	

2b: ADH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



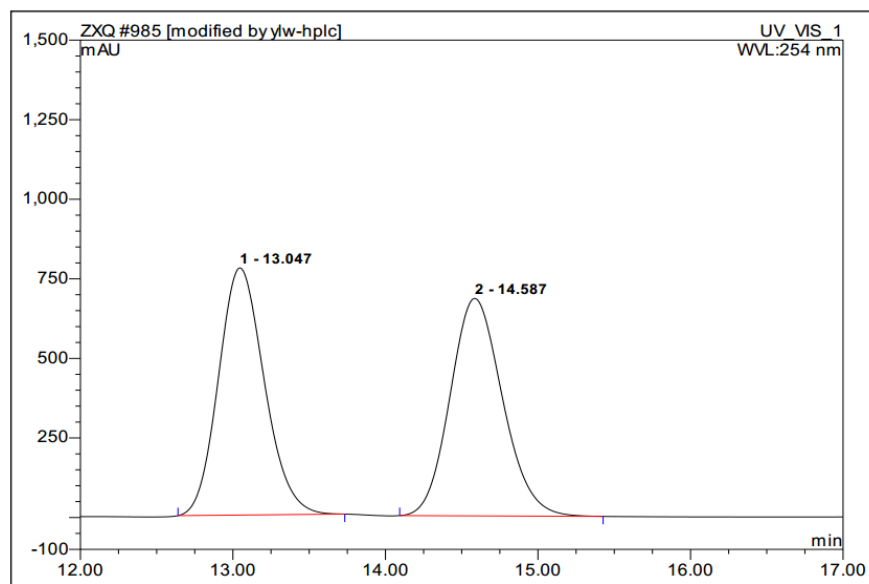
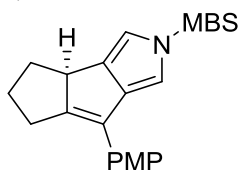
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.00	n.a.	58.158	67.162	50.81	n.a.	BMB*
2	27.60	n.a.	36.574	65.013	49.19	n.a.	BMB*
<b>Total:</b>			94.732	132.175	100.00	0.000	



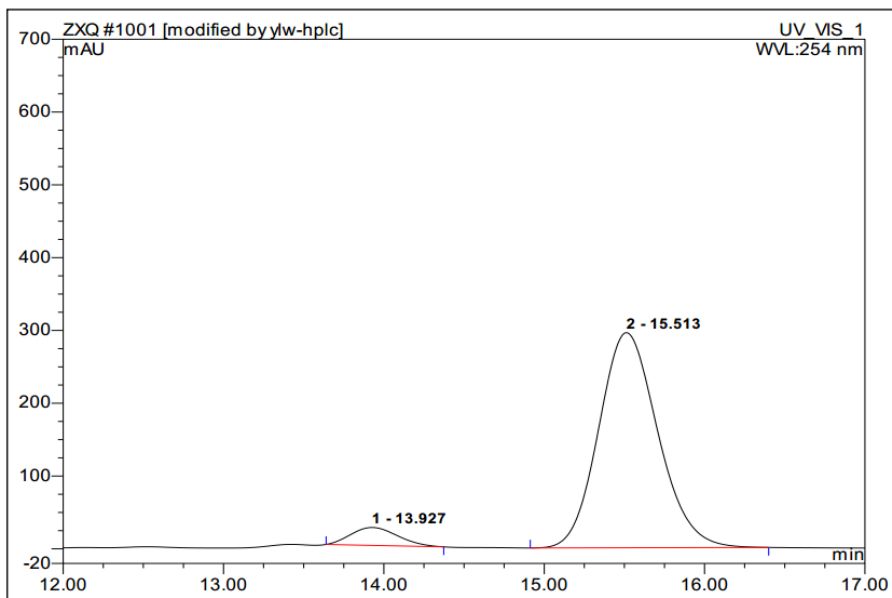
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.03	n.a.	217.635	269.093	94.88	n.a.	BMB*
2	27.53	n.a.	11.090	14.508	5.12	n.a.	BMB*
<b>Total:</b>			228.725	283.601	100.00	0.000	



2c: IC, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

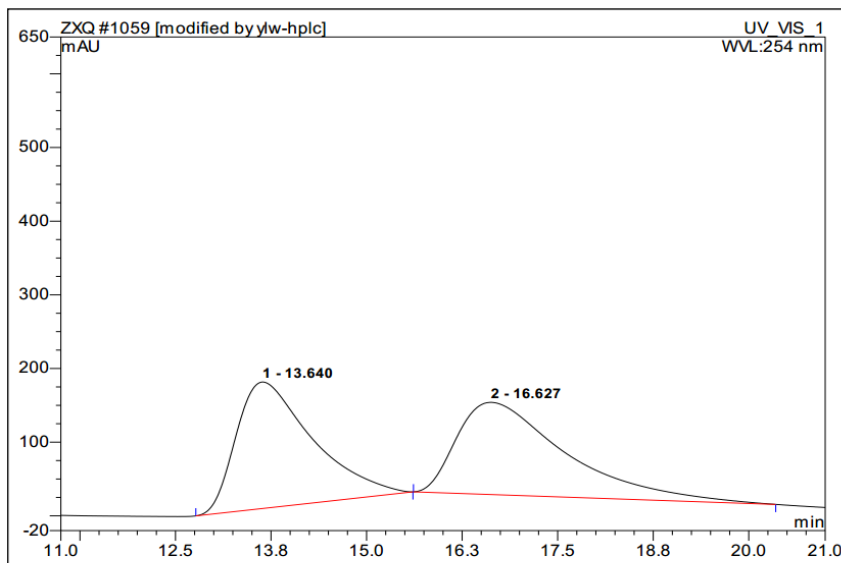
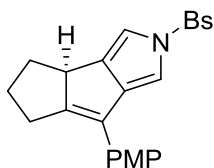


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.05	n.a.	776.578	270.480	49.89	n.a.	BMB*
2	14.59	n.a.	683.281	271.708	50.11	n.a.	BMB*
<b>Total:</b>			1459.859	542.188	100.00	0.000	

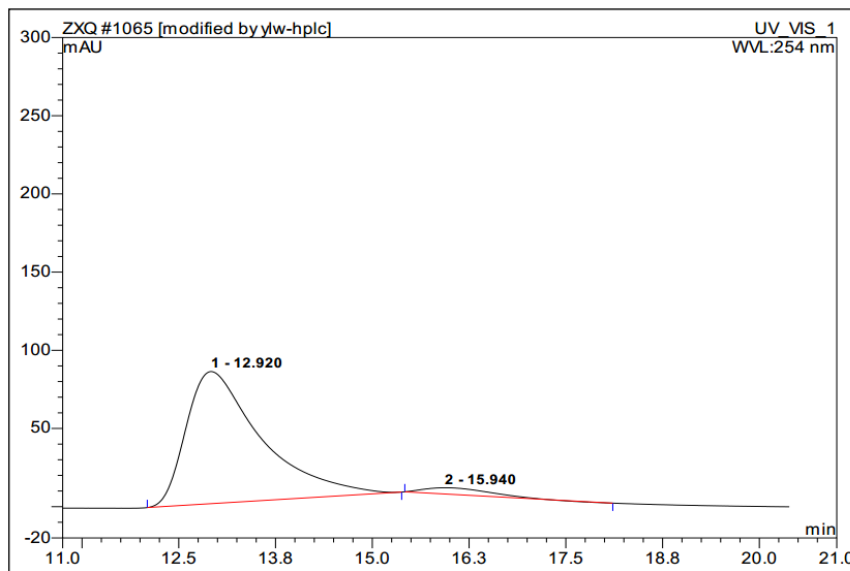


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.93	n.a.	24.603	8.303	6.17	n.a.	BMB*
2	15.51	n.a.	295.475	126.192	93.83	n.a.	BMB*
<b>Total:</b>			320.078	134.496	100.00	0.000	

2d: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

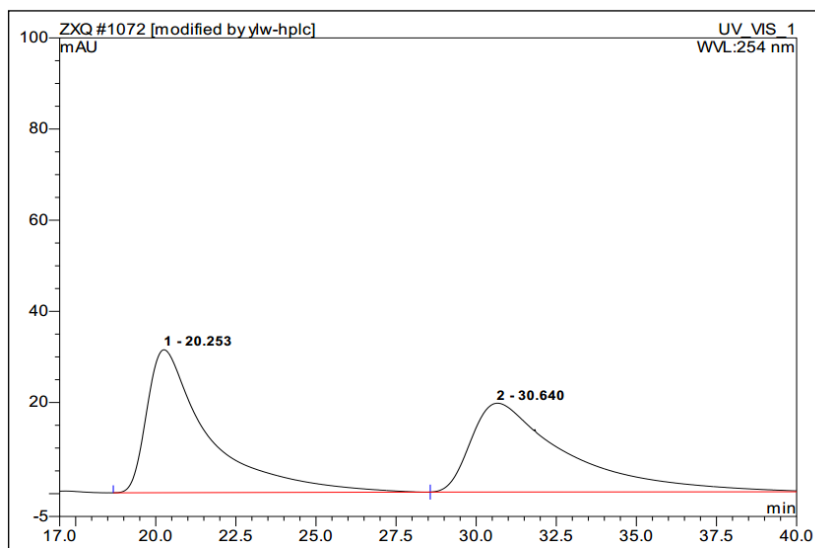
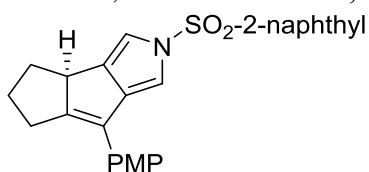


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.64	n.a.	171.672	198.084	49.11	n.a.	BMB*
2	16.63	n.a.	125.112	205.303	50.89	n.a.	BMB*
<b>Total:</b>			296.785	403.387	100.00	0.000	

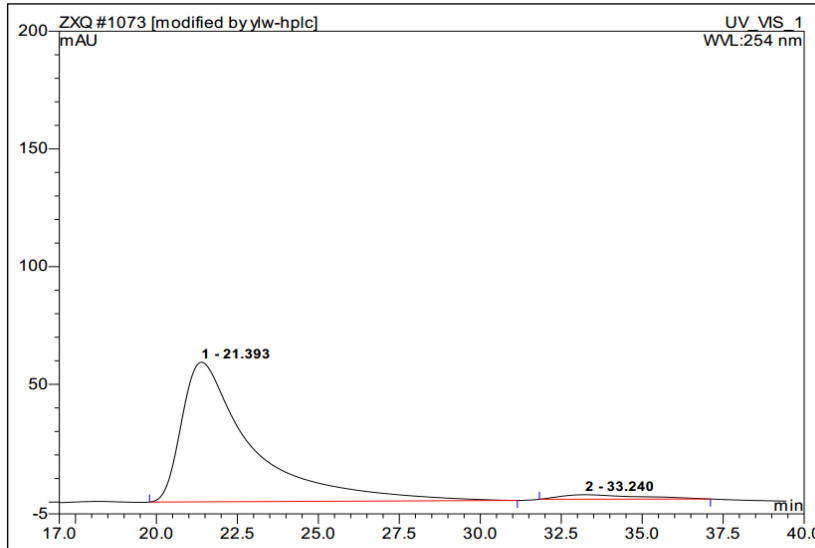


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.92	n.a.	84.469	94.677	96.01	n.a.	BMB*
2	15.94	n.a.	3.973	3.939	3.99	n.a.	BMB*
<b>Total:</b>			88.441	98.616	100.00	0.000	

2e: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

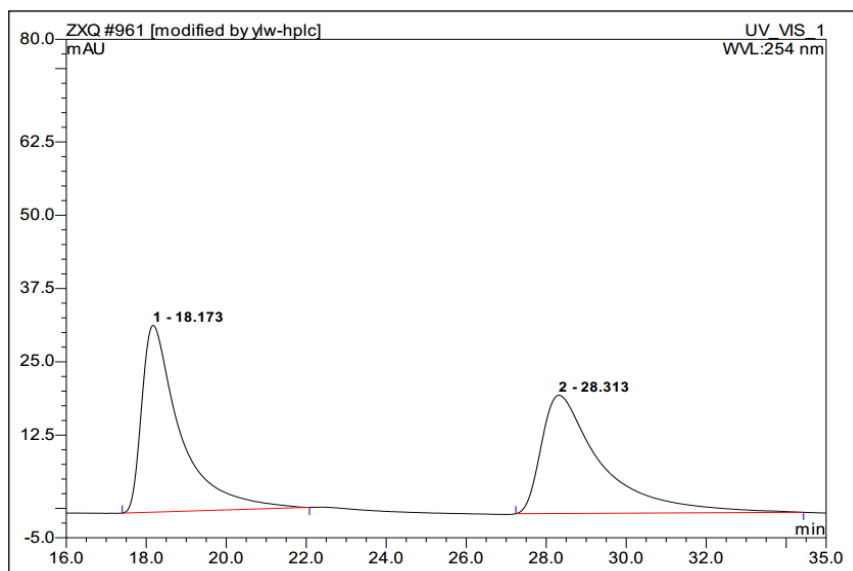
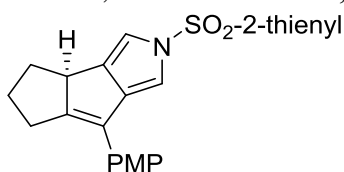


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	20.25	n.a.	31.365	69.632	50.90	n.a.	BMB*
2	30.64	n.a.	19.484	67.160	49.10	n.a.	bMB*
<b>Total:</b>			50.848	136.793	100.00	0.000	

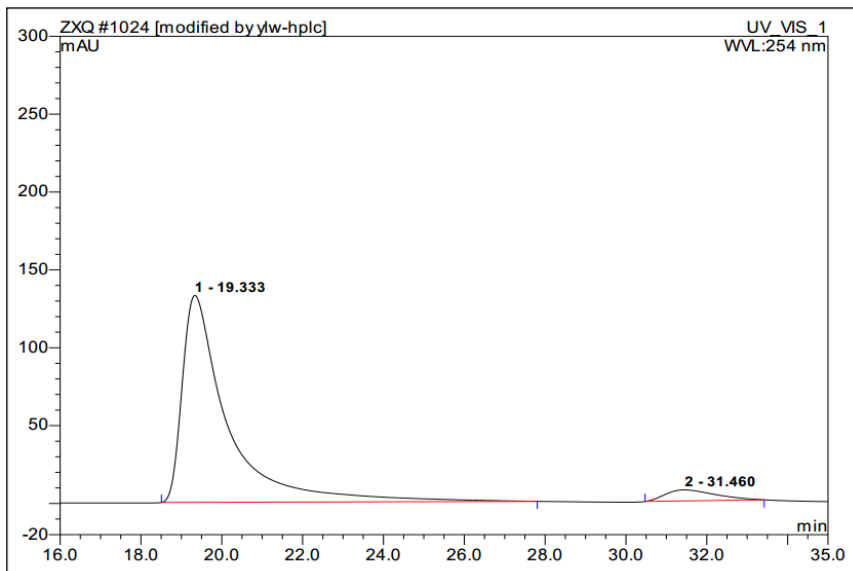


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	21.39	n.a.	59.301	148.437	96.50	n.a.	BMB*
2	33.24	n.a.	1.900	5.390	3.50	n.a.	BMB*
<b>Total:</b>			61.201	153.827	100.00	0.000	

2f: ADH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

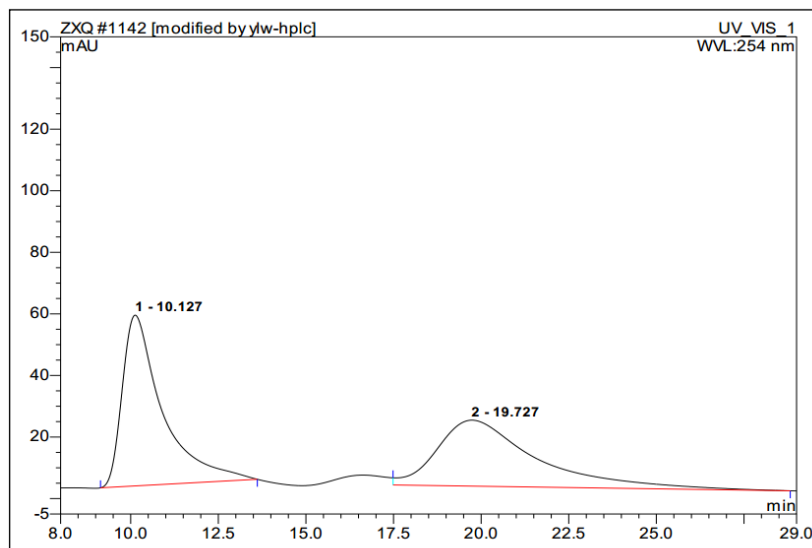
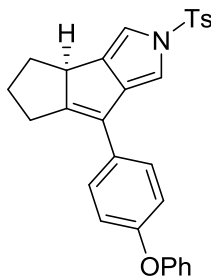


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.17	n.a.	31.850	35.527	50.37	n.a.	BMB*
2	28.31	n.a.	20.168	35.006	49.63	n.a.	BMB*
<b>Total:</b>			52.018	70.533	100.00	0.000	

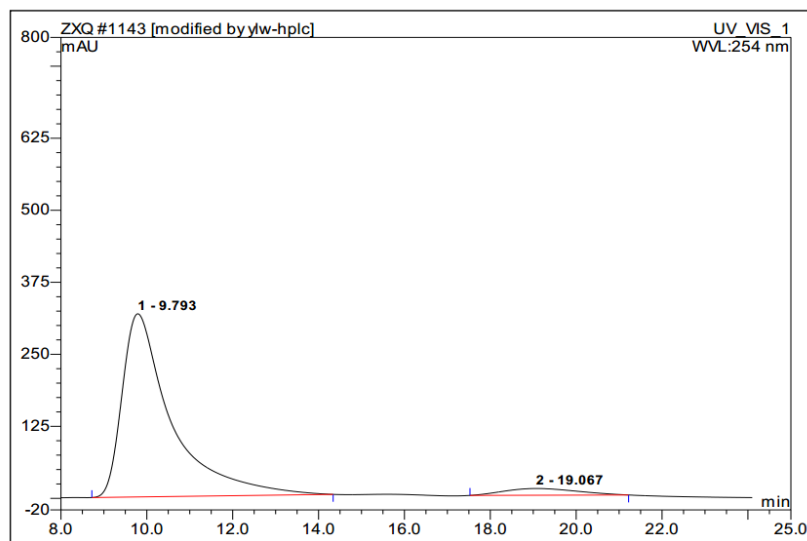


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.33	n.a.	132.876	173.074	94.48	n.a.	BMB*
2	31.46	n.a.	7.070	10.108	5.52	n.a.	BMB*
<b>Total:</b>			139.947	183.182	100.00	0.000	

2g: ASH, *n*-hexane/2-propanol = 50/50,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

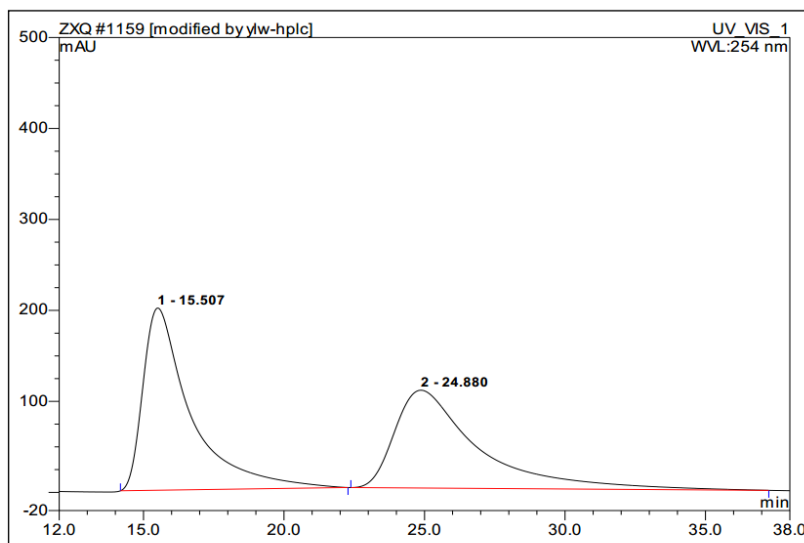
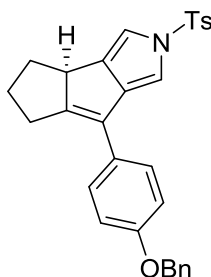


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.13	n.a.	55.480	73.674	51.28	n.a.	BMB*
2	19.73	n.a.	21.430	69.996	48.72	n.a.	MB*
<b>Total:</b>			76.910	143.670	100.00	0.000	

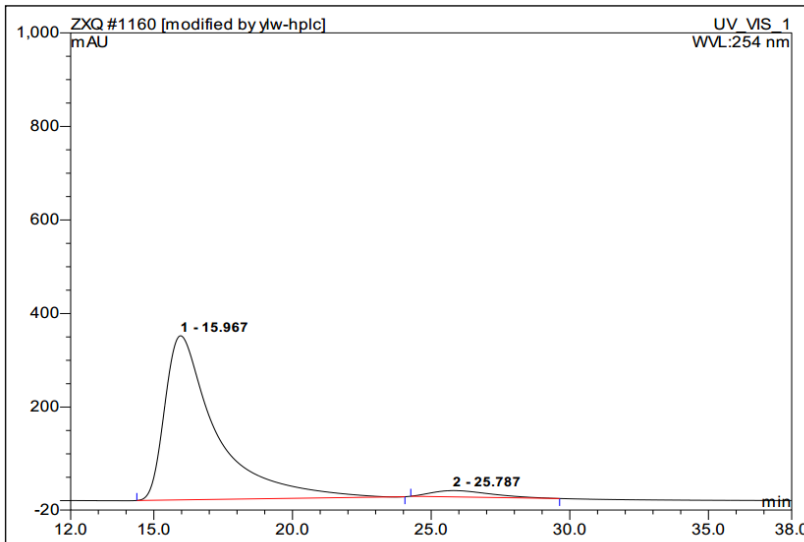


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.79	n.a.	317.848	422.696	94.85	n.a.	BMB*
2	19.07	n.a.	11.676	22.974	5.15	n.a.	BMB*
<b>Total:</b>			329.524	445.670	100.00	0.000	

**2h:** ASH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

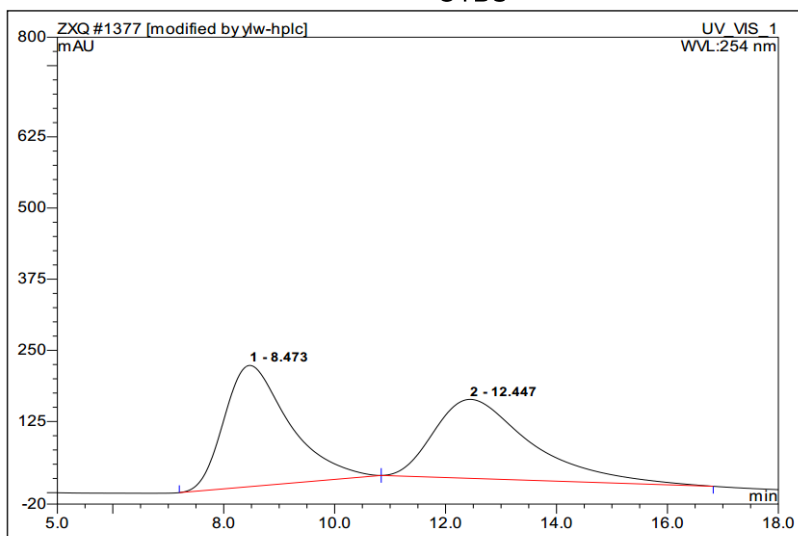
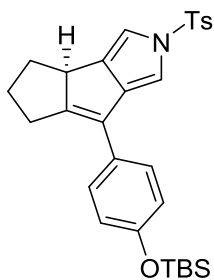


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.51	n.a.	200.286	394.761	51.82	n.a.	BMB*
2	24.88	n.a.	107.519	367.019	48.18	n.a.	BMB*
<b>Total:</b>			307.805	761.780	100.00	0.000	

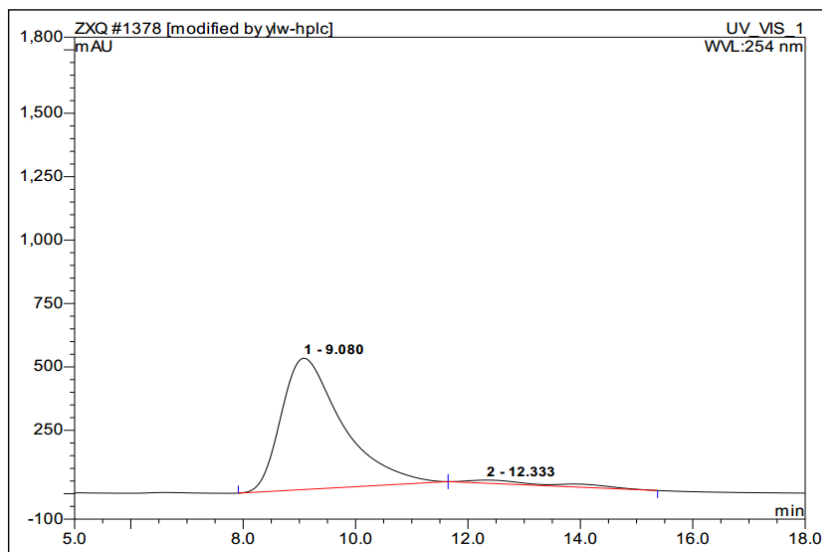


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.97	n.a.	350.786	756.062	95.77	n.a.	BMB*
2	25.79	n.a.	13.421	33.395	4.23	n.a.	BMB*
<b>Total:</b>			364.208	789.457	100.00	0.000	

2i: ASH, *n*-hexane/2-propanol = 98/2,  $\nu = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

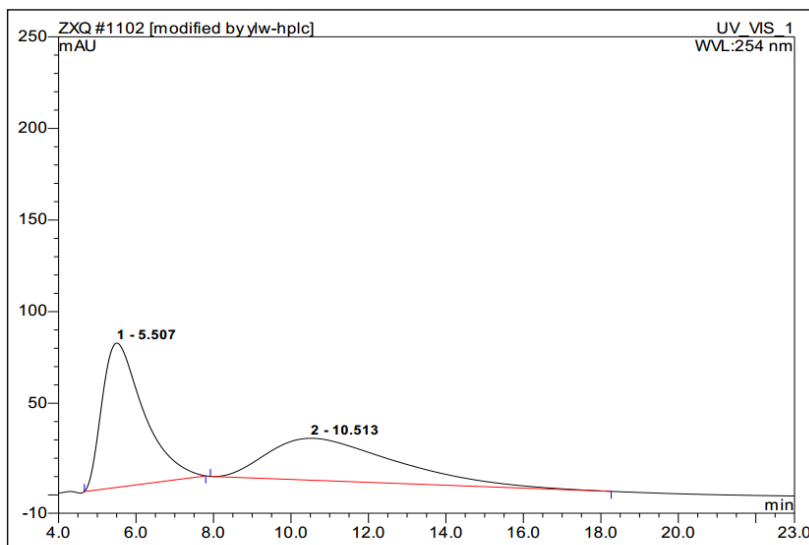
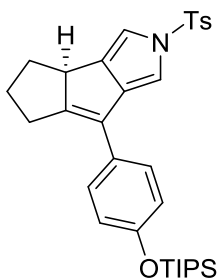


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.47	n.a.	212.818	288.667	50.74	n.a.	BMb*
2	12.45	n.a.	138.685	280.194	49.26	n.a.	bMB*
<b>Total:</b>			351.502	568.861	100.00	0.000	

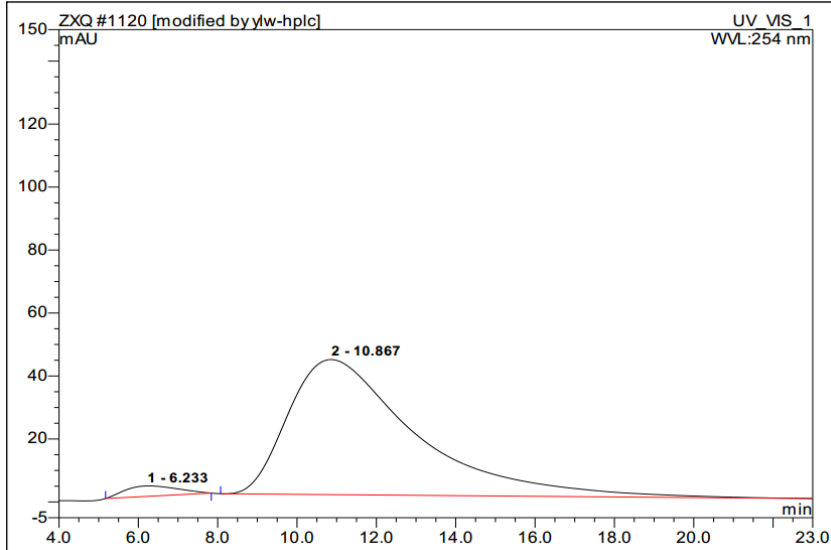


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.08	n.a.	517.614	653.385	96.09	n.a.	BMb*
2	12.33	n.a.	12.494	26.573	3.91	n.a.	bMB*
<b>Total:</b>			530.108	679.957	100.00	0.000	

2j: ASH, *n*-hexane/2-propanol = 99/1,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



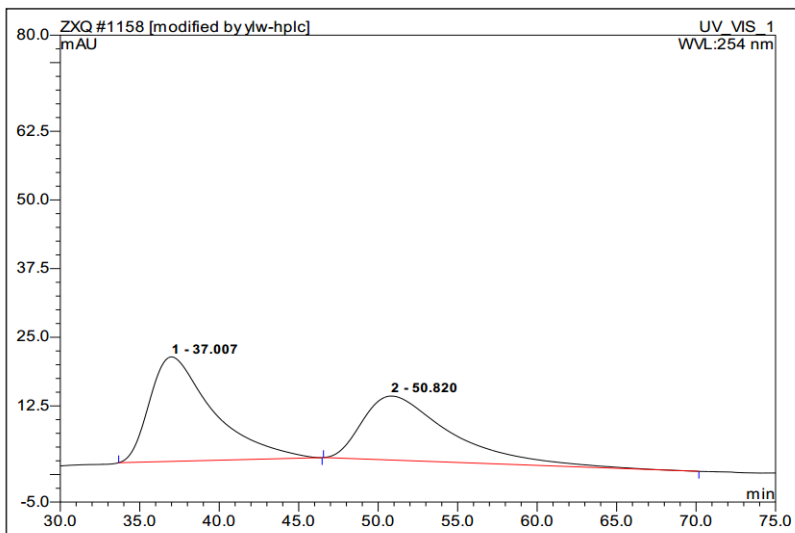
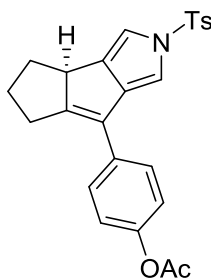
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	5.51	n.a.	78.713	98.058	52.68	n.a.	BMB*
2	10.51	n.a.	22.841	88.072	47.32	n.a.	BMB*
<b>Total:</b>			101.554	186.130	100.00	0.000	



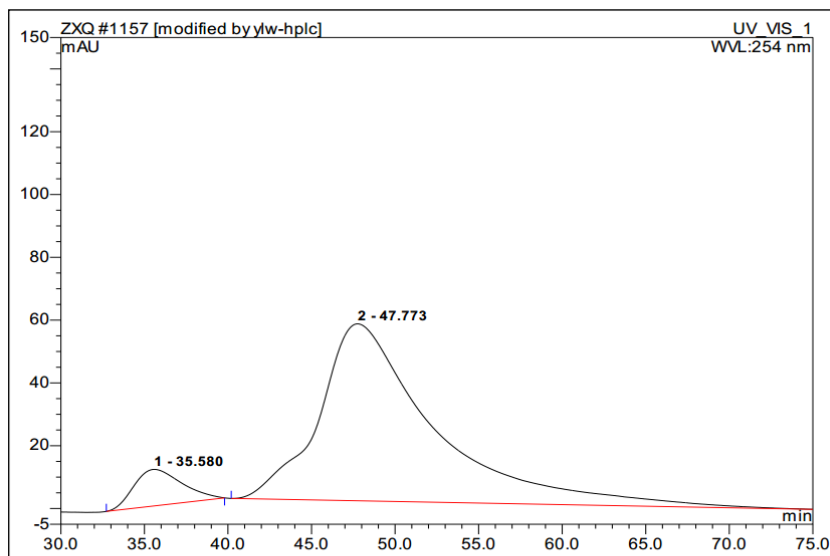
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.23	n.a.	3.309	5.082	3.10	n.a.	BMB*
2	10.87	n.a.	42.897	158.894	96.90	n.a.	BMB*
<b>Total:</b>			46.206	163.976	100.00	0.000	



**2k:** ASH, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

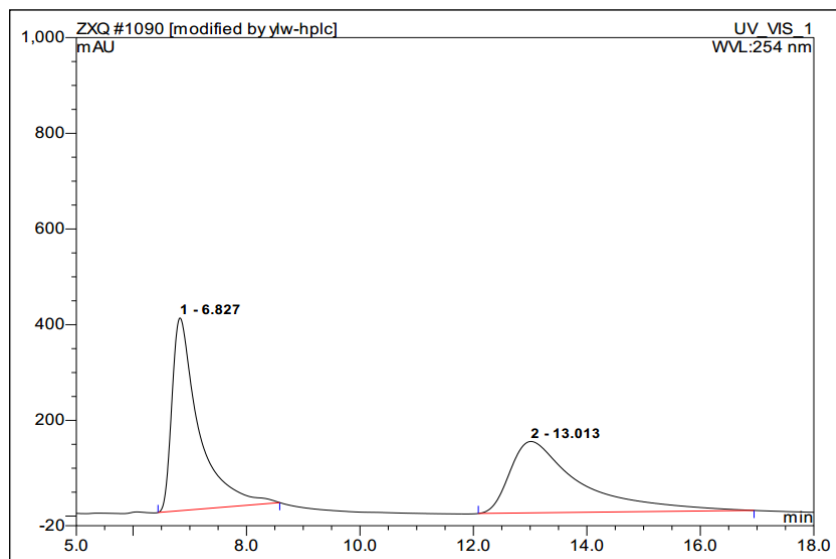
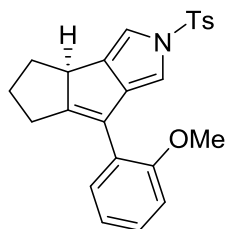


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	37.01	n.a.	19.027	87.679	54.01	n.a.	BMB*
2	50.82	n.a.	11.652	74.664	45.99	n.a.	BMB*
<b>Total:</b>			30.678	162.343	100.00	0.000	

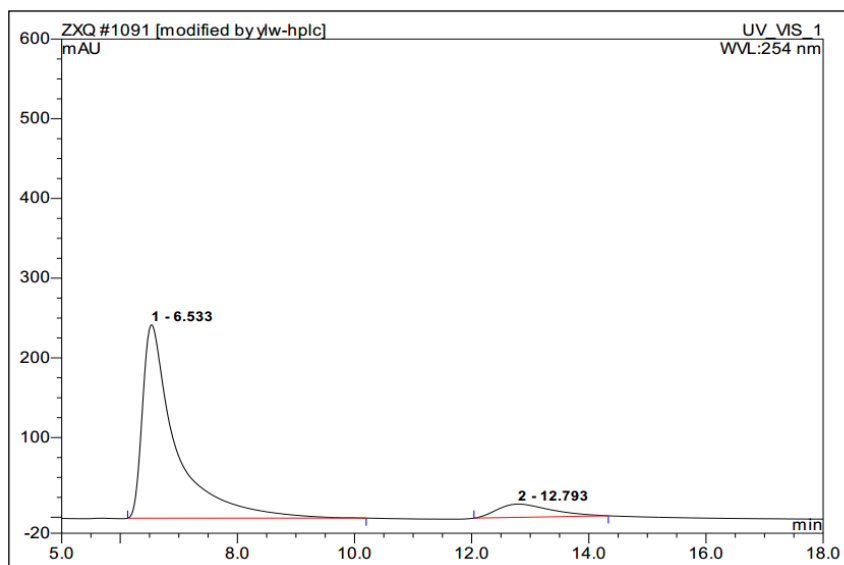


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	35.58	n.a.	11.632	38.534	7.91	n.a.	BMB*
2	47.77	n.a.	56.353	448.628	92.09	n.a.	BMB*
<b>Total:</b>			67.986	487.162	100.00	0.000	

2l: ASH, *n*-hexane/2-propanol = 50/50,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

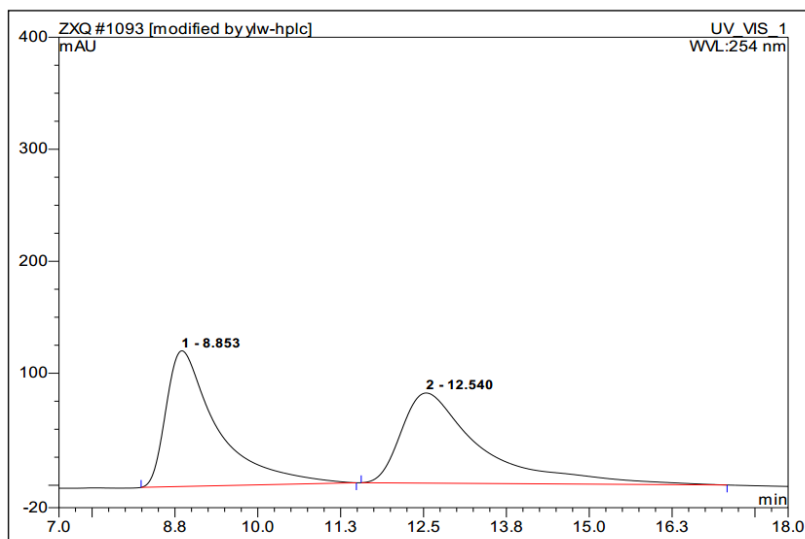
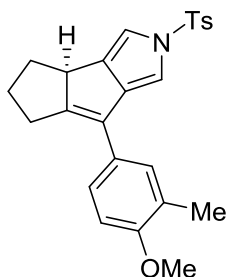


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.83	n.a.	402.794	222.206	51.12	n.a.	BMB*
2	13.01	n.a.	149.220	212.441	48.88	n.a.	BMB*
<b>Total:</b>			552.014	434.647	100.00	0.000	

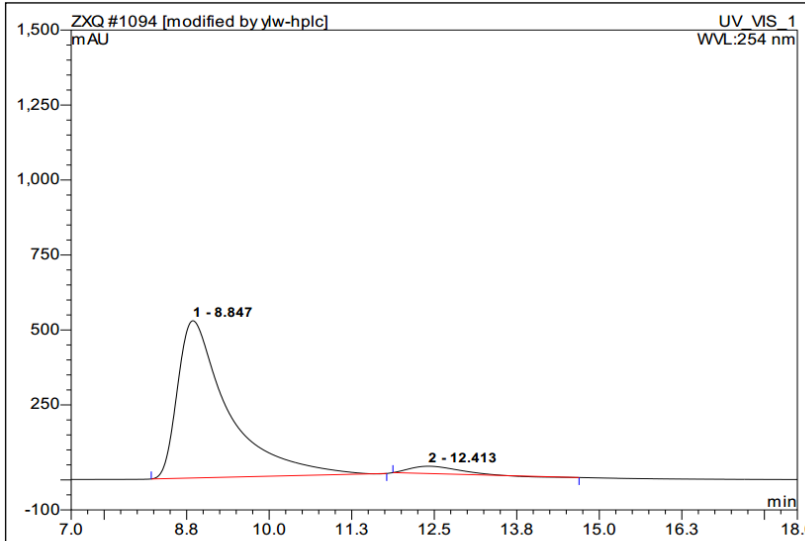


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.53	n.a.	242.594	160.414	90.09	n.a.	BMB*
2	12.79	n.a.	16.628	17.639	9.91	n.a.	BMB*
<b>Total:</b>			259.222	178.053	100.00	0.000	

**2m:** ASH, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

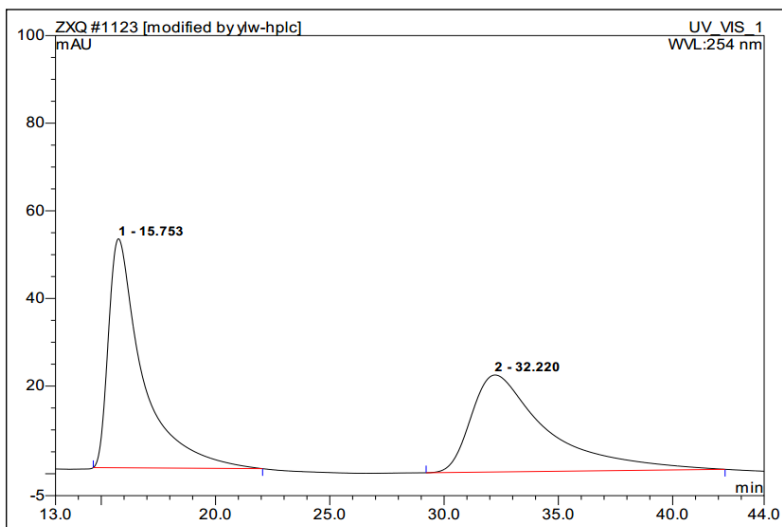
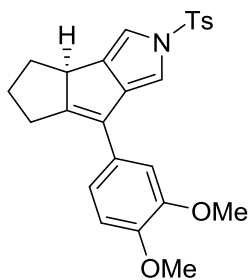


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.85	n.a.	121.132	108.500	49.43	n.a.	BMB*
2	12.54	n.a.	80.474	110.987	50.57	n.a.	BMB*
<b>Total:</b>			201.606	219.487	100.00	0.000	

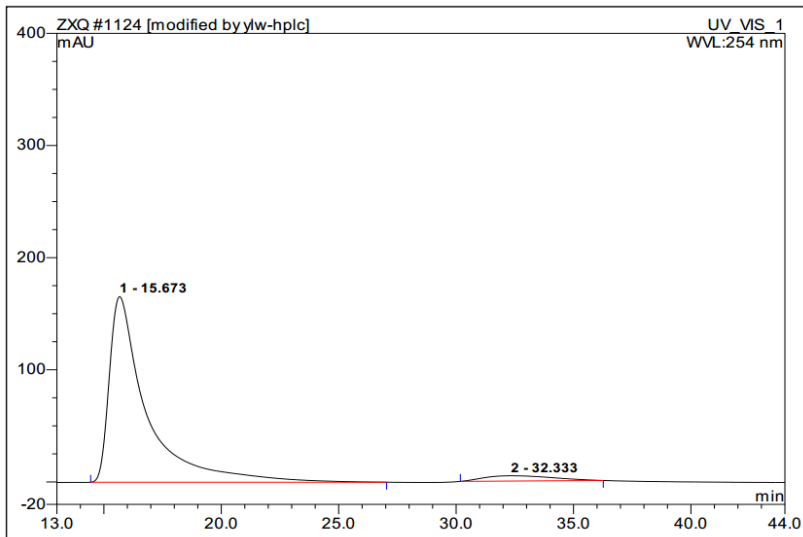


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.85	n.a.	524.266	466.048	95.90	n.a.	BMB*
2	12.41	n.a.	24.443	19.931	4.10	n.a.	BMB*
<b>Total:</b>			548.710	485.979	100.00	0.000	

**2n**: ASH, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

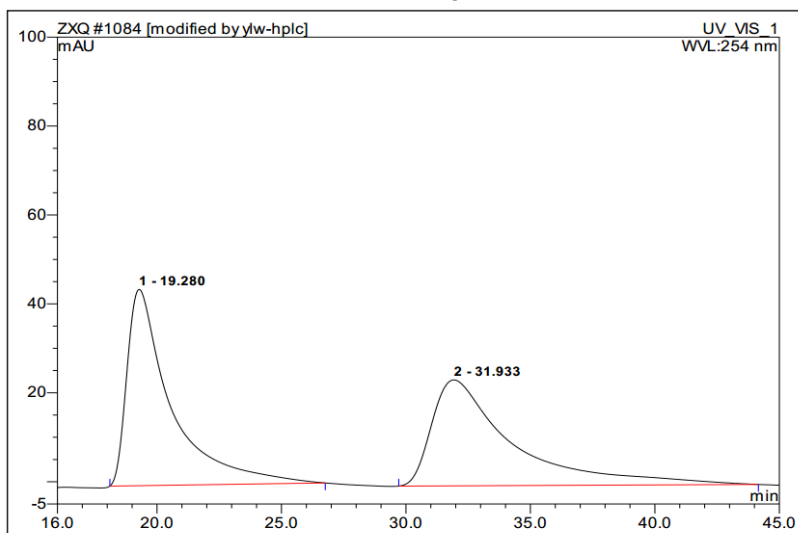
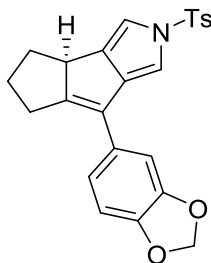


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.75	n.a.	52.254	90.423	51.65	n.a.	BMB*
2	32.22	n.a.	22.132	84.659	48.35	n.a.	BMB*
<b>Total:</b>			74.385	175.082	100.00	0.000	

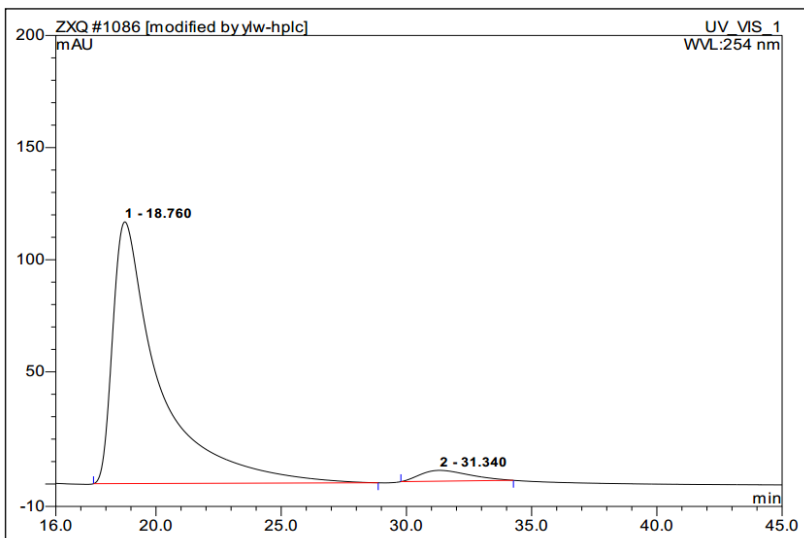


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.67	n.a.	165.442	306.673	95.06	n.a.	BMB*
2	32.33	n.a.	4.705	15.925	4.94	n.a.	BMB*
<b>Total:</b>			170.148	322.598	100.00	0.000	

2o: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

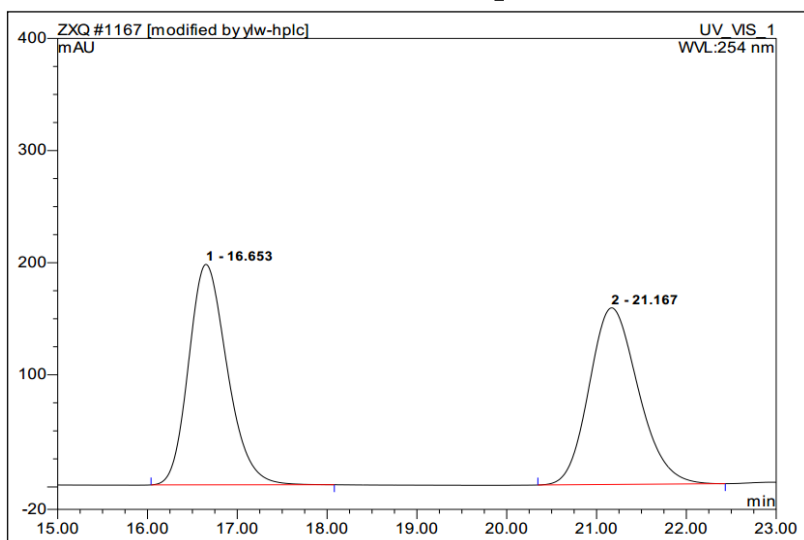
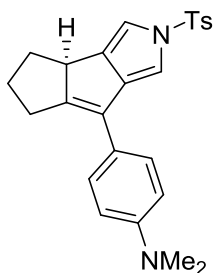


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.28	n.a.	44.143	90.668	50.53	n.a.	BMB*
2	31.93	n.a.	23.827	88.751	49.47	n.a.	BMB*
<b>Total:</b>			67.971	179.419	100.00	0.000	

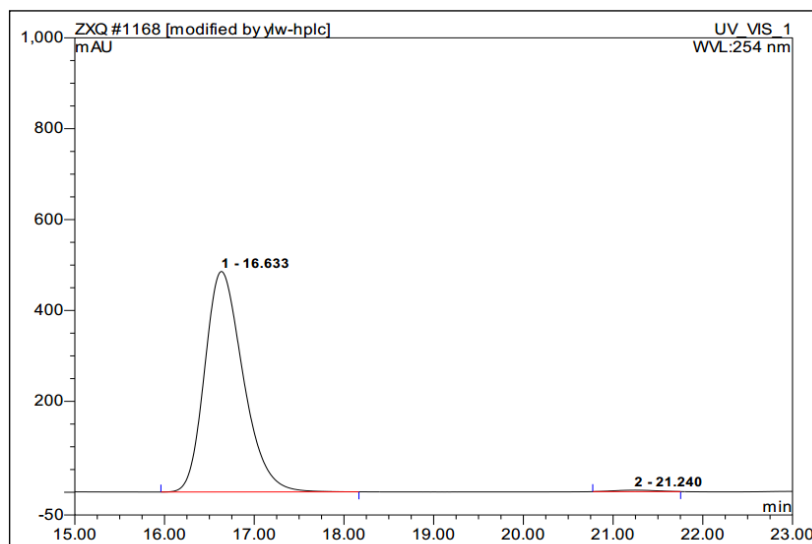


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.76	n.a.	116.710	251.741	95.82	n.a.	BMB*
2	31.34	n.a.	4.824	10.979	4.18	n.a.	BMB*
<b>Total:</b>			121.534	262.720	100.00	0.000	

**2p:** IC, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

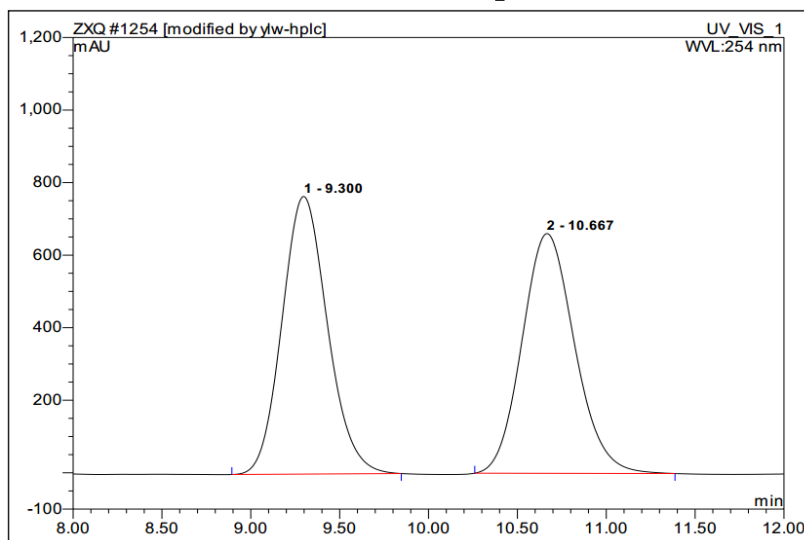
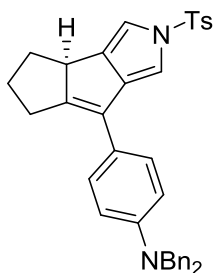


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.65	n.a.	196.581	97.908	49.48	n.a.	BMB*
2	21.17	n.a.	157.504	99.951	50.52	n.a.	BMB*
<b>Total:</b>			354.085	197.859	100.00	0.000	

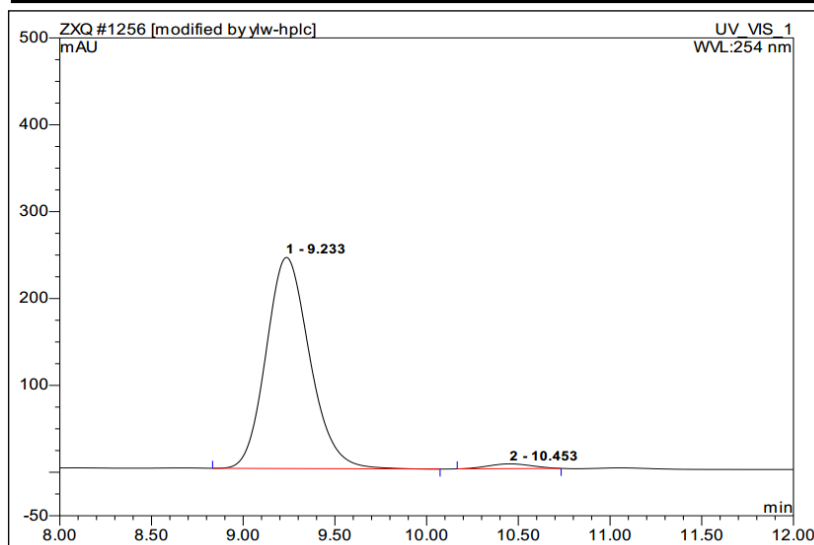


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.63	n.a.	485.274	241.175	99.32	n.a.	BMB*
2	21.24	n.a.	3.124	1.659	0.68	n.a.	BMB*
<b>Total:</b>			488.397	242.834	100.00	0.000	

2q: IC, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

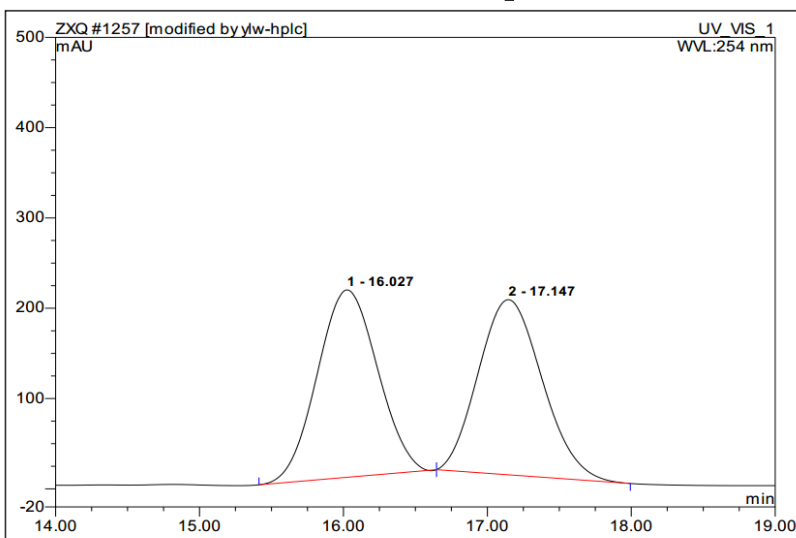
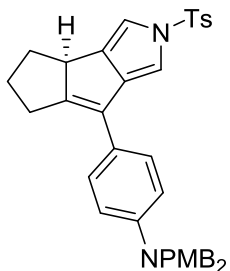


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.30	n.a.	765.335	227.052	50.06	n.a.	BMB*
2	10.67	n.a.	660.933	226.507	49.94	n.a.	BMB*
<b>Total:</b>			1426.269	453.558	100.00	0.000	

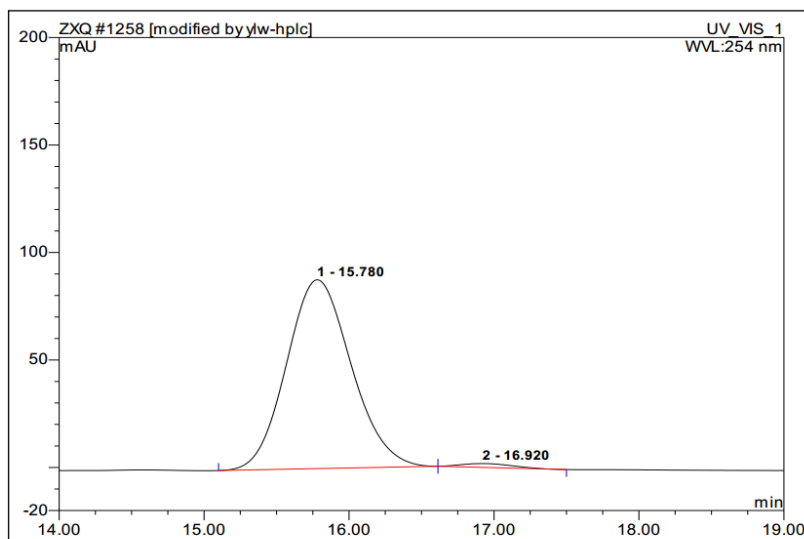


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.23	n.a.	242.999	67.084	97.79	n.a.	BMB*
2	10.45	n.a.	5.495	1.518	2.21	n.a.	BMB*
<b>Total:</b>			248.494	68.601	100.00	0.000	

2r: IC, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



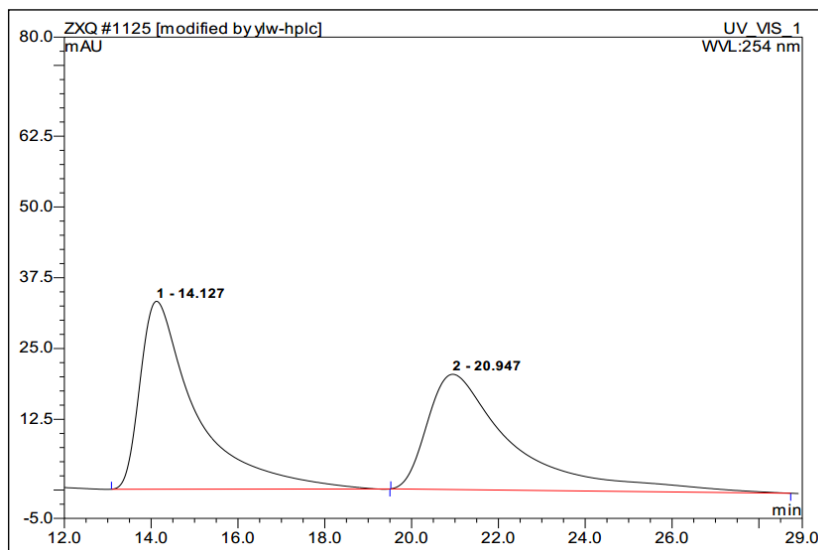
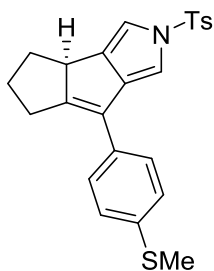
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.03	n.a.	207.465	100.403	50.16	n.a.	BMb*
2	17.15	n.a.	193.899	99.774	49.84	n.a.	bMB*
<b>Total:</b>			401.363	200.176	100.00	0.000	



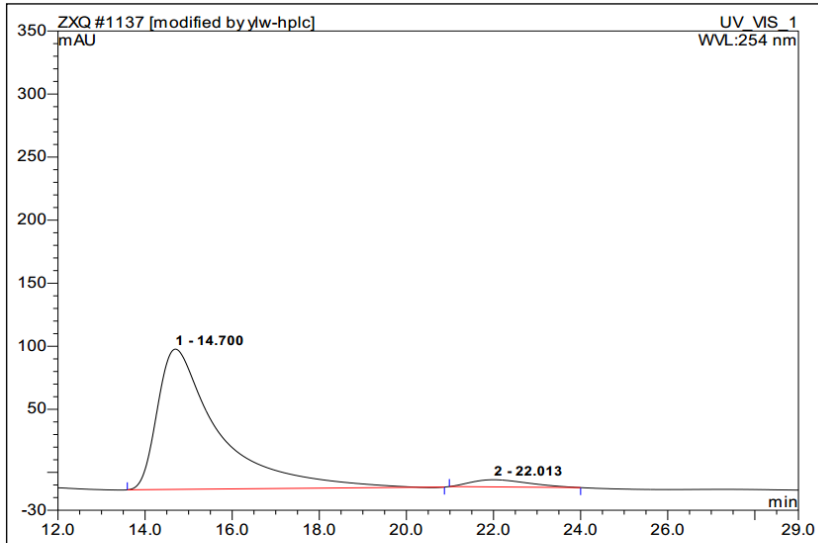
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.78	n.a.	87.824	45.464	98.41	n.a.	BMb*
2	16.92	n.a.	1.780	0.734	1.59	n.a.	bMB*
<b>Total:</b>			89.603	46.198	100.00	0.000	



2s: ASH, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

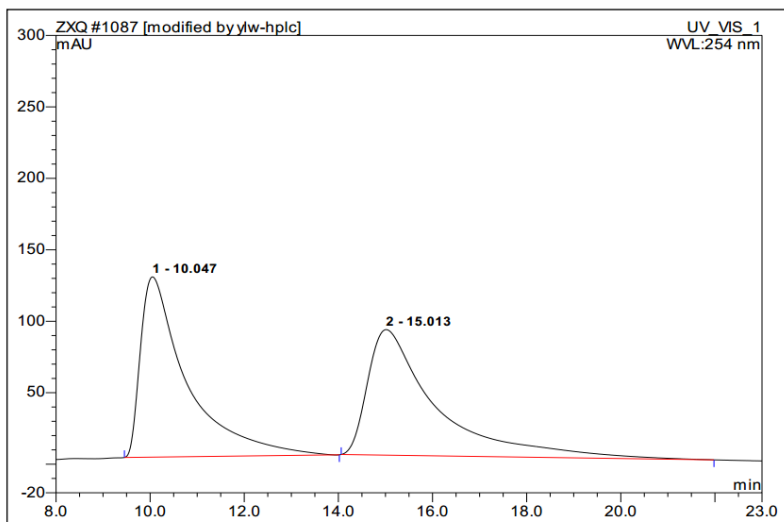
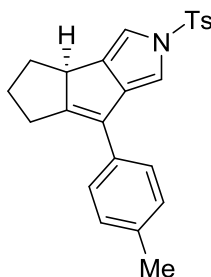


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.13	n.a.	33.190	49.631	51.84	n.a.	BMB*
2	20.95	n.a.	20.349	46.105	48.16	n.a.	BMB*
<b>Total:</b>			53.539	95.736	100.00	0.000	

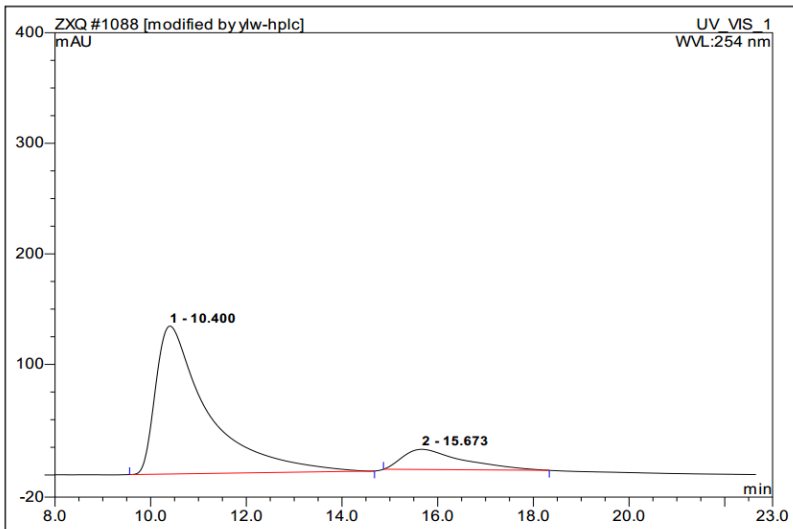


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.70	n.a.	111.242	180.955	95.39	n.a.	BMB*
2	22.01	n.a.	5.700	8.753	4.61	n.a.	BMB*
<b>Total:</b>			116.942	189.708	100.00	0.000	

2t: ASH, *n*-hexane/2-propanol = 90/10,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

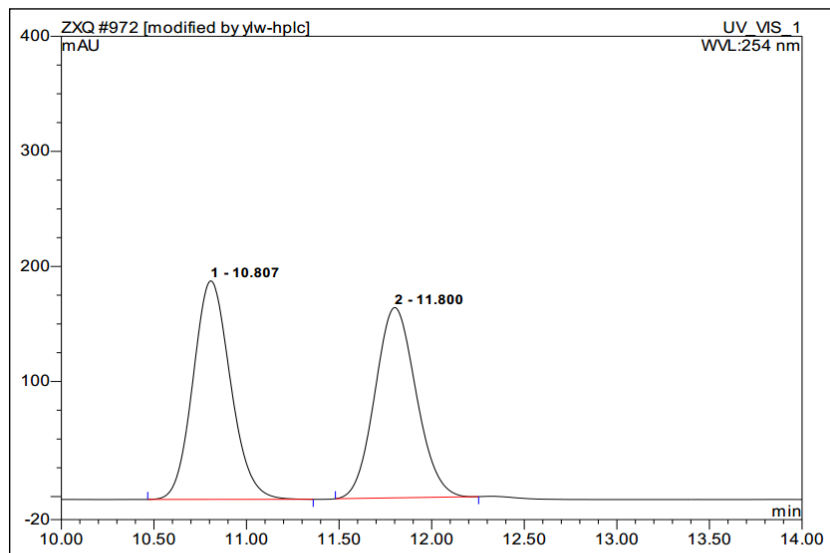
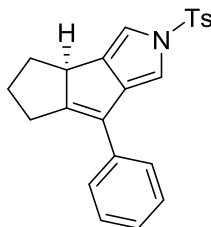


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.05	n.a.	126.117	143.579	49.45	n.a.	BMB*
2	15.01	n.a.	87.815	146.752	50.55	n.a.	BMB*
<b>Total:</b>			213.932	290.331	100.00	0.000	

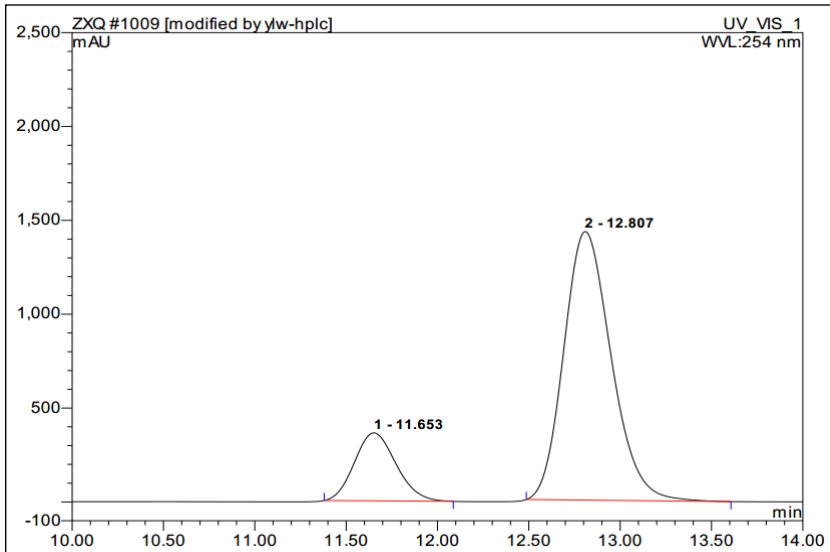


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.40	n.a.	133.773	169.413	86.42	n.a.	BMB*
2	15.67	n.a.	18.255	26.611	13.58	n.a.	BMB*
<b>Total:</b>			152.028	196.024	100.00	0.000	

**2u:** IC, *n*-hexane/2-propanol = 90/10,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

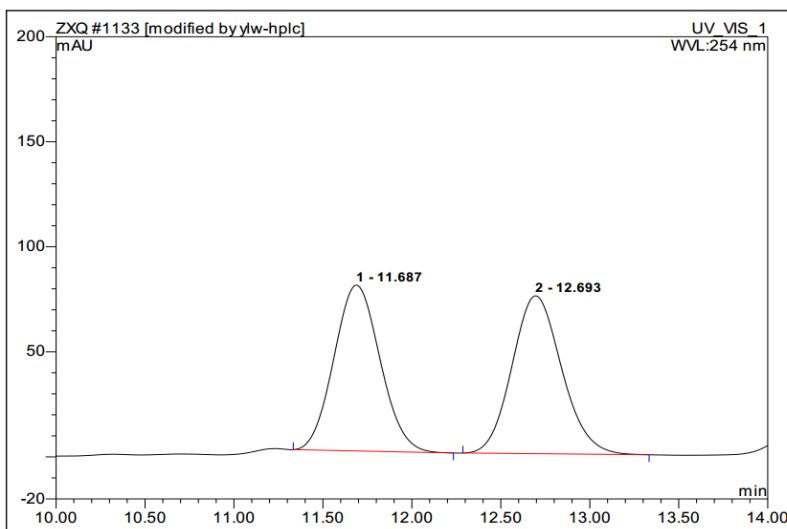
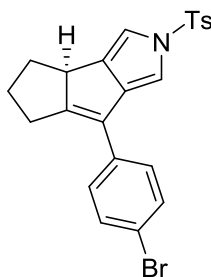


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.81	n.a.	189.939	44.554	51.08	n.a.	BMB*
2	11.80	n.a.	165.423	42.667	48.92	n.a.	BMB*
<b>Total:</b>			<b>355.362</b>	<b>87.221</b>	<b>100.00</b>	<b>0.000</b>	

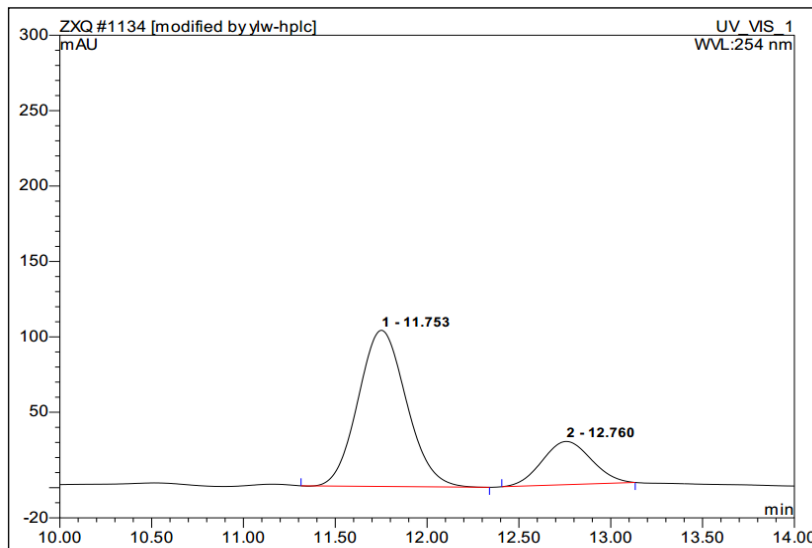


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.65	n.a.	361.887	95.392	18.15	n.a.	BMB*
2	12.81	n.a.	1430.263	430.212	81.85	n.a.	BMB*
<b>Total:</b>			<b>1792.150</b>	<b>525.604</b>	<b>100.00</b>	<b>0.000</b>	

2v: IC, *n*-hexane/2-propanol = 90/10,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

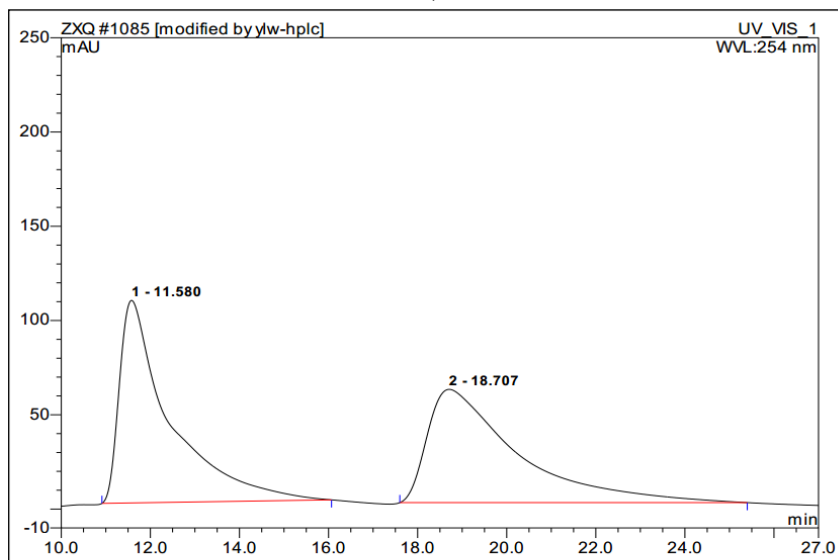
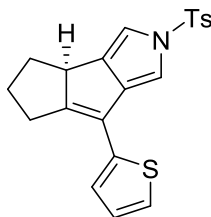


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.69	n.a.	78.918	23.701	49.36	n.a.	BMB*
2	12.69	n.a.	75.121	24.316	50.64	n.a.	BMB*
<b>Total:</b>			154.039	48.017	100.00	0.000	

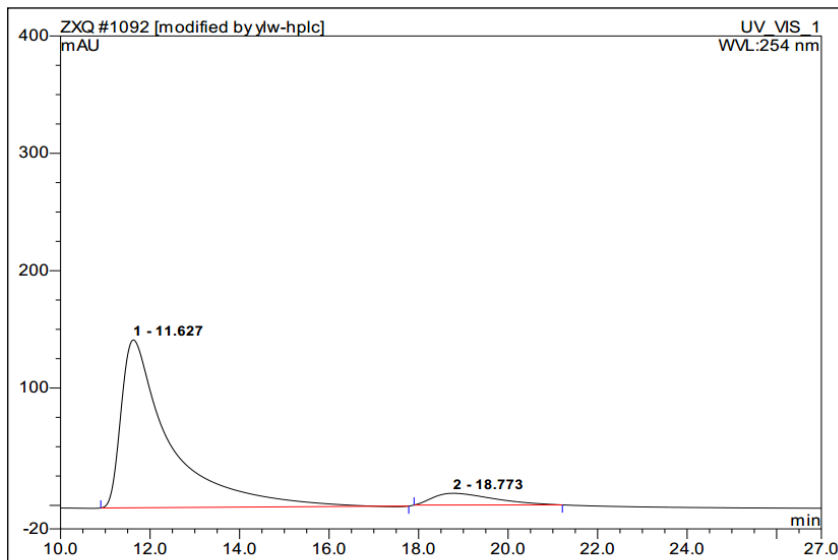


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.75	n.a.	103.540	31.580	77.99	n.a.	BMB*
2	12.76	n.a.	28.643	8.912	22.01	n.a.	BMB*
<b>Total:</b>			132.183	40.492	100.00	0.000	

2w: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

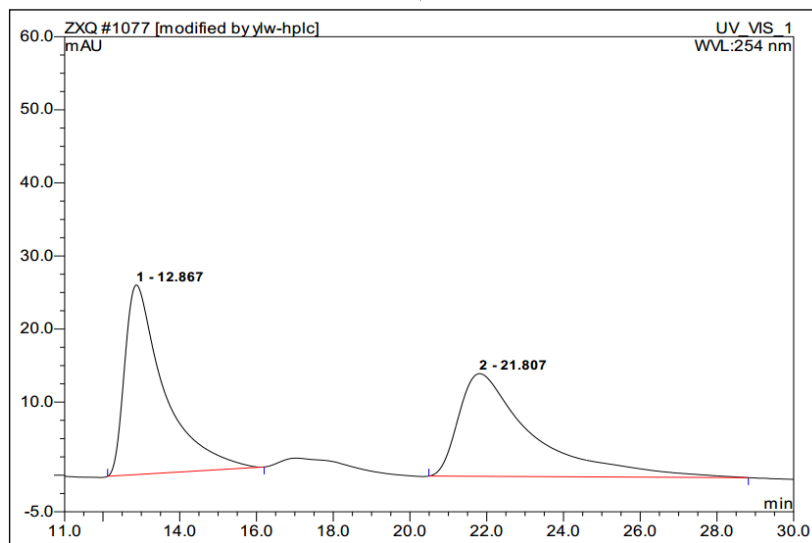
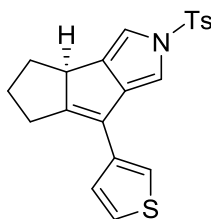


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.58	n.a.	107.410	140.577	50.32	n.a.	BMB*
2	18.71	n.a.	60.069	138.779	49.68	n.a.	BMB*
<b>Total:</b>			167.479	279.356	100.00	0.000	

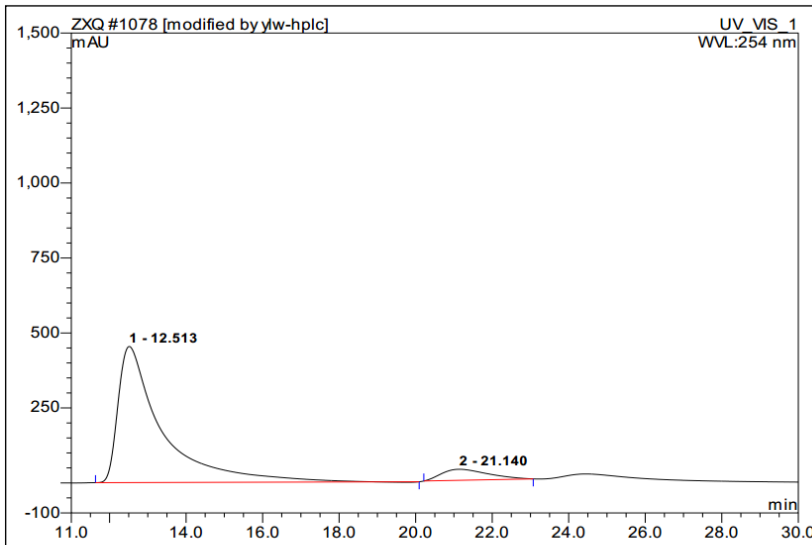


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.63	n.a.	143.051	181.003	91.99	n.a.	BMB*
2	18.77	n.a.	9.979	15.759	8.01	n.a.	BMB*
<b>Total:</b>			153.029	196.762	100.00	0.000	

2x: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

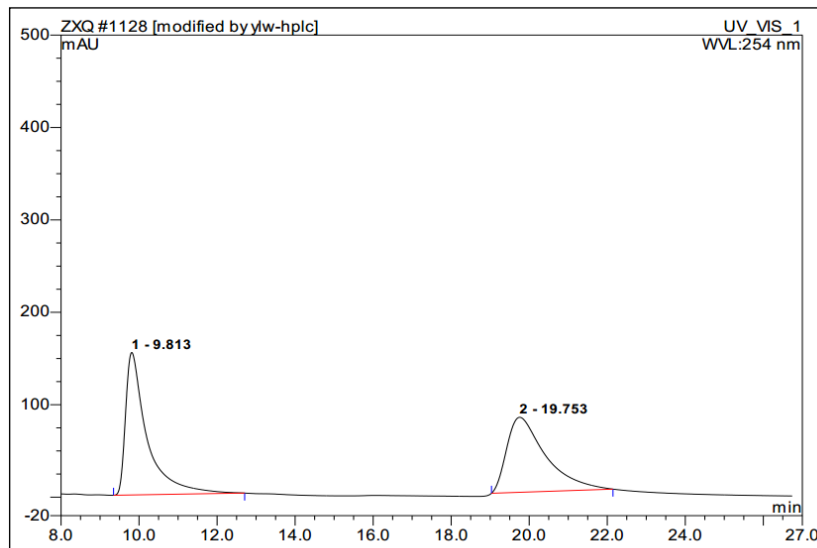
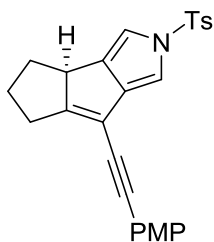


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.87	n.a.	25.942	30.873	49.74	n.a.	BMB*
2	21.81	n.a.	14.052	31.193	50.26	n.a.	BMB*
<b>Total:</b>			39.994	62.066	100.00	0.000	

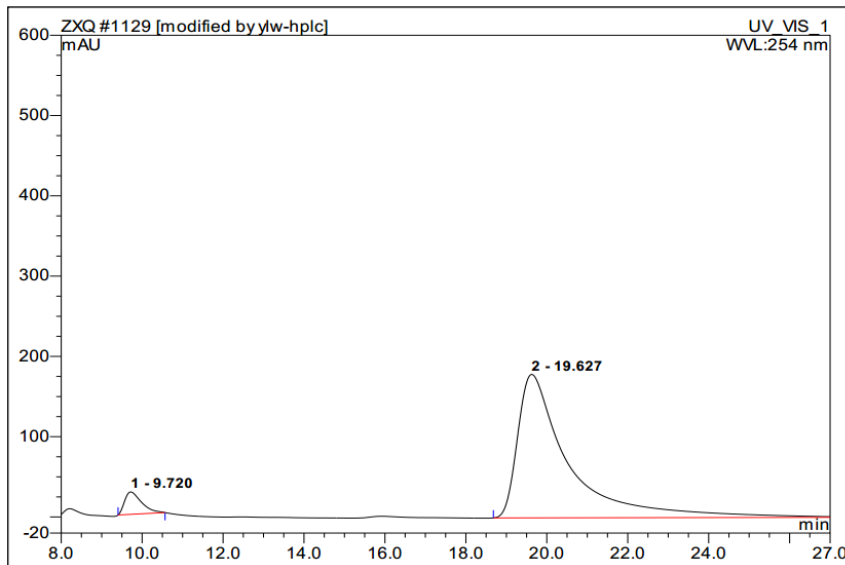


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.51	n.a.	453.705	604.053	92.13	n.a.	BMB*
2	21.14	n.a.	36.789	51.627	7.87	n.a.	BMB*
<b>Total:</b>			490.494	655.680	100.00	0.000	

2y: ADH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

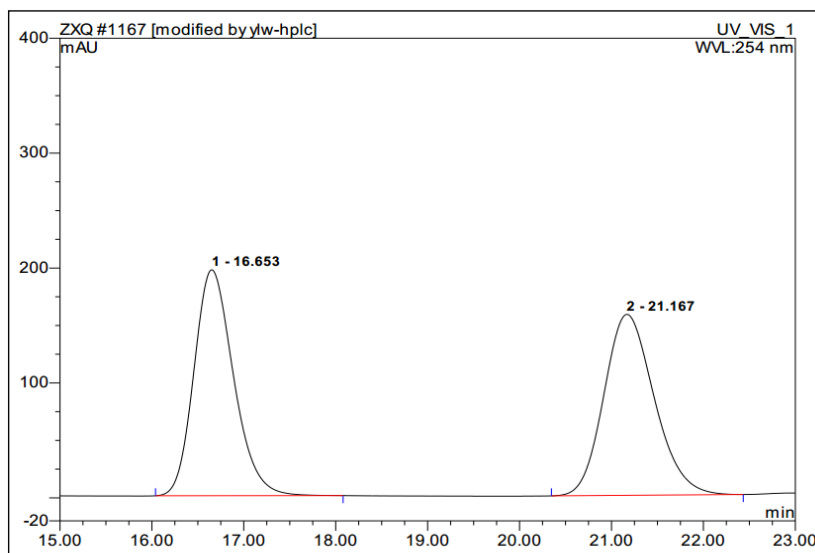
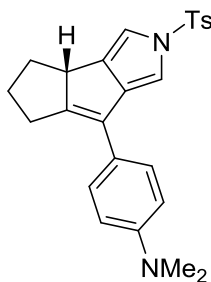


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.81	n.a.	154.146	98.126	51.23	n.a.	BMB*
2	19.75	n.a.	81.175	93.417	48.77	n.a.	BMB*
<b>Total:</b>			235.321	191.543	100.00	0.000	

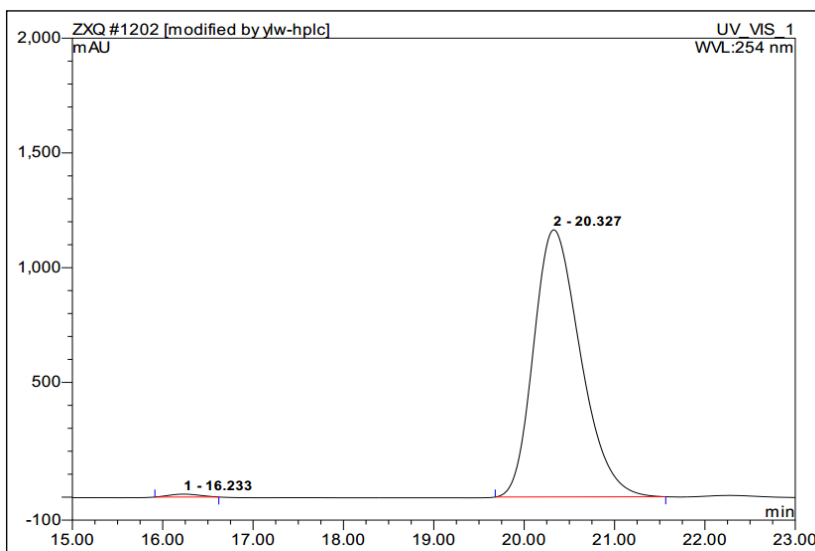


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.72	n.a.	27.877	13.464	4.90	n.a.	BMB*
2	19.63	n.a.	178.713	261.385	95.10	n.a.	BMB*
<b>Total:</b>			206.591	274.848	100.00	0.000	

2z: IC, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



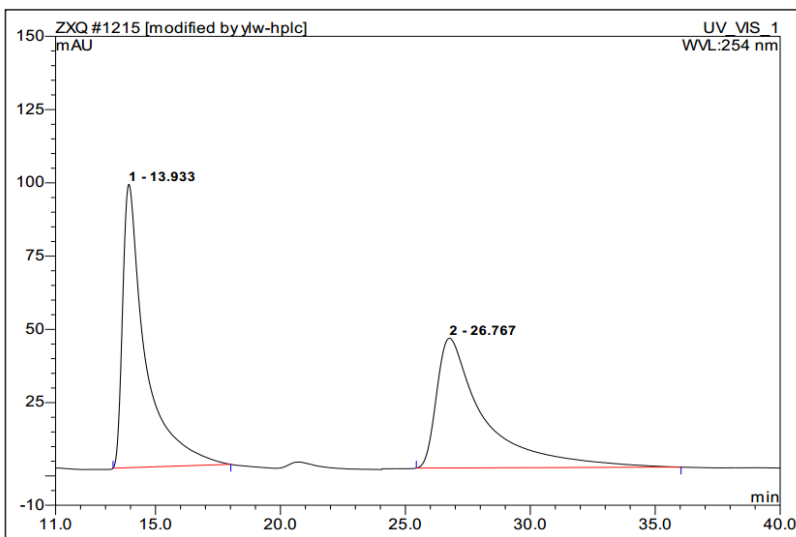
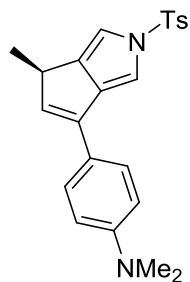
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.65	n.a.	196.581	97.908	49.48	n.a.	BMB*
2	21.17	n.a.	157.504	99.951	50.52	n.a.	BMB*
<b>Total:</b>			354.085	197.859	100.00	0.000	



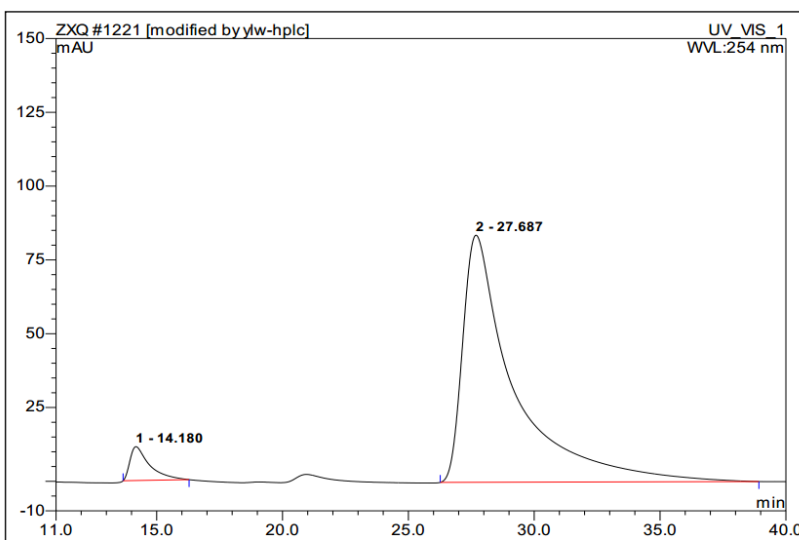
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.23	n.a.	12.570	4.879	0.69	n.a.	BMB*
2	20.33	n.a.	1163.953	699.593	99.31	n.a.	BMB*
<b>Total:</b>			1176.523	704.472	100.00	0.000	



**2aa:** ADH, *n*-hexane/2-propanol = 60/40,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

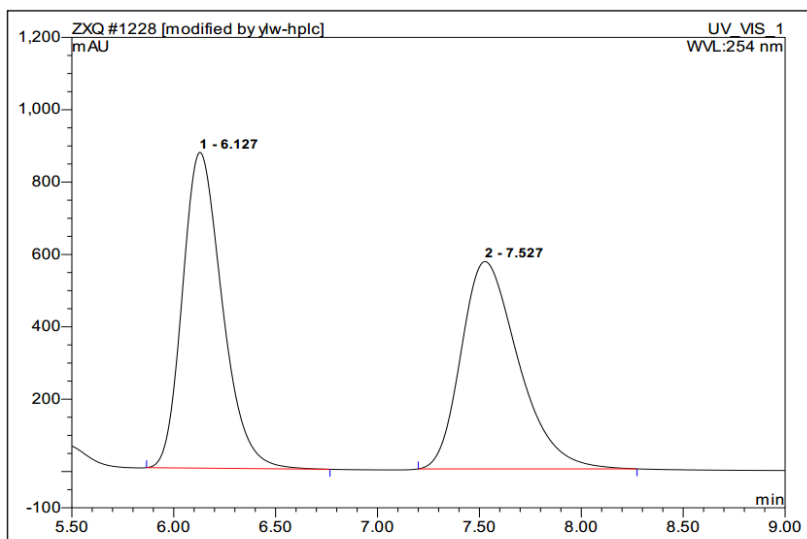
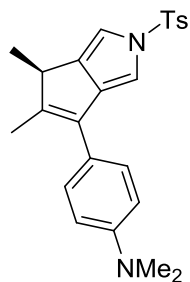


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.93	n.a.	96.689	101.581	50.89	n.a.	BMB*
2	26.77	n.a.	44.268	98.046	49.11	n.a.	BMB*
<b>Total:</b>			140.957	199.628	100.00	0.000	

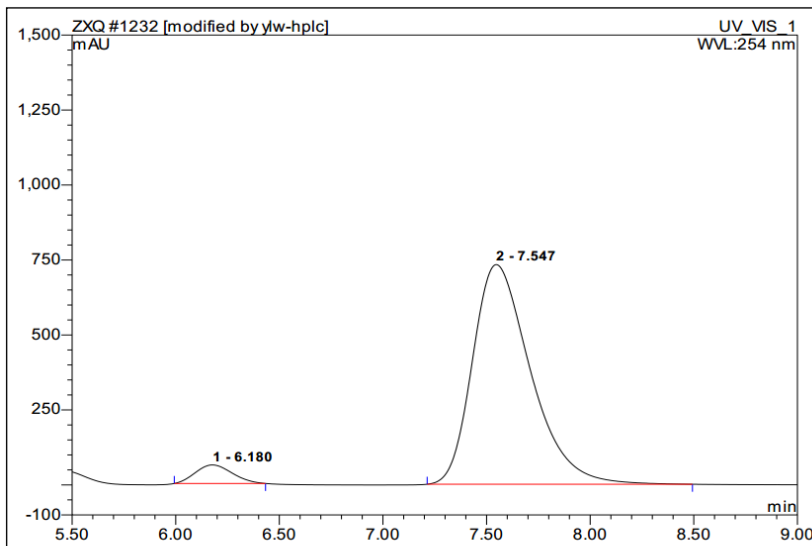


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.18	n.a.	11.465	10.320	4.95	n.a.	BMB*
2	27.69	n.a.	83.722	198.068	95.05	n.a.	BMB*
<b>Total:</b>			95.187	208.388	100.00	0.000	

**2ab:** ODH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

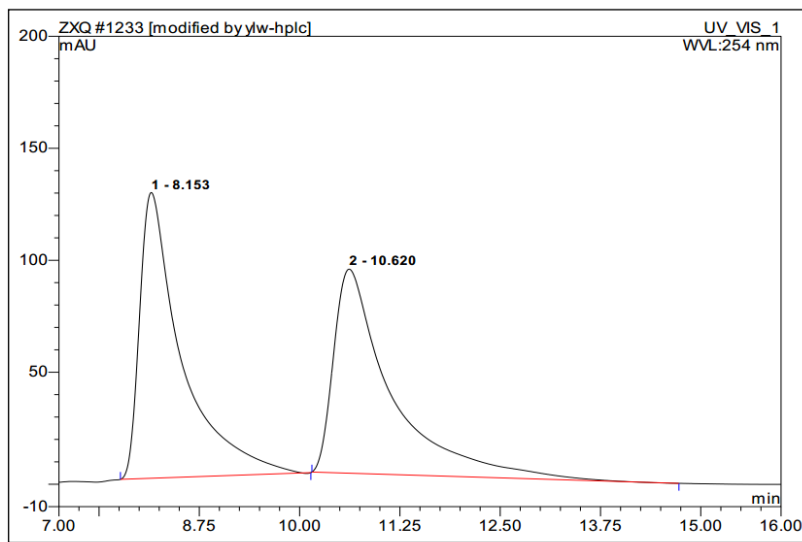
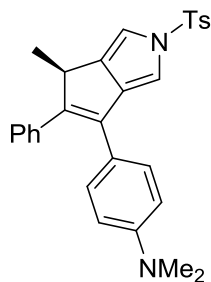


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.13	n.a.	872.811	197.332	51.37	n.a.	BMB*
2	7.53	n.a.	573.107	186.821	48.63	n.a.	BMB*
<b>Total:</b>			1445.918	384.153	100.00	0.000	

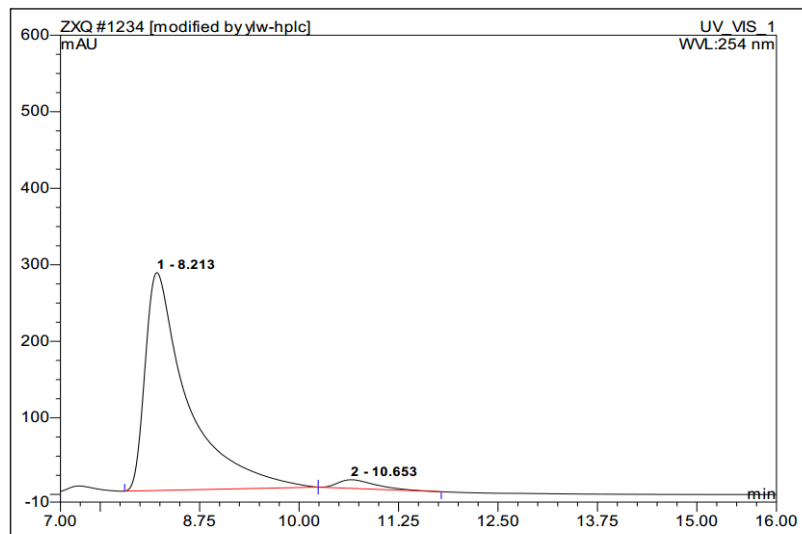


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.18	n.a.	61.808	12.719	5.07	n.a.	BMB*
2	7.55	n.a.	732.558	237.928	94.93	n.a.	BMB*
<b>Total:</b>			794.365	250.647	100.00	0.000	

**2ac:** ADH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

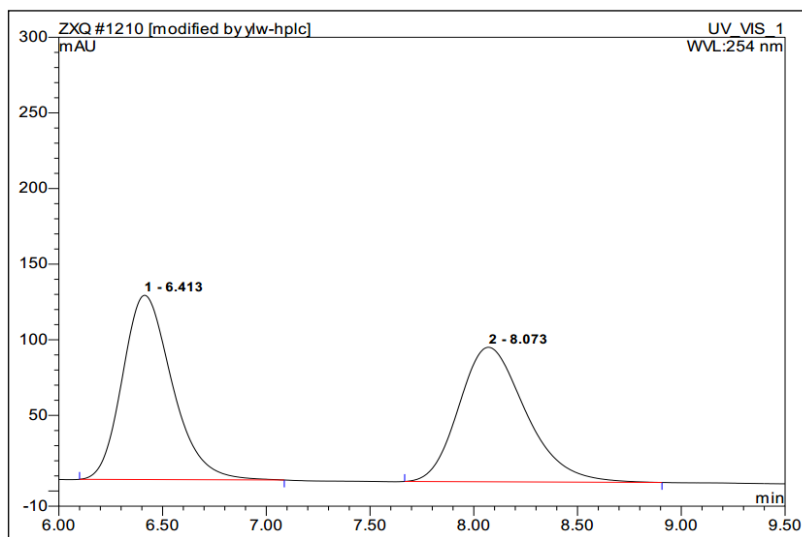
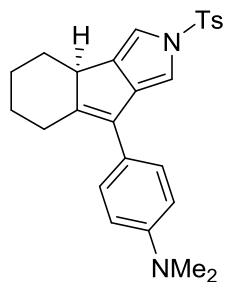


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.15	n.a.	127.565	76.852	50.45	n.a.	BMB*
2	10.62	n.a.	91.103	75.473	49.55	n.a.	BMB*
<b>Total:</b>			218.668	152.325	100.00	0.000	

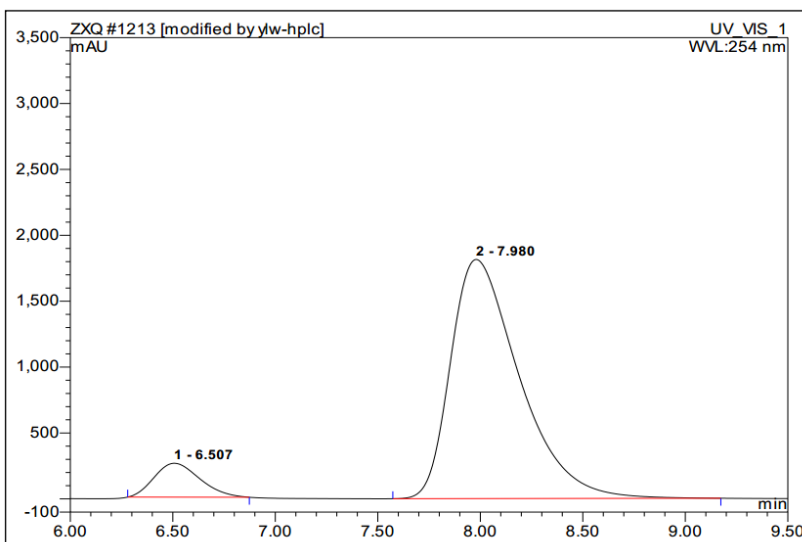


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.21	n.a.	284.655	175.764	96.55	n.a.	BMB*
2	10.65	n.a.	11.274	6.272	3.45	n.a.	bMB*
<b>Total:</b>			295.929	182.036	100.00	0.000	

2ad: ODH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

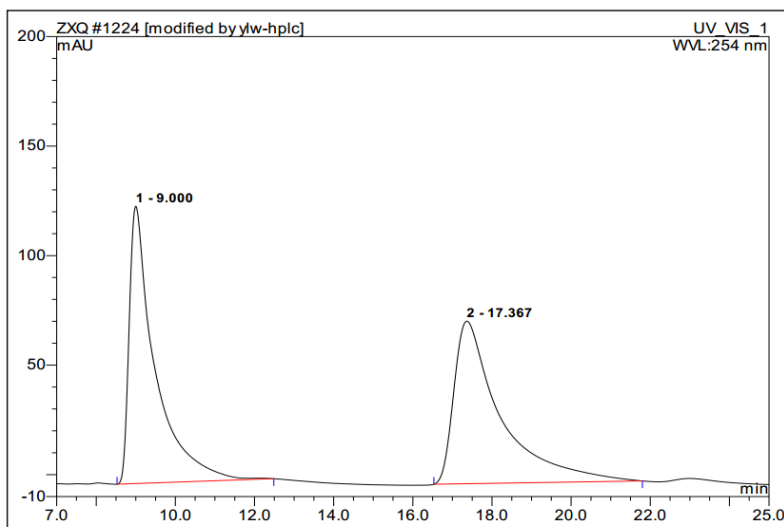
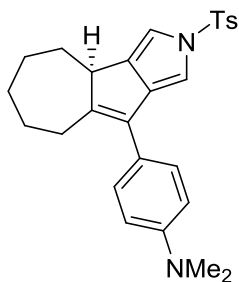


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.41	n.a.	121.824	33.883	50.51	n.a.	BMB*
2	8.07	n.a.	88.915	33.198	49.49	n.a.	BMB*
<b>Total:</b>			<b>210.739</b>	<b>67.081</b>	<b>100.00</b>	<b>0.000</b>	

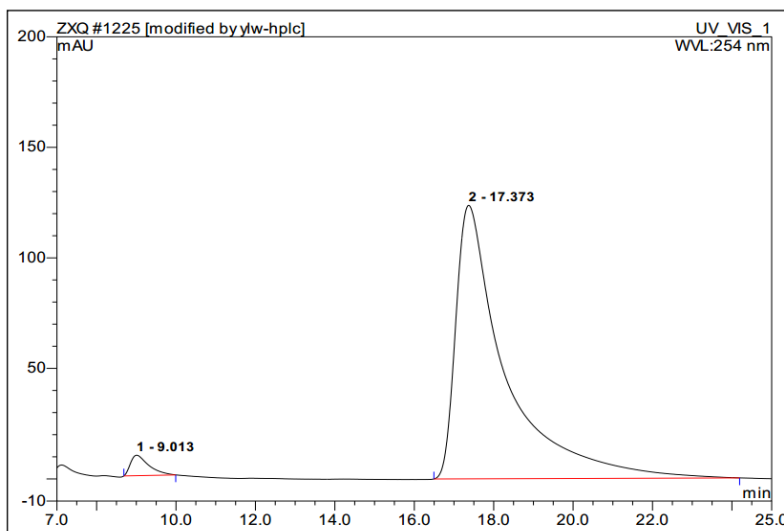


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.51	n.a.	257.274	66.278	8.60	n.a.	BMB*
2	7.98	n.a.	1814.616	704.338	91.40	n.a.	BMB*
<b>Total:</b>			<b>2071.891</b>	<b>770.616</b>	<b>100.00</b>	<b>0.000</b>	

**2ae**: ADH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

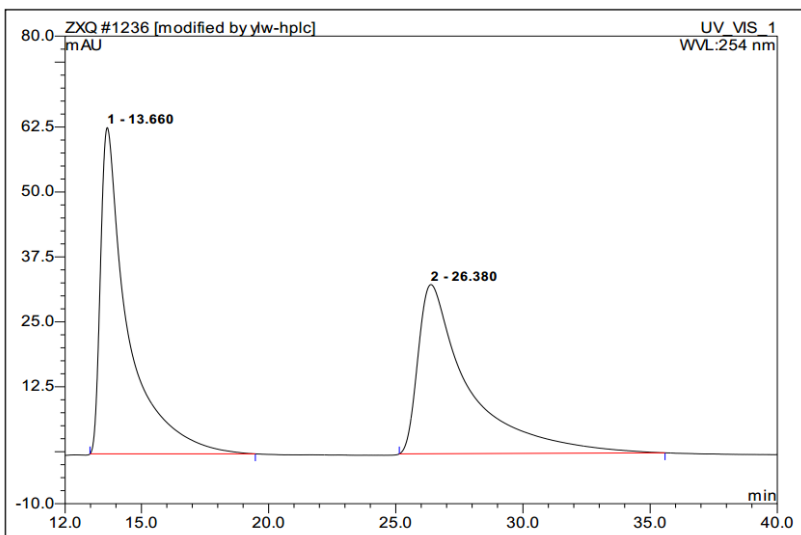
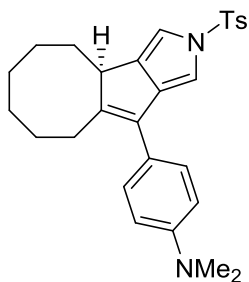


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.00	n.a.	126.585	95.483	48.55	n.a.	BMB*
2	17.37	n.a.	74.224	101.172	51.45	n.a.	BMB*
<b>Total:</b>			200.809	196.654	100.00	0.000	

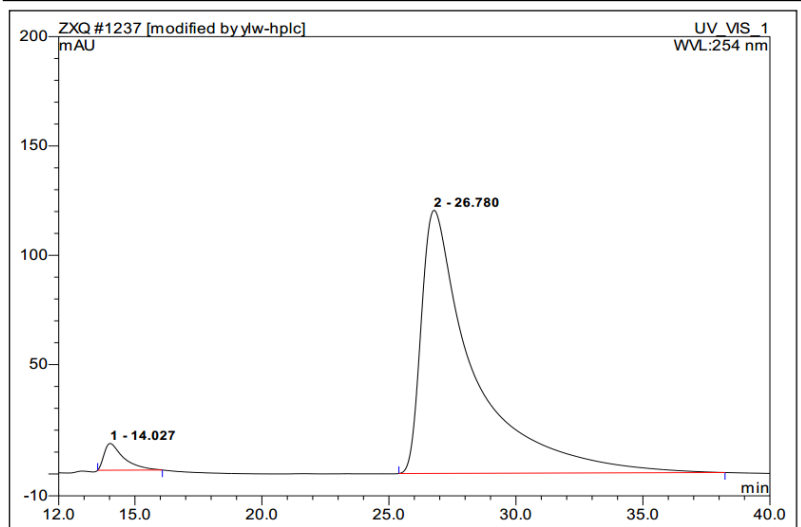


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.01	n.a.	9.239	4.930	2.69	n.a.	BMB*
2	17.37	n.a.	123.727	178.626	97.31	n.a.	BMB*
<b>Total:</b>			132.966	183.556	100.00	0.000	

**2af:** ADH, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

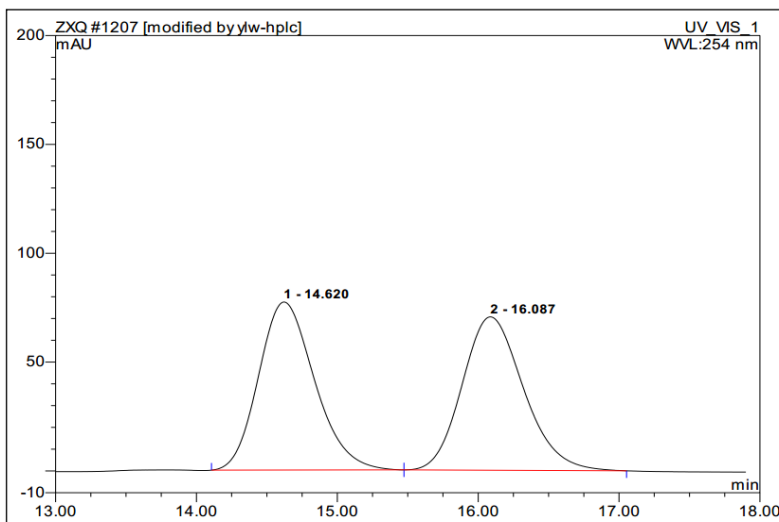
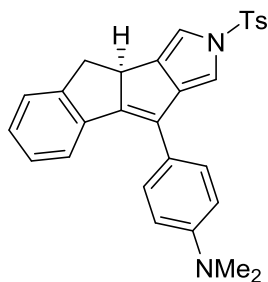


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.66	n.a.	62.809	77.758	50.82	n.a.	BMB*
2	26.38	n.a.	32.565	75.245	49.18	n.a.	BMB*
<b>Total:</b>			95.375	153.003	100.00	0.000	

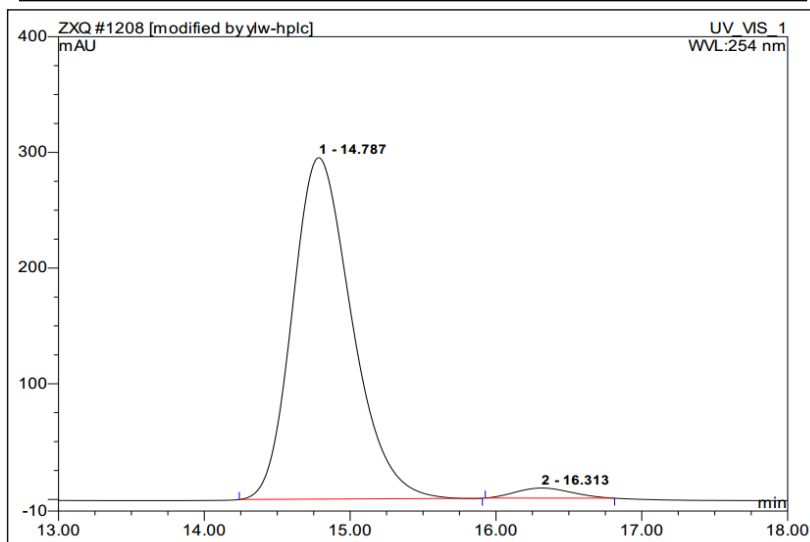


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.03	n.a.	12.233	10.939	3.64	n.a.	BMB*
2	26.78	n.a.	120.336	289.943	96.36	n.a.	BMB*
<b>Total:</b>			132.569	300.882	100.00	0.000	

**2ag**: IC, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

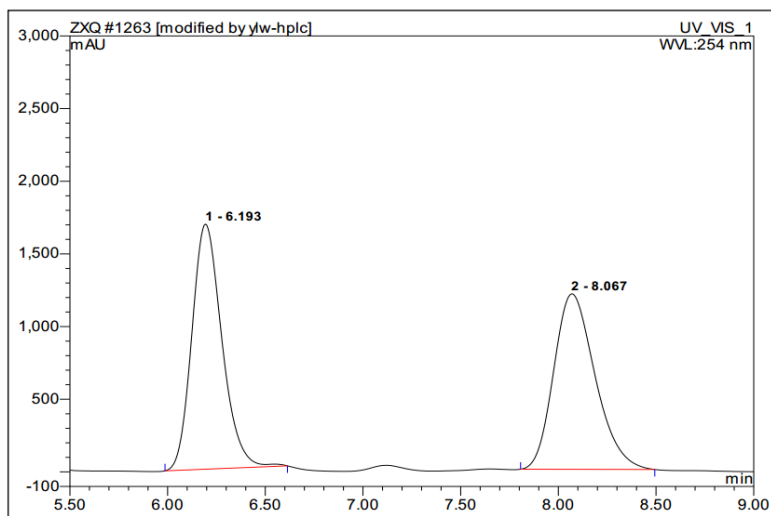
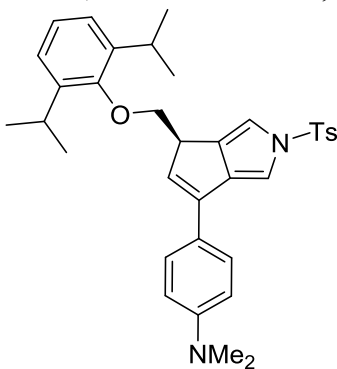


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.62	n.a.	77.171	35.528	49.99	n.a.	BMB*
2	16.09	n.a.	70.456	35.537	50.01	n.a.	bMB*
<b>Total:</b>			147.627	71.065	100.00	0.000	

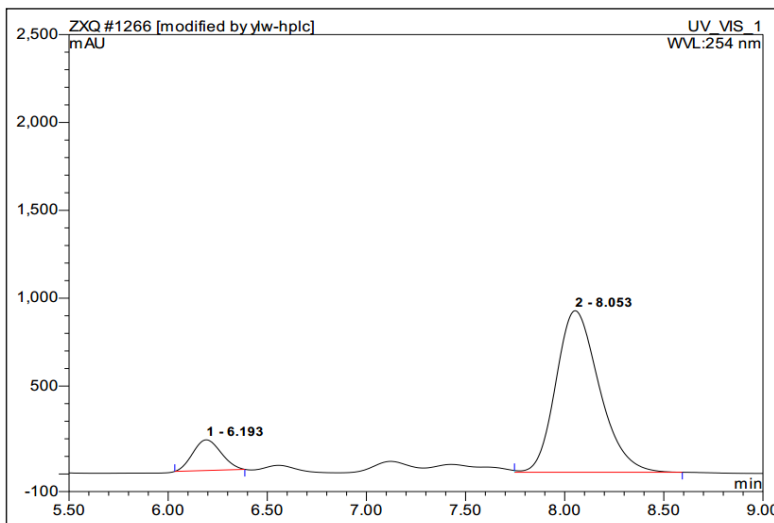


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.79	n.a.	295.110	138.853	97.30	n.a.	BMB*
2	16.31	n.a.	8.714	3.852	2.70	n.a.	BMB*
<b>Total:</b>			303.824	142.705	100.00	0.000	

**2ah**: IC, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



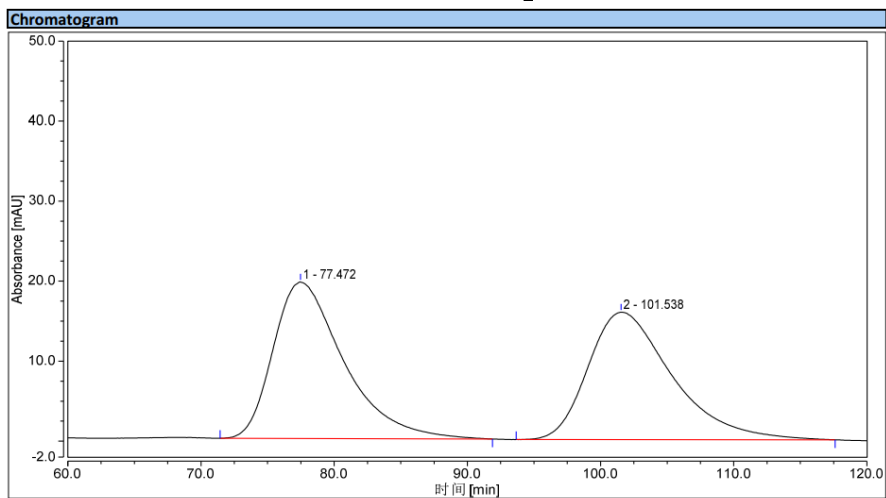
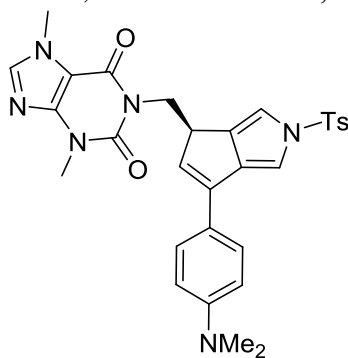
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.19	n.a.	1686.820	300.387	50.38	n.a.	BMB*
2	8.07	n.a.	1207.037	295.909	49.62	n.a.	BMB*
<b>Total:</b>			2893.857	596.296	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.19	n.a.	174.542	28.813	10.99	n.a.	BMB*
2	8.05	n.a.	919.355	233.249	89.01	n.a.	MB*
<b>Total:</b>			1093.897	262.062	100.00	0.000	

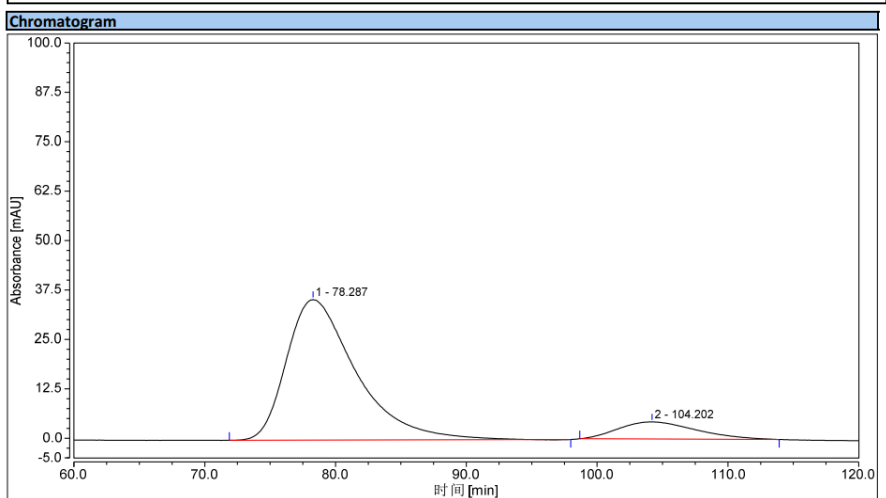


2ai: IC, *n*-hexane/2-propanol = 50/50,  $v = 1.5 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



**Integration Results**

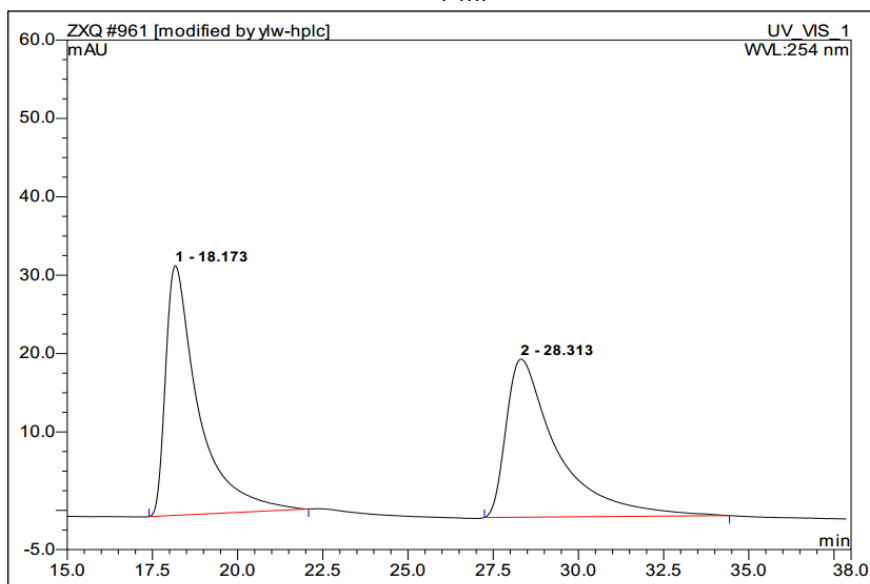
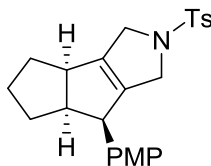
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		77.472	120.126	19.572	50.77	55.10	n.a.
2		101.538	116.498	15.946	49.23	44.90	n.a.
<b>Total:</b>			<b>236.624</b>	<b>35.517</b>	<b>100.00</b>	<b>100.00</b>	



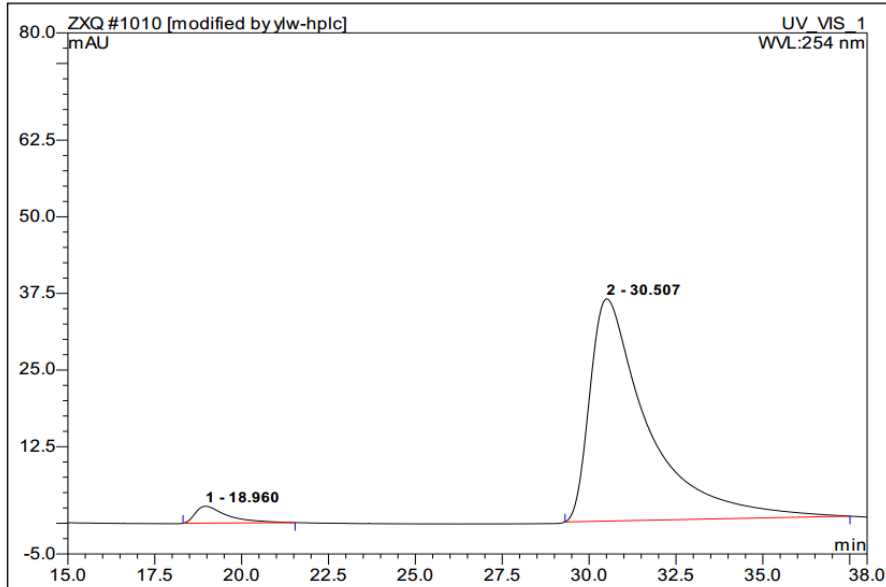
**Integration Results**

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		78.287	218.884	35.579	88.03	89.14	n.a.
2		104.202	29.774	4.334	11.97	10.86	n.a.
<b>Total:</b>			<b>248.659</b>	<b>39.913</b>	<b>100.00</b>	<b>100.00</b>	

**3aa:** ADH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

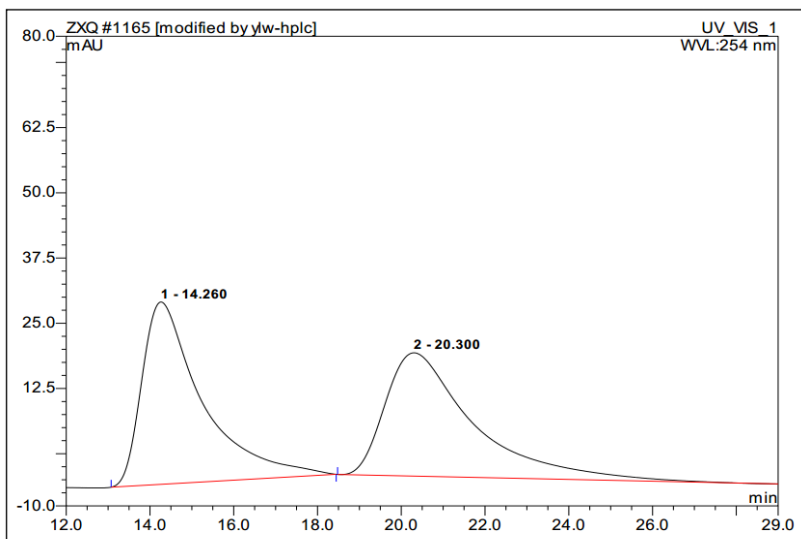
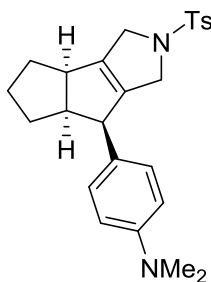


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.17	n.a.	31.850	35.527	50.37	n.a.	BMB*
2	28.31	n.a.	20.168	35.006	49.63	n.a.	BMB*
<b>Total:</b>			52.018	70.533	100.00	0.000	

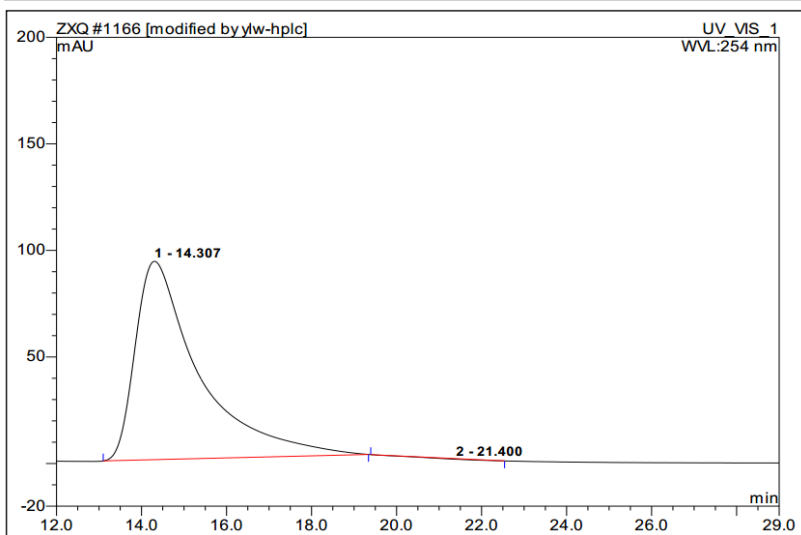


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.96	n.a.	2.754	2.929	3.98	n.a.	BMB*
2	30.51	n.a.	36.255	70.581	96.02	n.a.	BMB*
<b>Total:</b>			39.008	73.509	100.00	0.000	

3pa: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

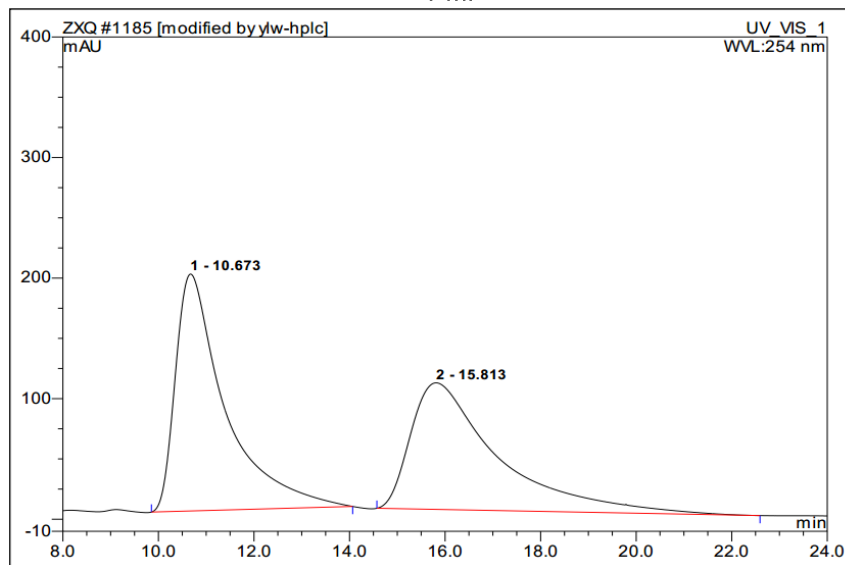
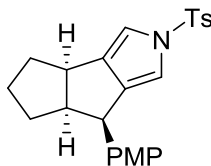


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.26	n.a.	34.948	58.253	50.44	n.a.	BMB*
2	20.30	n.a.	23.625	57.226	49.56	n.a.	BMB*
<b>Total:</b>			<b>58.573</b>	<b>115.479</b>	<b>100.00</b>	<b>0.000</b>	

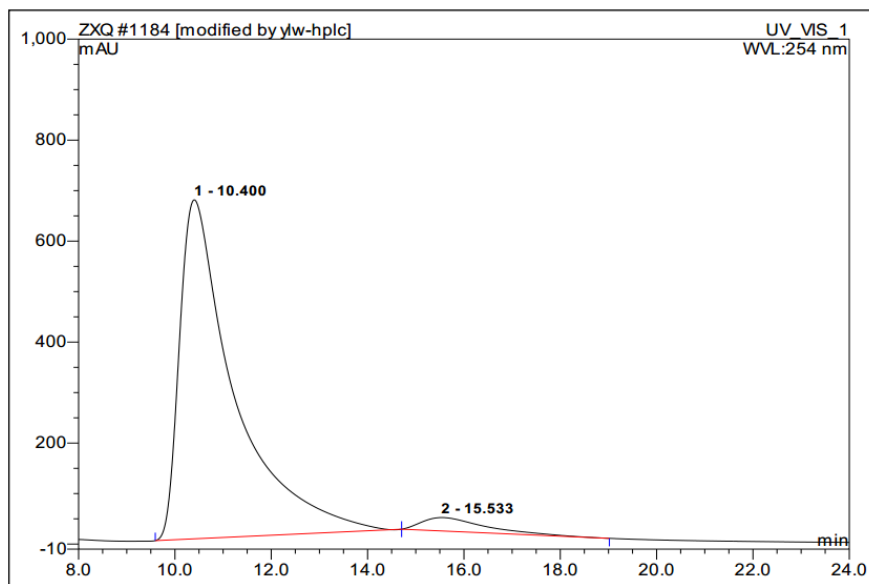


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.31	n.a.	93.070	161.692	99.68	n.a.	BMB*
2	21.40	n.a.	0.289	0.514	0.32	n.a.	BMB*
<b>Total:</b>			<b>93.359</b>	<b>162.206</b>	<b>100.00</b>	<b>0.000</b>	

**3ab**: ASH, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

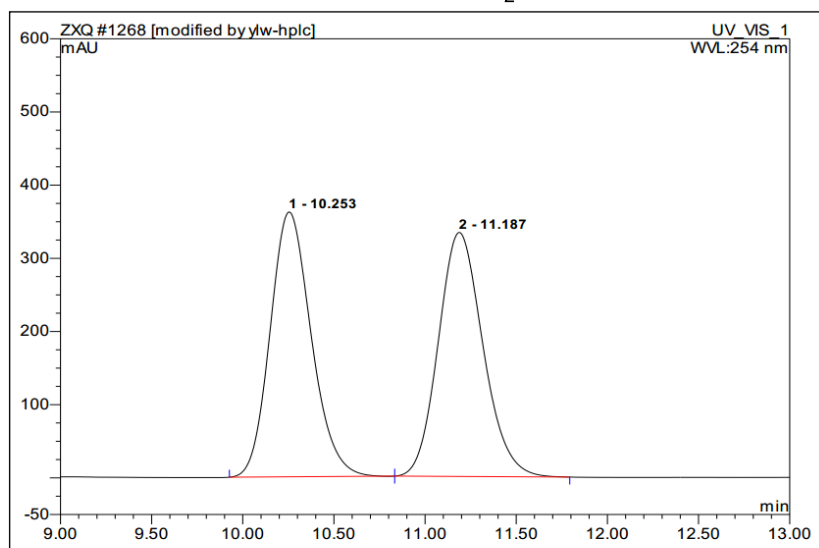
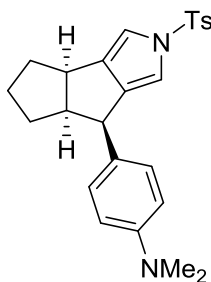


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.67	n.a.	196.502	236.457	51.83	n.a.	BMB*
2	15.81	n.a.	104.987	219.755	48.17	n.a.	BMB*
<b>Total:</b>			301.490	456.212	100.00	0.000	

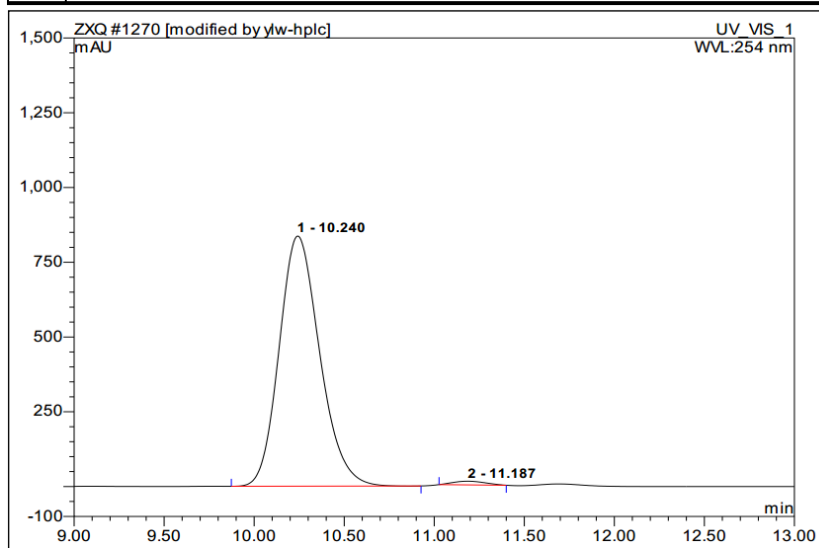


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.40	n.a.	671.279	881.395	95.57	n.a.	BMB*
2	15.53	n.a.	26.483	40.877	4.43	n.a.	bMB*
<b>Total:</b>			697.762	922.272	100.00	0.000	

**3pb**: IC, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

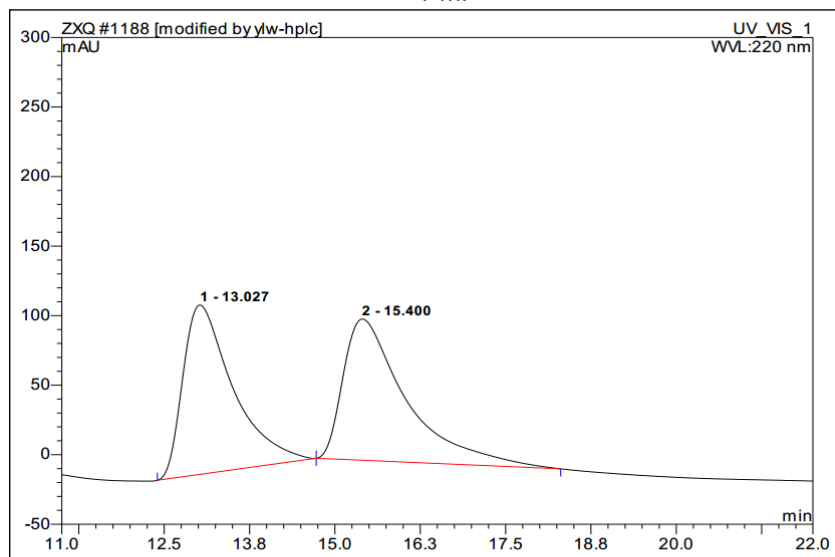
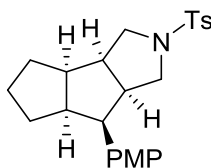


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.25	n.a.	361.943	94.293	49.91	n.a.	BMB*
2	11.19	n.a.	333.497	94.624	50.09	n.a.	bMB*
<b>Total:</b>			695.440	188.918	100.00	0.000	

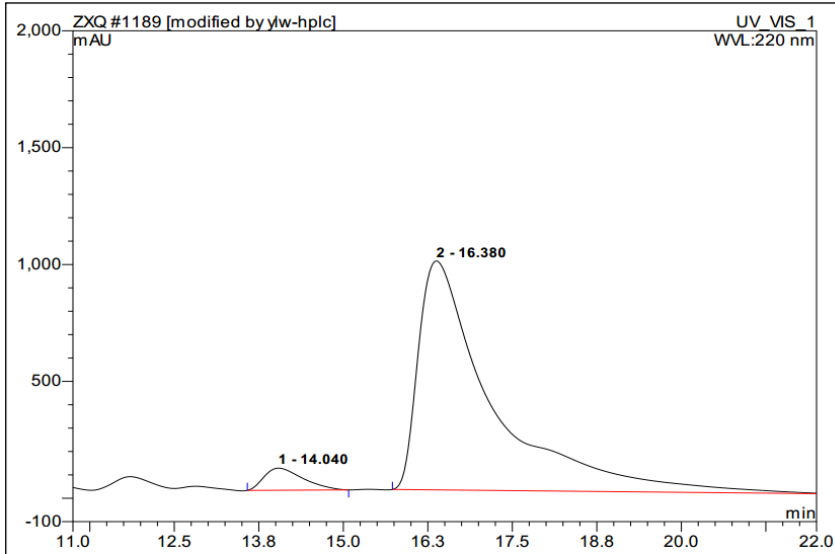


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.24	n.a.	836.631	218.272	98.84	n.a.	BMB*
2	11.19	n.a.	12.310	2.569	1.16	n.a.	BMB*
<b>Total:</b>			848.941	220.841	100.00	0.000	

**3ac:** ADH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

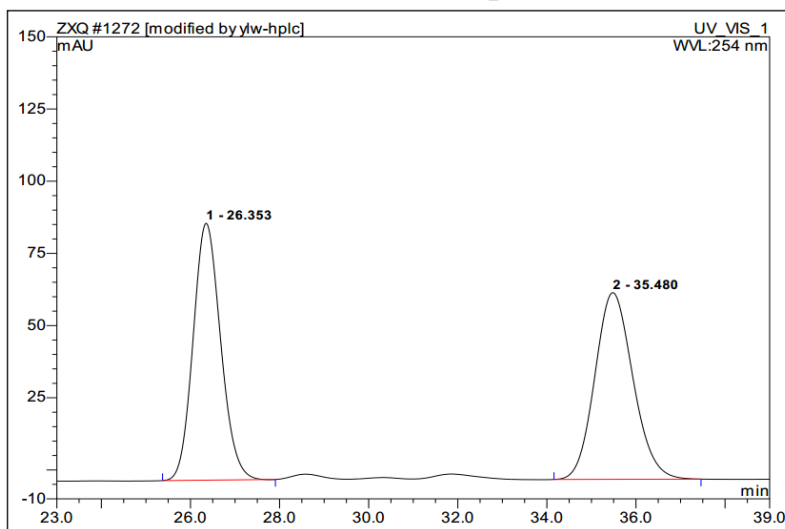
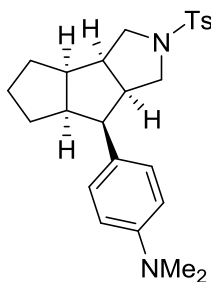


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.03	n.a.	121.754	103.037	48.80	n.a.	BMB*
2	15.40	n.a.	101.551	108.107	51.20	n.a.	bMB*
<b>Total:</b>			223.305	211.144	100.00	0.000	

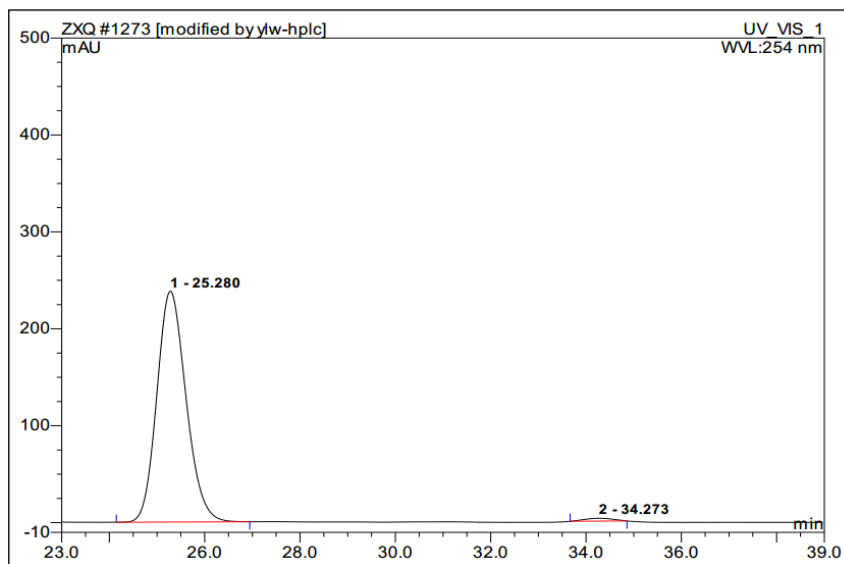


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.04	n.a.	94.501	62.737	4.80	n.a.	BMB*
2	16.38	n.a.	979.294	1244.434	95.20	n.a.	BMB*
<b>Total:</b>			1073.795	1307.171	100.00	0.000	

**3pc**: IC, *n*-hexane/2-propanol = 70/30,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

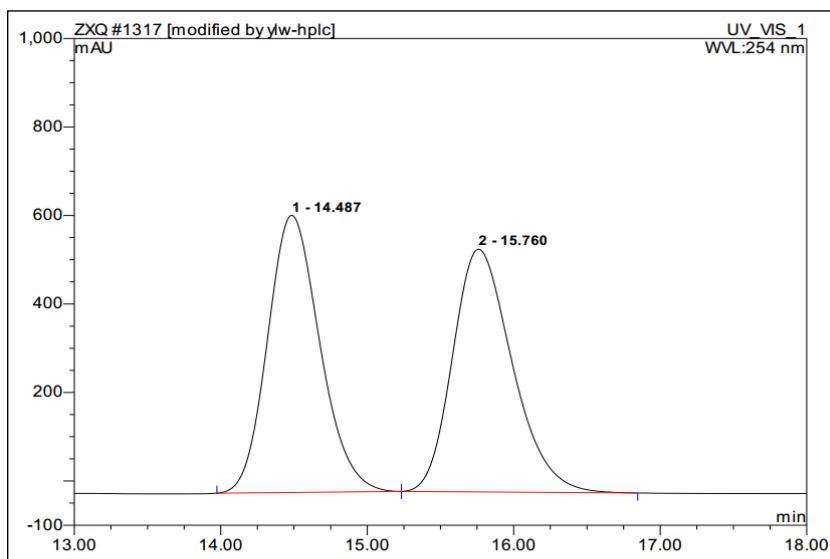
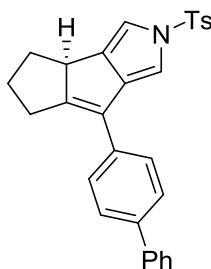


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	26.35	n.a.	88.947	63.703	49.82	n.a.	BMB*
2	35.48	n.a.	64.641	64.158	50.18	n.a.	BMB*
<b>Total:</b>			153.588	127.861	100.00	0.000	

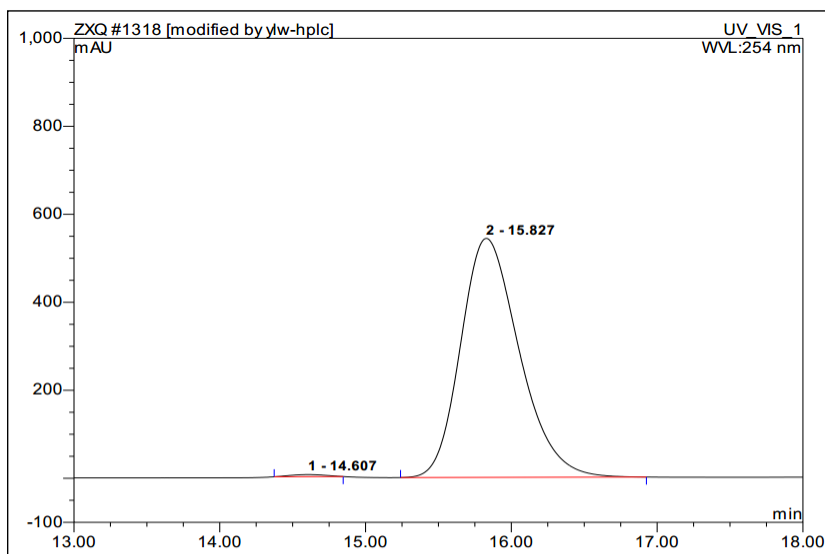


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	25.28	n.a.	238.185	168.961	98.81	n.a.	BMB*
2	34.27	n.a.	2.924	2.036	1.19	n.a.	BMB*
<b>Total:</b>			241.109	170.996	100.00	0.000	

3pd: IC, *n*-hexane/2-propanol = 80/20,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$



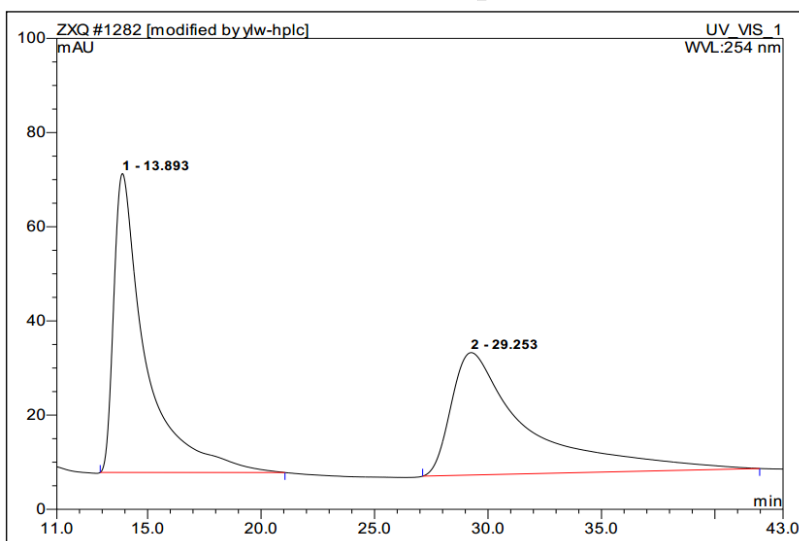
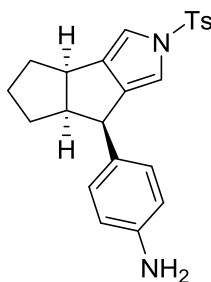
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.49	n.a.	626.332	258.369	49.99	n.a.	BMB*
2	15.76	n.a.	548.630	258.507	50.01	n.a.	bMB*
<b>Total:</b>			1174.962	516.876	100.00	0.000	



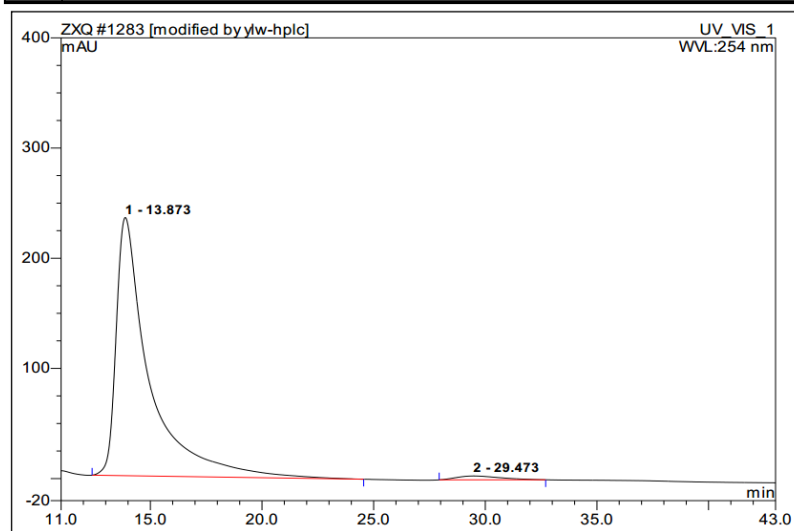
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.61	n.a.	4.756	1.328	0.52	n.a.	BMB*
2	15.83	n.a.	543.225	252.893	99.48	n.a.	BMB*
<b>Total:</b>			547.981	254.221	100.00	0.000	



3qa: ASH, *n*-hexane/2-propanol = 50/50,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

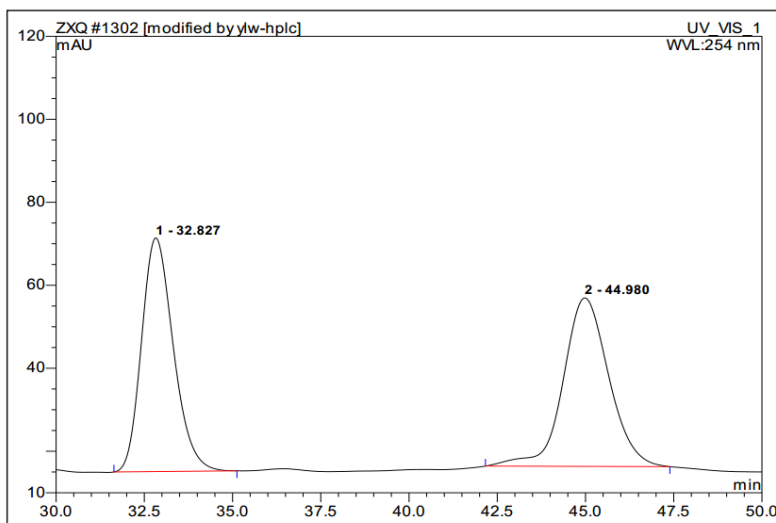
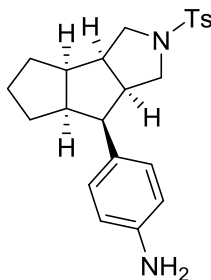


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.89	n.a.	63.466	102.959	50.45	n.a.	BMB*
2	29.25	n.a.	25.999	101.110	49.55	n.a.	BMB*
<b>Total:</b>			89.466	204.069	100.00	0.000	

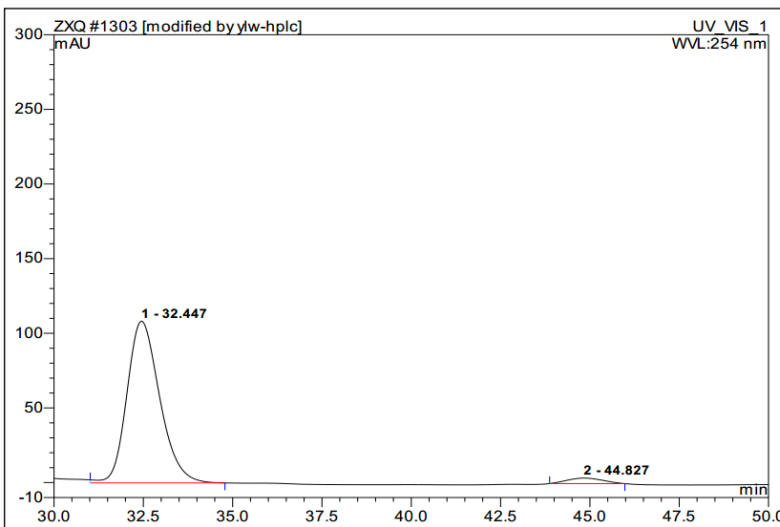


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.87	n.a.	234.278	403.800	98.07	n.a.	BMB*
2	29.47	n.a.	3.508	7.958	1.93	n.a.	BMB*
<b>Total:</b>			237.786	411.758	100.00	0.000	

**3qb:** IC, *n*-hexane/2-propanol = 50/50,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

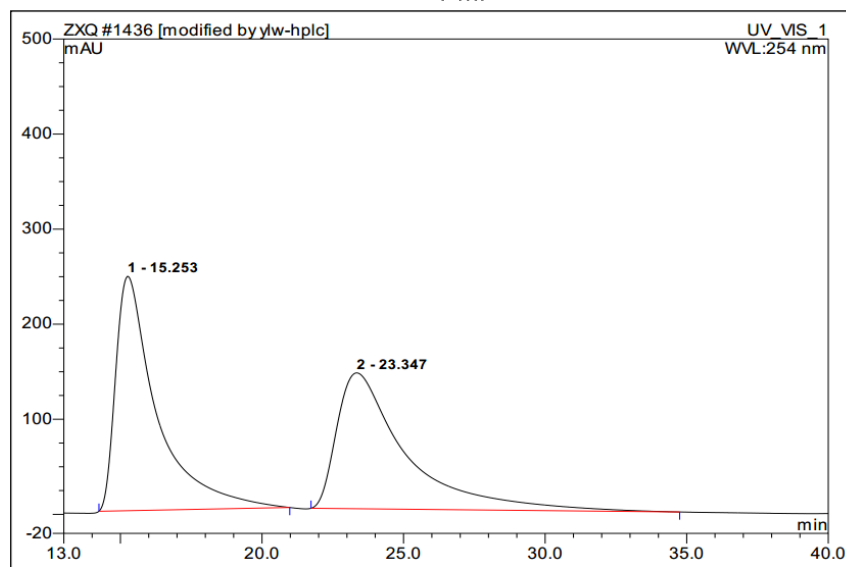
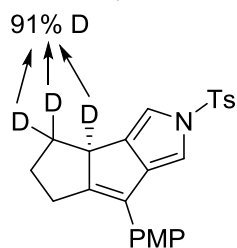


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	32.83	n.a.	56.300	58.798	49.12	n.a.	BMB*
2	44.98	n.a.	40.590	60.901	50.88	n.a.	BMB*
<b>Total:</b>			96.890	119.699	100.00	0.000	

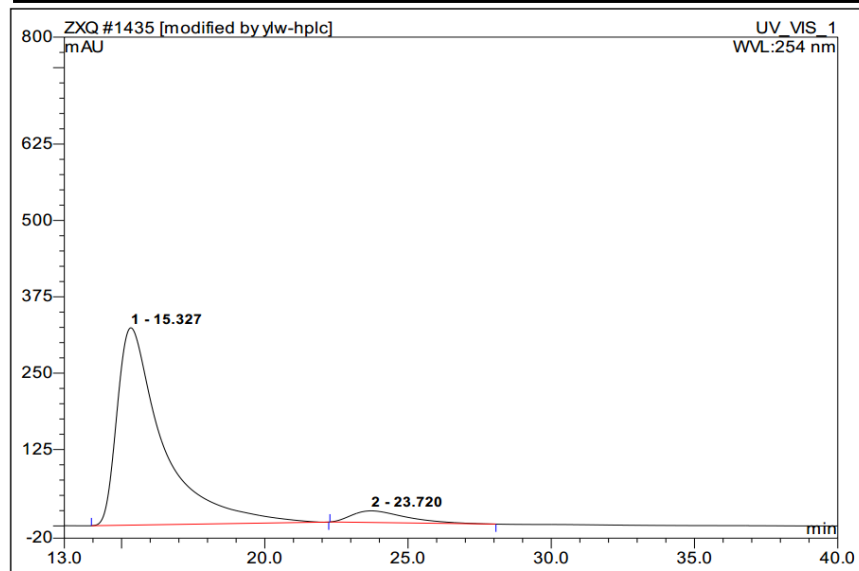


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	32.45	n.a.	108.382	115.588	96.46	n.a.	MB*
2	44.83	n.a.	3.676	4.241	3.54	n.a.	BMB*
<b>Total:</b>			112.058	119.829	100.00	0.000	

[D<sub>3</sub>]-2a: ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

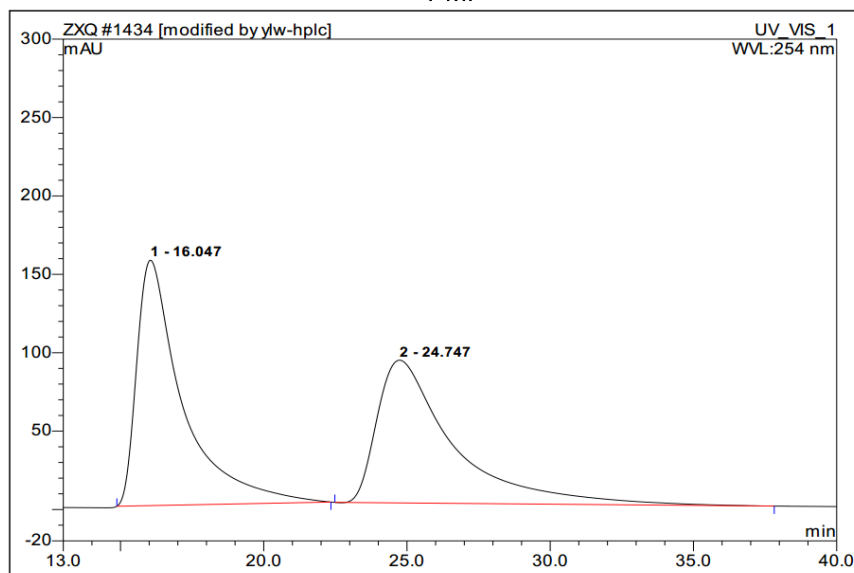
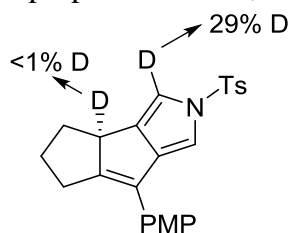


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.25	n.a.	246.552	414.671	50.79	n.a.	BMB*
2	23.35	n.a.	142.874	401.720	49.21	n.a.	BMB*
<b>Total:</b>			389.426	816.391	100.00	0.000	

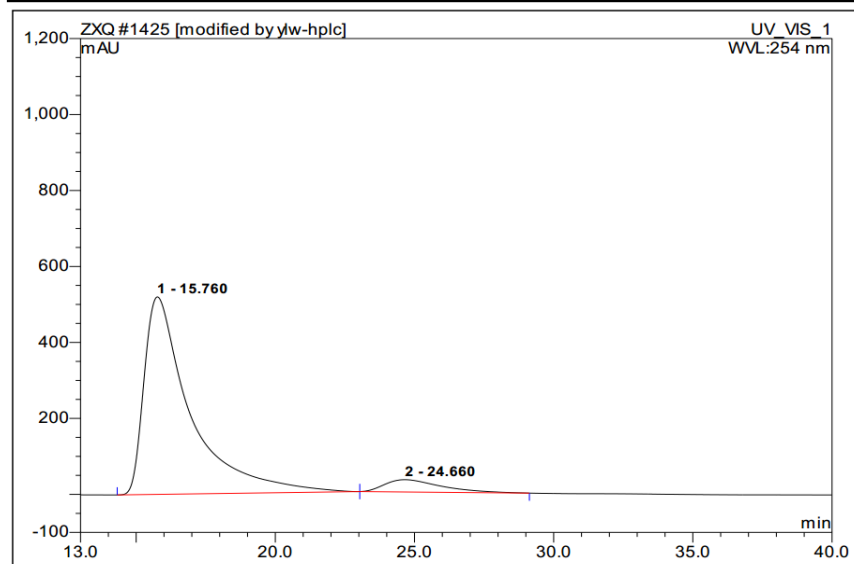


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.33	n.a.	322.927	600.385	93.46	n.a.	BMB*
2	23.72	n.a.	19.020	41.980	6.54	n.a.	BMB*
<b>Total:</b>			341.947	642.365	100.00	0.000	

[D]-2a (29% D): ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

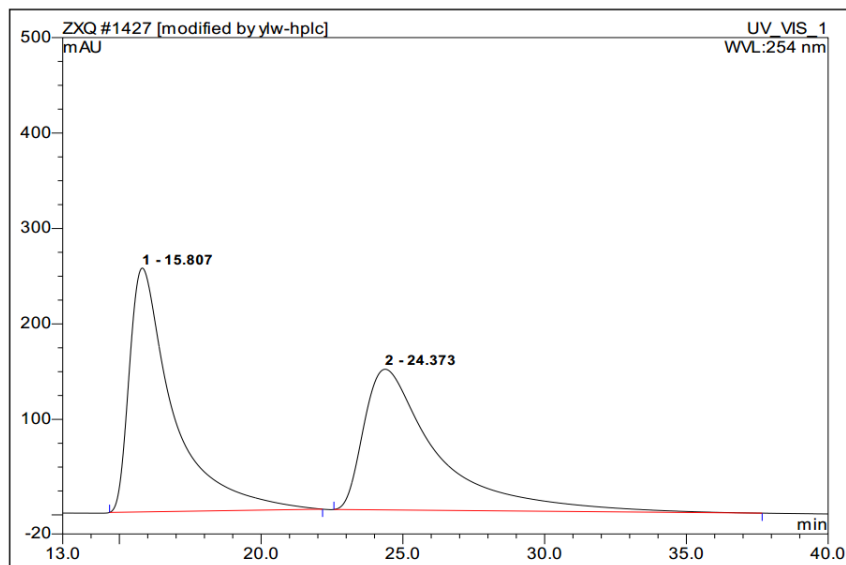
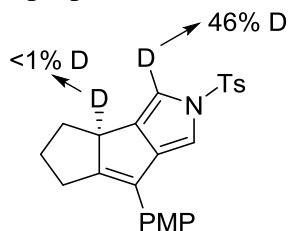


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.05	n.a.	156.485	289.613	50.92	n.a.	BMB*
2	24.75	n.a.	91.036	279.095	49.08	n.a.	BMB*
<b>Total:</b>			247.520	568.708	100.00	0.000	

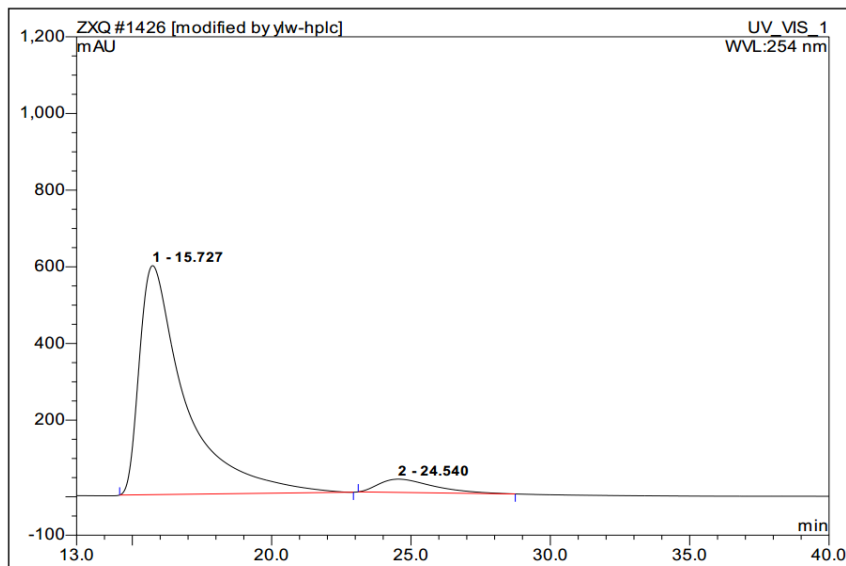


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.76	n.a.	519.832	1001.240	92.99	n.a.	BMB*
2	24.66	n.a.	32.292	75.525	7.01	n.a.	bMB*
<b>Total:</b>			552.124	1076.765	100.00	0.000	

[D]-2a (46% D): ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

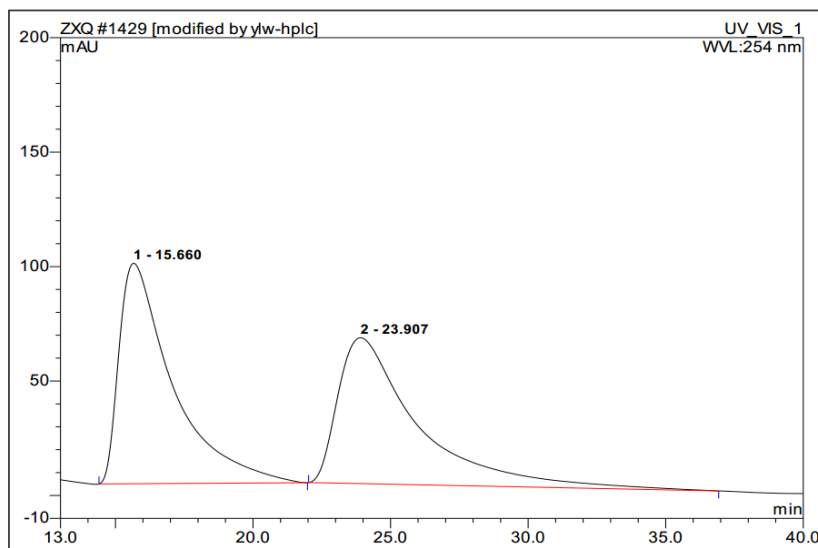
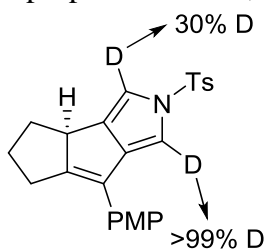


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.81	n.a.	255.473	457.902	50.89	n.a.	BMB*
2	24.37	n.a.	147.365	441.908	49.11	n.a.	BMB*
<b>Total:</b>			402.838	899.810	100.00	0.000	

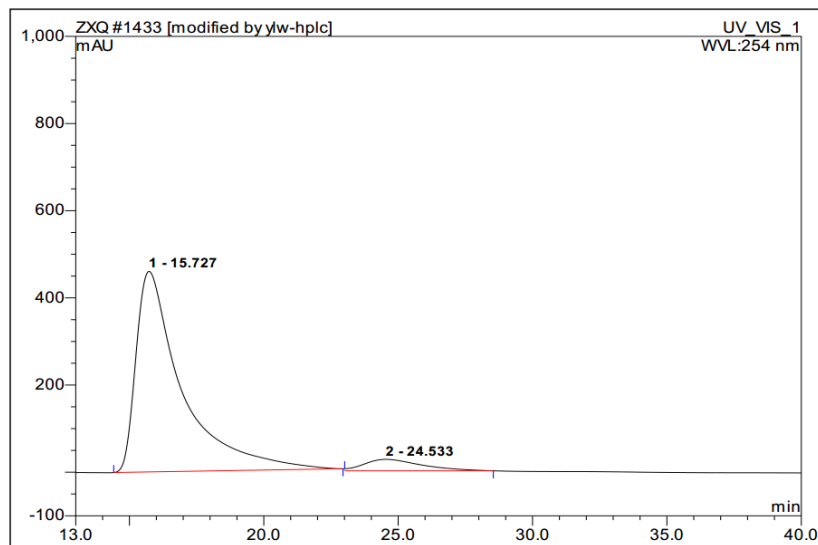


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.73	n.a.	597.314	1141.499	93.57	n.a.	BMB*
2	24.54	n.a.	34.434	78.410	6.43	n.a.	BMB*
<b>Total:</b>			631.748	1219.909	100.00	0.000	

[D<sub>2</sub>]-**2a** (30% D): ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

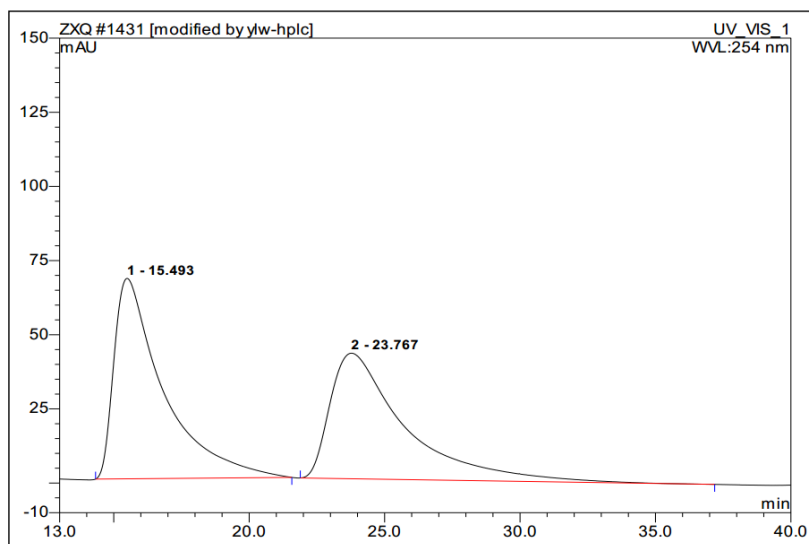
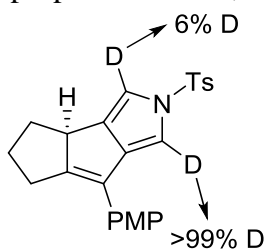


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.66	n.a.	96.311	217.085	50.58	n.a.	BMB*
2	23.91	n.a.	63.714	212.107	49.42	n.a.	BMB*
<b>Total:</b>			160.024	429.192	100.00	0.000	

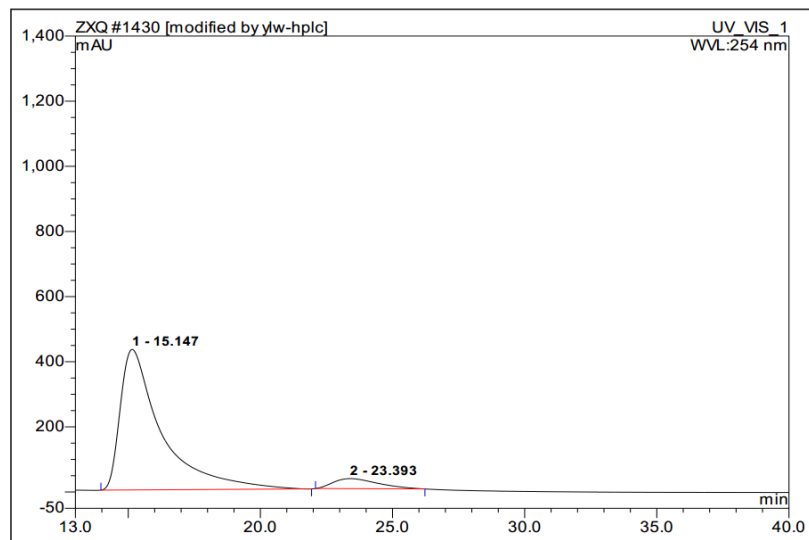


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.73	n.a.	460.148	911.268	93.33	n.a.	BMB*
2	24.53	n.a.	26.270	65.136	6.67	n.a.	MB*
<b>Total:</b>			486.418	976.404	100.00	0.000	

[D<sub>2</sub>]-**2a** (6% D): ASH, *n*-hexane/2-propanol = 85/15,  $v = 1.0 \text{ mL min}^{-1}$ ,  $\lambda = 254 \text{ nm}$

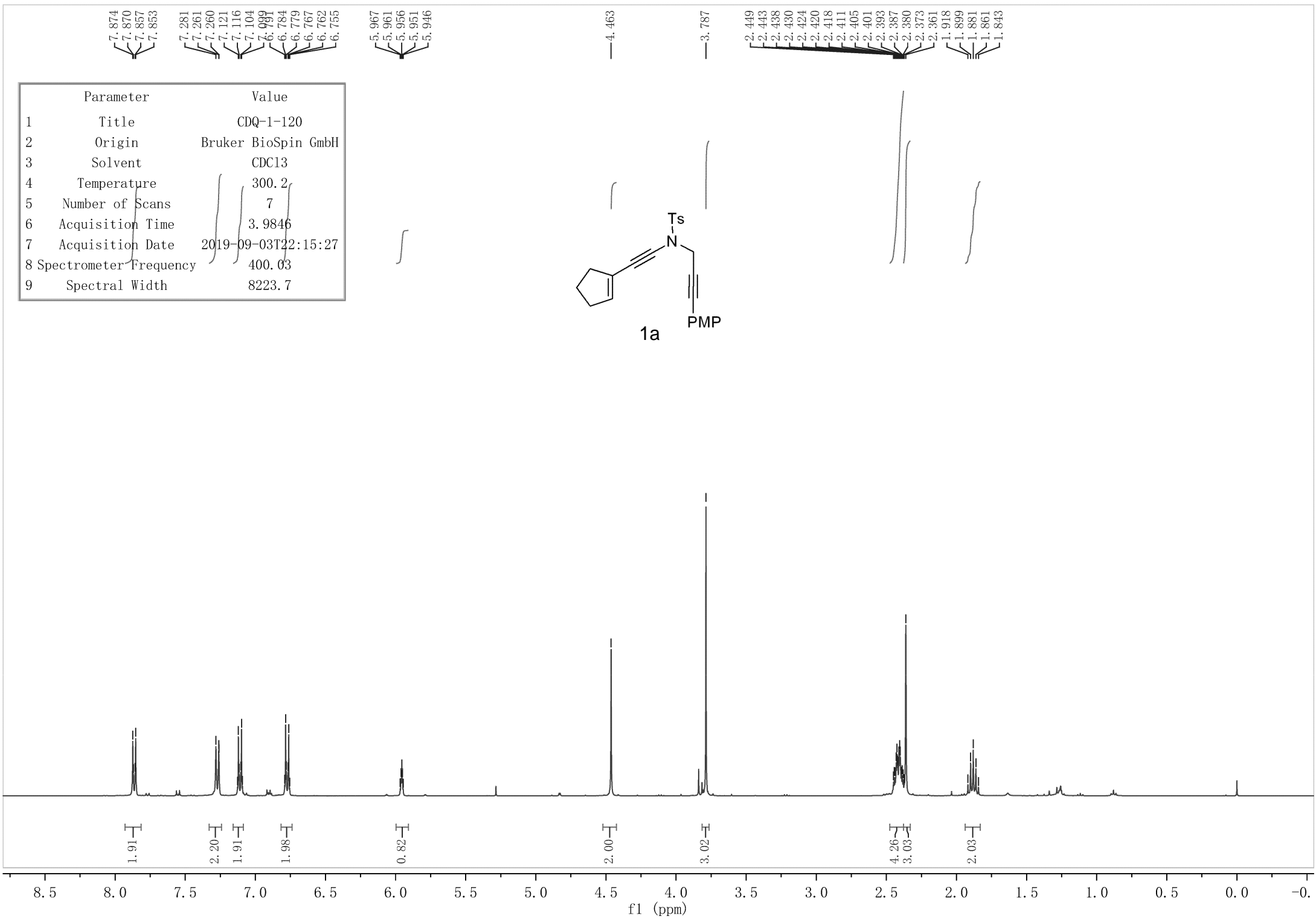
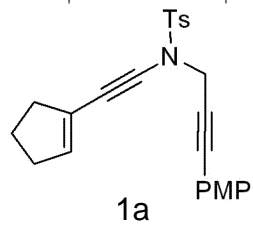


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.49	n.a.	67.562	142.198	51.41	n.a.	BMB*
2	23.77	n.a.	42.332	134.401	48.59	n.a.	BMB*
<b>Total:</b>			109.893	276.599	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.15	n.a.	431.362	782.915	92.82	n.a.	BMB*
2	23.39	n.a.	30.812	60.600	7.18	n.a.	BMB*
<b>Total:</b>			462.174	843.514	100.00	0.000	

Parameter	Value
1 Title	CDQ-1-120
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.2
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2019-09-03T22:15:27
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



7.874  
7.870  
7.857  
7.853

7.281  
7.261  
7.260  
7.121  
7.116  
7.104

6.989  
6.981  
6.784  
6.779  
6.767  
6.762  
6.755

5.967  
5.961  
5.956  
5.951  
5.946

4.463

3.787

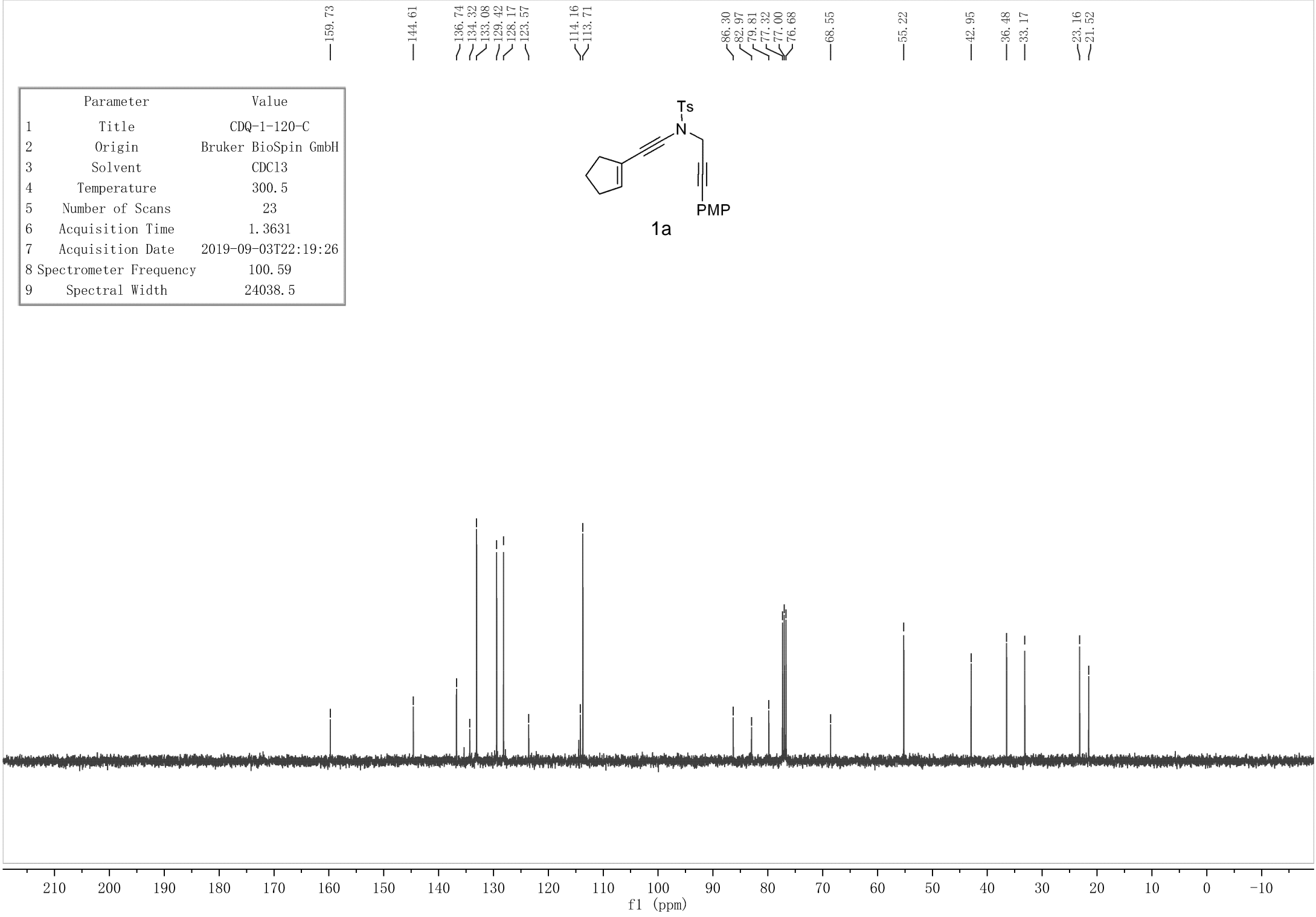
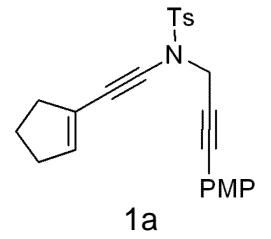
2.449  
2.443  
2.438  
2.430  
2.424  
2.420  
2.418  
2.411  
2.405  
2.401

2.393  
2.387  
2.380  
2.373  
2.361

1.918  
1.899  
1.881  
1.861  
1.843



Parameter	Value
1 Title	CDQ-1-120-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.5
5 Number of Scans	23
6 Acquisition Time	1.3631
7 Acquisition Date	2019-09-03T22:19:26
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-20-9
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2020-04-06T14:16:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

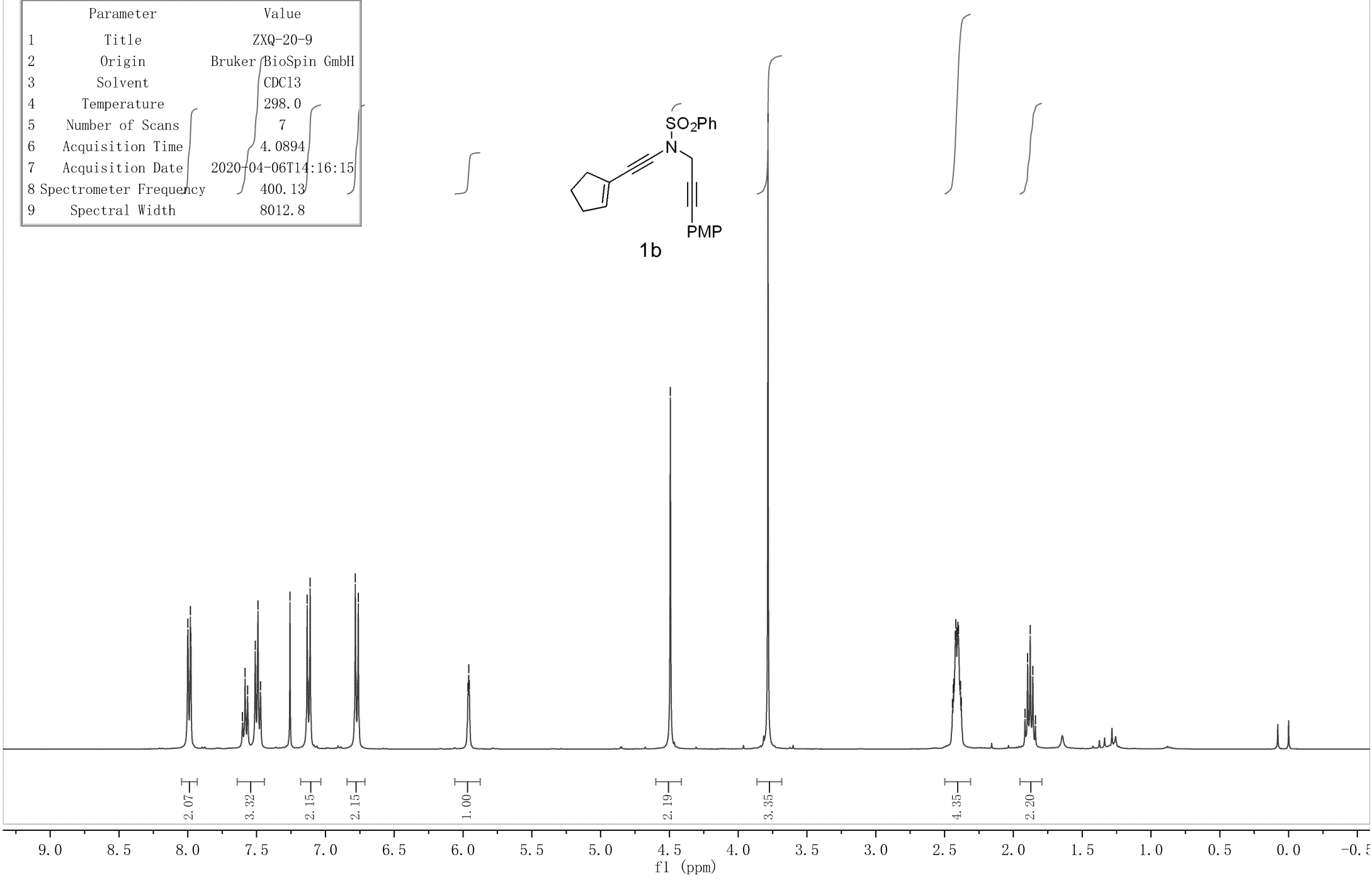
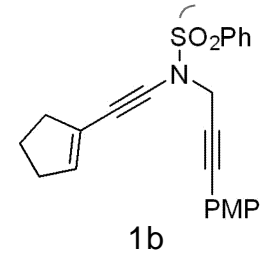
8.000  
7.981  
7.978  
7.584  
7.510  
7.510  
7.490  
7.478  
7.458  
7.133  
7.111  
6.783  
6.761

5.964  
5.959  
5.954

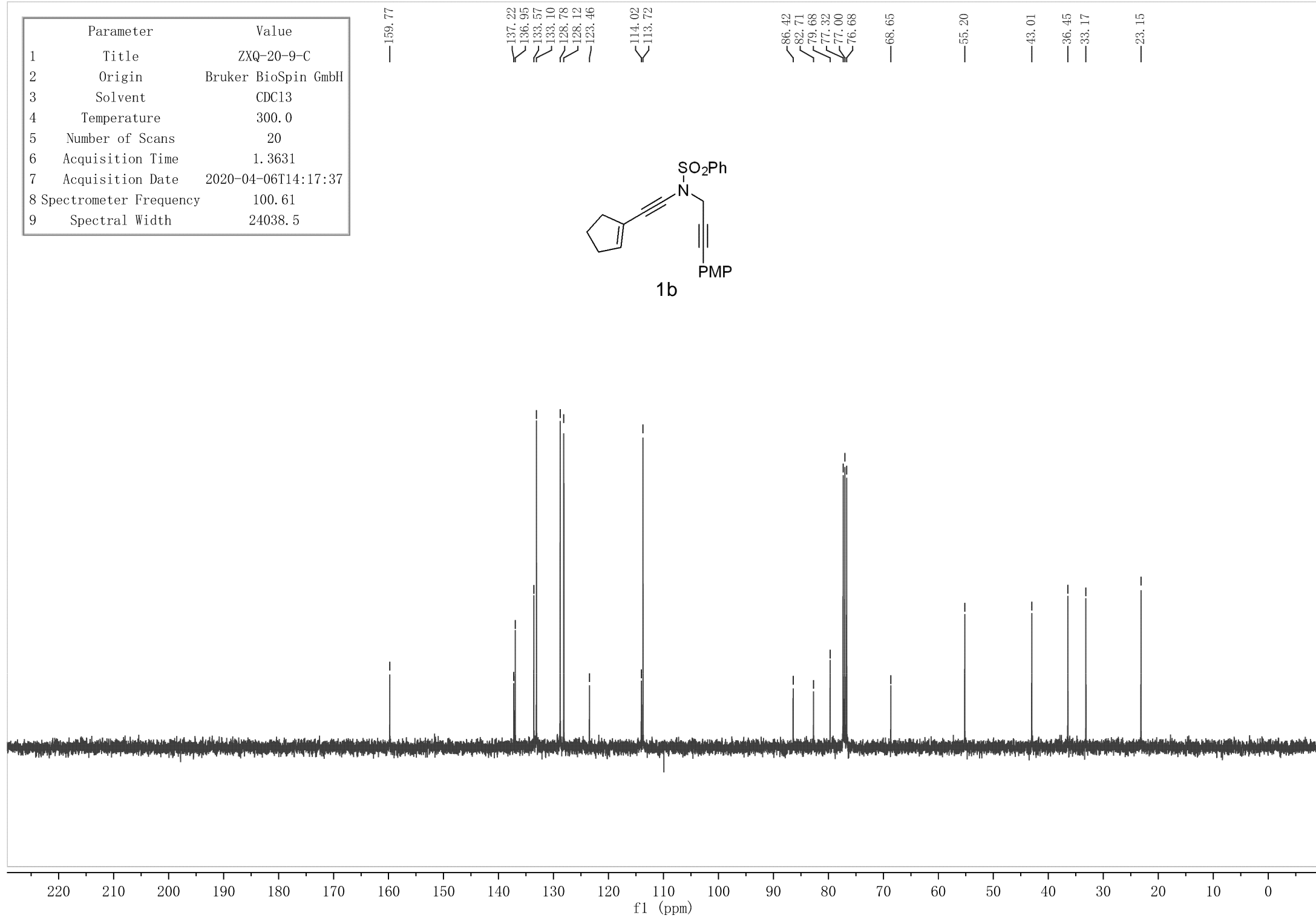
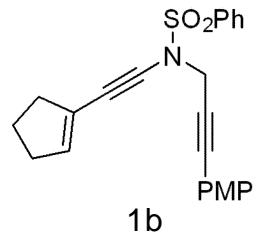
4.493

3.784

2.442  
2.437  
2.432  
2.422  
2.417  
2.409  
2.404  
2.399  
2.385  
2.379  
1.916  
1.896  
1.878  
1.859  
1.840



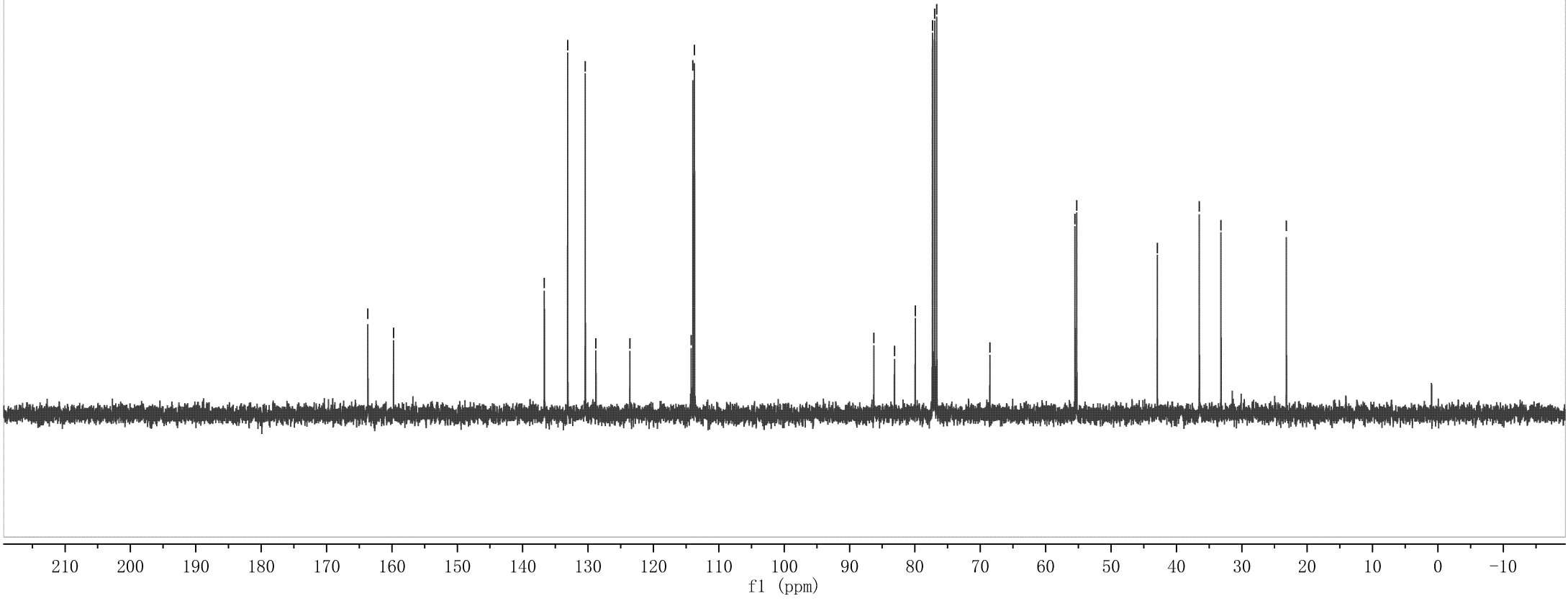
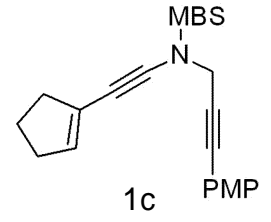
Parameter	Value
1 Title	ZXQ-20-9-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	20
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-06T14:17:37
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

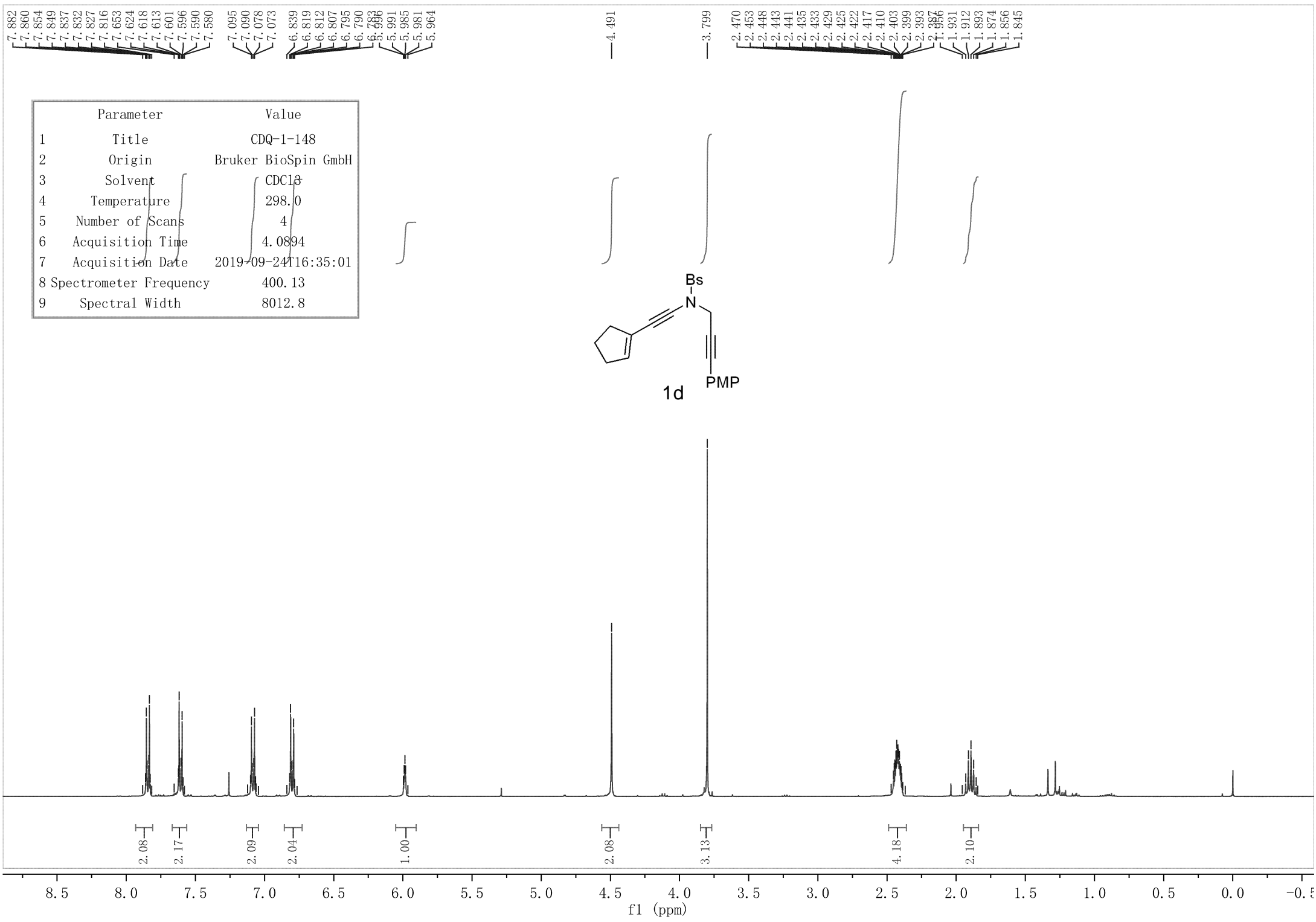




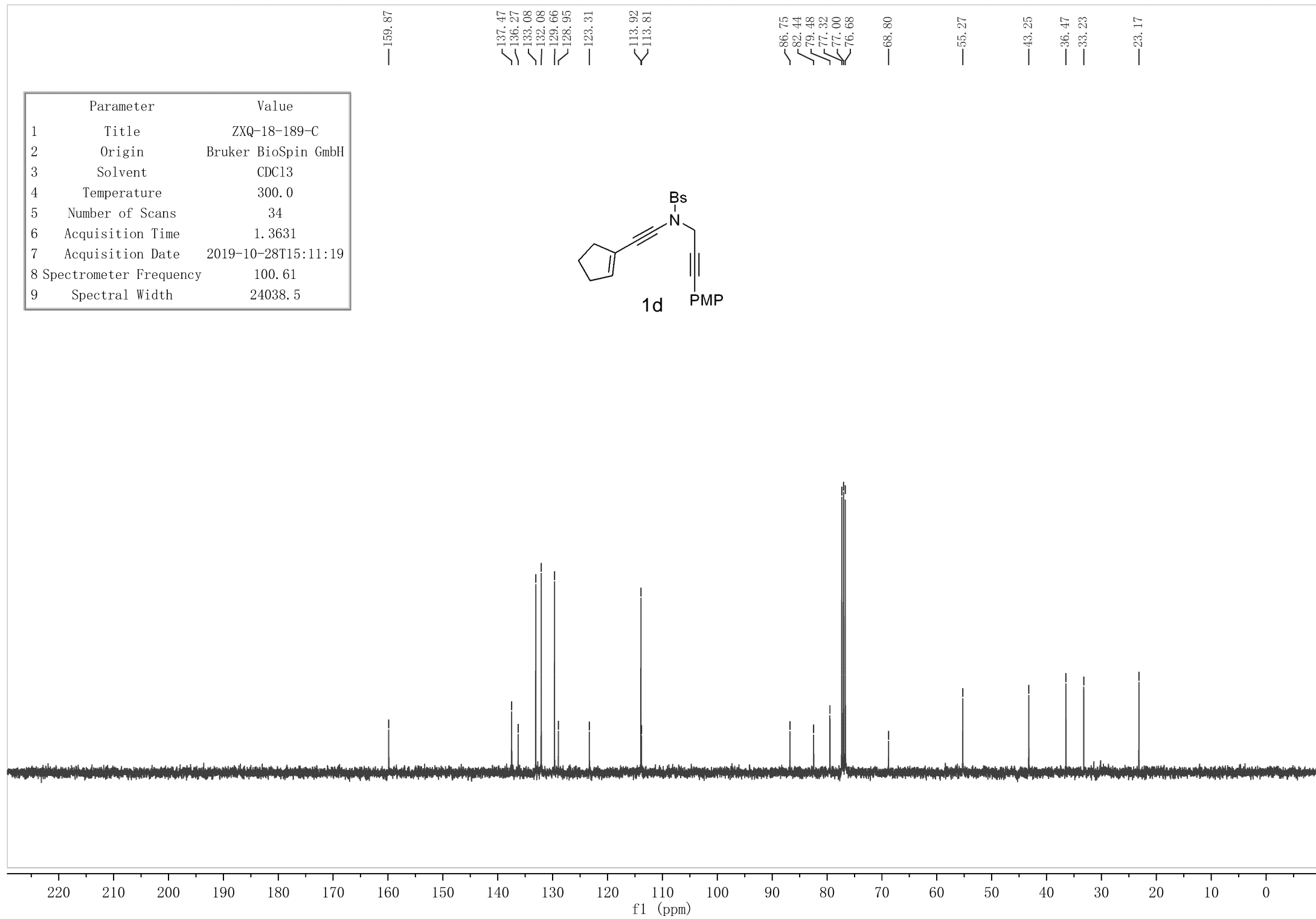
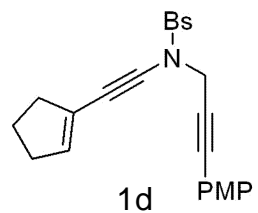
163.68  
 159.75  
 136.69  
 133.12  
 130.43  
 128.80  
 123.60  
 114.22  
 113.96  
 113.72  
 86.29  
 83.13  
 79.95  
 77.32  
 77.00  
 76.68  
 68.54  
 55.52  
 55.25  
 42.92  
 36.50  
 33.18  
 23.18

Parameter	Value
1 Title	ZXQ-20-202-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.4
5 Number of Scans	49
6 Acquisition Time	1.3631
7 Acquisition Date	2020-05-19T14:09:07
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



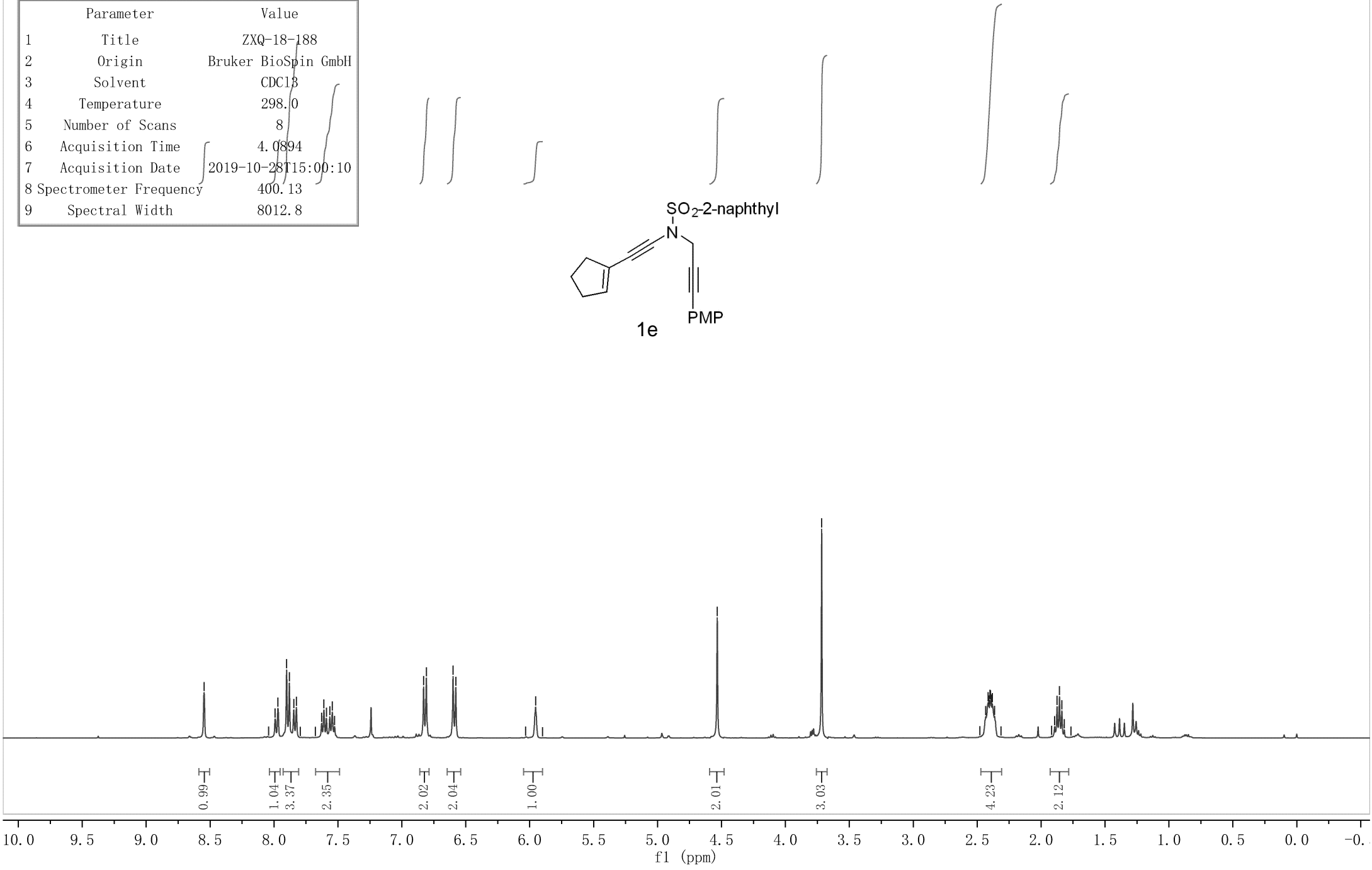
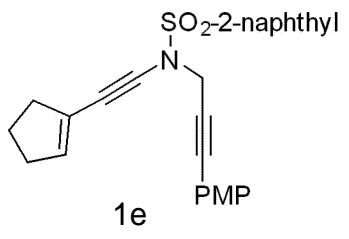


Parameter	Value
1 Title	ZXQ-18-189-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	34
6 Acquisition Time	1.3631
7 Acquisition Date	2019-10-28T15:11:19
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



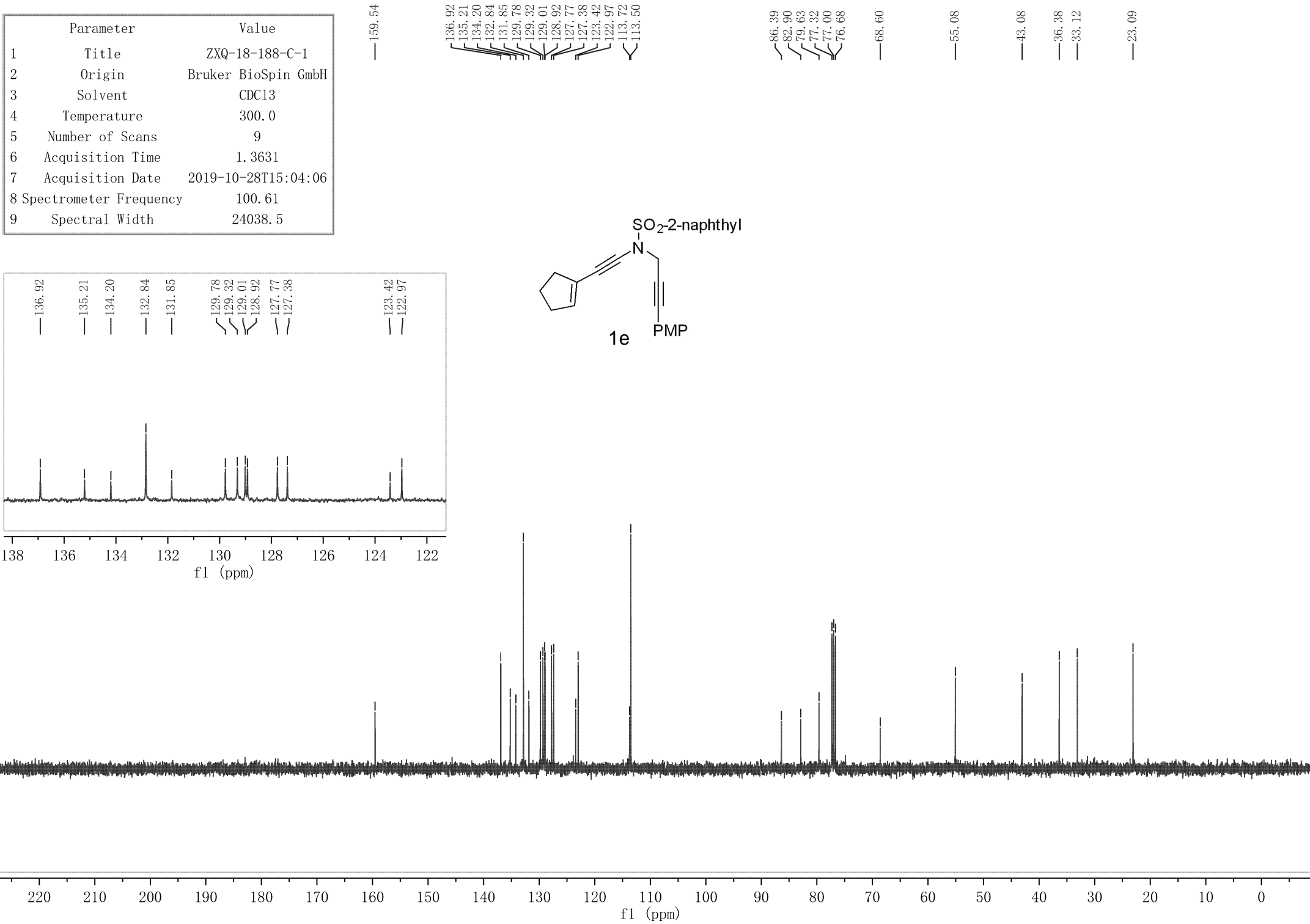
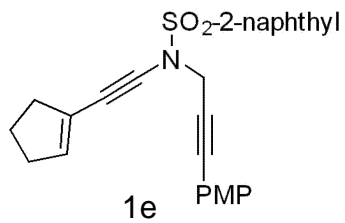
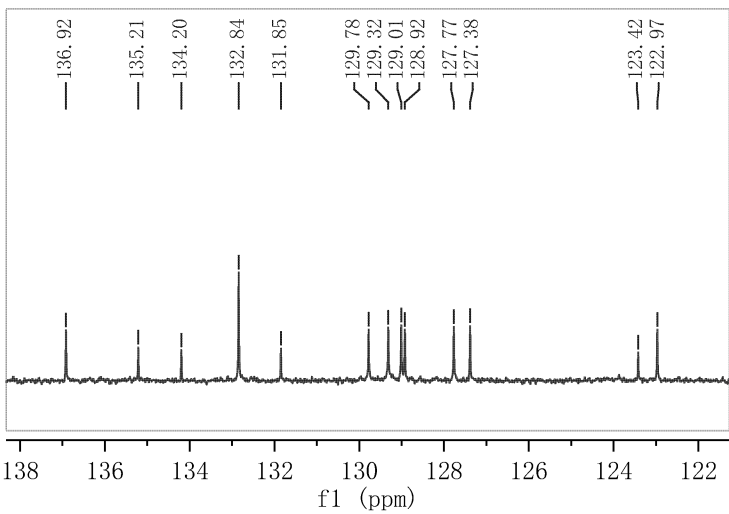
8.547  
 7.991  
 7.970  
 7.901  
 7.880  
 7.845  
 7.825  
 7.827  
 7.610  
 7.590  
 7.590  
 7.563  
 7.544  
 7.536  
 6.808  
 6.600  
 6.578  
 6.033  
 5.954  
 5.900  
 4.533  
 3.716  
 2.480  
 2.433  
 2.415  
 2.408  
 2.400  
 2.395  
 2.389  
 2.382  
 2.364  
 2.314  
 1.918  
 1.894  
 1.875  
 1.856  
 1.837  
 1.819  
 1.767

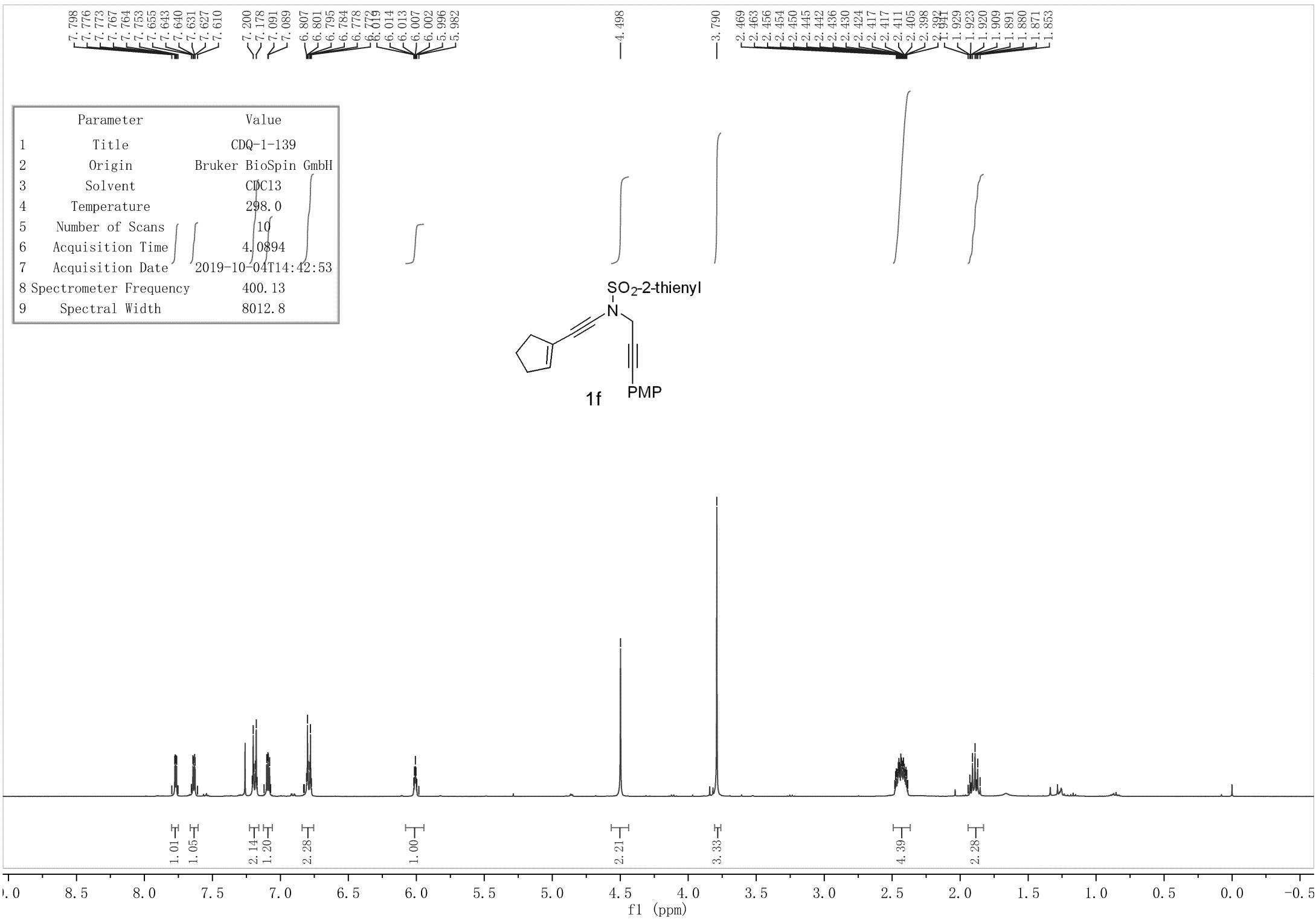
Parameter	Value
1 Title	ZXQ-18-188
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2019-10-28T15:00:10
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8





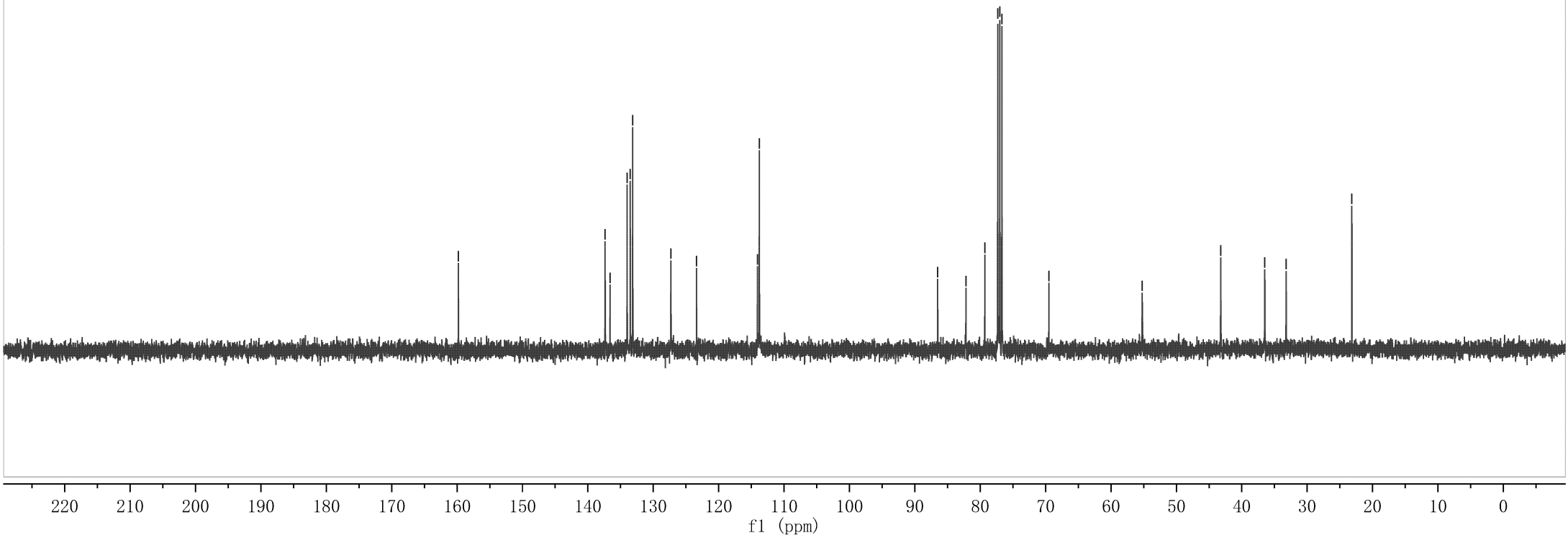
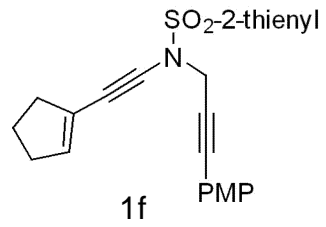
Parameter	Value
1 Title	ZXQ-18-188-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	9
6 Acquisition Time	1.3631
7 Acquisition Date	2019-10-28T15:04:06
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



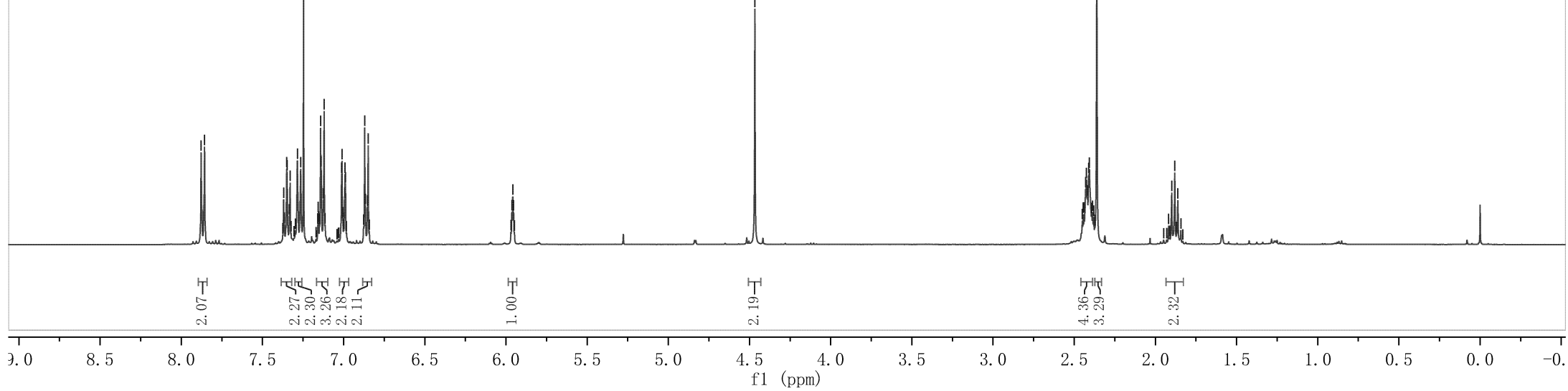
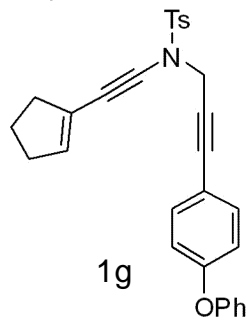
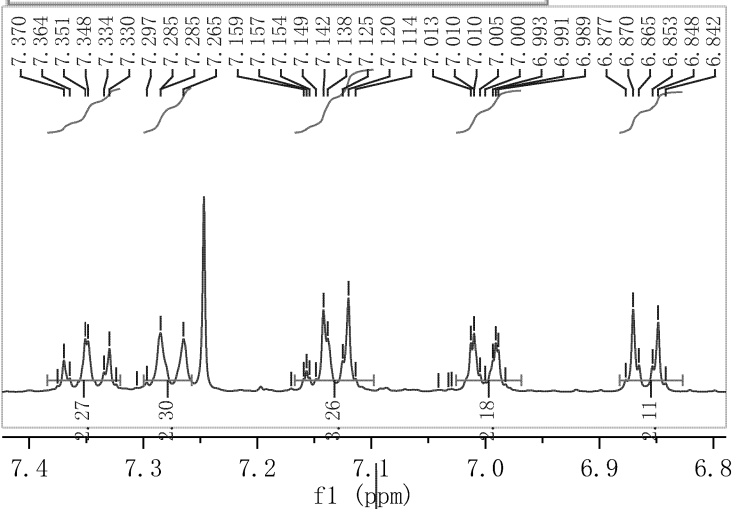


Parameter	Value
1 Title	CDQ-1-139-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	20
6 Acquisition Time	1.3631
7 Acquisition Date	2019-10-04T14:45:45
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

159.80  
 137.37  
 136.61  
 133.99  
 133.52  
 133.15  
 127.30  
 123.38  
 114.06  
 113.78  
 86.50  
 82.19  
 79.30  
 77.32  
 77.00  
 76.68  
 69.50  
 55.23  
 43.22  
 36.48  
 33.21  
 23.16



Parameter	Value
1 Title	ZXQ-19-66
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	301.5
5 Number of Scans	11
6 Acquisition Time	3.9846
7 Acquisition Date	2019-11-27T14:01:03
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

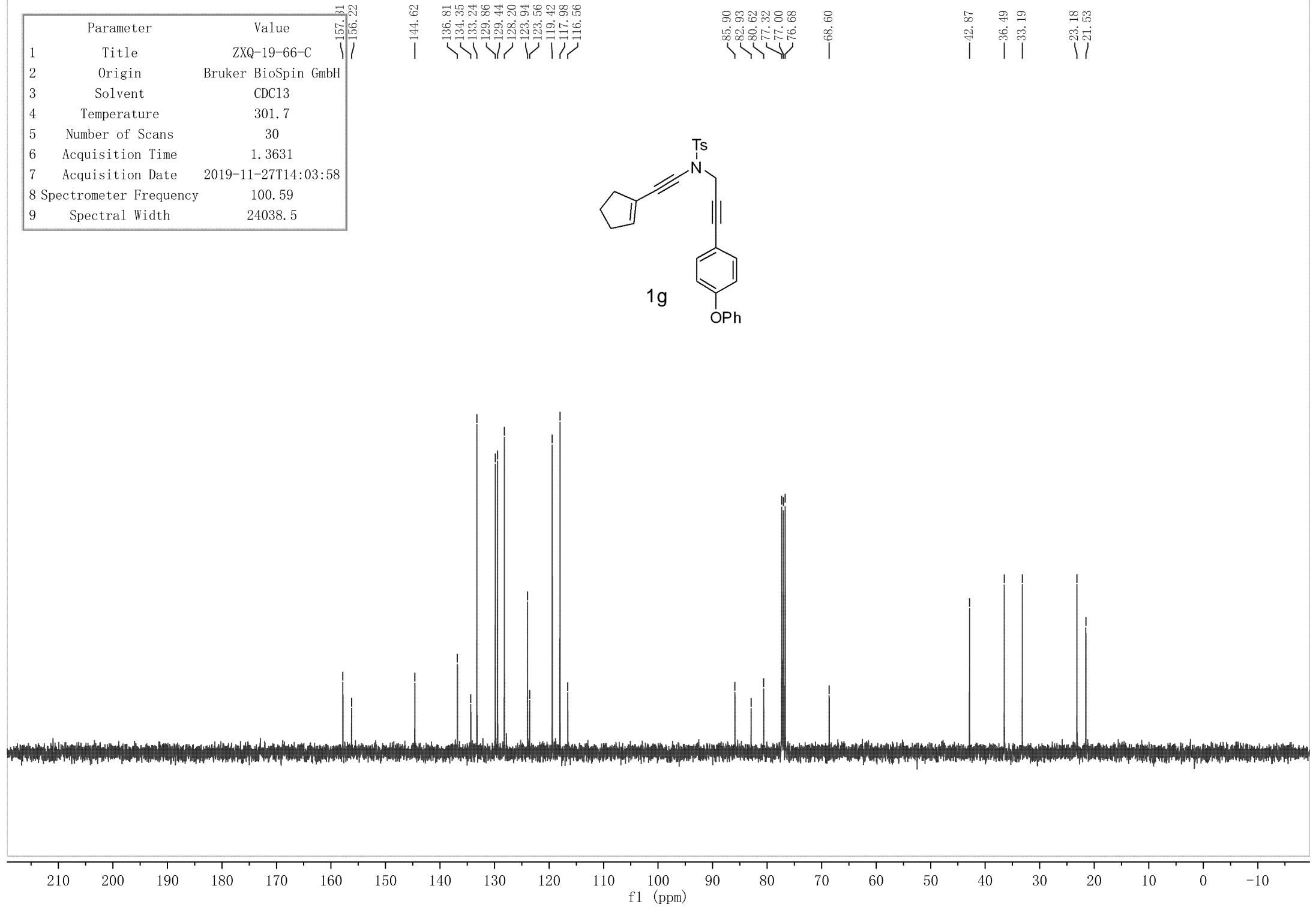
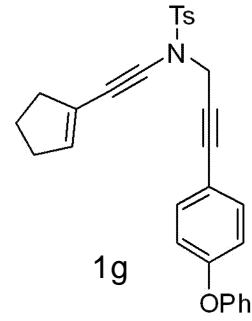


7.878  
7.857  
7.351  
7.348  
7.330  
7.285  
7.265  
7.142  
7.138  
7.120  
7.013  
7.010  
7.010  
6.991  
6.989  
6.870  
6.869  
6.863  
5.958  
5.953  
5.948

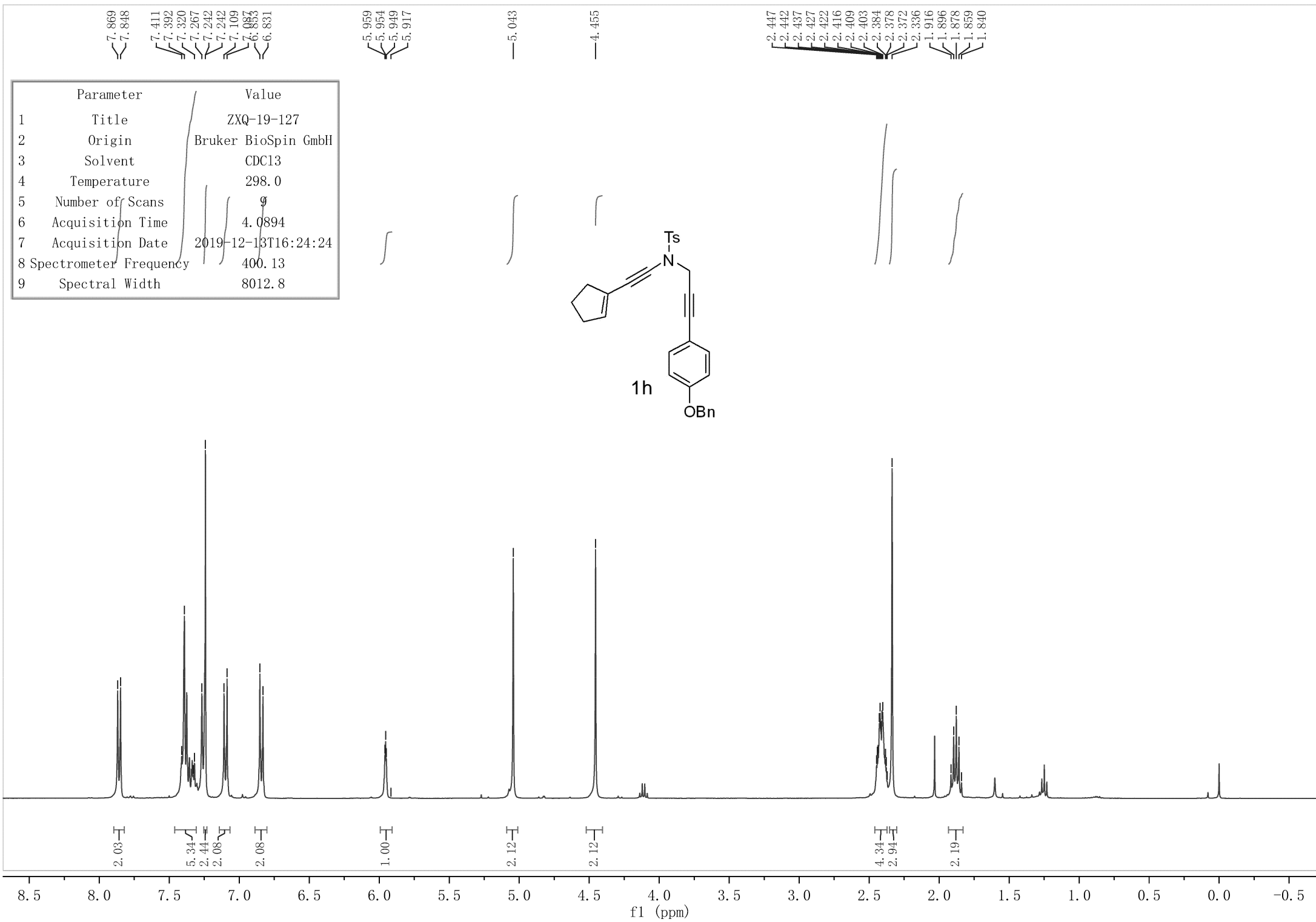
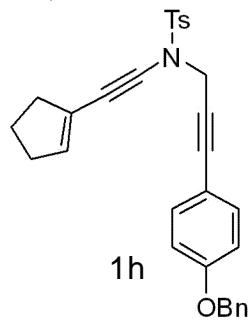
4.467

2.450  
2.444  
2.439  
2.430  
2.425  
2.418  
2.411  
2.406  
2.392  
2.387  
2.380  
2.373  
2.361  
1.949  
1.930  
1.919  
1.912  
1.899  
1.881  
1.870  
1.862  
1.843  
1.831

Parameter	Value
1 Title	ZXQ-19-66-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	301.7
5 Number of Scans	30
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-27T14:03:58
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

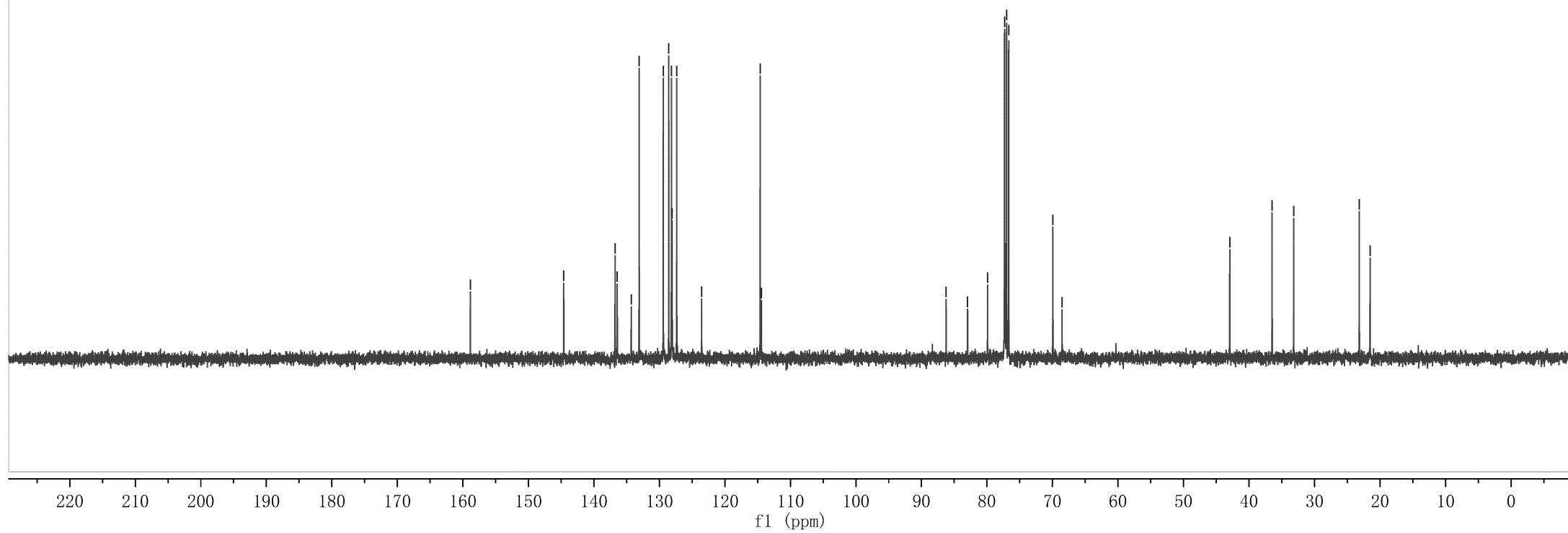
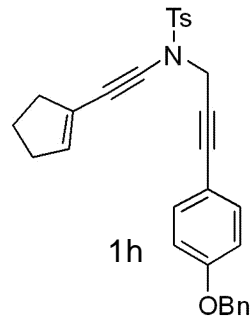


Parameter	Value
1 Title	ZXQ-19-127
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-13T16:24:24
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

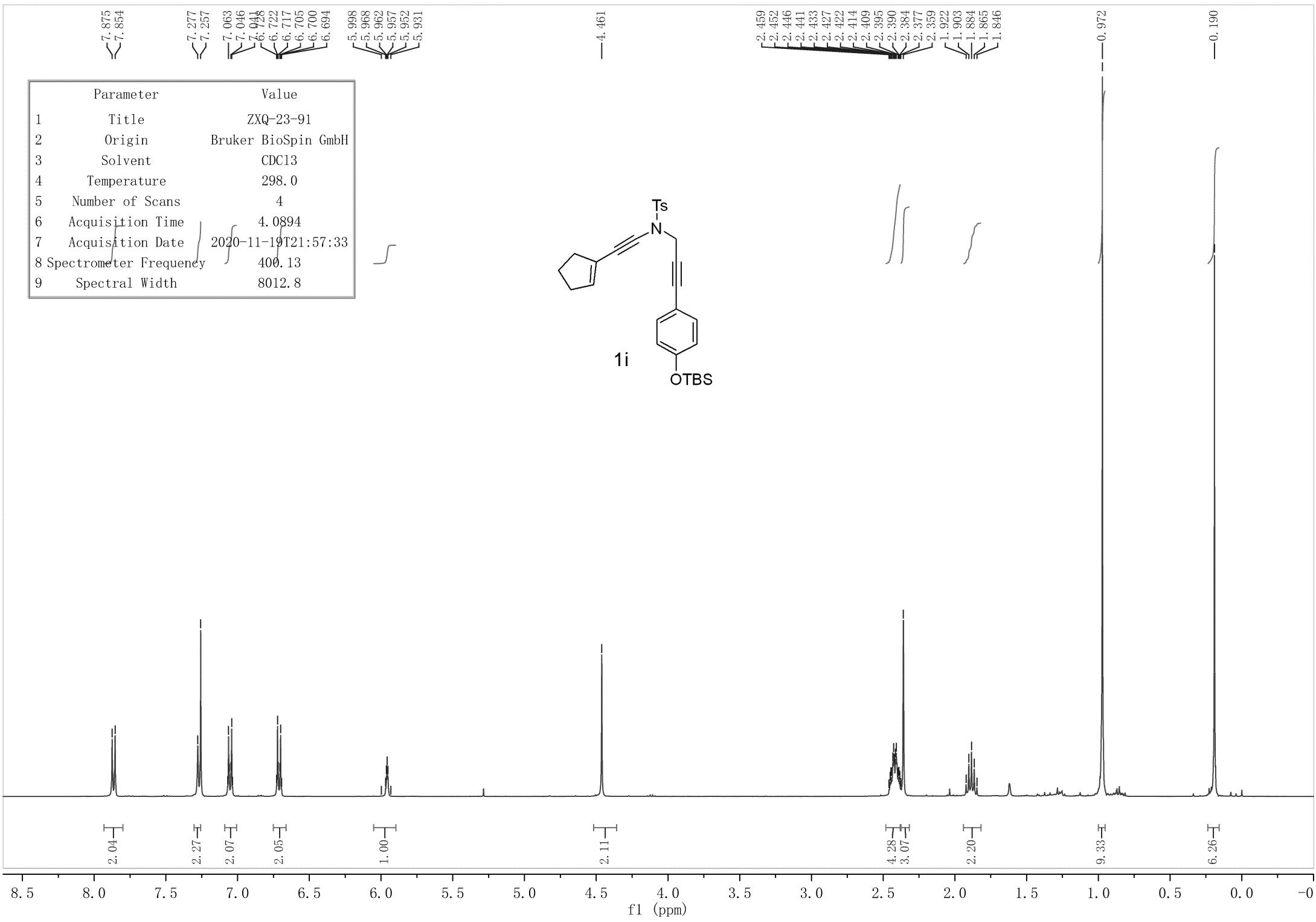
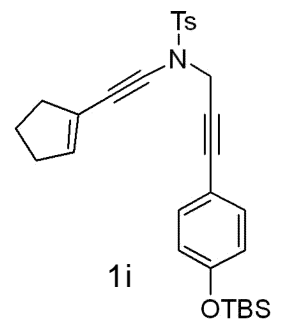


Parameter	Value
1 Title	ZXQ-19-127-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	31
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-13T16:25:48
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.85  
 144.60  
 136.76  
 136.43  
 134.30  
 133.09  
 129.41  
 128.57  
 128.16  
 128.05  
 127.36  
 123.55  
 114.61  
 114.43  
 86.23  
 82.95  
 79.90  
 77.32  
 77.00  
 76.68  
 69.94  
 68.52  
 42.93  
 36.47  
 33.17  
 23.16  
 21.52



Parameter	Value
1 Title	ZXQ-23-91
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2020-11-19T21:57:33
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.875  
7.854  
7.277  
7.257  
7.063  
7.046  
6.928  
6.928  
6.722  
6.717  
6.705  
6.700  
6.694  
5.998  
5.968  
5.962  
5.957  
5.952  
5.931

4.461

2.459  
2.452  
2.446  
2.441  
2.433  
2.427  
2.422  
2.414  
2.409  
2.395  
2.390  
2.384  
2.377  
2.359  
1.922  
1.903  
1.884  
1.865  
1.846

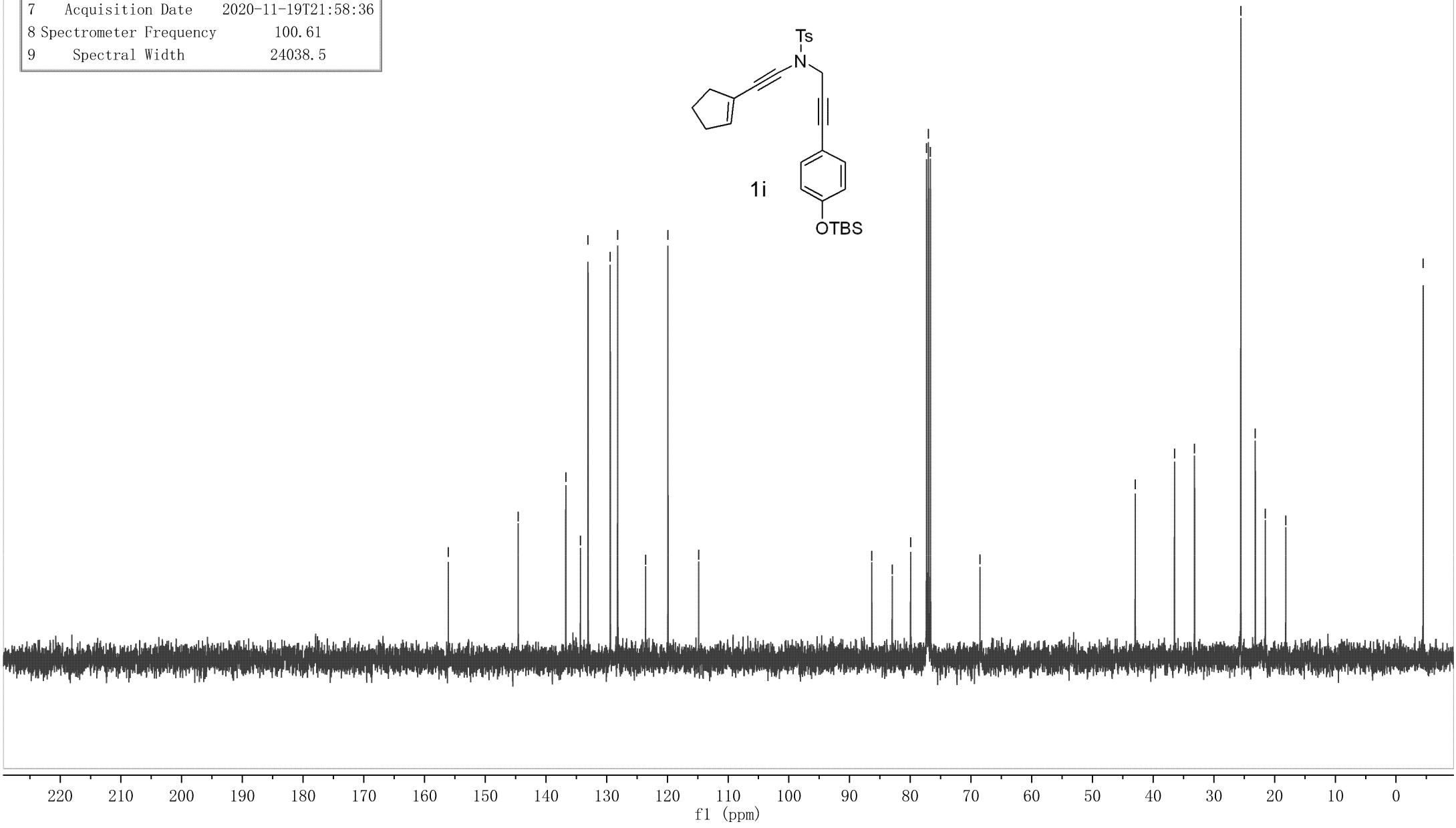
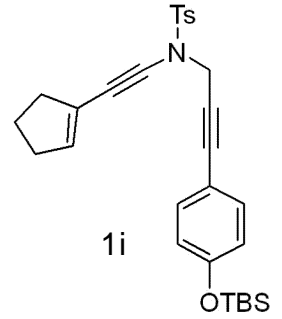
0.972

0.190

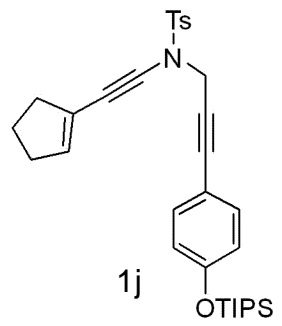


Parameter	Value
1 Title	ZXQ-23-91-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	14
6 Acquisition Time	1.3631
7 Acquisition Date	2020-11-19T21:58:36
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

- 156.09
- 144.57
- 136.73
- 134.33
- 133.07
- 129.41
- 128.20
- 123.59
- 119.91
- 114.84
- 86.34
- 82.97
- 79.95
- 77.32
- 77.00
- 76.68
- 68.53
- 42.95
- 36.48
- 33.18
- 25.56
- 23.18
- 21.53
- 18.16
- 4.47

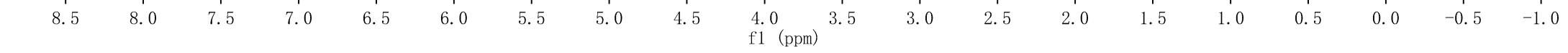


Parameter	Value
1 Title	ZXQ-19-17
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-13T11:33:35
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



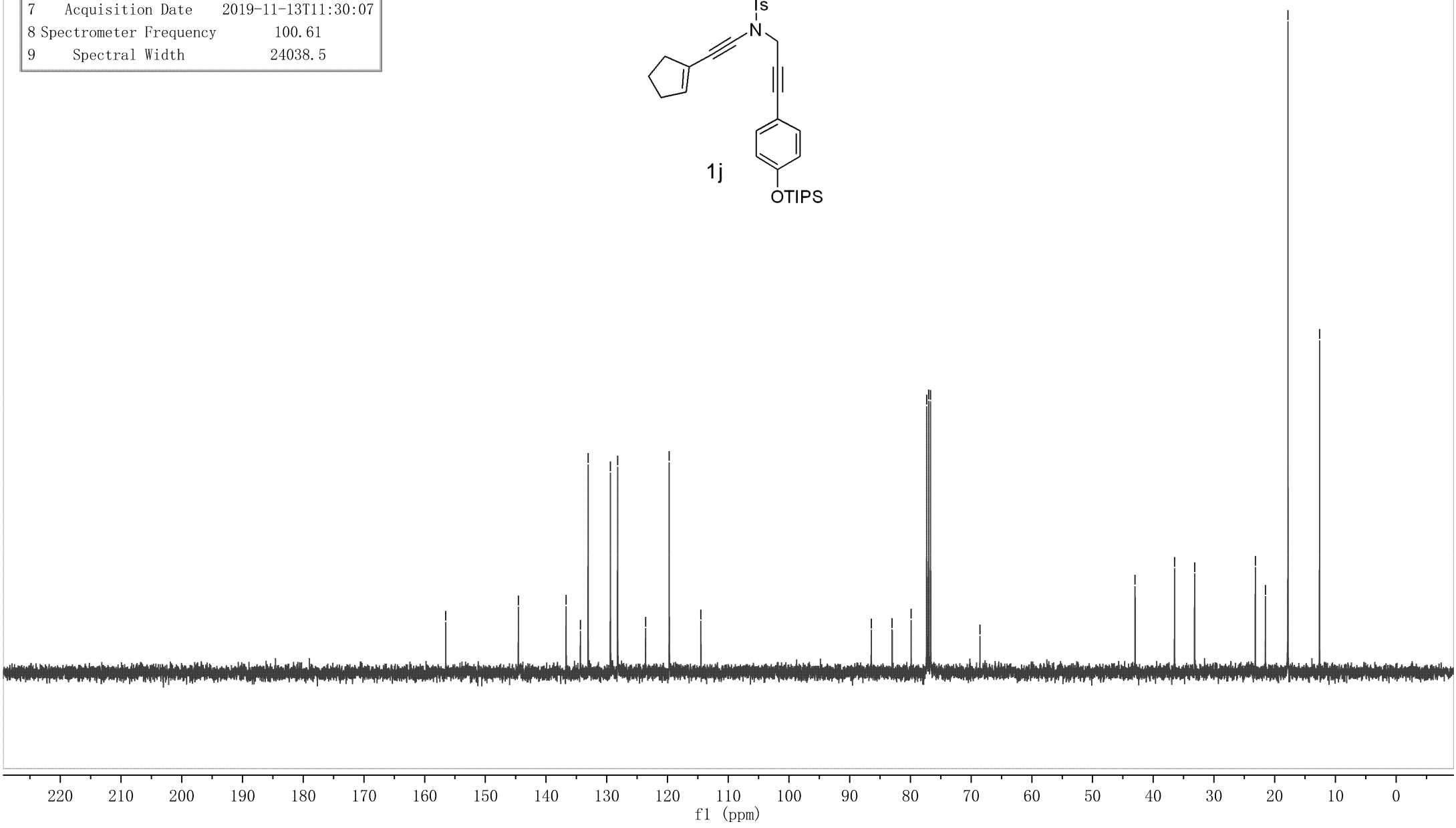
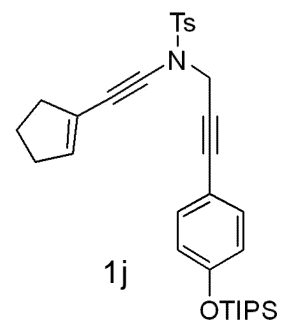
7.876  
7.855  
7.299  
7.274  
7.274  
7.057  
6.986  
6.760  
6.755  
6.743  
6.738  
6.732  
5.967  
5.961  
5.956  
5.951  
5.930  
4.463  
2.451  
2.446  
2.441  
2.432  
2.427  
2.422  
2.415  
2.408  
2.396  
2.391  
2.358  
1.922  
1.903  
1.884  
1.866  
1.847  
1.803  
1.284  
1.272  
1.268  
1.264  
1.254  
1.251  
1.246  
1.236  
1.232  
1.227  
1.218  
1.209  
1.192  
1.098  
1.080

2.07  
2.35  
2.17  
2.09  
1.00  
2.11  
4.35  
2.89  
2.16  
3.20  
18.17



Parameter	Value
1 Title	ZXQ-19-17-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-13T11:30:07
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

- 156.53
- 144.56
- 136.71
- 134.85
- 133.08
- 129.41
- 128.22
- 123.61
- 119.72
- 114.50
- 86.44
- 83.00
- 79.89
- 77.32
- 77.00
- 76.68
- 68.54
- 42.99
- 36.50
- 33.19
- 23.19
- 21.53
- 17.82
- 12.61



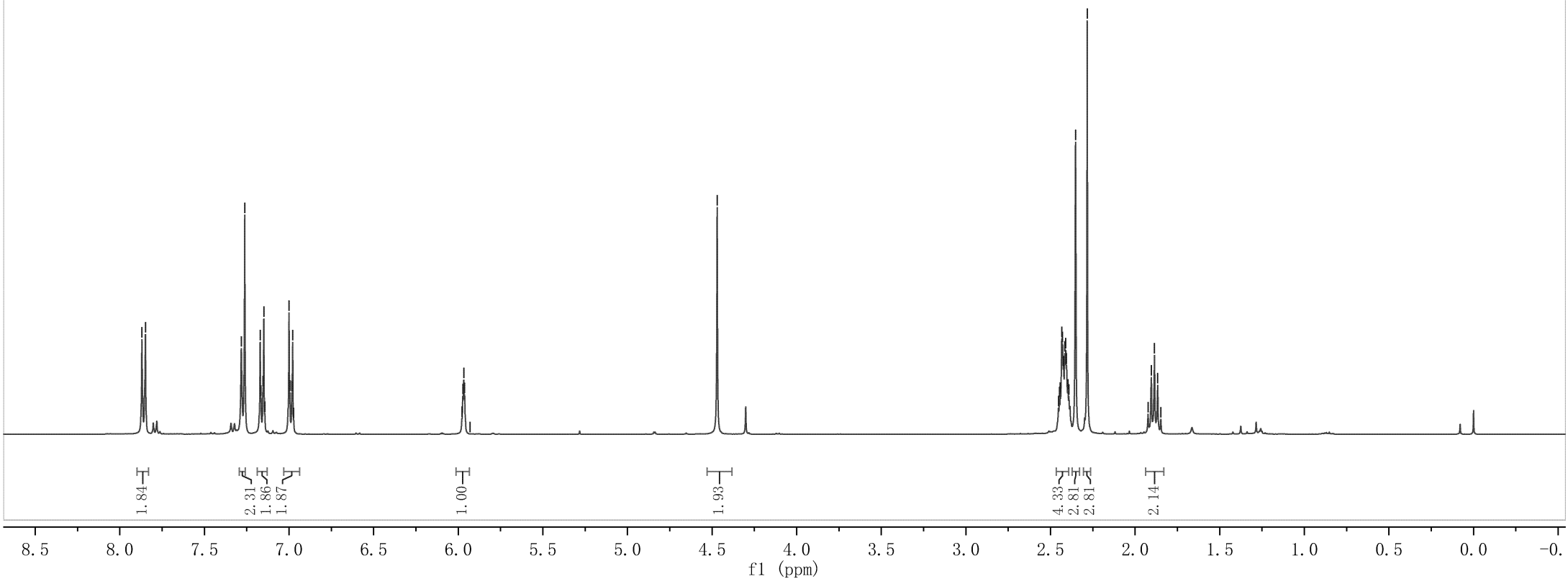
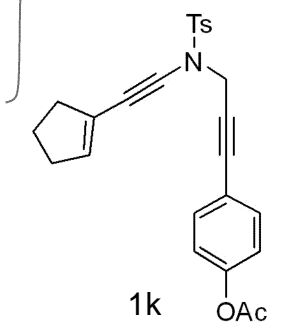
Parameter	Value
1 Title	ZXQ-19-87
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-03T11:35:55
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

7.870  
7.849  
7.282  
7.262  
7.171  
7.166  
7.154  
7.149  
7.143  
7.000  
6.995  
6.983  
6.978  
6.973

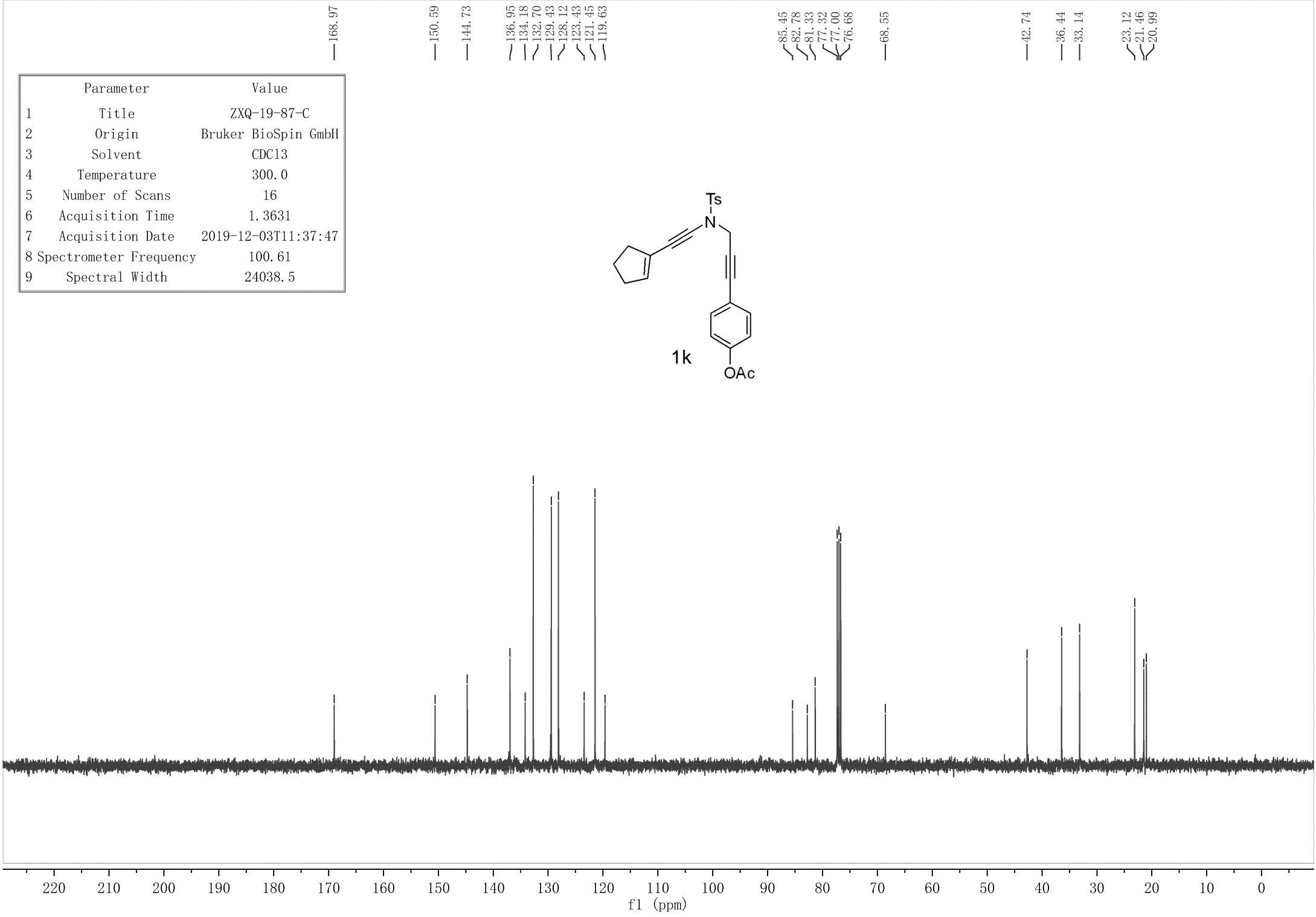
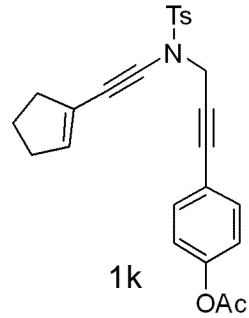
5.978  
5.973  
5.968  
5.963  
5.963  
5.931

4.470

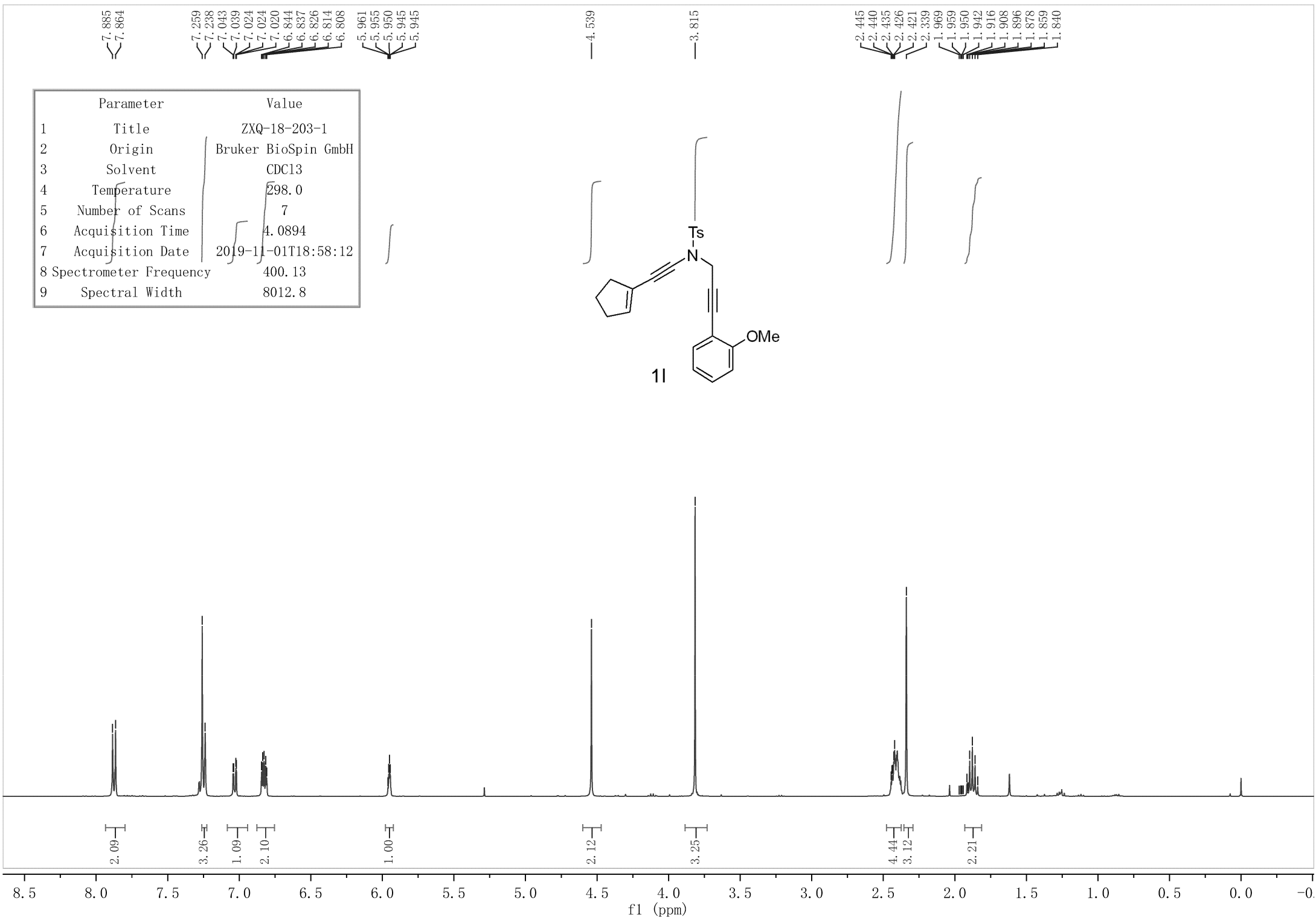
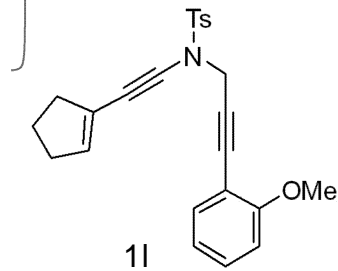
2.453  
2.447  
2.442  
2.433  
2.429  
2.423  
2.416  
2.410  
2.406  
2.397  
2.392  
2.352  
2.283  
1.924  
1.924  
1.904  
1.886  
1.886  
1.867  
1.848



Parameter	Value
1 Title	ZXQ-19-87-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	16
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-03T11:37:47
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-18-203-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-01T18:58:12
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.885  
7.864

7.259  
7.238  
7.043  
7.039  
7.024  
7.024  
7.020  
6.844  
6.837  
6.826  
6.814  
6.808

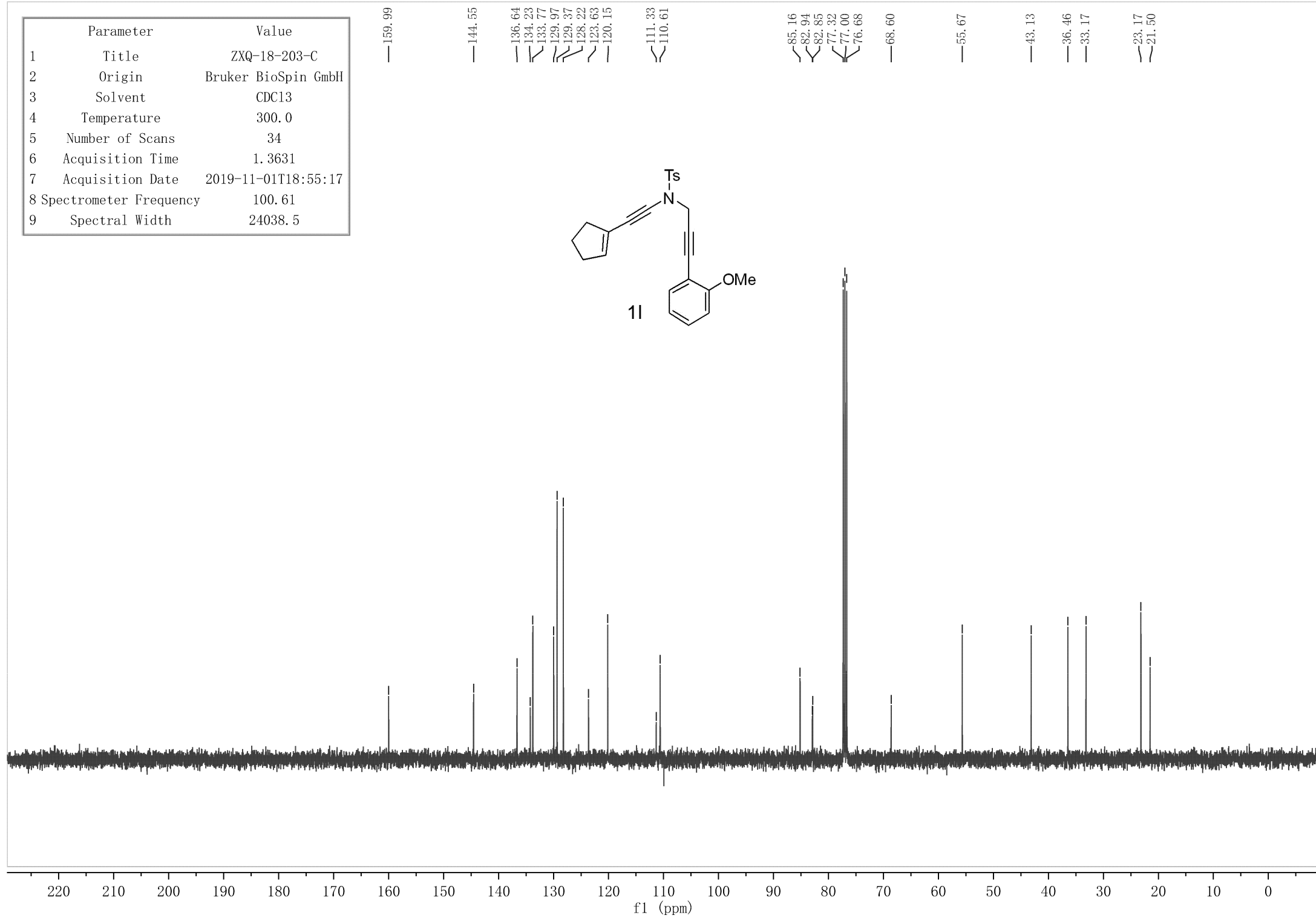
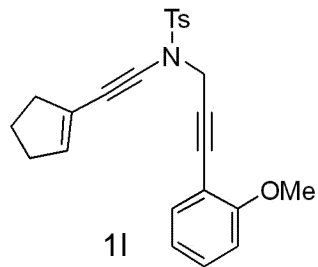
5.961  
5.955  
5.950  
5.945  
5.945

4.539

3.815

2.445  
2.440  
2.435  
2.426  
2.421  
2.339  
1.969  
1.959  
1.950  
1.942  
1.916  
1.908  
1.896  
1.878  
1.859  
1.840

Parameter	Value
1 Title	ZXQ-18-203-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	34
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-01T18:55:17
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



7.879  
7.858

7.289  
7.269  
7.255

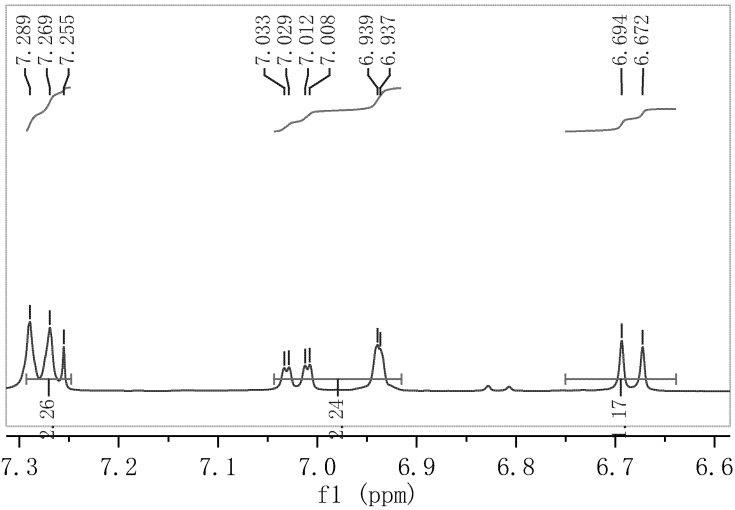
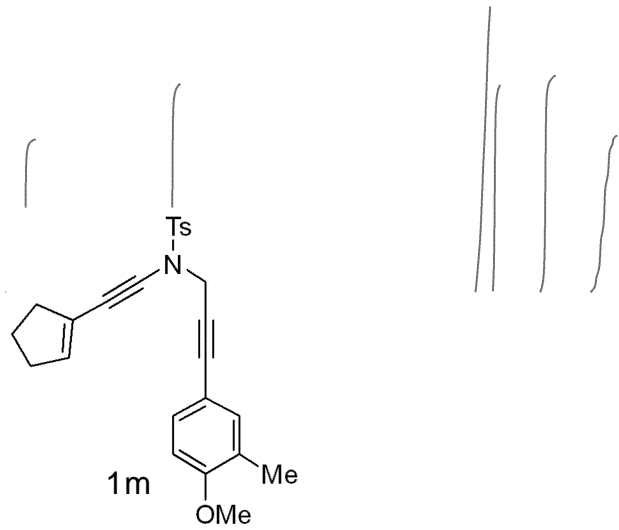
7.008  
6.939  
6.937  
6.672

5.969  
5.963  
5.958  
5.953  
5.947

4.463

3.808  
2.452  
2.447  
2.442  
2.431  
2.428  
2.425  
2.412  
2.412  
2.409  
2.406  
2.404  
2.394  
2.388  
2.380  
2.371  
2.145  
1.919  
1.900  
1.881  
1.881  
1.871  
1.862  
1.844

Parameter	Value
1 Title	ZXQ-18-241-H2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-09T18:49:24
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2.21

2.26

2.24

1.17

1.00

2.32

3.16

4.34

3.14

3.29

2.38

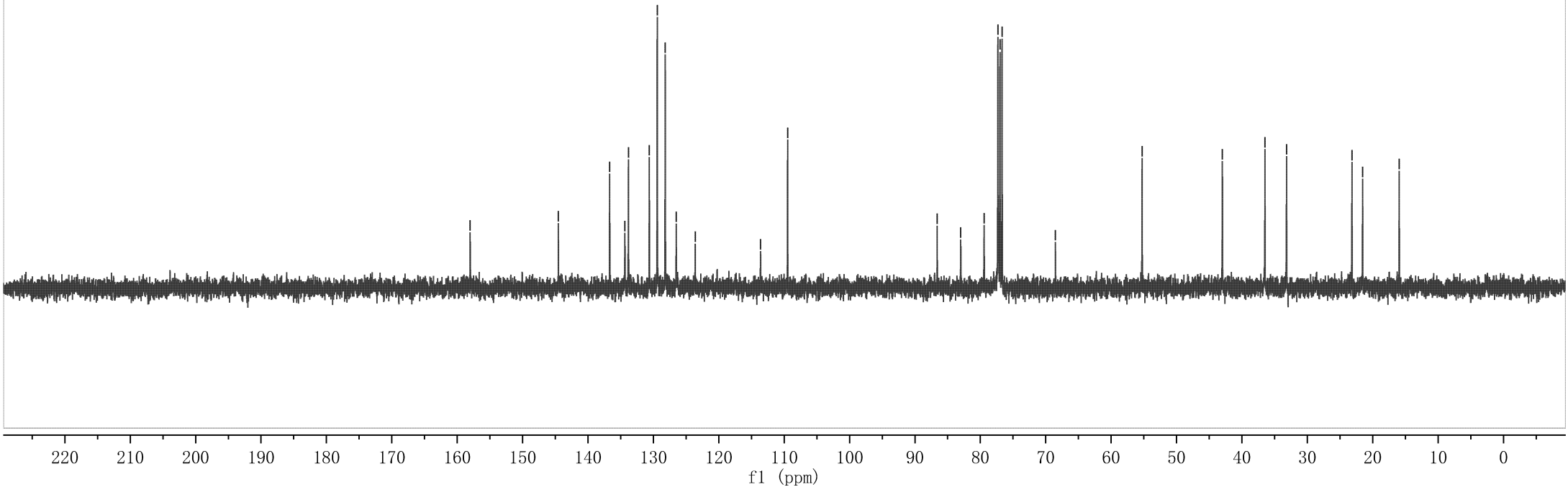
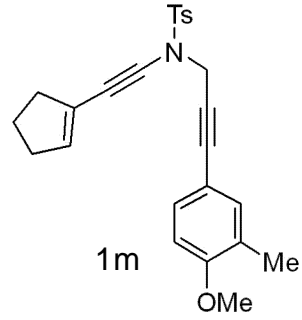
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)



Parameter	Value
1 Title	ZXQ-18-241
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	42
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-09T17:47:18
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

- 158.02
- 144.54
- 136.69
- 134.36
- 133.82
- 130.63
- 129.41
- 128.19
- 126.51
- 123.60
- 113.61
- 109.47
- 86.60
- 83.00
- 79.42
- 77.32
- 77.00
- 76.68
- 68.52
- 55.27
- 42.98
- 36.47
- 33.17
- 23.17
- 21.54
- 15.94



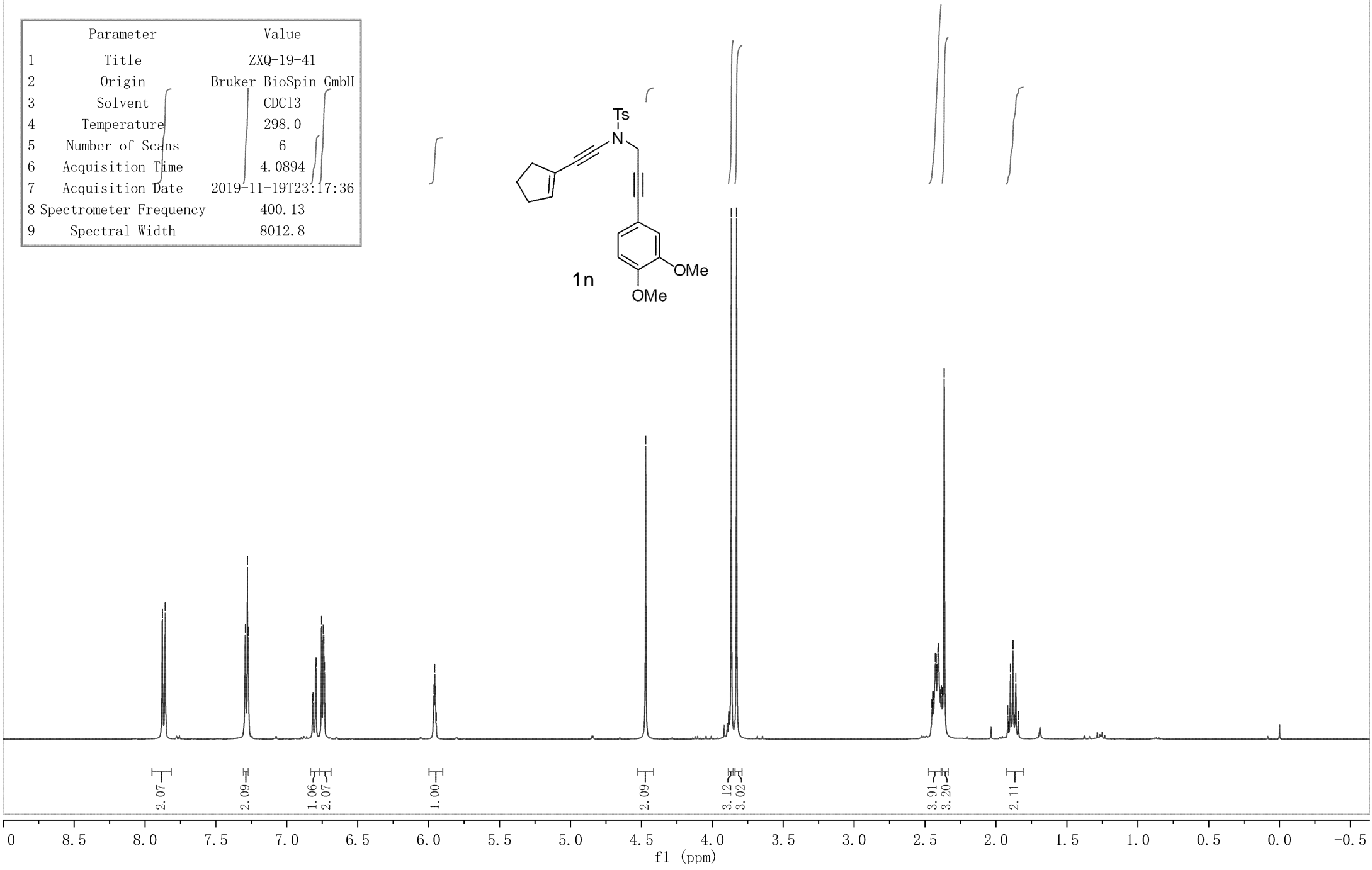
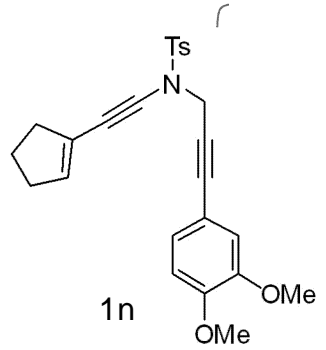
7.878  
7.857  
7.292  
7.278  
7.272  
6.814  
6.814  
6.798  
6.793  
6.755  
6.744  
6.739  
6.734  
6.734  
5.962  
5.957  
5.952  
5.946

4.470

3.866  
3.829

2.452  
2.446  
2.441  
2.428  
2.422  
2.415  
2.409  
2.404  
2.391  
2.385  
2.378  
2.365  
1.917  
1.908  
1.898  
1.879  
1.868  
1.860  
1.860  
1.841

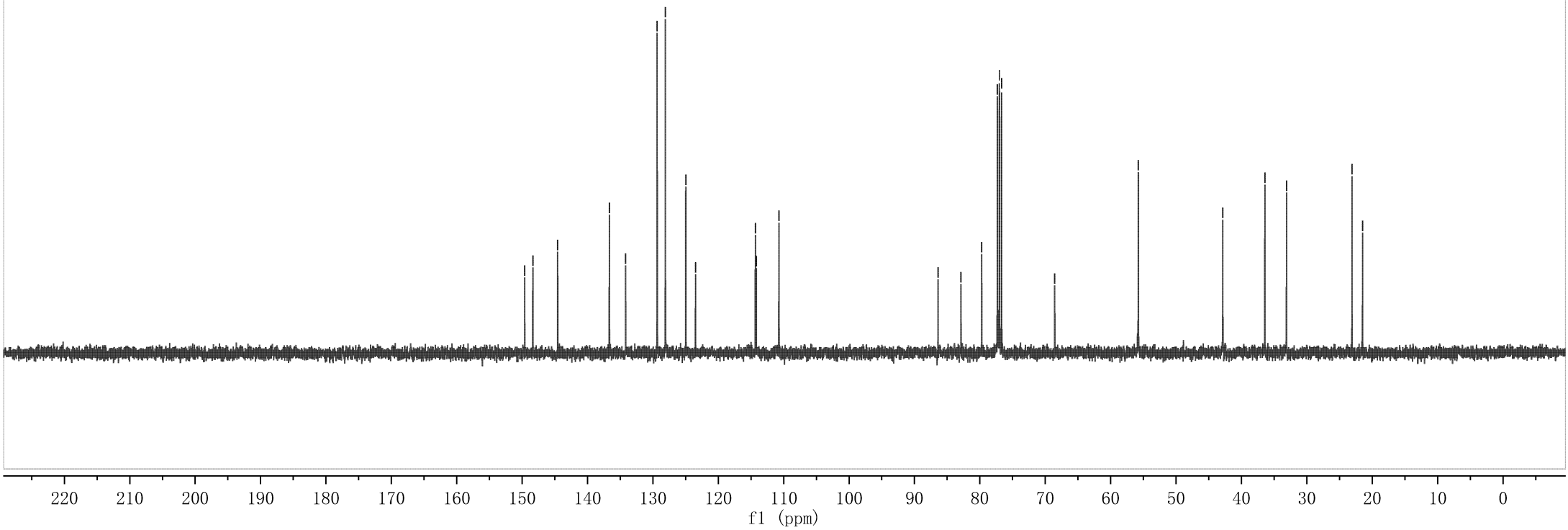
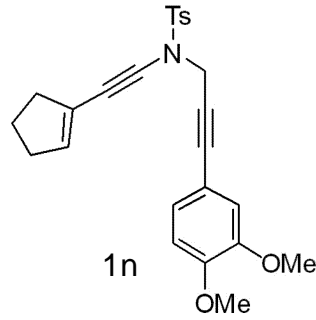
Parameter	Value
1 Title	ZXQ-19-41
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-19T23:17:36
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

Parameter	Value
1 Title	ZXQ-19-41-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	17
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-19T23:19:11
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

- 149.61
- 148.36
- 144.56
- 136.66
- 134.18
- 129.35
- 128.09
- 124.97
- 123.49
- 114.33
- 114.19
- 110.73
- 86.39
- 82.89
- 79.72
- 77.32
- 77.00
- 76.68
- 68.55
- 55.77
- 42.85
- 36.42
- 33.10
- 23.09
- 21.48

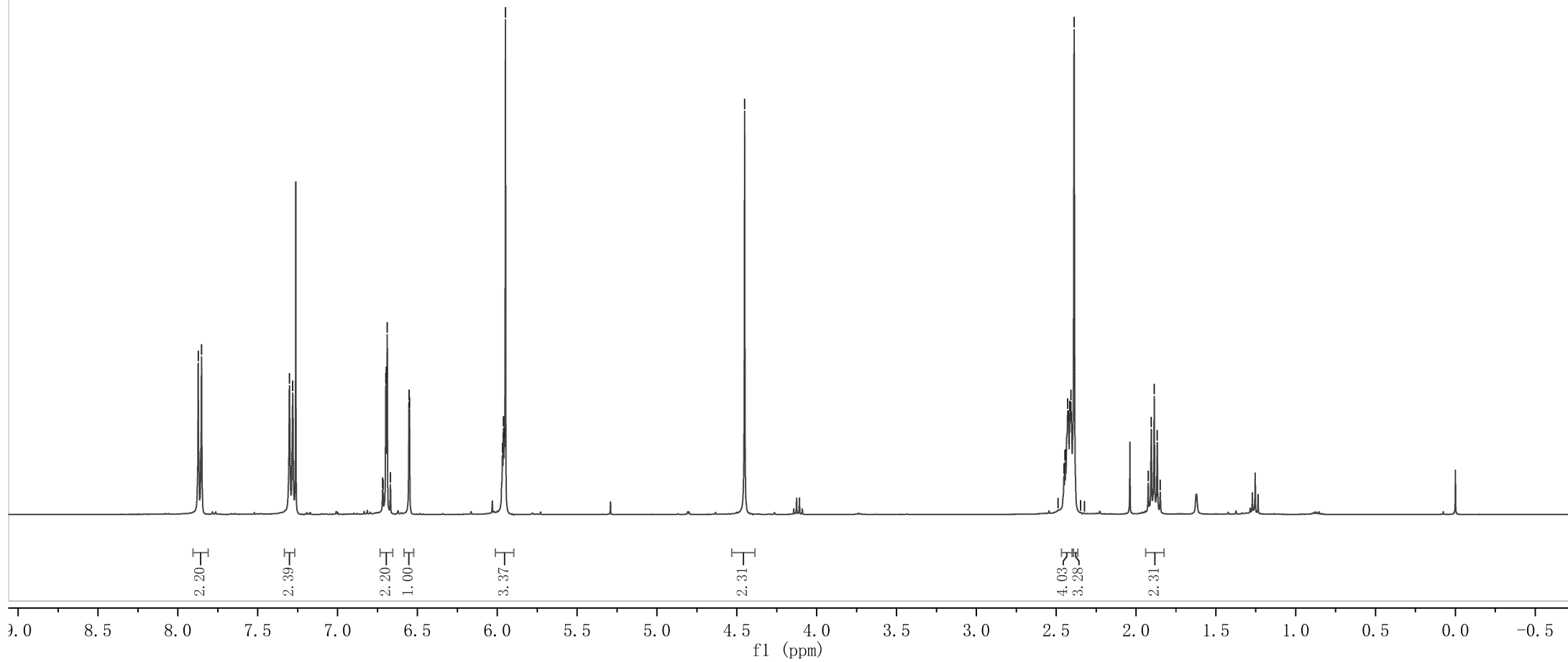
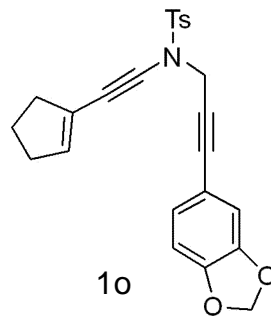


7.873  
7.852  
7.301  
7.281  
6.718  
6.715  
6.698  
6.695  
6.689  
6.669  
6.553  
6.550  
5.967  
5.961  
5.956  
5.949

4.451

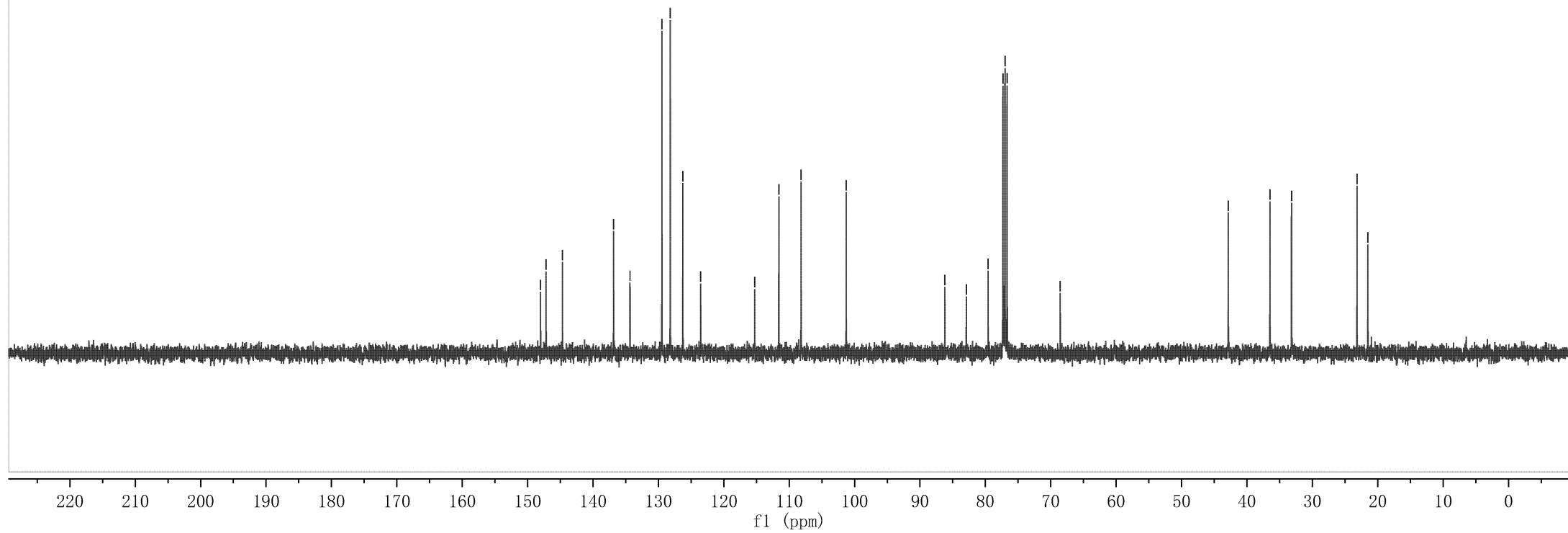
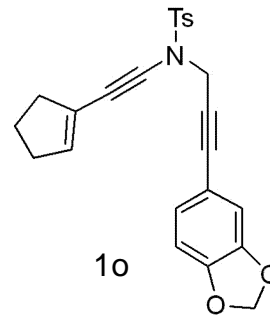
2.488  
2.451  
2.446  
2.441  
2.428  
2.422  
2.416  
2.412  
2.408  
2.388  
2.347  
2.323  
1.924  
1.904  
1.886  
1.867  
1.848

Parameter	Value
1 Title	ZXQ-18-215-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-04T16:21:23
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

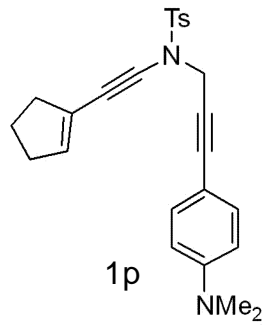


Parameter	Value
1 Title	ZXQ-18-215-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-04T16:23:53
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

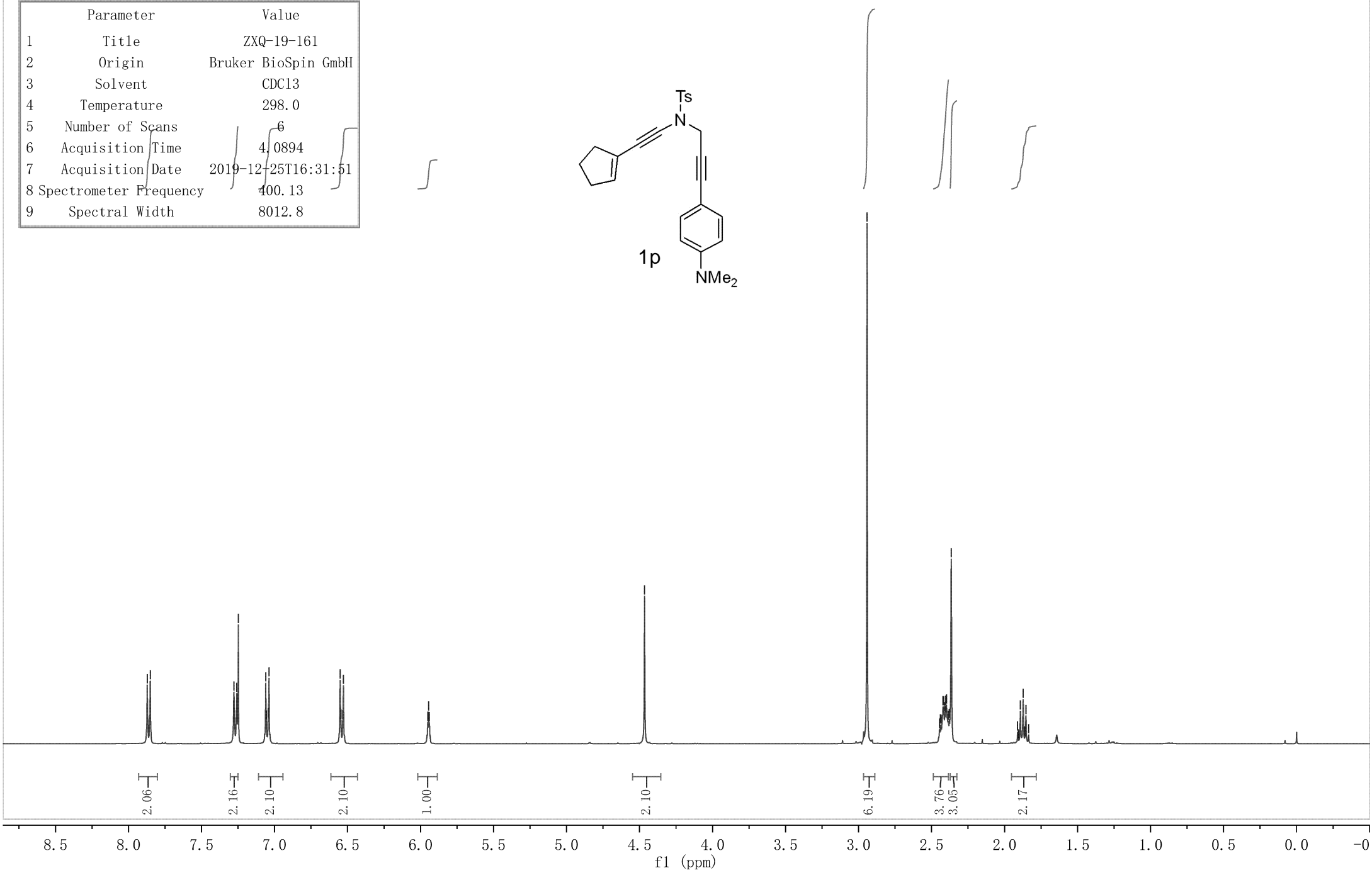
148.02 147.18 144.68 136.86 134.34 129.46 128.18 126.27 123.54 115.27 111.58 108.19 101.28 86.20 82.91 79.59 77.32 77.00 76.68 68.55 42.86 36.48 33.18 23.17 21.51



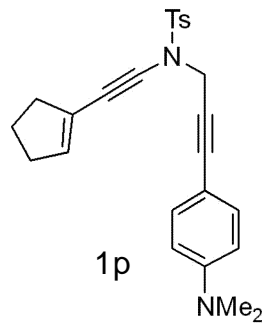
Parameter	Value
1 Title	ZXQ-19-161
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-25T16:31:51
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



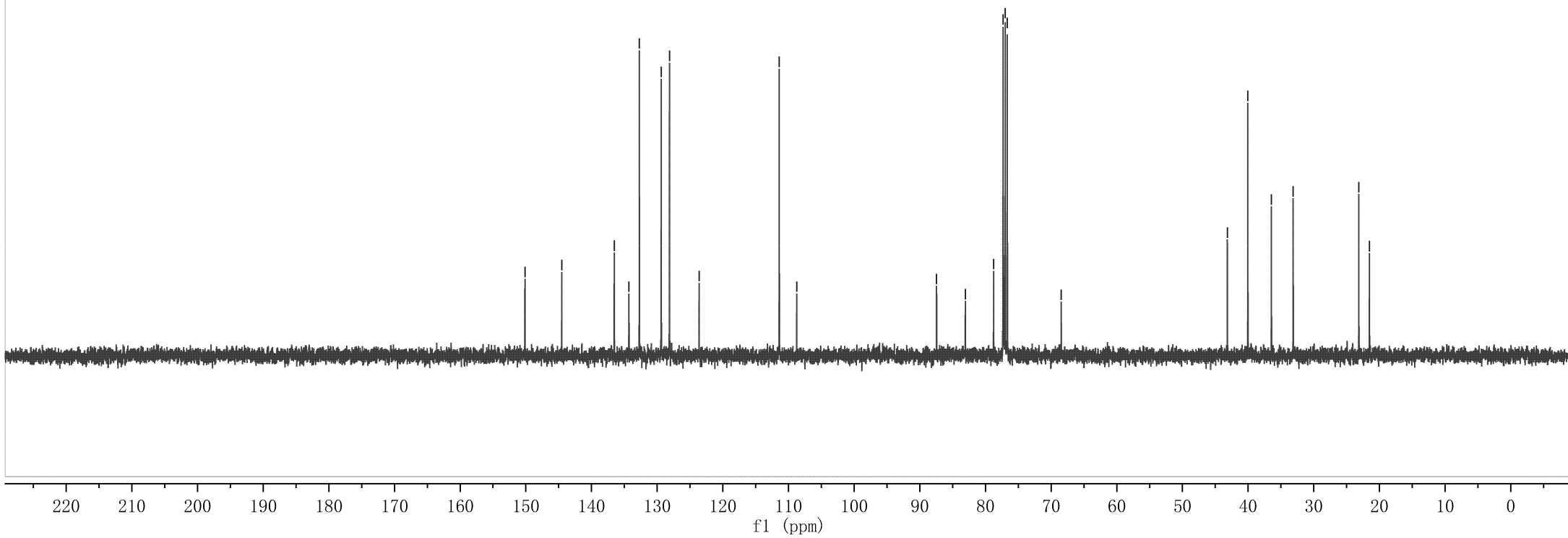
7.872  
7.851  
7.278  
7.258  
7.247  
7.060  
7.055  
7.043  
7.038  
6.550  
6.545  
6.533  
6.528  
5.950  
5.945  
5.940  
4.466  
2.942  
2.422  
2.416  
2.408  
2.403  
2.398  
2.385  
2.379  
2.365  
1.904  
1.891  
1.873  
1.862  
1.853  
1.835



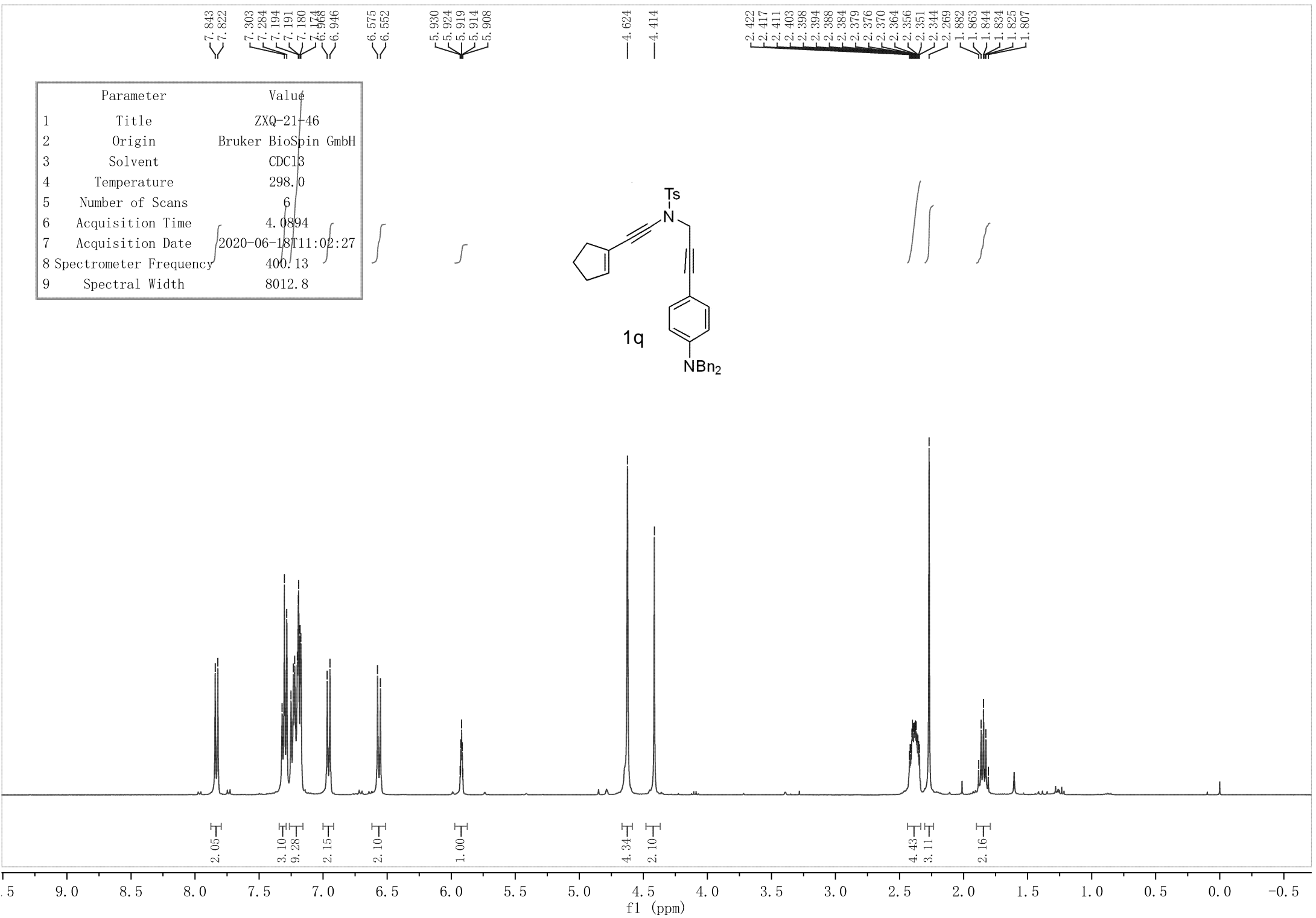
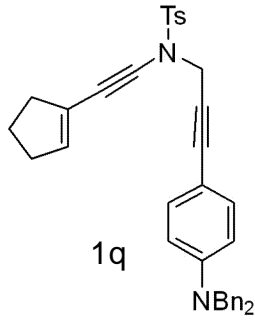
Parameter	Value
1 Title	ZXQ-19-161-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-25T16:33:25
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



150.14    144.52    136.54    134.30    132.71    129.38    128.12    123.61    111.41    108.74    87.44    83.07    78.76    77.32    77.00    76.68    68.46    43.17    40.05    36.45    33.14    23.14    21.53



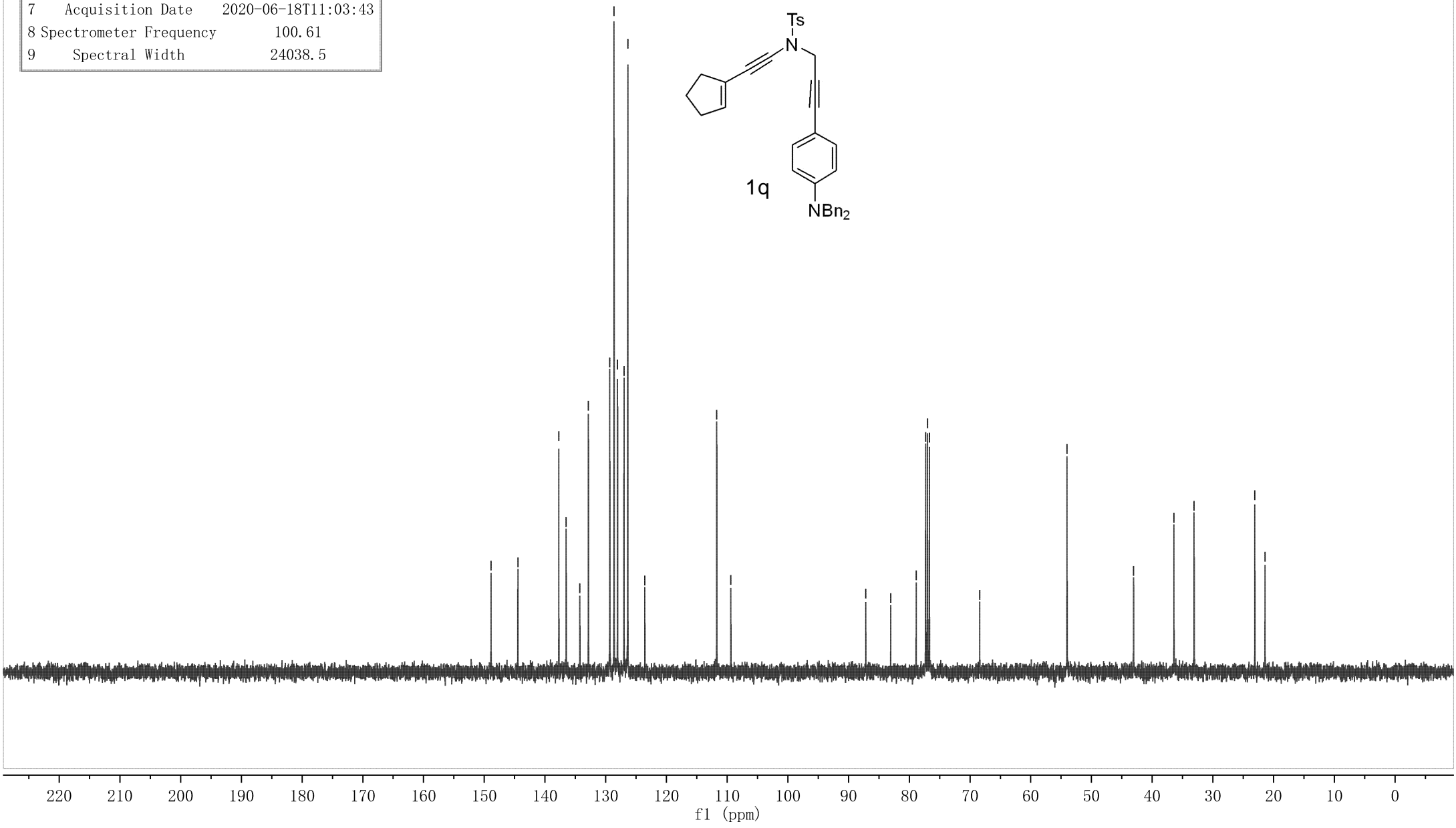
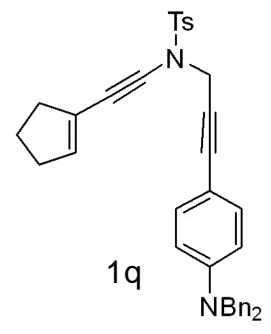
Parameter	Value
1 Title	ZXQ-21-46
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2020-06-18 11:02:27
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8





Parameter	Value
1 Title	ZXQ-21-46-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	10
6 Acquisition Time	1.3631
7 Acquisition Date	2020-06-18T11:03:43
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

- 148.88
- 144.46
- 137.71
- 136.51
- 134.26
- 132.84
- 129.32
- 128.62
- 128.05
- 126.99
- 126.35
- 123.55
- 111.71
- 109.39
- 87.16
- 83.05
- 78.87
- 77.32
- 77.00
- 76.68
- 68.40
- 54.03
- 43.06
- 36.41
- 33.09
- 23.09
- 21.42



Parameter	Value
1 Title	ZXQ-21-84
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.9
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-06-27T16:35:35
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

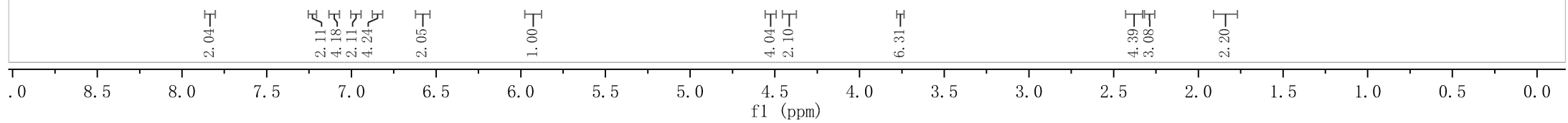
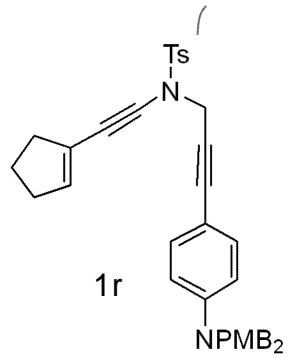
7.844  
7.824  
7.235  
7.214  
7.138  
7.103  
7.082  
6.975  
6.953  
6.854  
6.847  
6.826  
6.593  
6.570

5.932  
5.926  
5.921  
5.916  
5.910

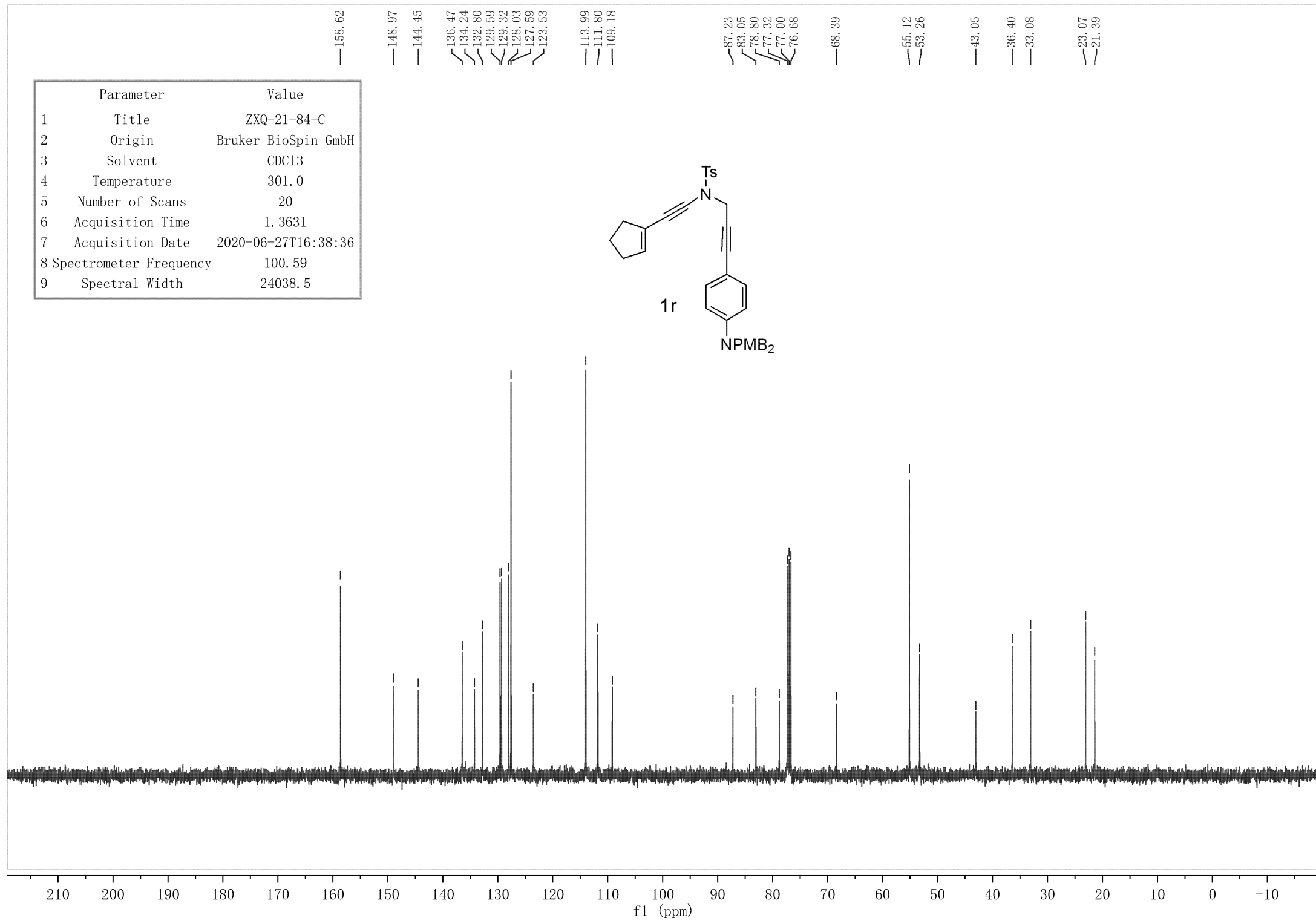
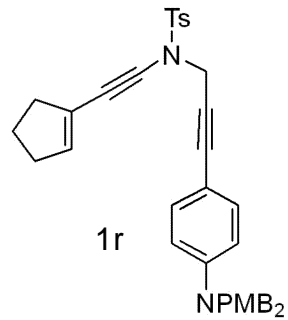
4.535  
4.421

3.751

2.425  
2.419  
2.414  
2.404  
2.400  
2.397  
2.391  
2.386  
2.379  
2.373  
2.367  
2.361  
2.354  
2.347  
2.286  
1.886  
1.866  
1.848  
1.829  
1.810



Parameter	Value
1 Title	ZXQ-21-84-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	301.0
5 Number of Scans	20
6 Acquisition Time	1.3631
7 Acquisition Date	2020-06-27T16:38:36
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



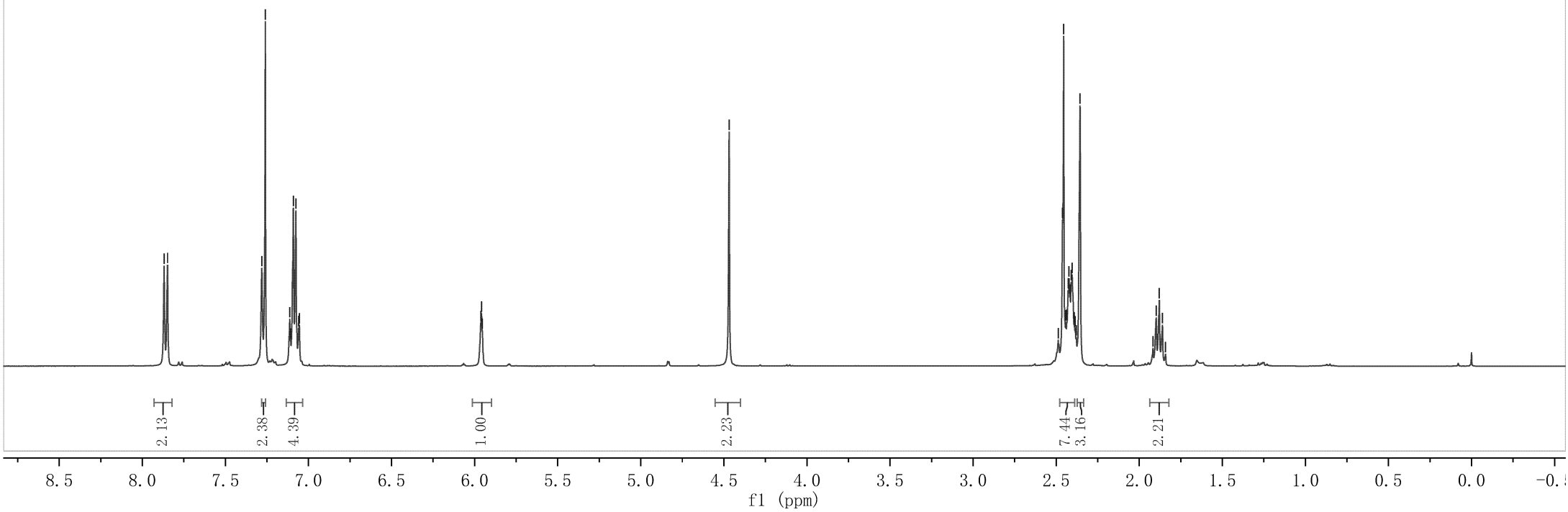
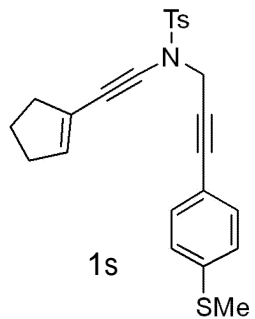
7.869  
7.848  
7.281  
7.260  
7.113  
7.108  
7.091  
7.076  
7.059  
7.055

5.963  
5.958  
5.954

4.468

2.488  
2.462  
2.455  
2.441  
2.436  
2.428  
2.422  
2.417  
2.409  
2.404  
2.391  
2.385  
2.379  
2.356  
1.917  
1.898  
1.879  
1.860  
1.842

Parameter	Value
1 Title	ZXQ-19-39
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-19T16:14:26
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



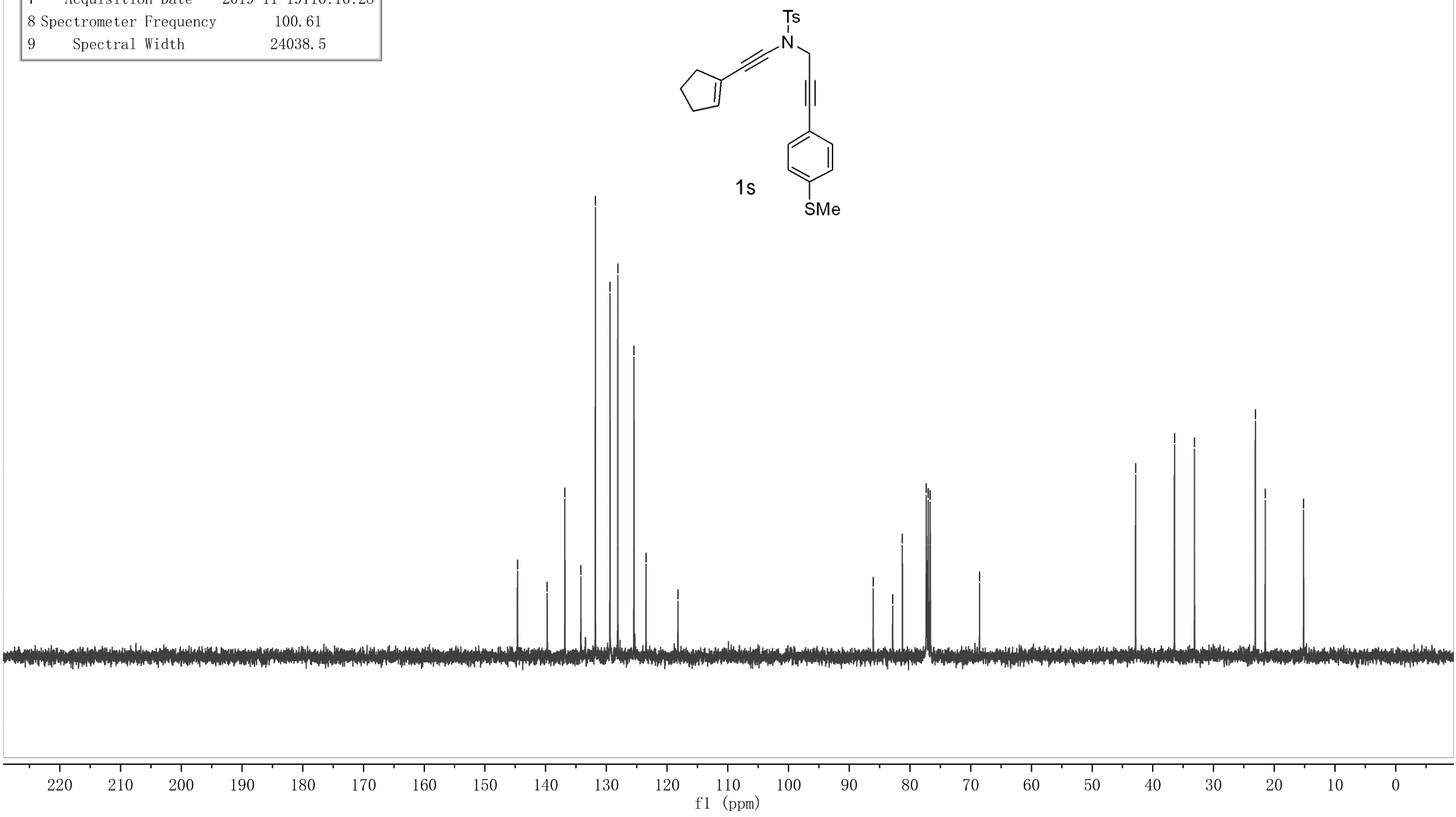
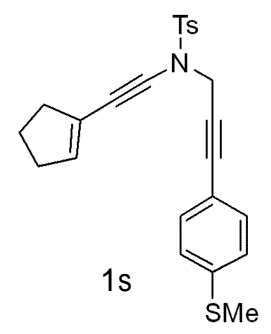
Parameter	Value
1 Title	ZXQ-19-39-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	29
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-19T16:16:28
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.64  
139.75  
136.84  
134.20  
131.82  
129.40  
128.12  
125.45  
123.47  
118.21

86.06  
82.86  
81.25  
77.32  
77.00  
76.68  
68.55

42.84  
36.44  
33.14

23.12  
21.49  
15.17



Parameter	Value
1 Title	ZXQ-18-225
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-06T11:26:18
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

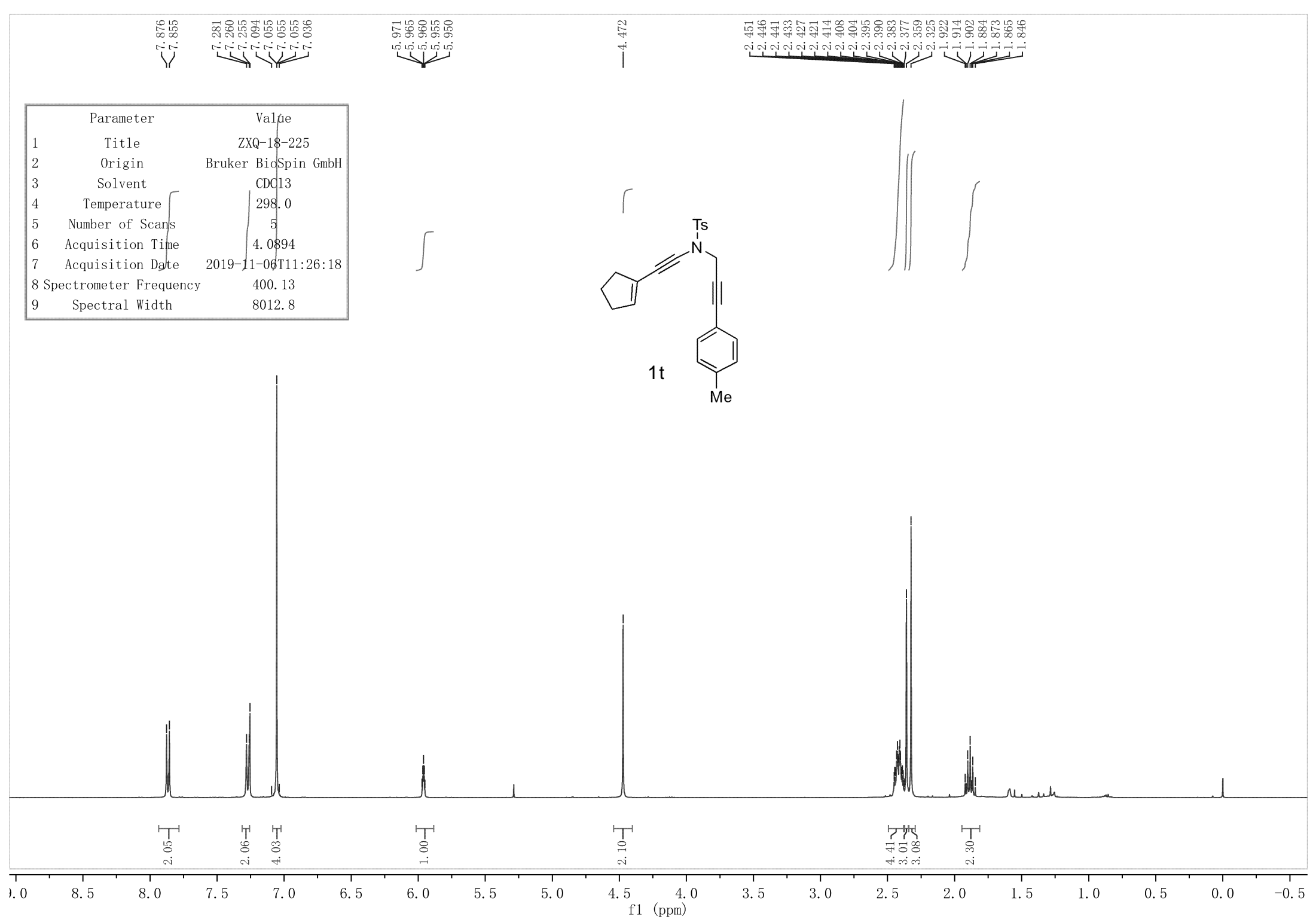
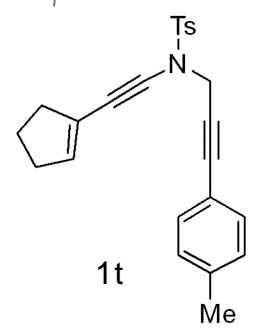
7.876  
7.855

7.281  
7.260  
7.255  
7.094  
7.055  
7.055  
7.036

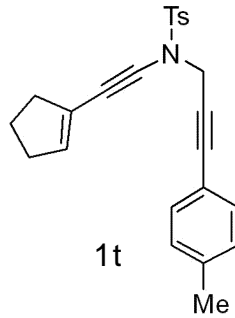
5.971  
5.965  
5.960  
5.955  
5.950

4.472

2.451  
2.446  
2.441  
2.433  
2.427  
2.421  
2.414  
2.408  
2.404  
2.395  
2.390  
2.383  
2.377  
2.359  
2.325  
1.922  
1.914  
1.902  
1.884  
1.873  
1.865  
1.846



Parameter	Value
1 Title	ZXQ-18-225-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	38
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-06T11:28:28
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

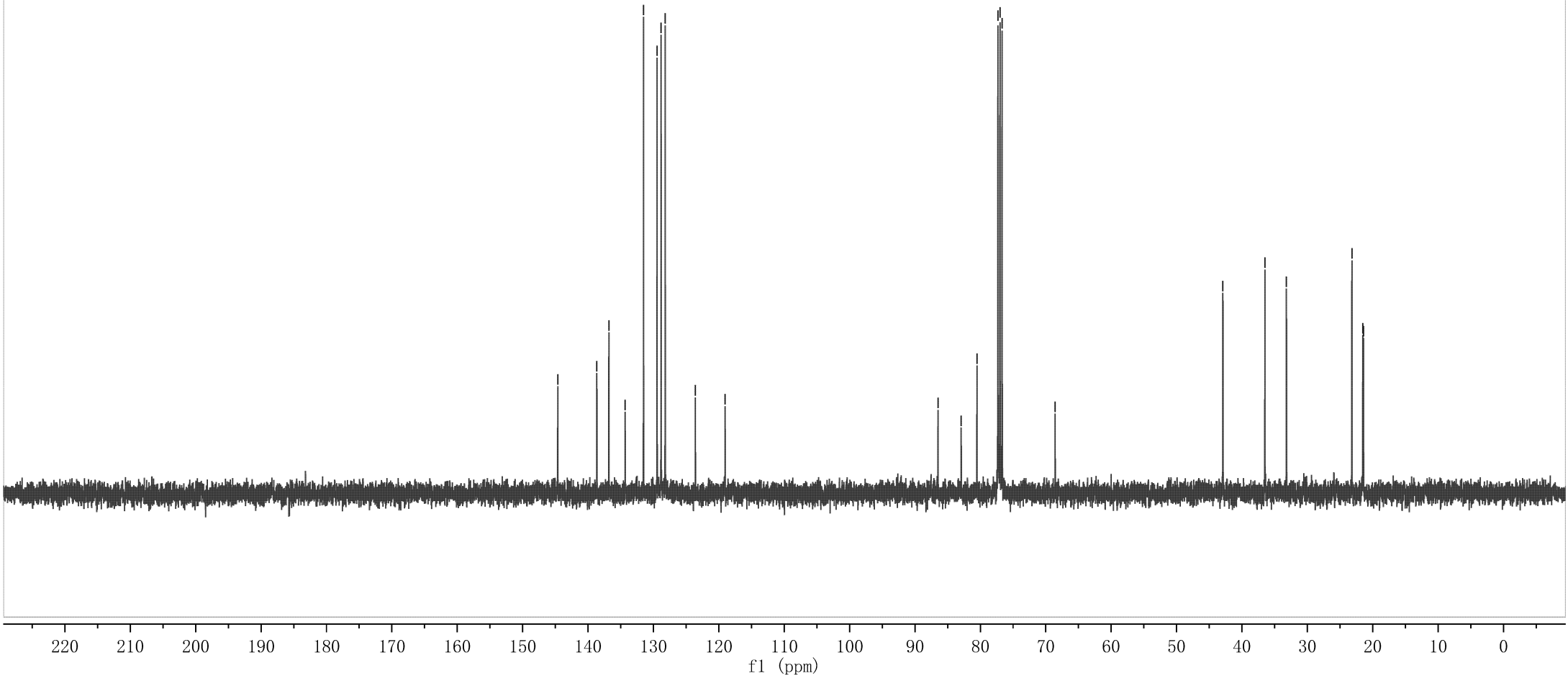


144.63  
138.65  
136.81  
134.32  
131.51  
129.45  
128.83  
128.20  
123.58  
119.03

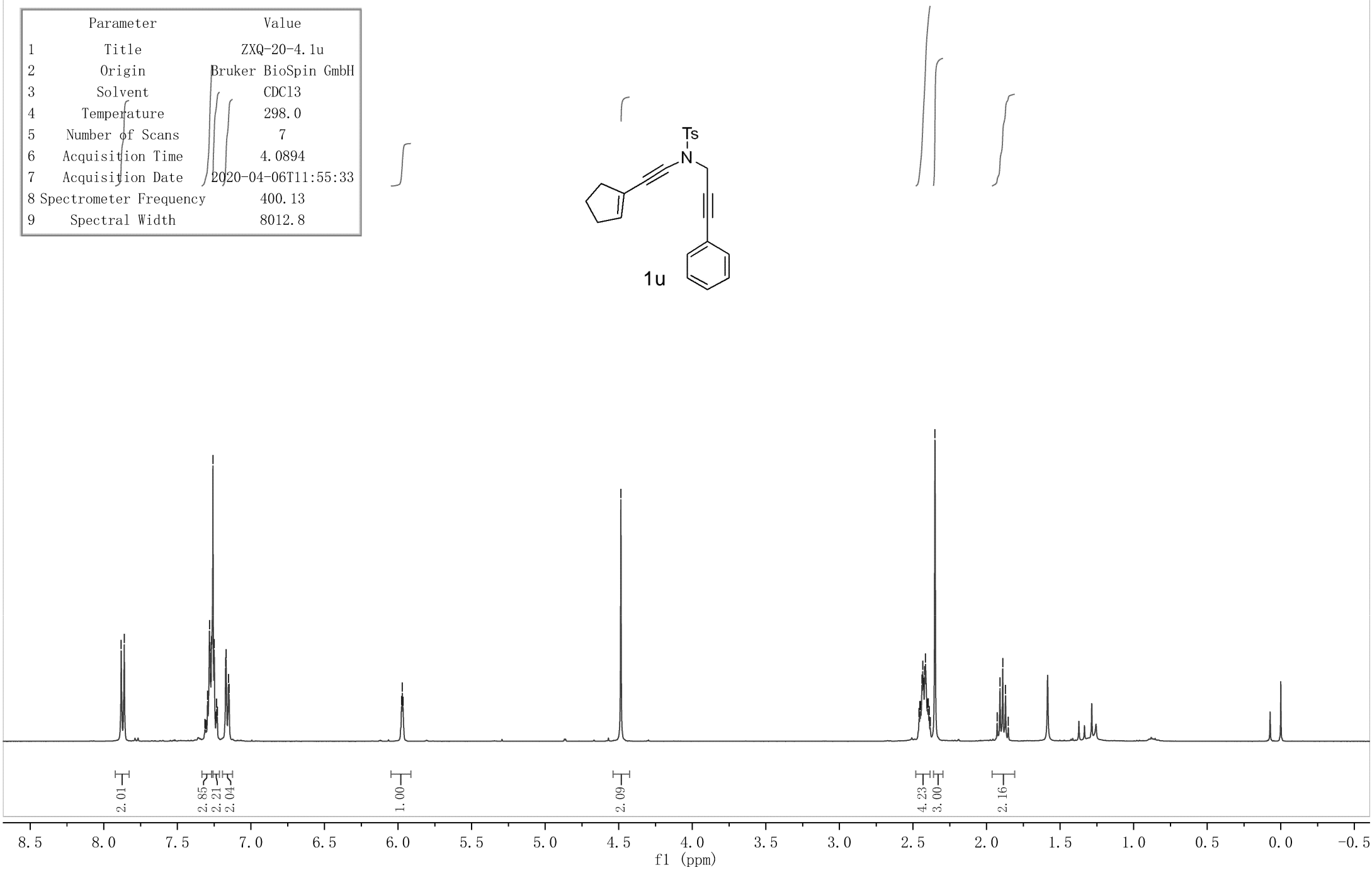
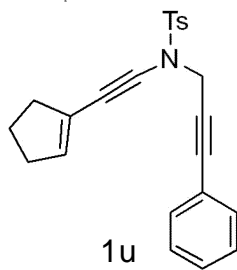
86.48  
82.93  
80.52  
77.32  
77.00  
76.68  
68.56

42.91  
36.49  
33.19

23.19  
21.53  
21.41



Parameter	Value
1 Title	ZXQ-20-4.1u
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2020-04-06T11:55:33
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8





Parameter	Value
1 Title	ZXQ-20-4. 1u-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	112
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-06T14:20:02
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

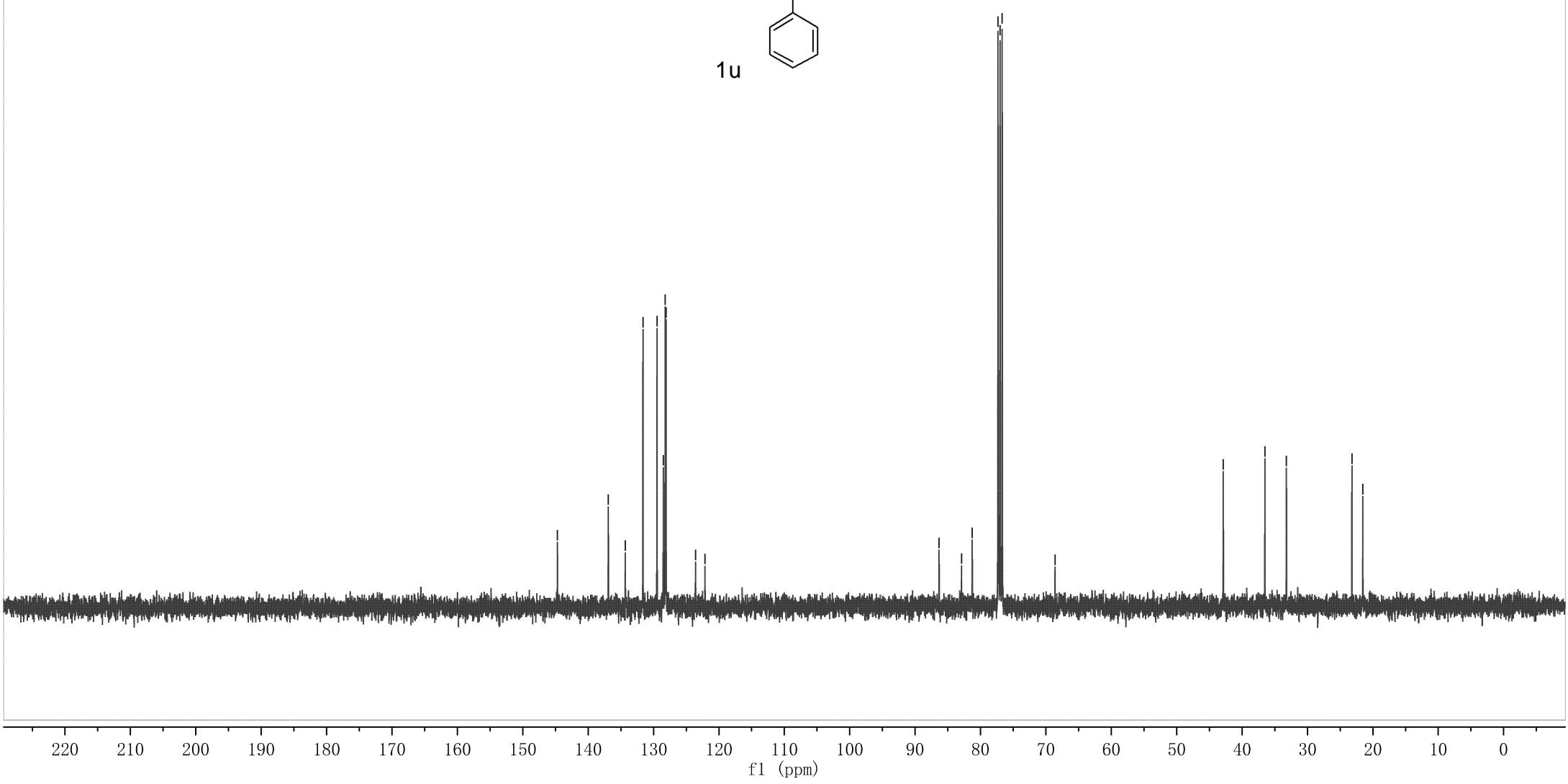
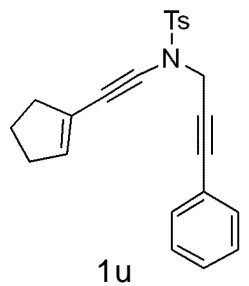
144.70  
136.92  
134.32  
131.62  
129.47  
128.51  
128.22  
128.09  
123.58  
122.13

86.33  
82.89  
81.26  
77.32  
77.00  
76.68

68.60

42.87  
36.51  
33.21

23.20  
21.53

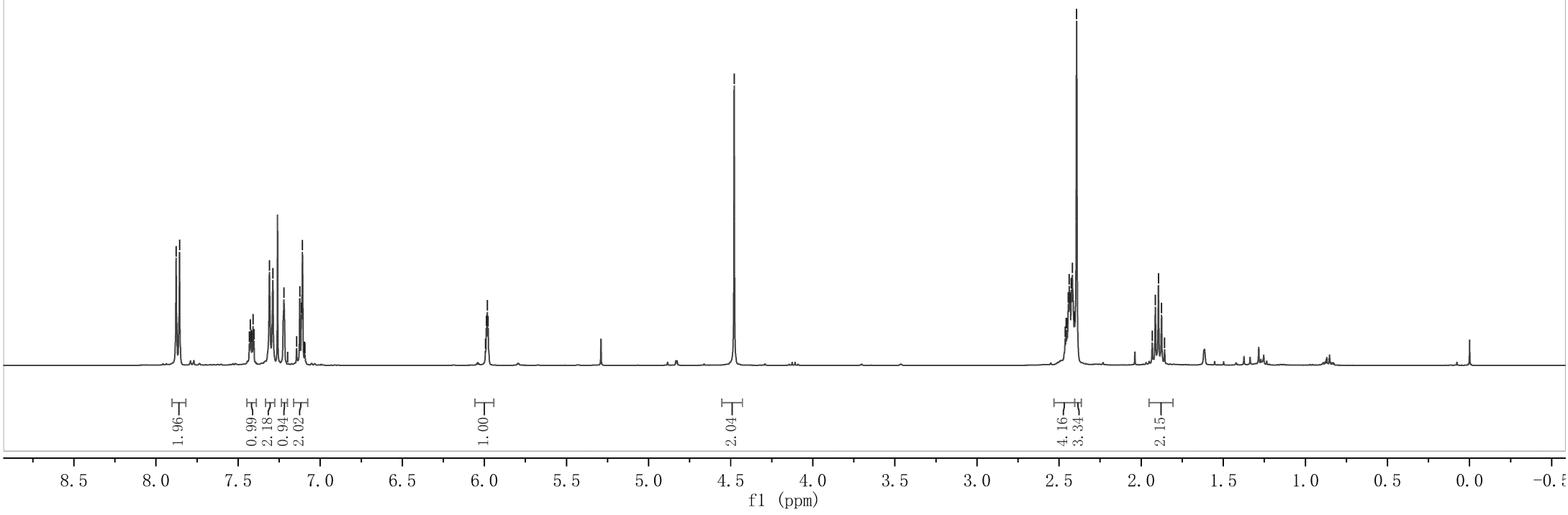
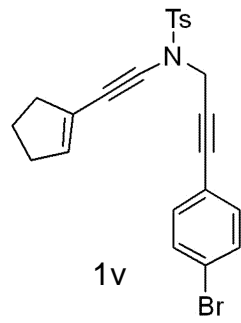


7.878  
7.857  
7.431  
7.431  
7.426  
7.420  
7.415  
7.409  
7.404  
7.309  
7.289  
7.221  
7.221  
7.144  
7.125  
7.115  
7.108  
5.994  
5.994  
5.982  
5.977

4.479

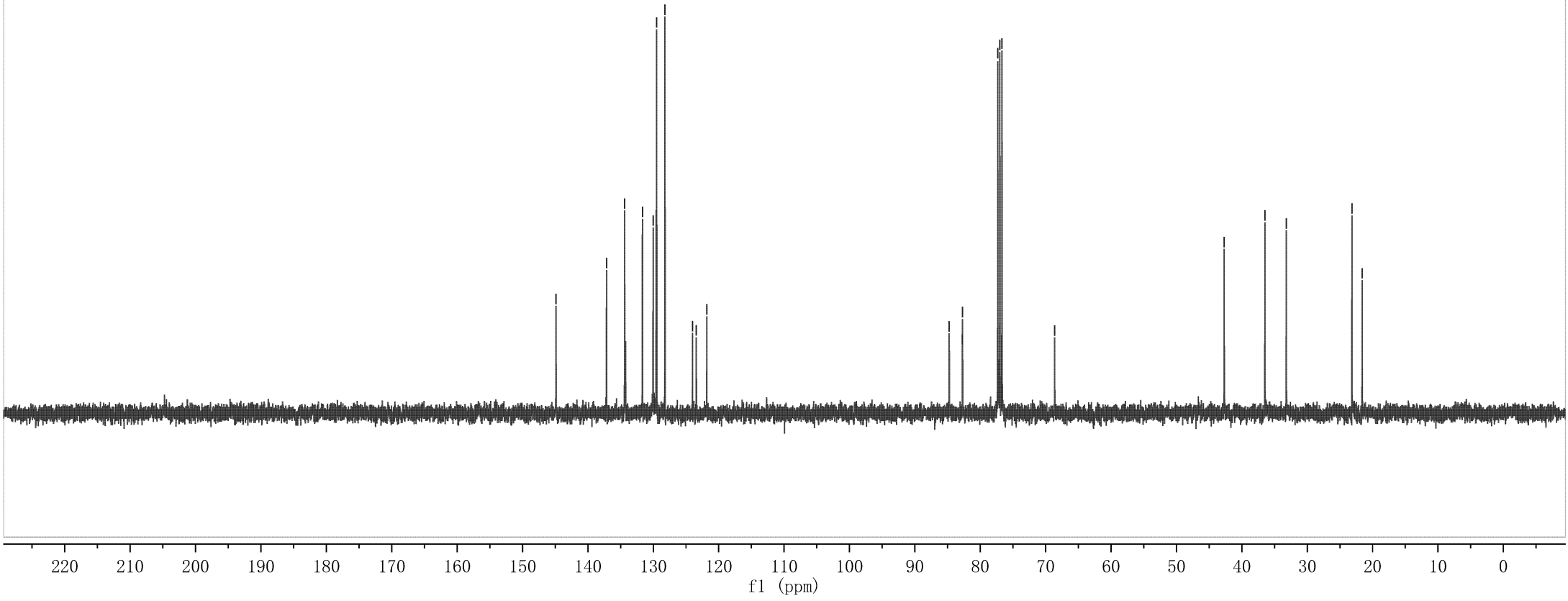
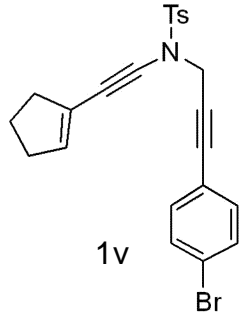
2.463  
2.457  
2.452  
2.444  
2.438  
2.433  
2.425  
2.419  
2.406  
2.393  
1.933  
1.913  
1.895  
1.876  
1.857

Parameter	Value
1 Title	ZXQ-19-10
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-12T11:31:46
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-10-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	25
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-12T11:33:12
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.88  
 137.15  
 134.38  
 131.65  
 130.03  
 129.48  
 128.21  
 124.00  
 123.43  
 121.82  
 84.74  
 82.75  
 82.71  
 77.32  
 77.00  
 76.68  
 68.62  
 42.70  
 36.48  
 33.20  
 23.16  
 21.61



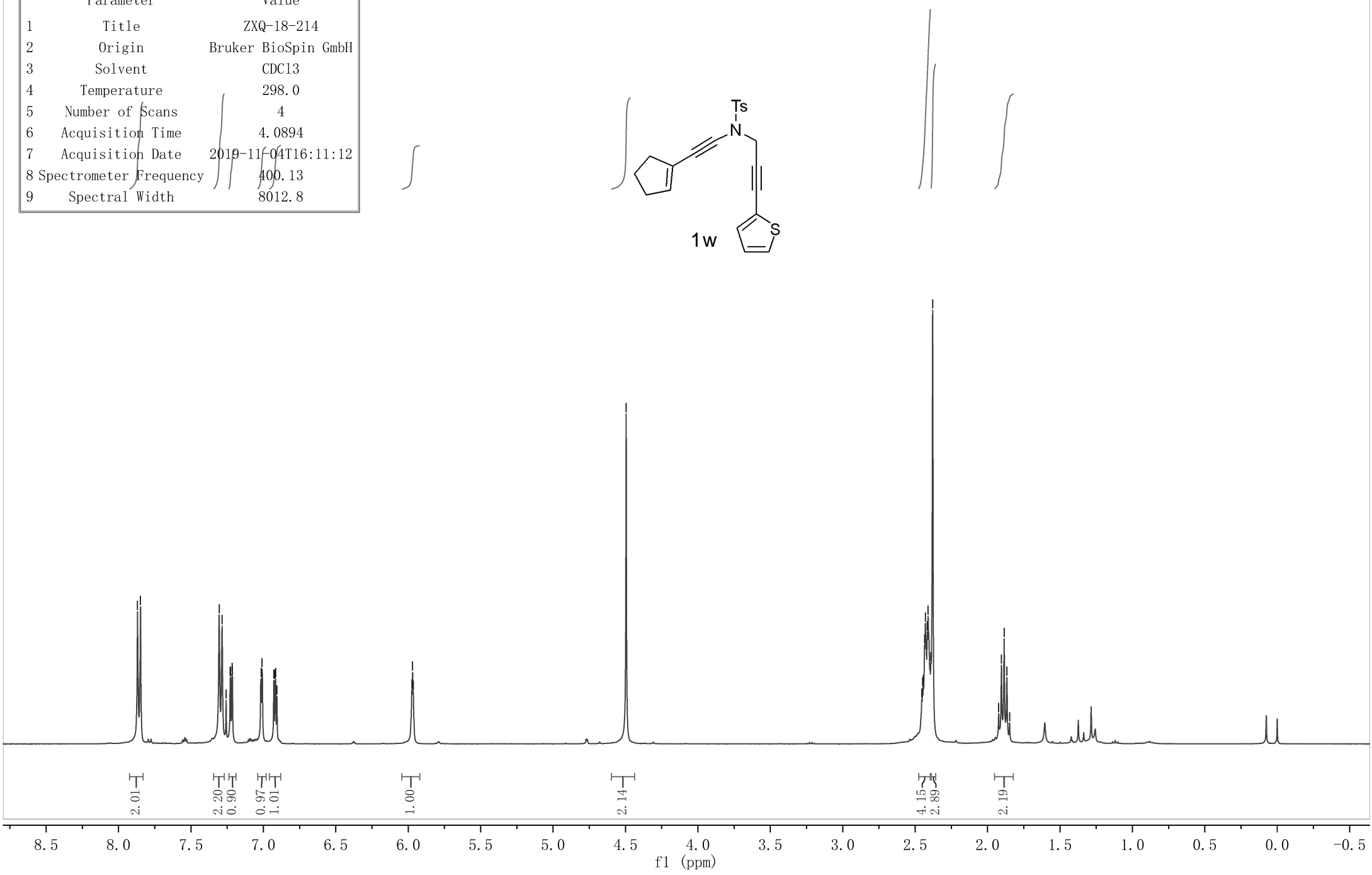
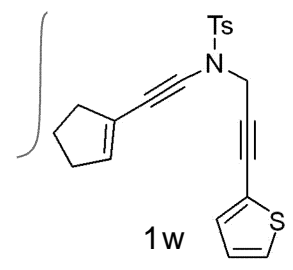
Parameter	Value
1 Title	ZXQ-18-214
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-04T16:11:12
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

7.869  
7.848  
7.305  
7.285  
7.227  
7.216  
7.214  
7.014  
7.009  
6.928  
6.919  
6.919  
6.915  
6.906

5.975  
5.970  
5.965

4.495

2.454  
2.449  
2.443  
2.435  
2.429  
2.416  
2.411  
2.391  
2.379  
1.923  
1.904  
1.885  
1.866  
1.848

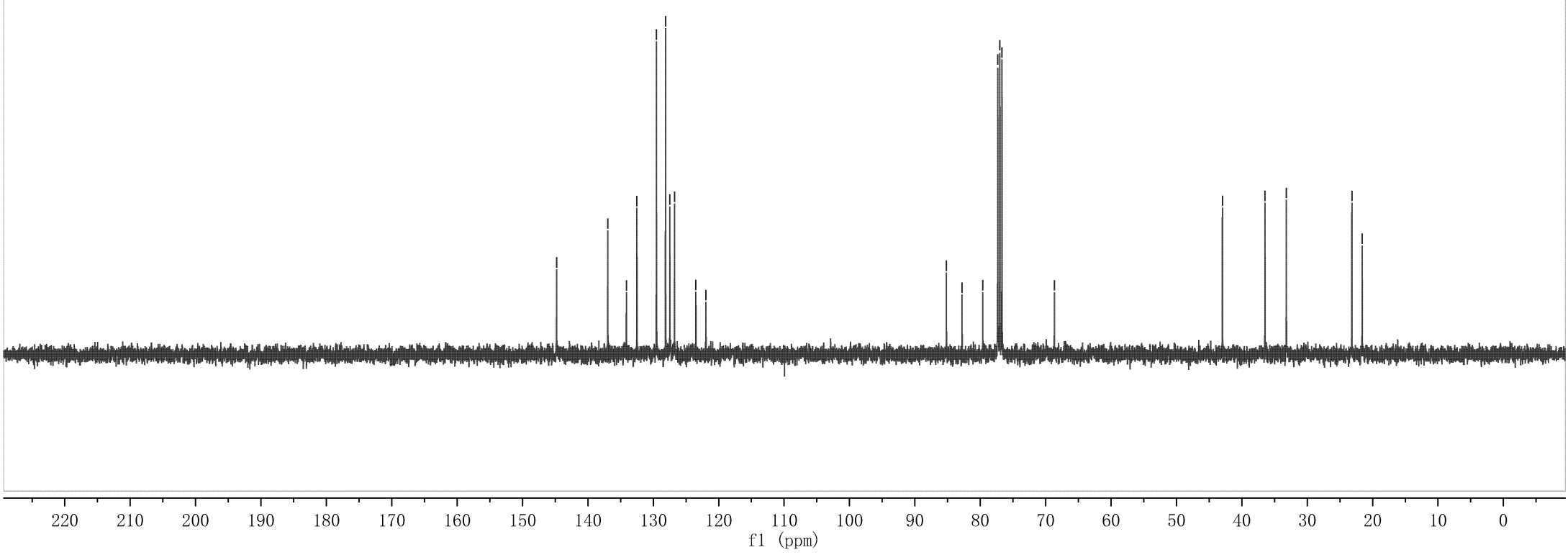
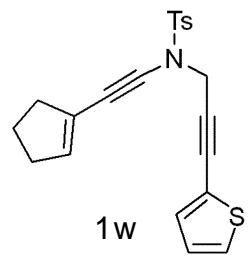


Parameter	Value
1 Title	ZXQ-18-214-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	27
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-04T16:13:37
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.79  
136.97  
134.12  
132.51  
129.52  
128.12  
127.48  
126.76  
123.49  
121.95

85.18  
82.79  
79.61  
77.32  
77.00  
76.68  
68.67

42.97  
36.46  
33.19  
23.17  
21.60



Parameter	Value
1 Title	ZXQ-18-210
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-02T17:37:29
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

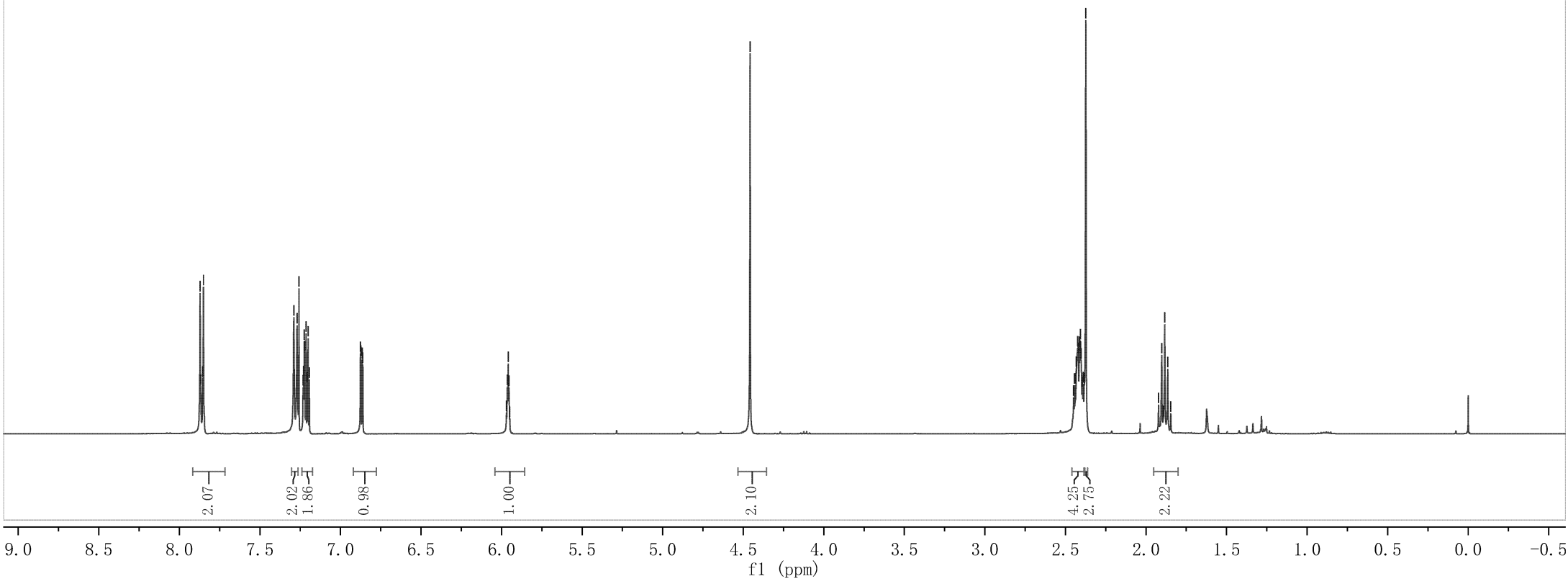
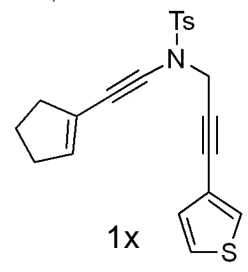
7.871  
7.867  
7.855  
7.850

7.290  
7.270  
7.258  
7.213  
7.201  
7.201  
6.873  
6.873  
6.864  
6.861  
6.861

5.970  
5.964  
5.959  
5.954  
5.949

4.458

2.449  
2.444  
2.439  
2.433  
2.424  
2.421  
2.414  
2.411  
2.408  
2.406  
2.403  
2.395  
2.390  
2.383  
2.373  
1.922  
1.902  
1.902  
1.892  
1.884  
1.865  
1.846

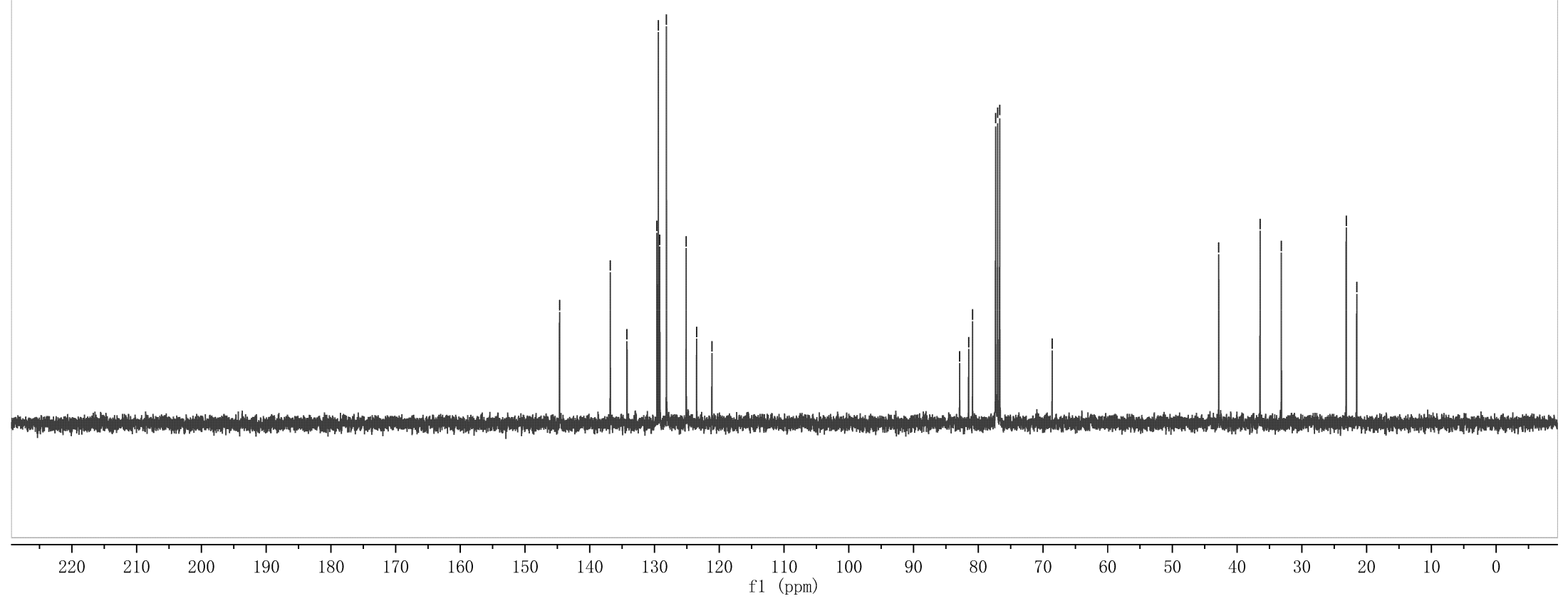
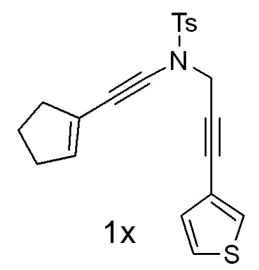


Parameter	Value
1 Title	ZXQ-18-210-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	21
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-02T17:41:29
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.67  
136.84  
134.25  
129.64  
129.41  
129.19  
128.16  
125.12  
123.51  
121.14

82.87  
81.48  
80.87  
77.32  
77.00  
76.68  
68.58

42.85  
36.46  
33.17  
23.16  
21.53



Parameter	Value
1 Title	ZXQ-19-38
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-19T21:29:36
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

7.862  
7.842

7.401  
7.379  
7.372  
7.352  
7.352

6.846  
6.825

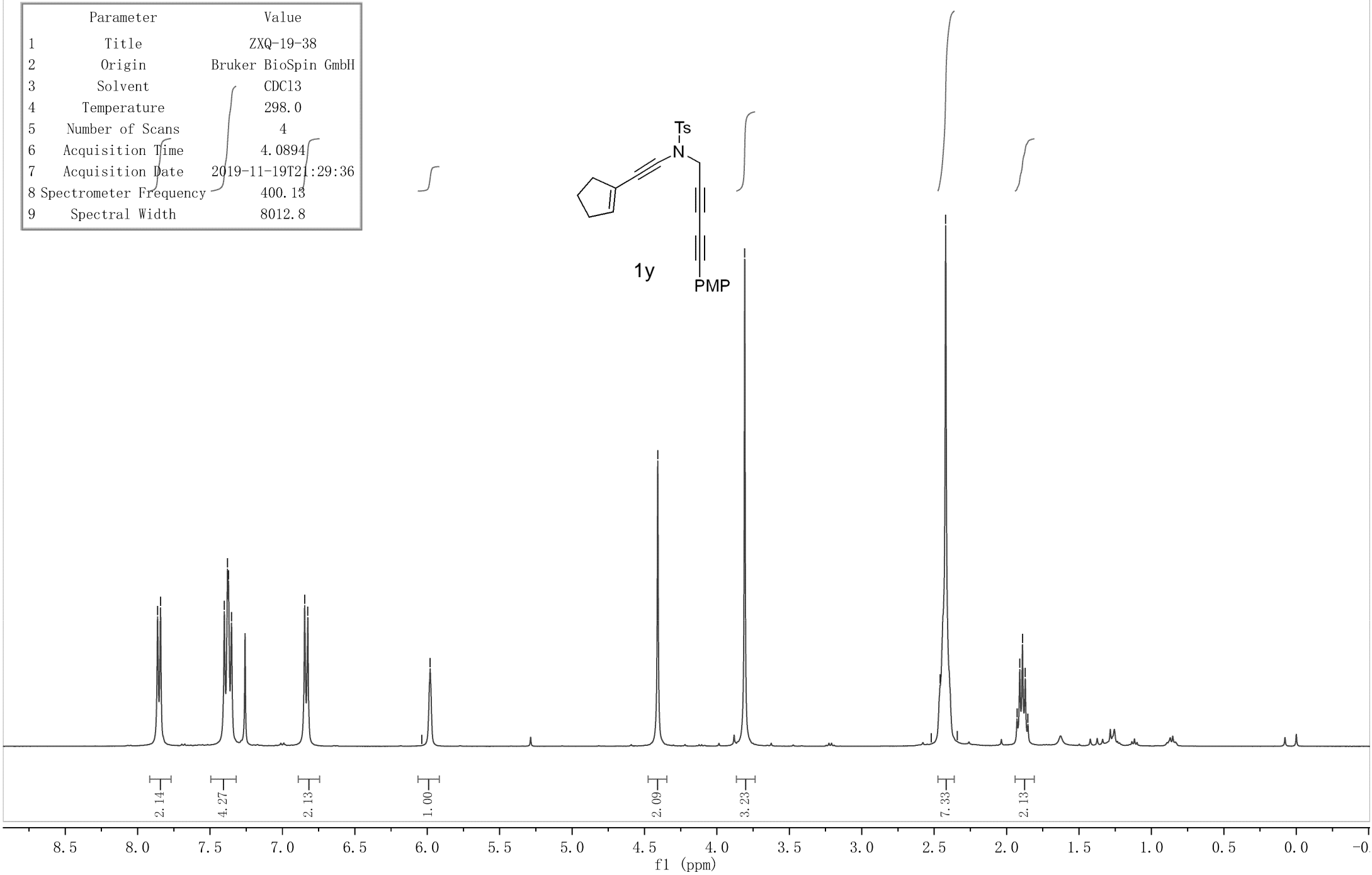
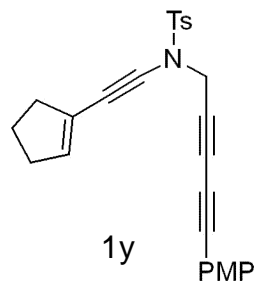
6.037  
5.980  
5.980  
5.980

4.408

3.808

2.520  
2.459  
2.421

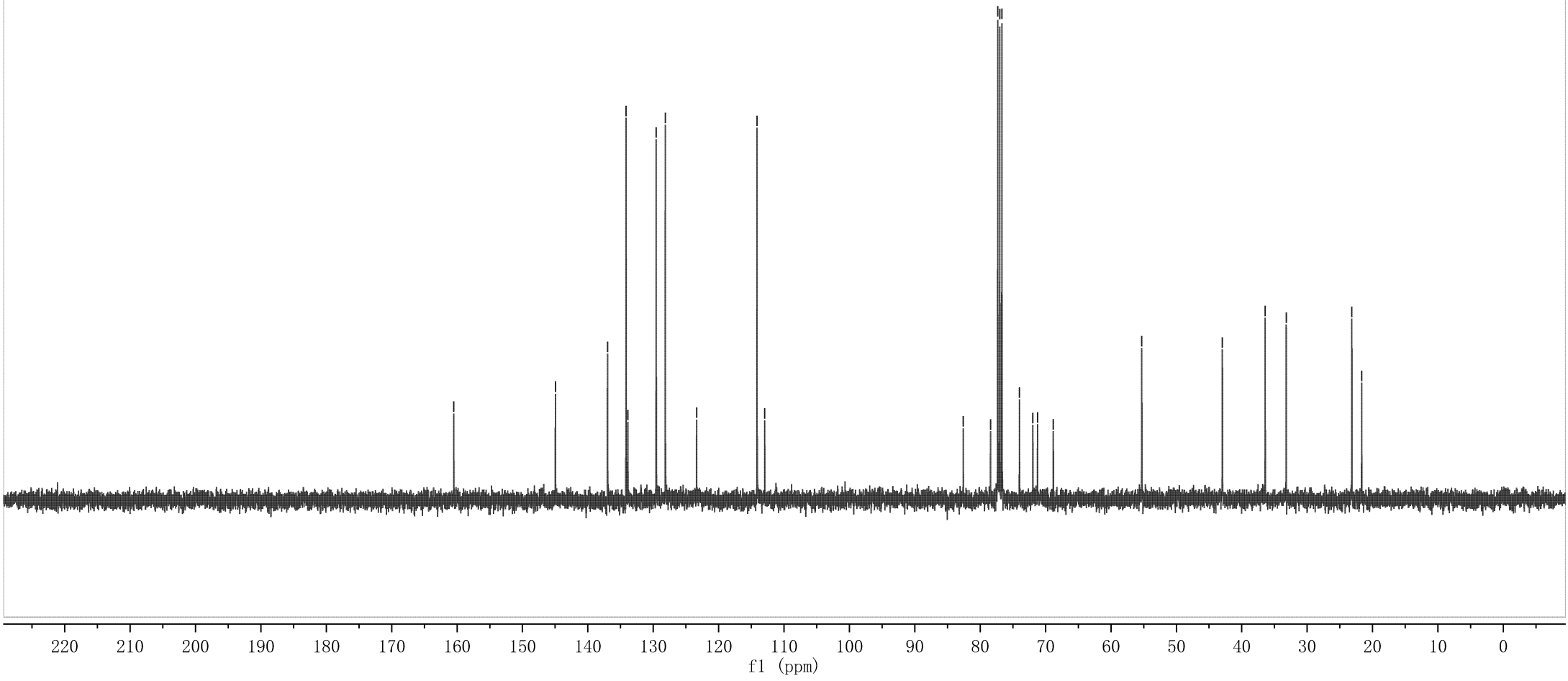
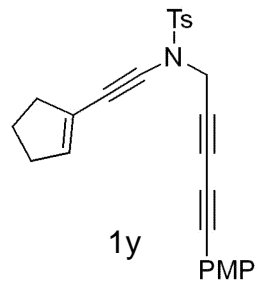
2.340  
1.928  
1.909  
1.890  
1.871  
1.853





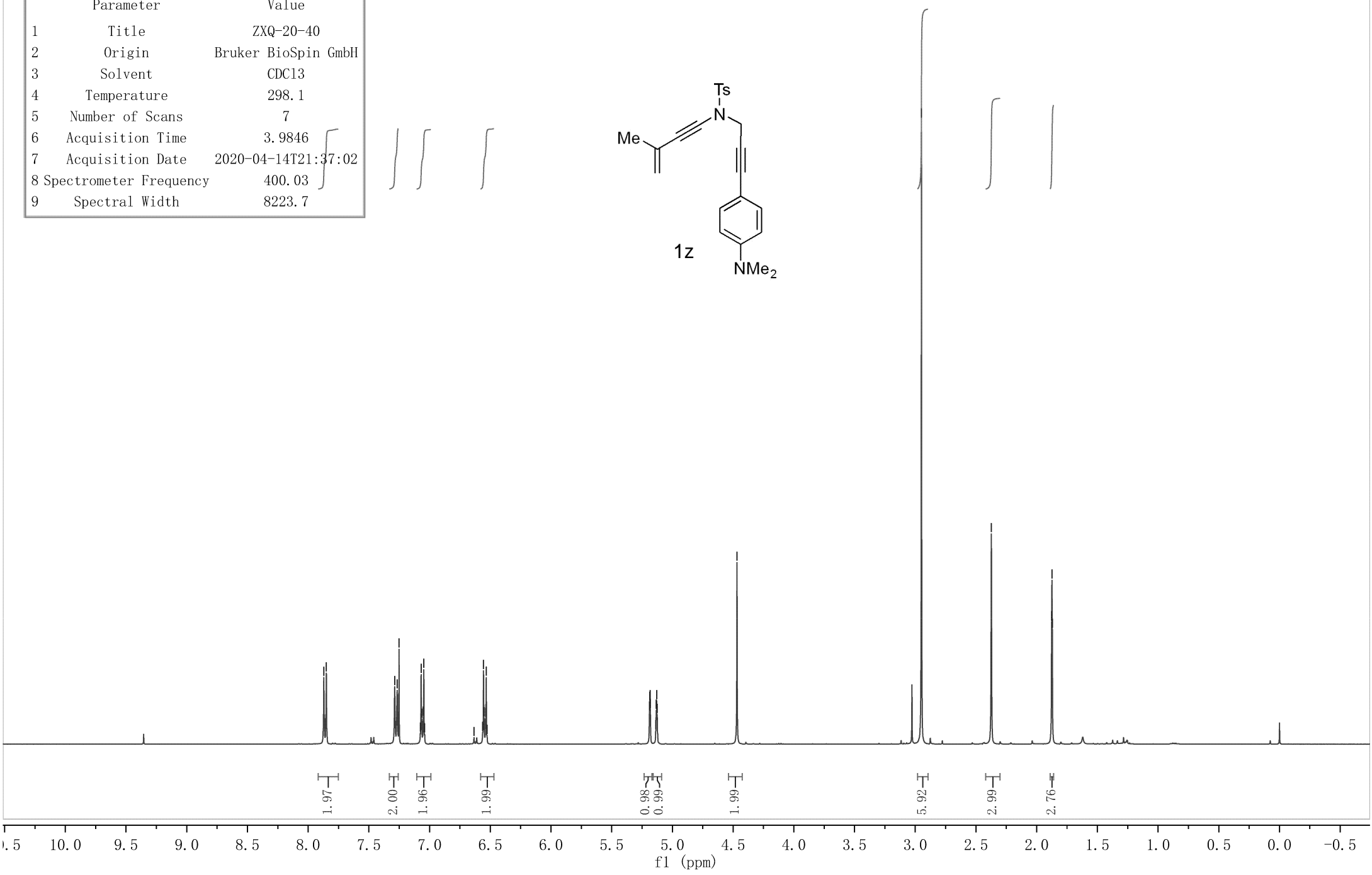
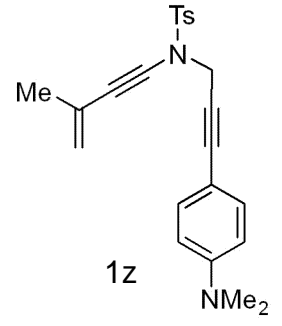
Parameter	Value
1 Title	ZXQ-19-38-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	30
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-19T21:31:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

160.51 —  
 144.96 —  
 137.00 —  
 134.16 —  
 133.89 —  
 129.55 —  
 128.16 —  
 123.37 —  
 114.13 —  
 112.95 —  
 82.60 —  
 78.42 —  
 77.32 —  
 77.00 —  
 76.68 —  
 74.00 —  
 71.95 —  
 71.23 —  
 68.82 —  
 55.29 —  
 42.96 —  
 36.42 —  
 33.20 —  
 23.17 —  
 21.66 —



7.871 7.850 7.287 7.267 7.251 7.076 7.070 7.065 7.052 6.834 6.834 6.562 6.556 6.551 6.538 6.533 6.527 5.189 5.186 5.184 5.182 5.137 5.134 5.129 5.125 4.468 2.949 2.373 1.877 1.874 1.871

Parameter	Value
1 Title	ZXQ-20-40
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-14T21:37:02
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

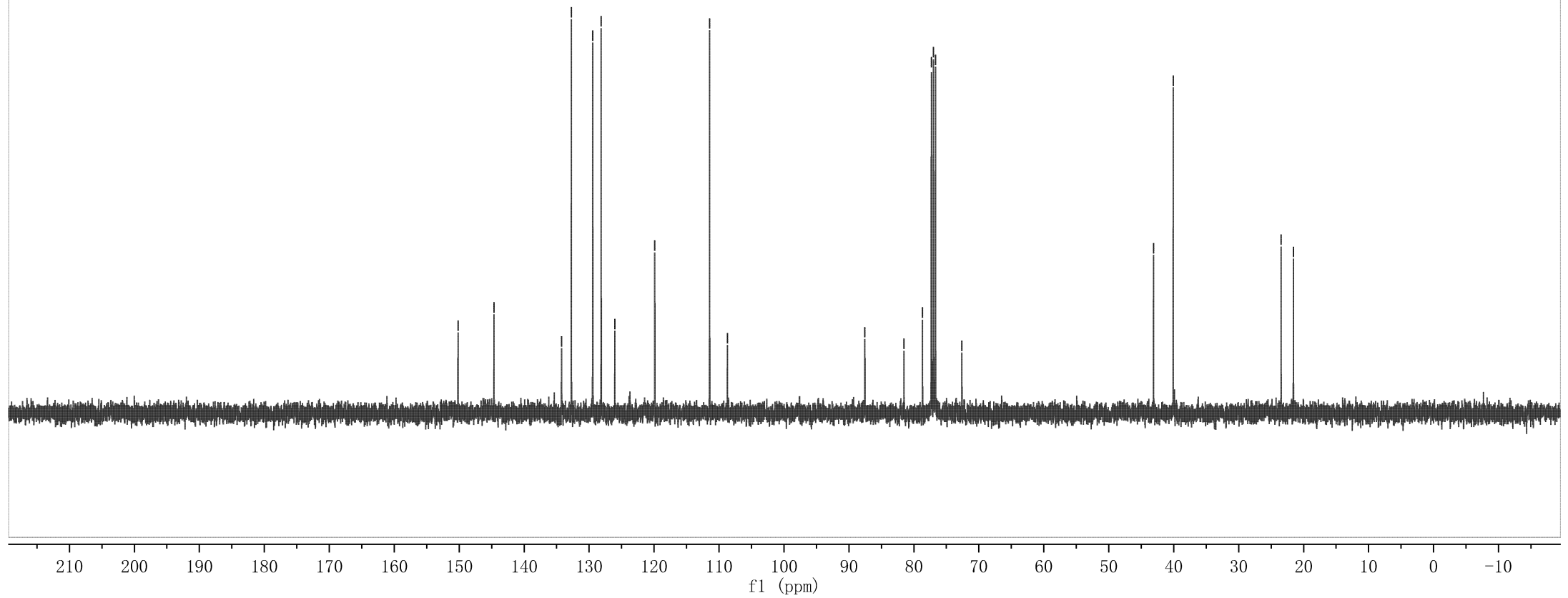
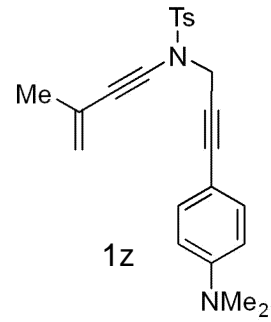


10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

Parameter	Value
1 Title	ZXQ-20-40
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-14T21:37:02
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

150.18 144.64 134.25 132.74 129.44 128.14 126.04 119.89 111.45 108.71 87.55 81.54 78.68 77.32 77.00 76.68 72.61 43.11 40.08 23.47 21.57



7.870  
7.866  
7.853  
7.849

7.277  
7.257

7.053  
7.036  
6.939  
6.937  
6.550  
6.545  
6.532  
6.527  
6.521

5.878  
5.874  
5.870  
5.864  
5.860  
5.856  
5.853  
5.846  
5.842  
5.839  
5.835  
5.828  
5.825  
5.821

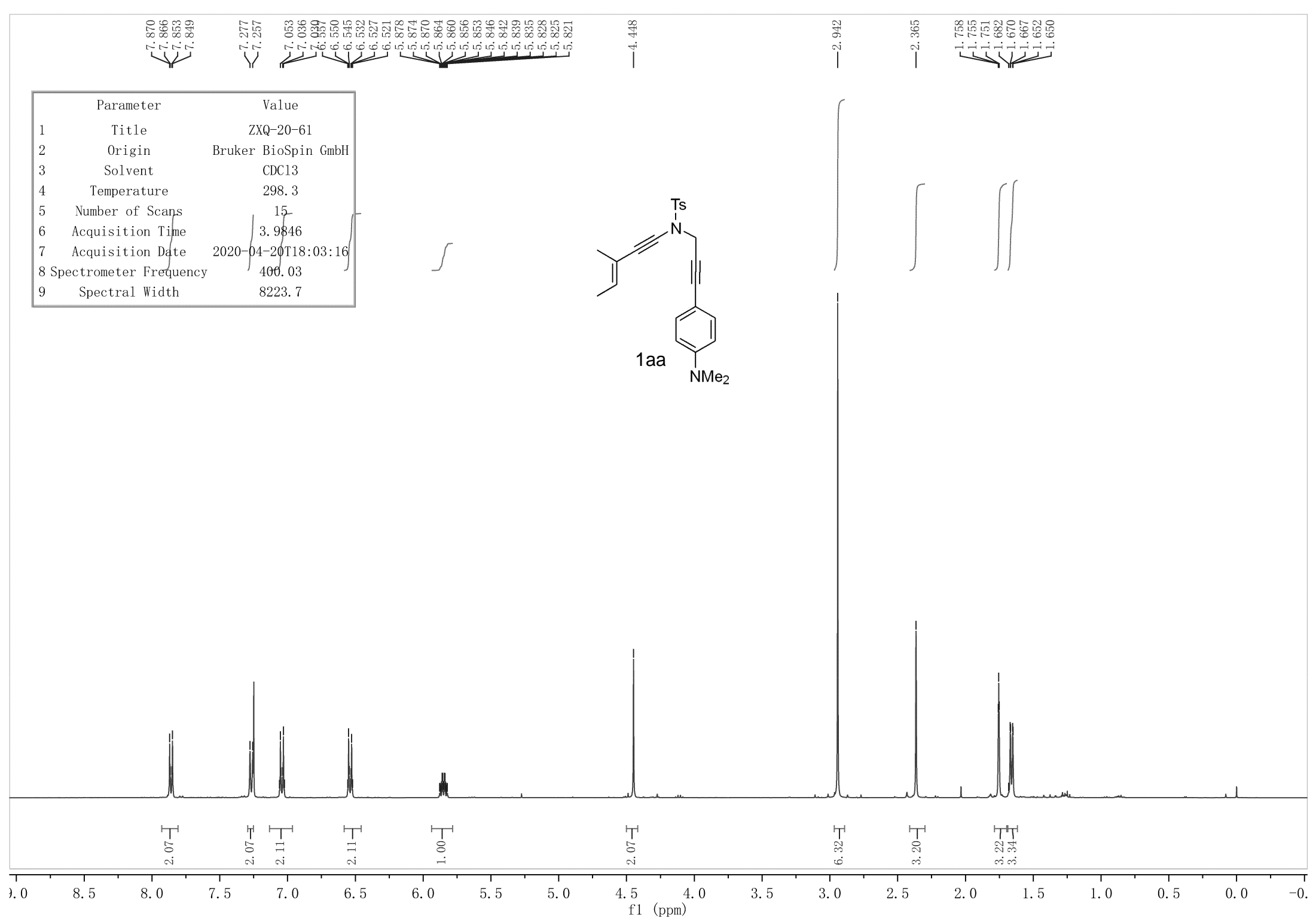
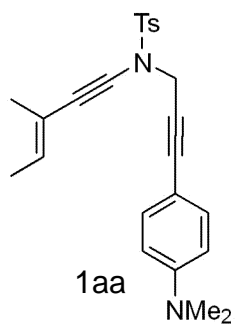
4.448

2.942

2.365

1.758  
1.755  
1.751  
1.682  
1.670  
1.667  
1.652  
1.650

Parameter	Value
1 Title	ZXQ-20-61
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.3
5 Number of Scans	15
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-20T18:03:16
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

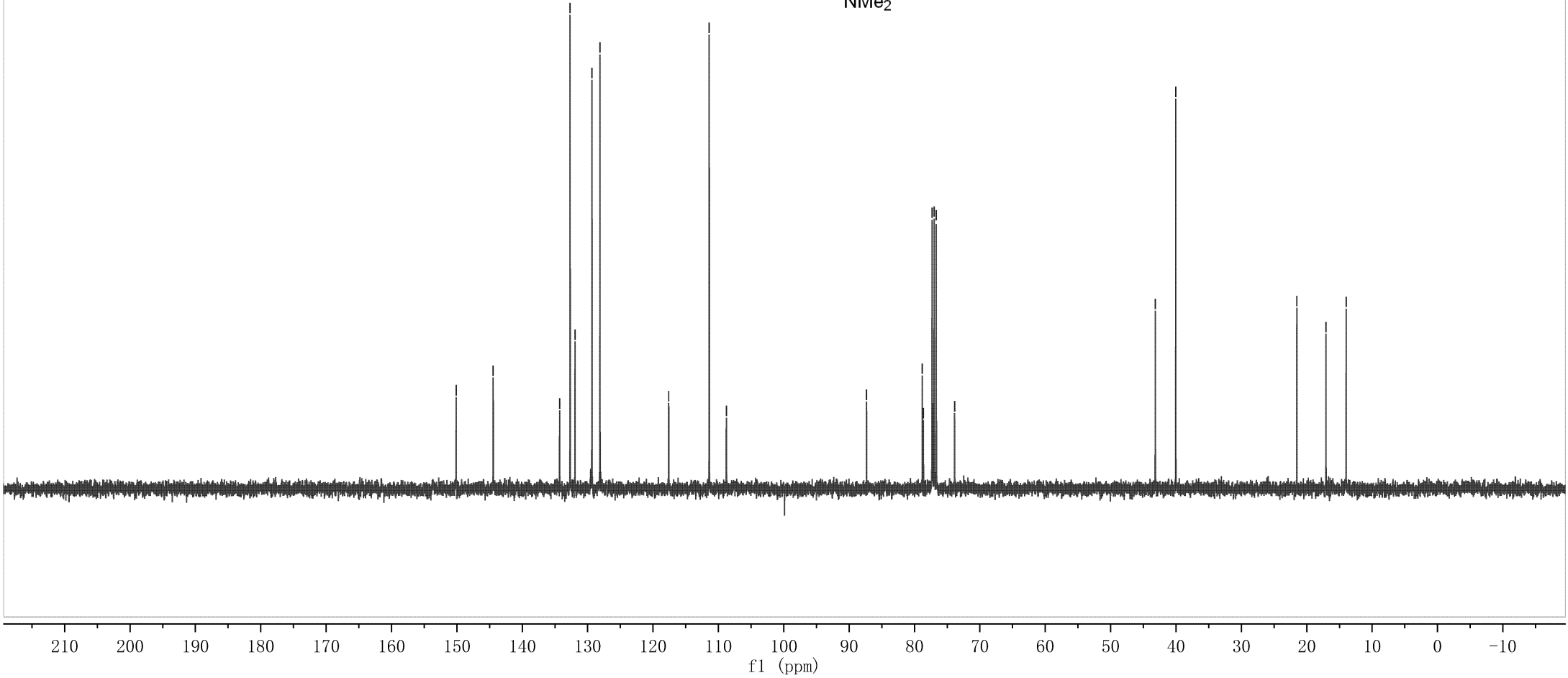
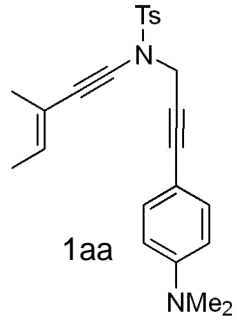


9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

Parameter	Value
1 Title	ZXQ-20-61-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.7
5 Number of Scans	27
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-20T18:06:30
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

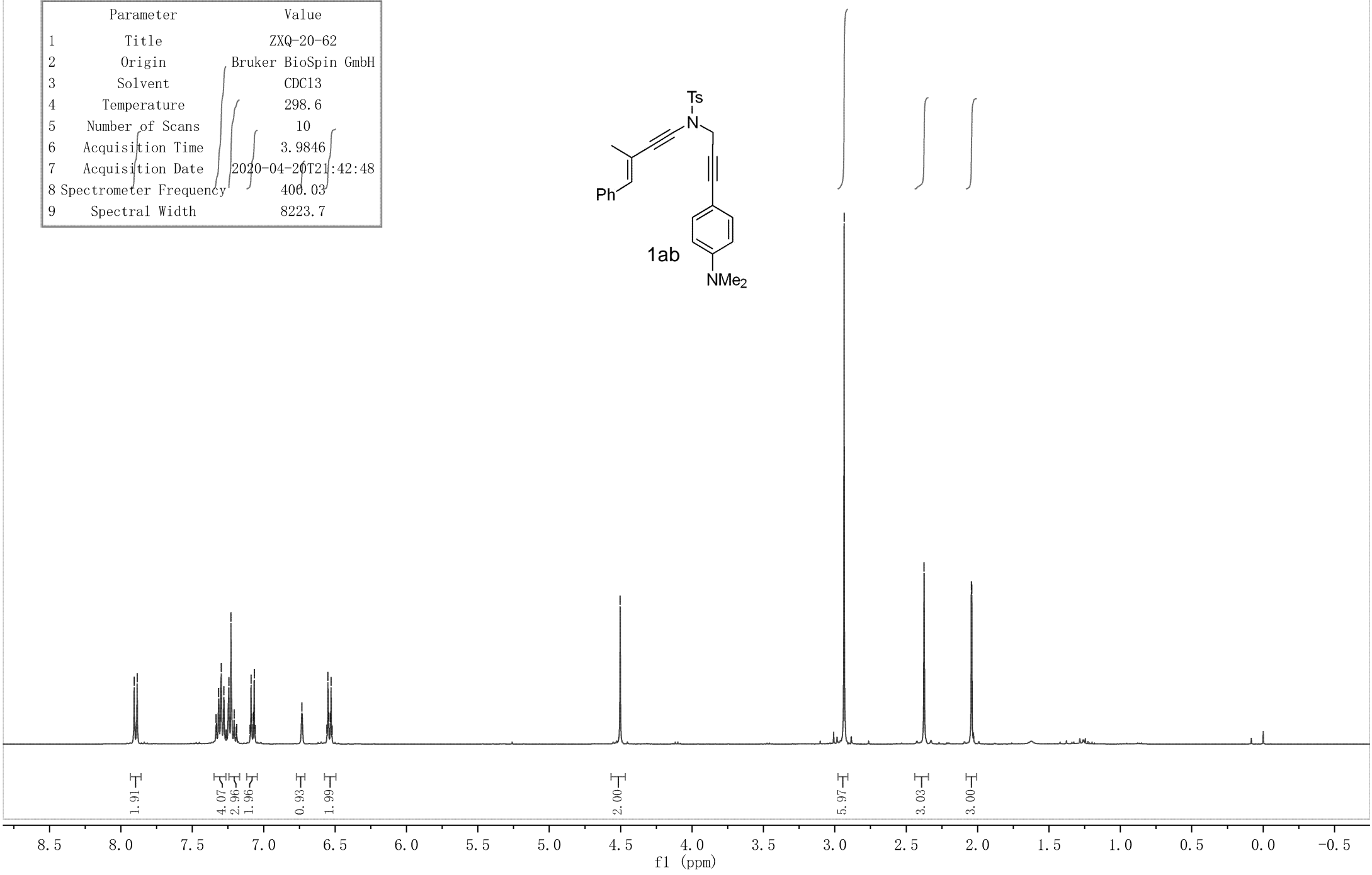
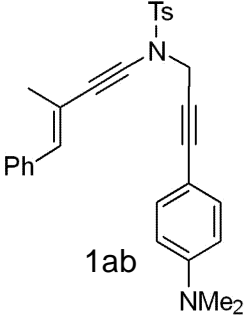
150.11 144.45 134.29 132.69 131.93 129.34 128.12 117.60 111.40 108.79 87.33 78.81 78.64 77.32 77.00 76.68 73.87 43.17 40.04 21.52 17.07 13.97



7.907  
7.886  
7.315  
7.297  
7.279  
7.244  
7.229  
7.207  
7.089  
7.071  
6.966  
6.732  
6.557  
6.551  
6.546  
6.533  
6.528  
6.521

4.503  
2.935  
2.375  
2.044  
2.040

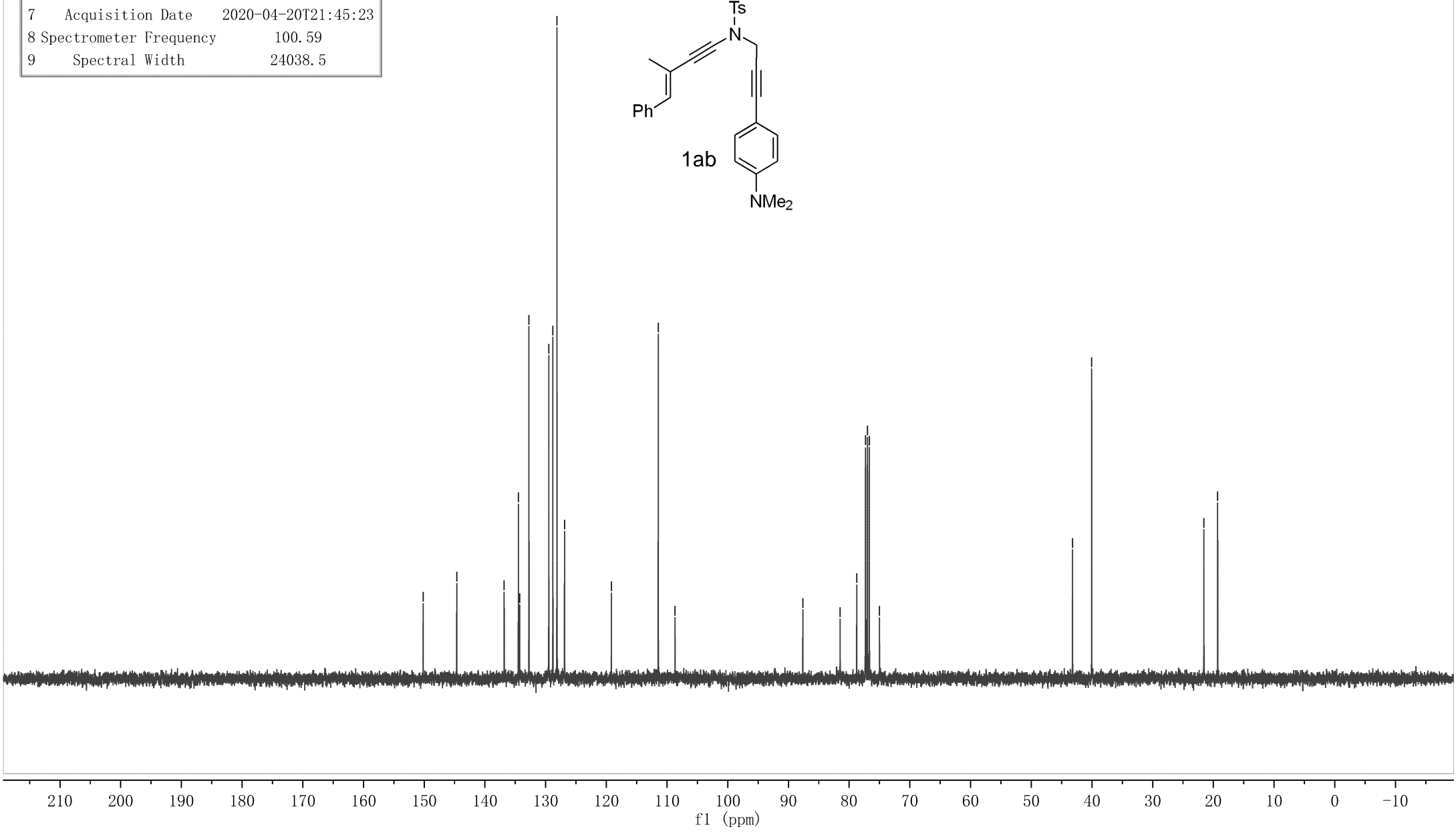
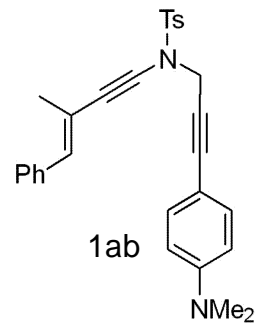
Parameter	Value
1 Title	ZXQ-20-62
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.6
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-20T21:42:48
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



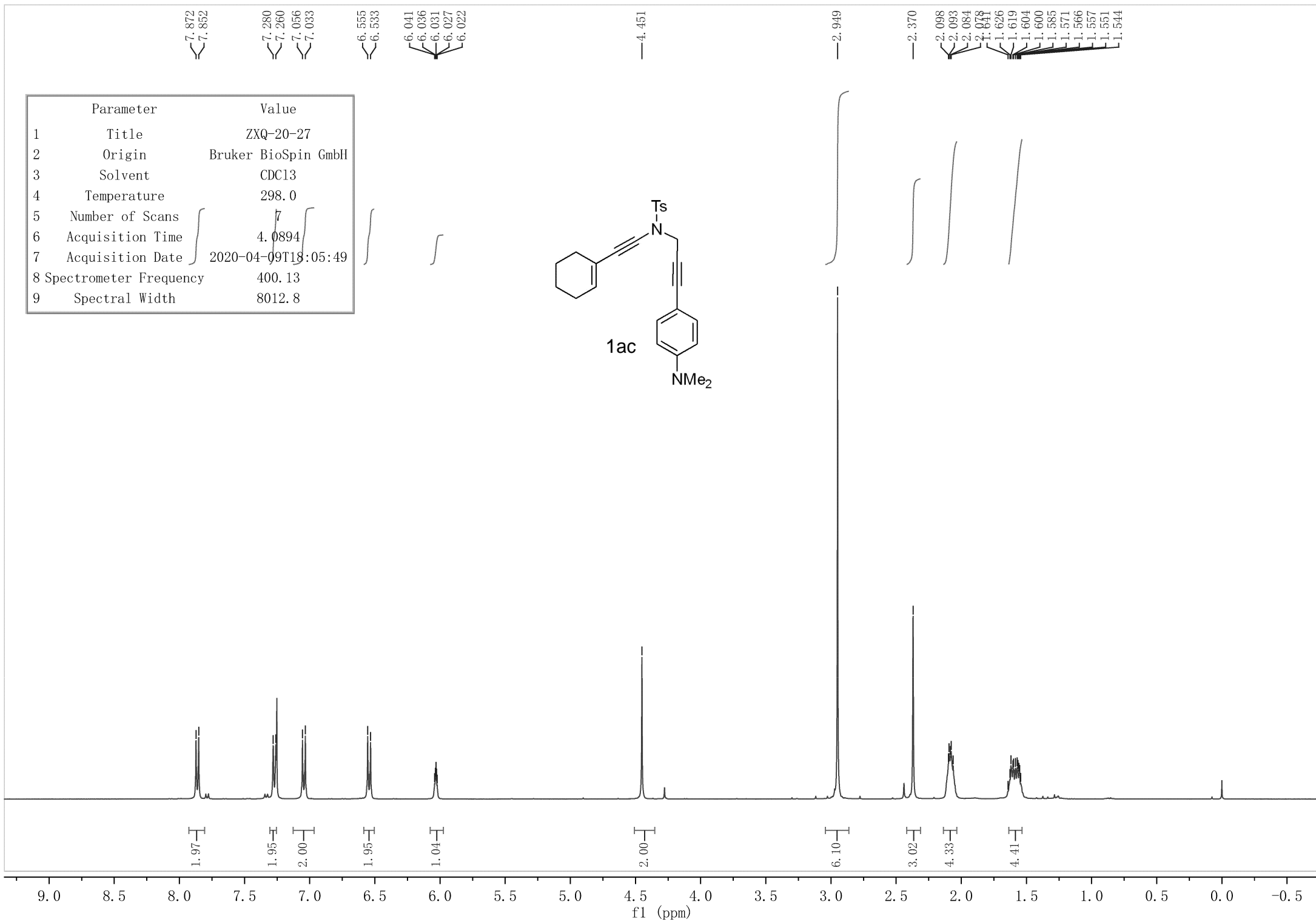
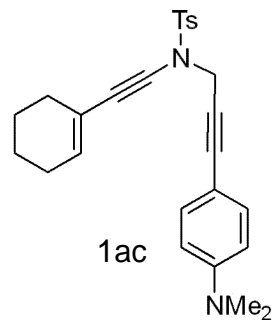
1.91  
4.07  
2.96  
1.96  
0.93  
1.99  
2.00  
5.97  
3.03  
3.00

Parameter	Value
1 Title	ZXQ-20-62-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.8
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-20T21:45:23
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

150.18 144.64 136.83 134.49 134.29 132.75 129.48 128.81 128.13 126.88 119.16 111.45 108.68 87.64 81.49 78.76 77.32 77.00 76.68 75.00 43.21 40.05 21.56 19.30

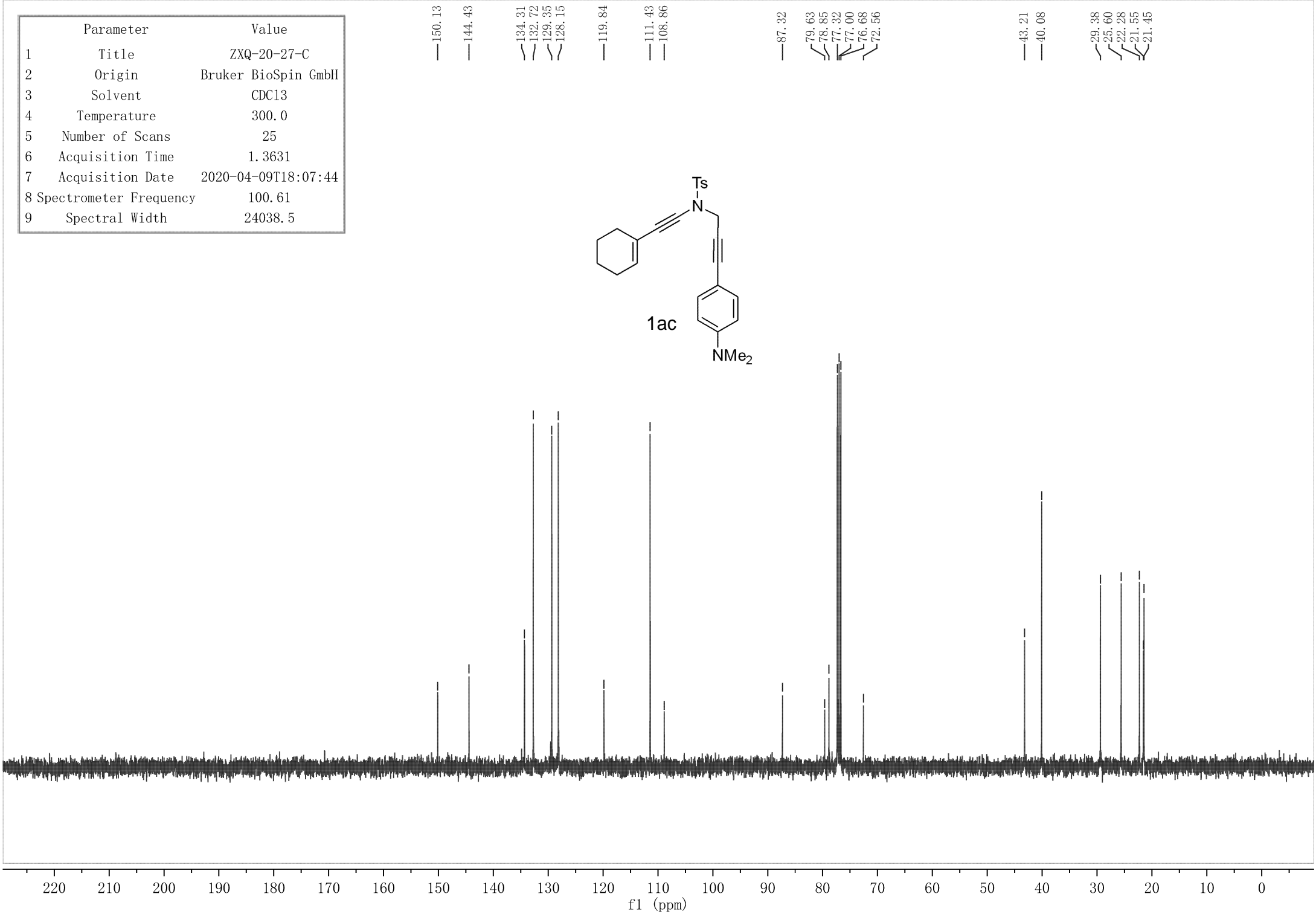
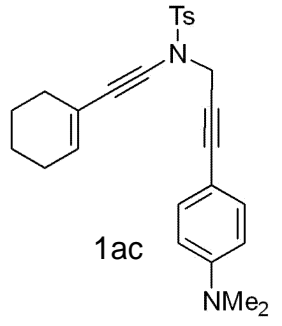


Parameter	Value
1 Title	ZXQ-20-27
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2020-04-09T18:05:49
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

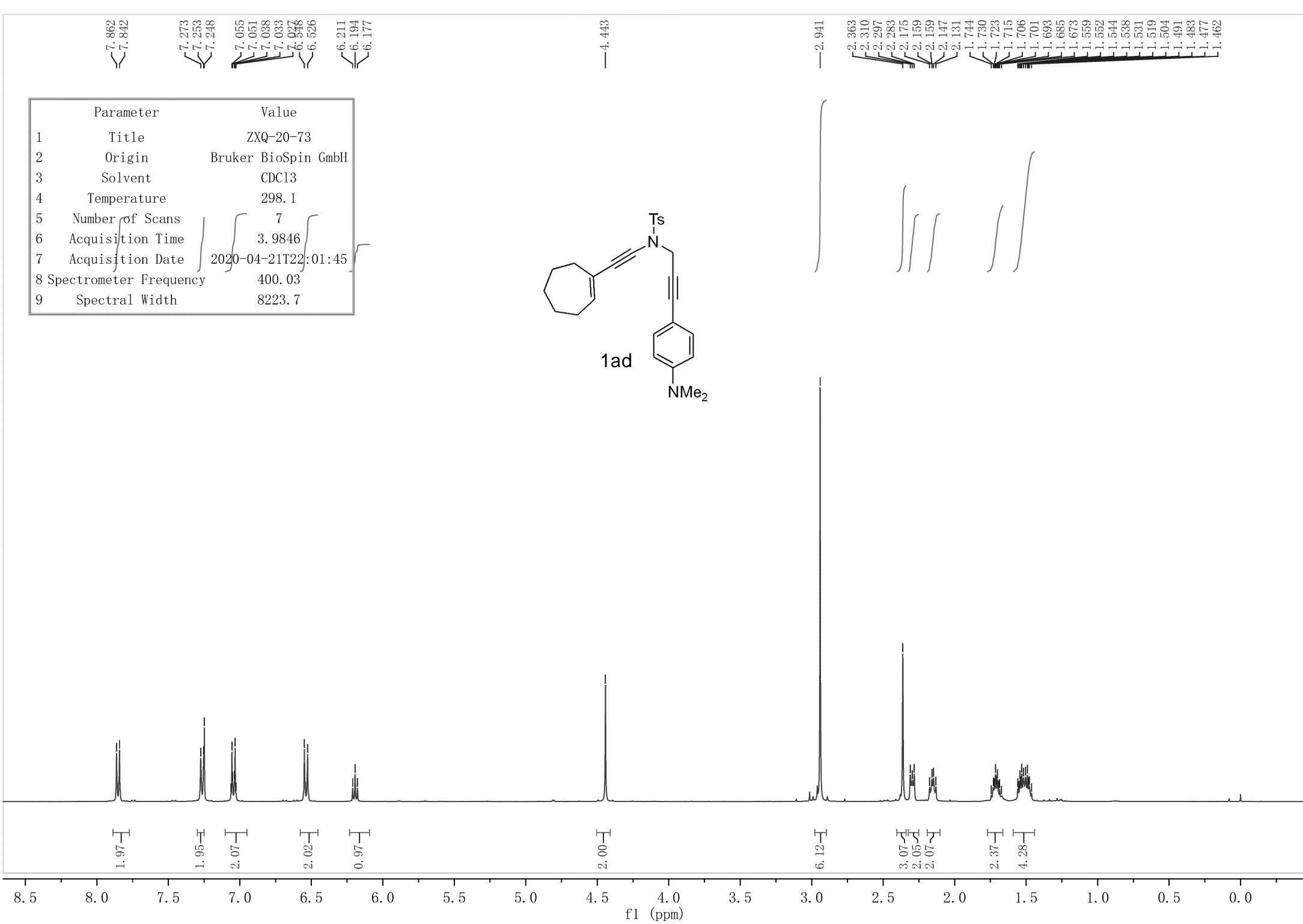
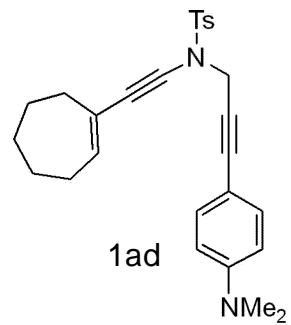




Parameter	Value
1 Title	ZXQ-20-27-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	25
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-09T18:07:44
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

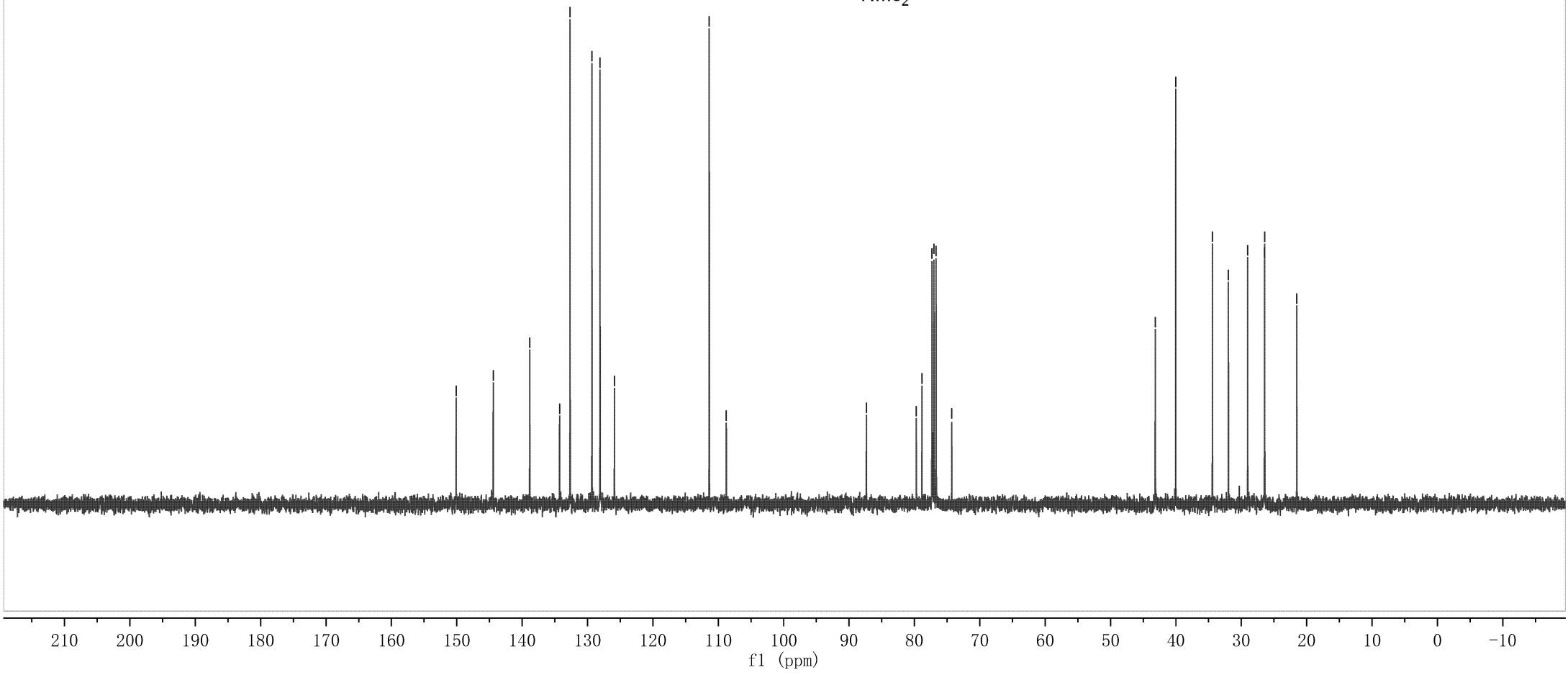
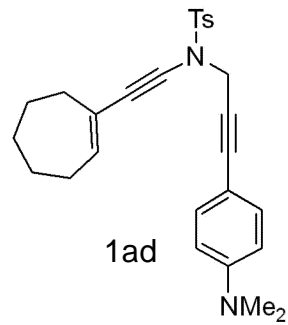


Parameter	Value
1 Title	ZXQ-20-73
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-21T22:01:45
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

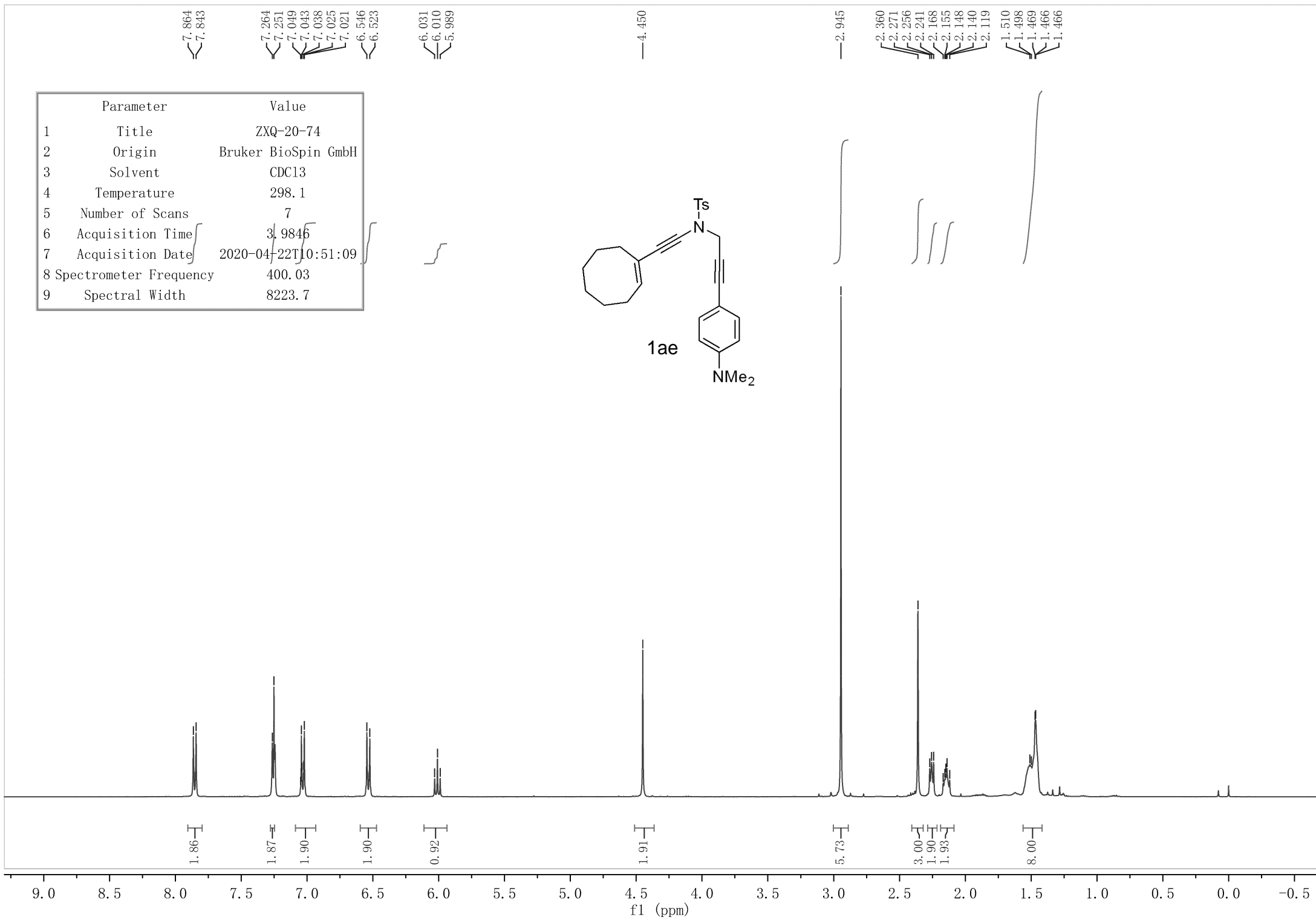
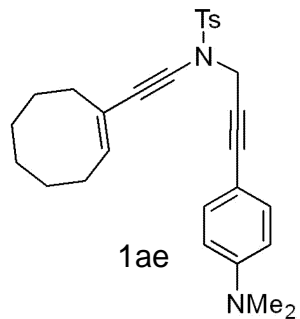


Parameter	Value
1 Title	ZXQ-20-73-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.6
5 Number of Scans	32
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-21T22:04:39
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

150.09 144.42 138.84 134.28 132.68 129.32 128.09 125.88  
 111.38 108.77 87.35 79.71 78.85 77.32 77.00 76.68 74.29  
 43.16 40.03 34.41 31.97 29.03 26.45 26.42 21.51



Parameter	Value
1 Title	ZXQ-20-74
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-22T10:51:09
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



7.864  
7.843

7.264  
7.251  
7.049  
7.038  
7.025  
7.021  
6.546  
6.523

6.031  
6.010  
5.989

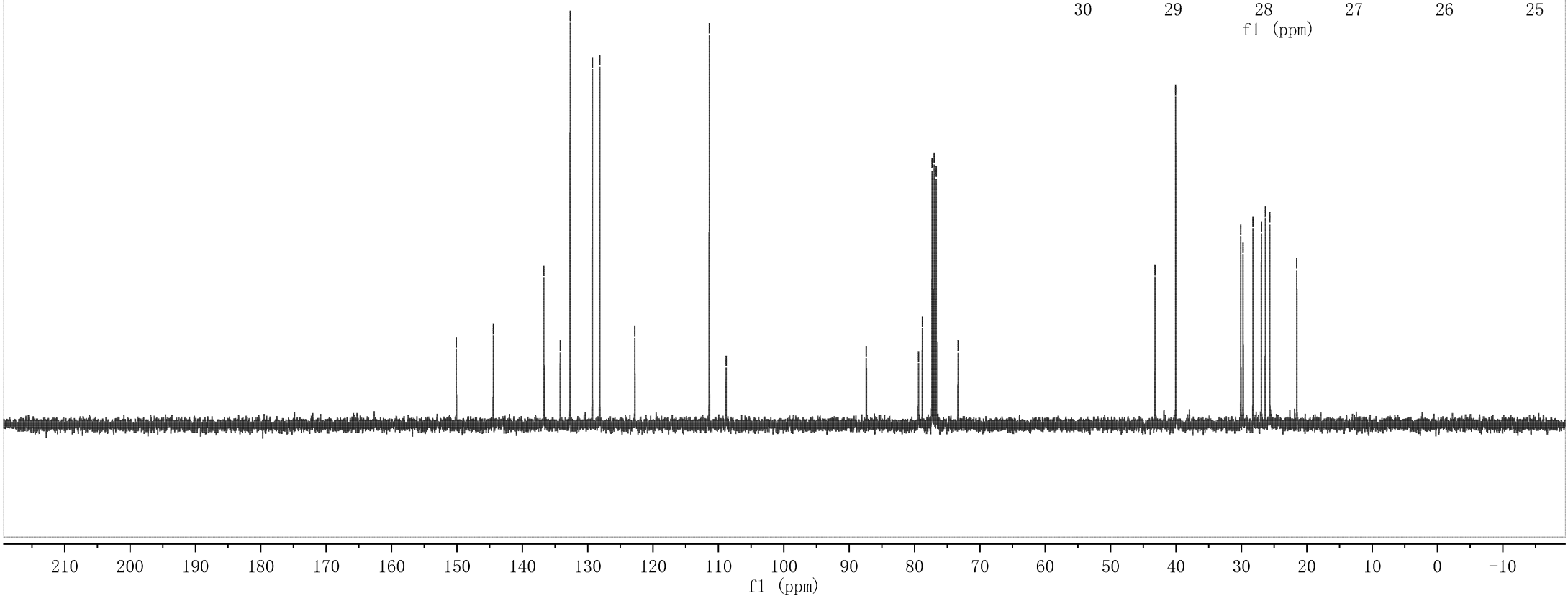
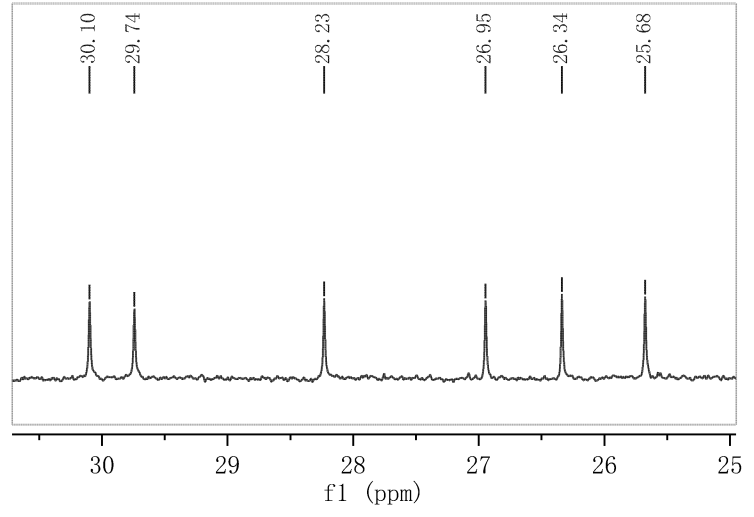
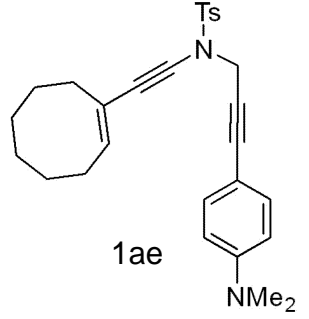
4.450

2.945

2.360  
2.271  
2.256  
2.241  
2.168  
2.155  
2.148  
2.140  
2.119  
1.510  
1.498  
1.469  
1.466  
1.466

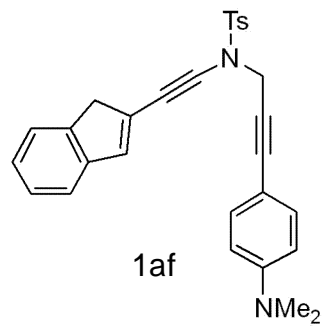
Parameter	Value
1 Title	ZXQ-20-74-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	29
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-22T10:54:03
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

150.10 144.43 136.71 134.19 132.67 129.29 128.17 122.79 111.39 108.82 87.37 79.40 78.81 77.32 77.00 76.68 73.34 43.21 40.06 30.10 29.74 28.23 26.95 26.34 25.68 21.53

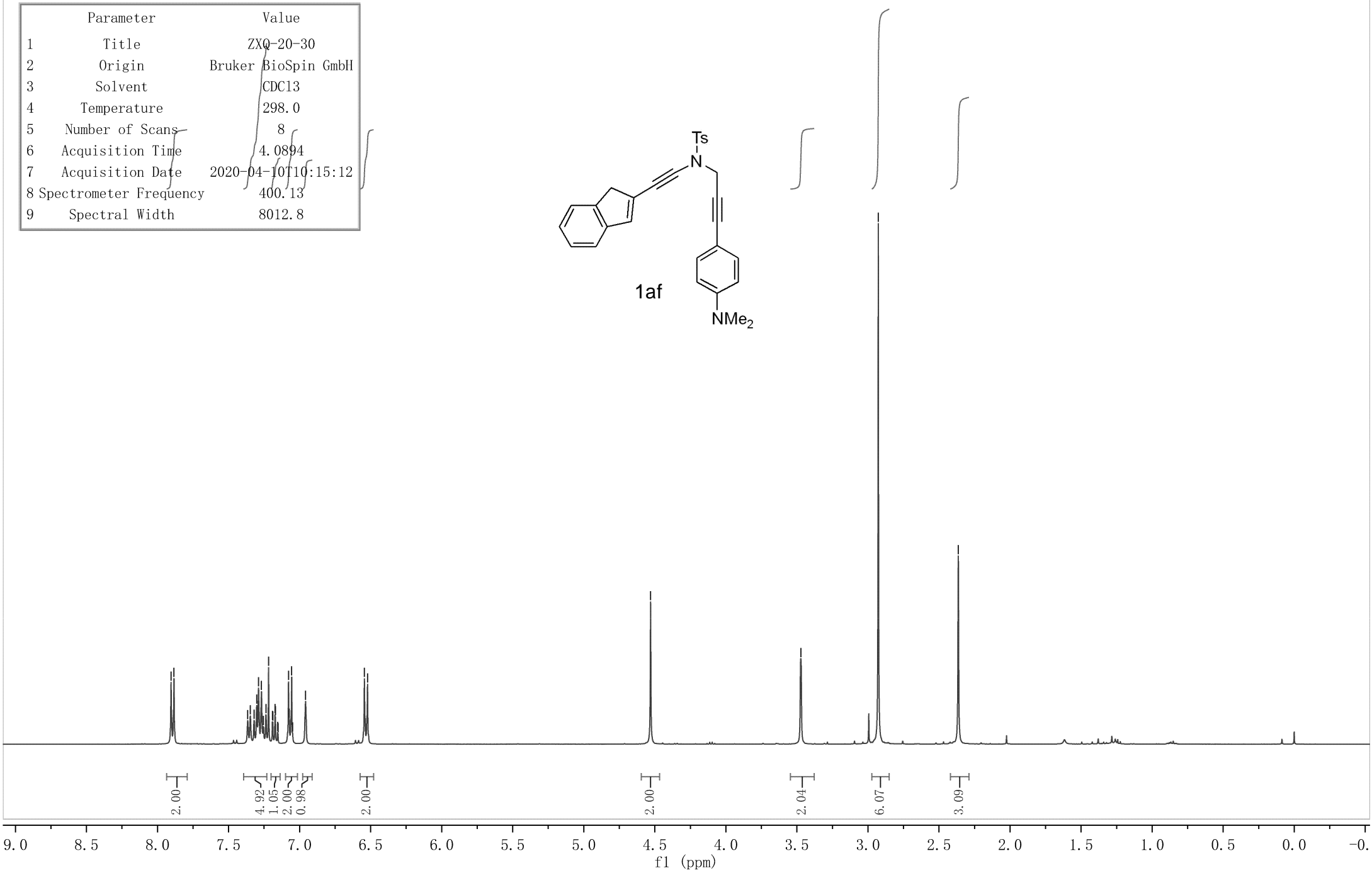


7.905  
7.884  
7.347  
7.302  
7.289  
7.269  
7.269  
7.237  
7.218  
7.173  
7.078  
7.056  
6.958  
6.934  
6.522

Parameter	Value
1 Title	ZXQ-20-30
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2020-04-10 10:15:12
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



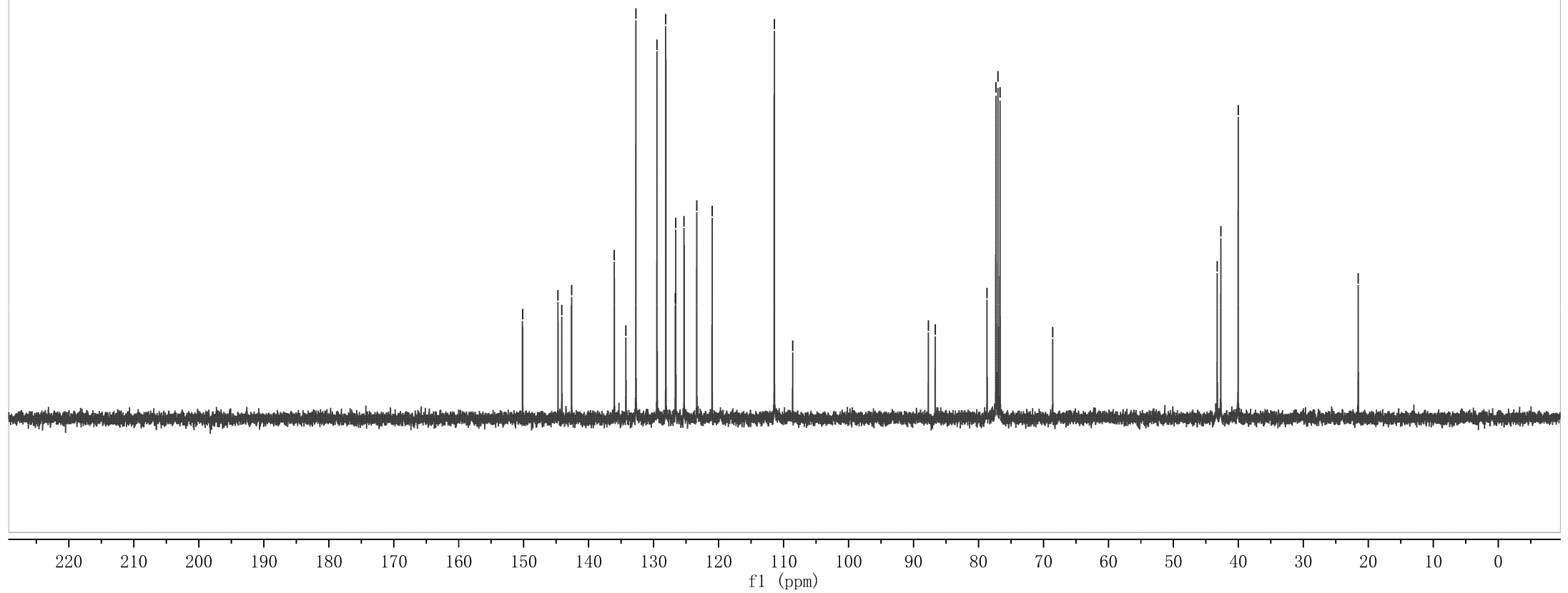
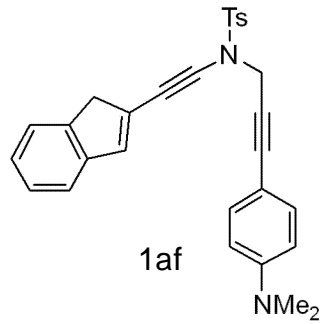
4.530  
3.472  
2.927  
2.364



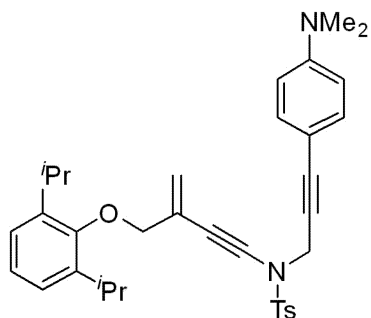
2.00  
4.92  
1.05  
2.00  
0.98  
2.00  
2.00  
2.04  
6.07  
3.09

Parameter	Value
1 Title	ZXQ-20-30-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	30
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-10T10:17:51
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

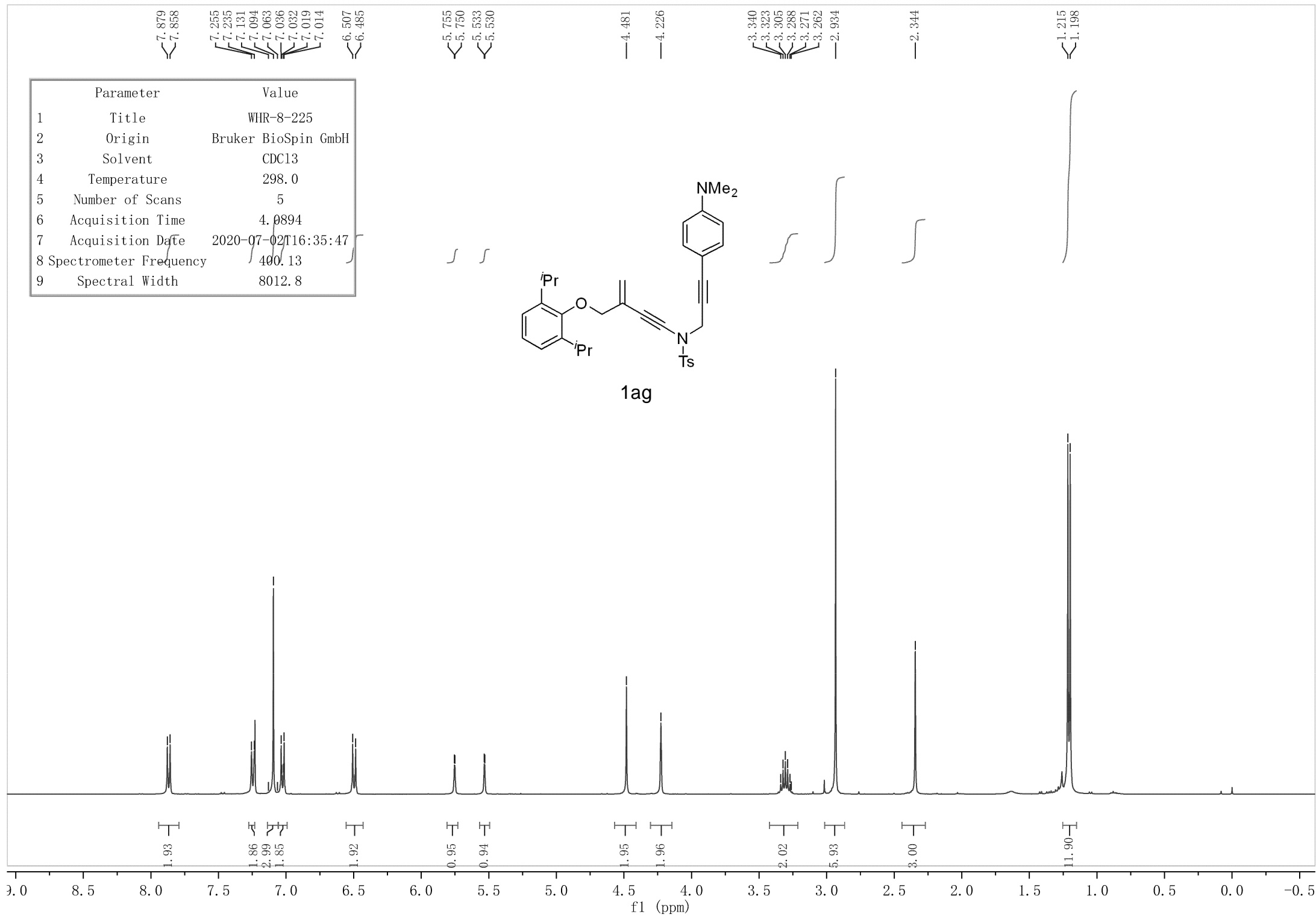
150.17  
 144.72  
 144.13  
 142.63  
 136.05  
 134.27  
 132.73  
 129.48  
 128.12  
 126.66  
 126.59  
 125.31  
 123.36  
 121.00  
 111.43  
 108.60  
 87.71  
 86.66  
 78.68  
 77.32  
 77.00  
 76.68  
 68.58  
 43.25  
 42.70  
 40.02  
 21.55



Parameter	Value
1 Title	WHR-8-225
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2020-07-02T16:35:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



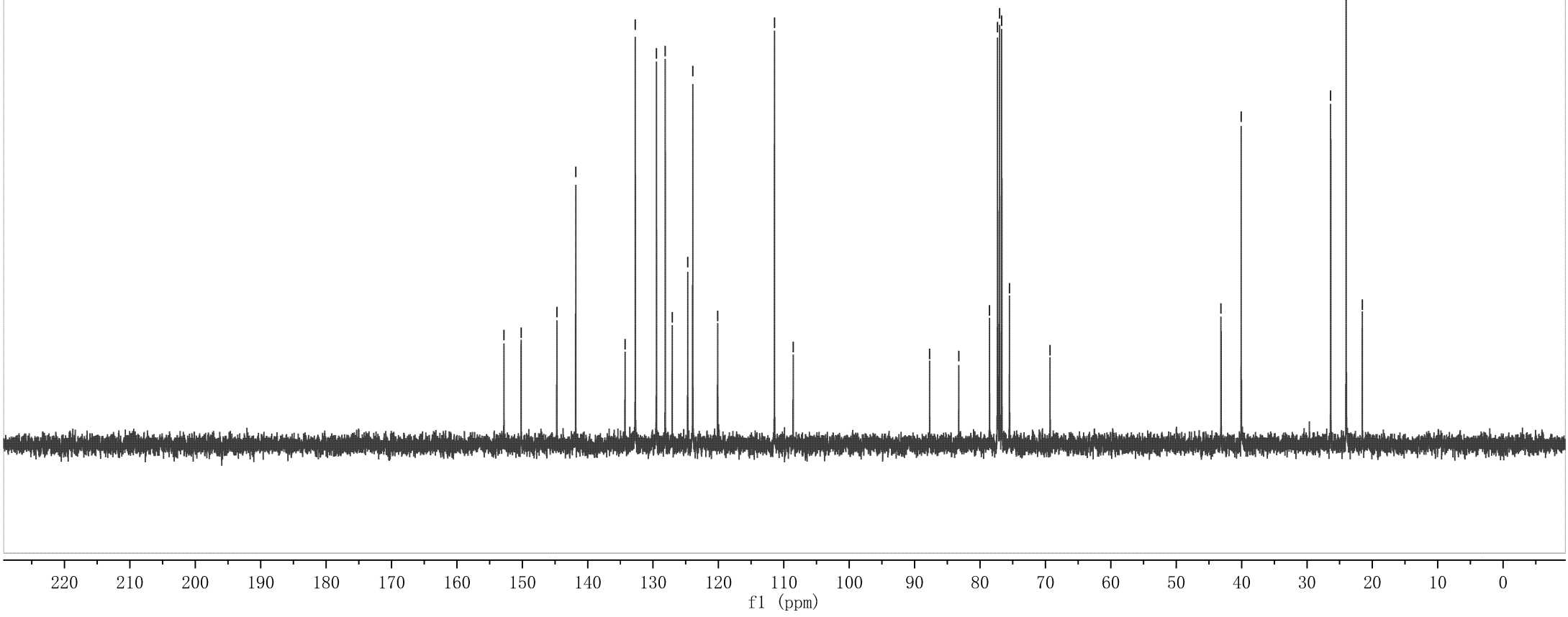
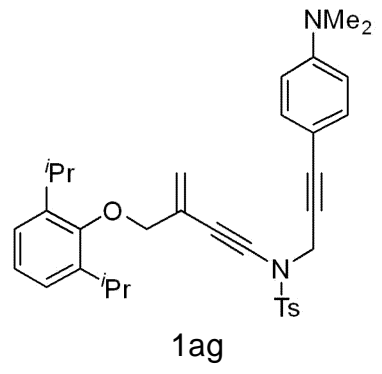
1ag



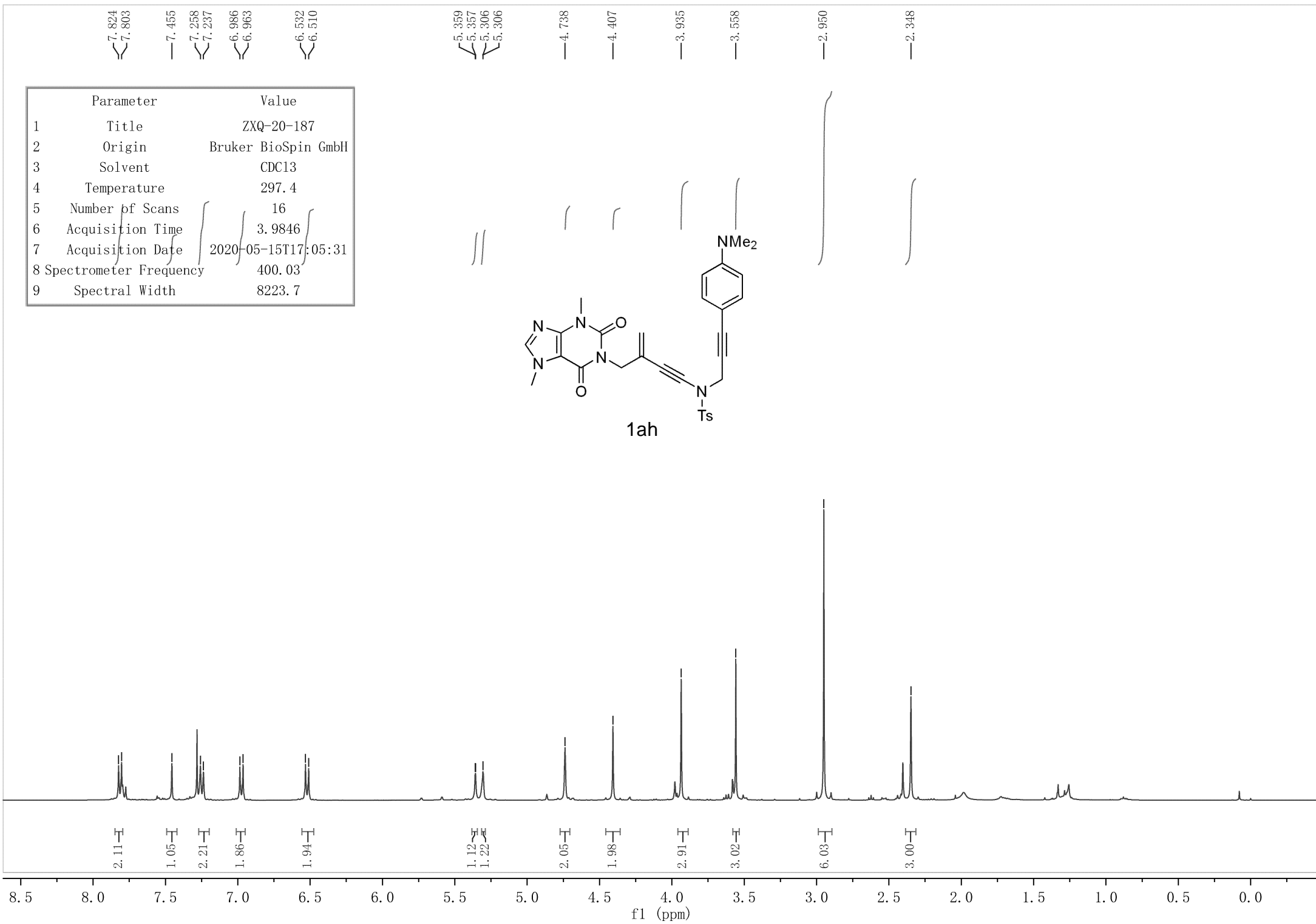
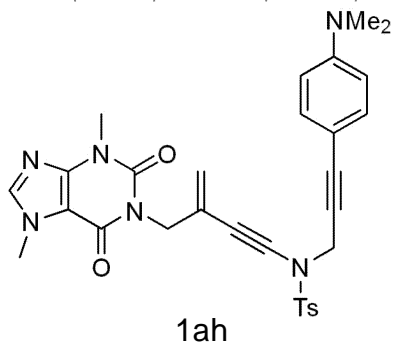


Parameter	Value
1 Title	WHR-8-225-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	21
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-02T16:36:55
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

- 152.80
- 150.18
- 144.71
- 141.82
- 134.28
- 132.72
- 129.48
- 128.14
- 127.07
- 124.70
- 123.93
- 120.12
- 111.43
- 108.57
- 87.71
- 83.25
- 78.55
- 77.32
- 77.00
- 76.68
- 75.50
- 69.29
- 43.14
- 40.06
- 26.38
- 24.02
- 21.54



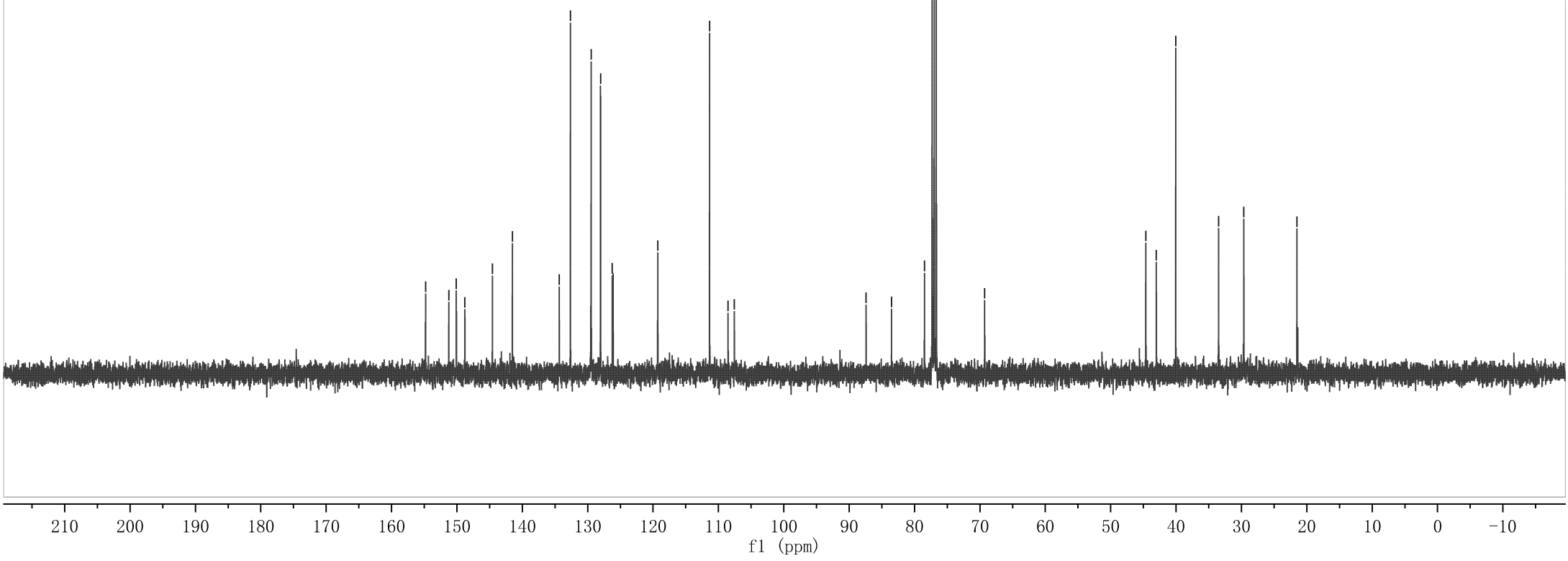
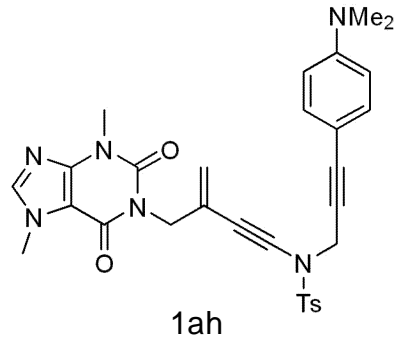
Parameter	Value
1 Title	ZXQ-20-187
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	297.4
5 Number of Scans	16
6 Acquisition Time	3.9846
7 Acquisition Date	2020-05-15T17:05:31
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



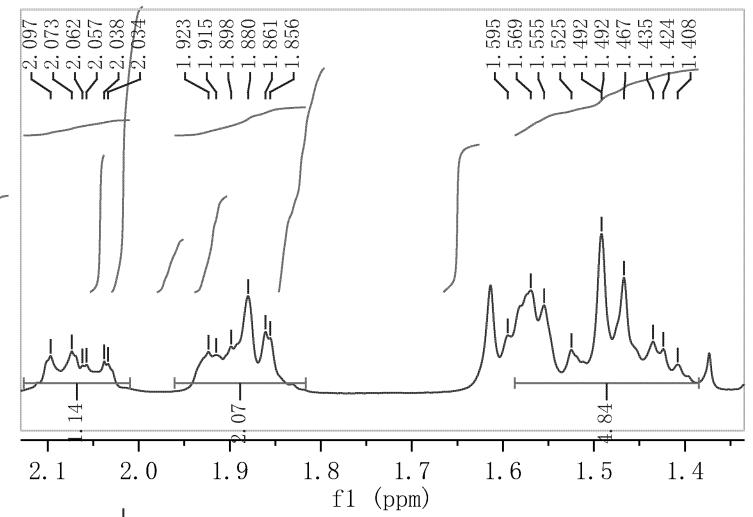
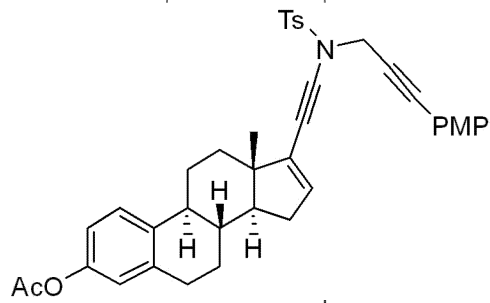
Parameter	Value
1 Title	ZXQ-20-187-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	297.8
5 Number of Scans	48
6 Acquisition Time	1.3631
7 Acquisition Date	2020-05-15T17:08:39
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

154.80 151.24 150.09 148.79 144.57 141.52 134.35 132.64 129.47 128.03 126.24 119.28 111.36 108.53 107.57 87.42 83.52 78.48 77.32 77.00 76.68 69.27

44.63 43.02 40.05 33.49 29.64 21.51



Parameter	Value
1 Title	ZXQ-19-155
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl <sub>3</sub>
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-21 16:03:02
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.892  
7.871

7.295  
7.275  
7.251  
7.233  
7.212  
7.107  
7.085

6.849  
6.844  
6.828  
6.823  
6.787  
6.765

5.963  
5.963  
5.959

4.542  
4.497  
4.489  
4.445

3.789

2.904  
2.878  
2.865

2.378  
2.301  
2.276  
2.253  
2.228  
2.223

1.898  
1.880  
1.861  
1.856

1.595  
1.569  
1.555  
1.525

1.492  
1.467  
1.435  
1.424  
1.408

2.02

2.12  
1.04  
2.02

4.00

1.00

2.01

3.15

2.08

2.96  
6.16  
1.14  
2.07

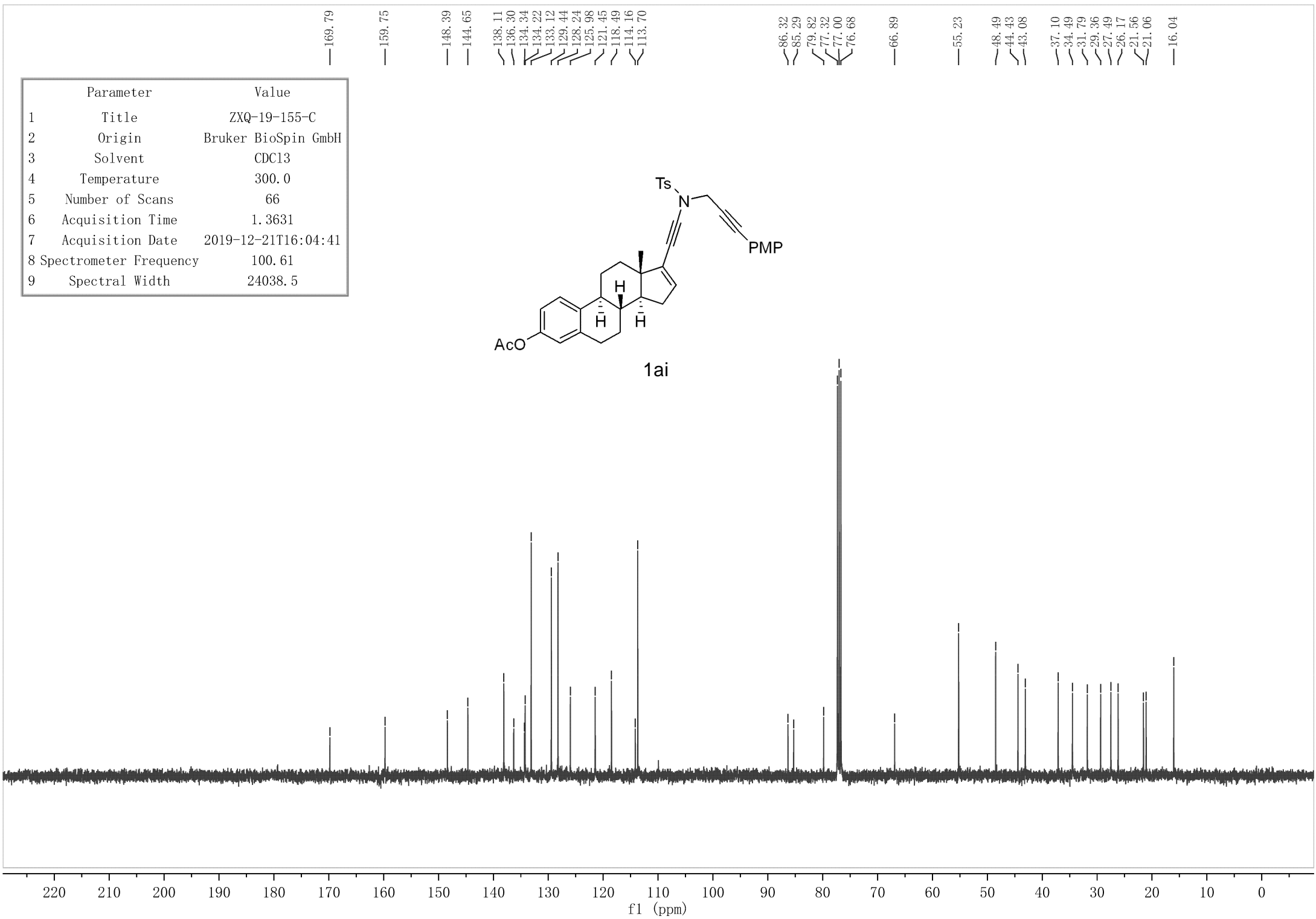
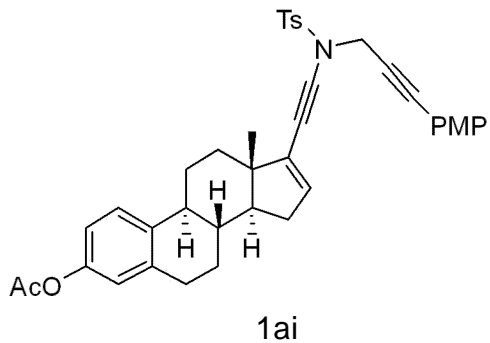
4.84

3.18

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

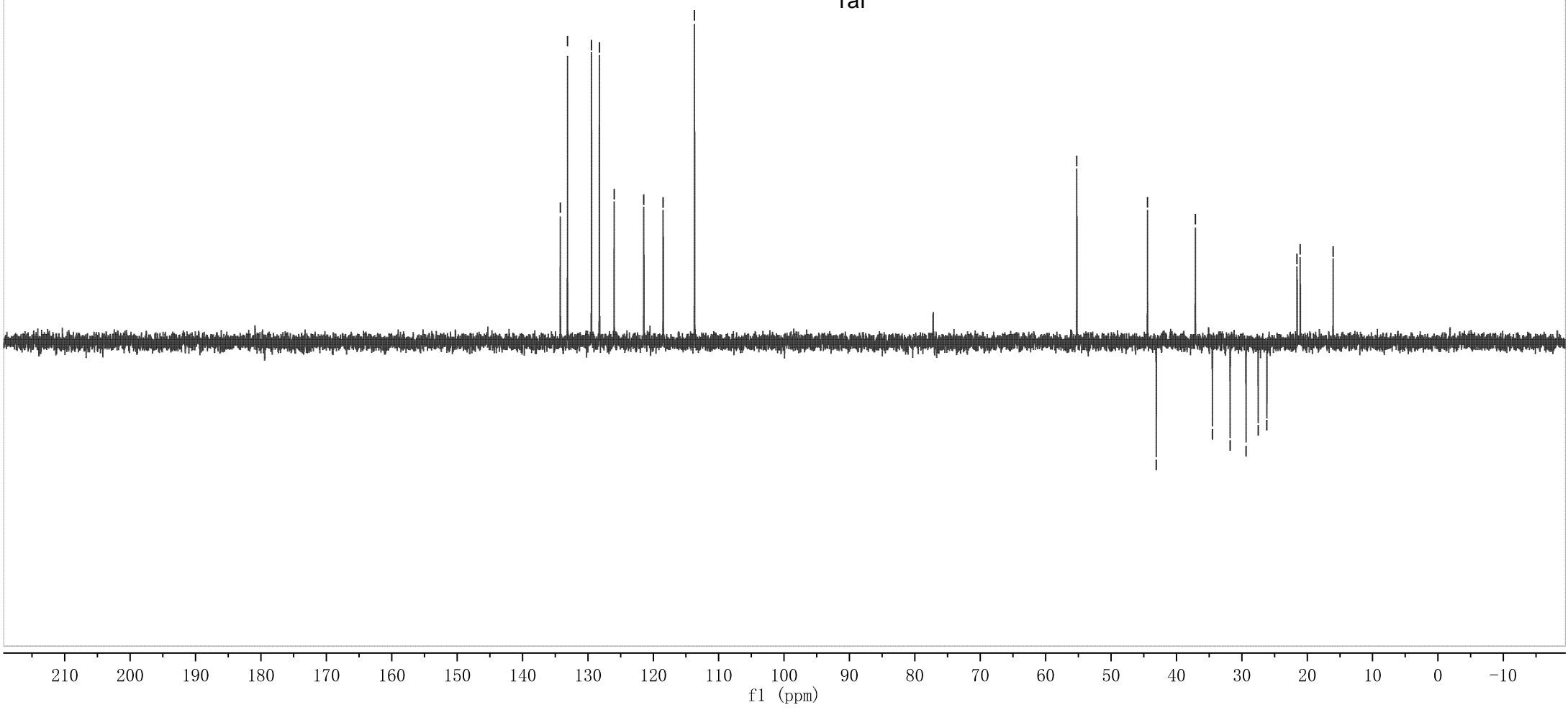
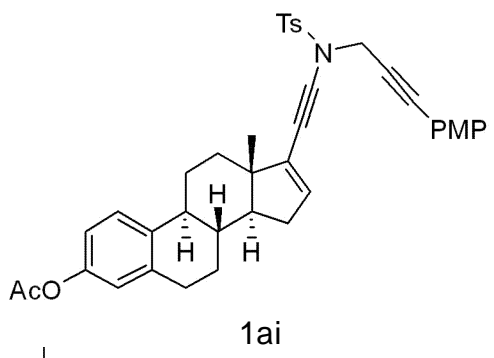
Parameter	Value
1 Title	ZXQ-19-155-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	66
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-21T16:04:41
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



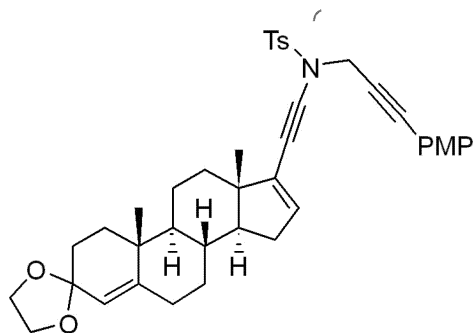
Parameter	Value
1 Title	ZXQ-19-155-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	14
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-21T16:09:17
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

134.22  
133.12  
129.45  
128.24  
125.98  
121.45  
118.49  
113.70

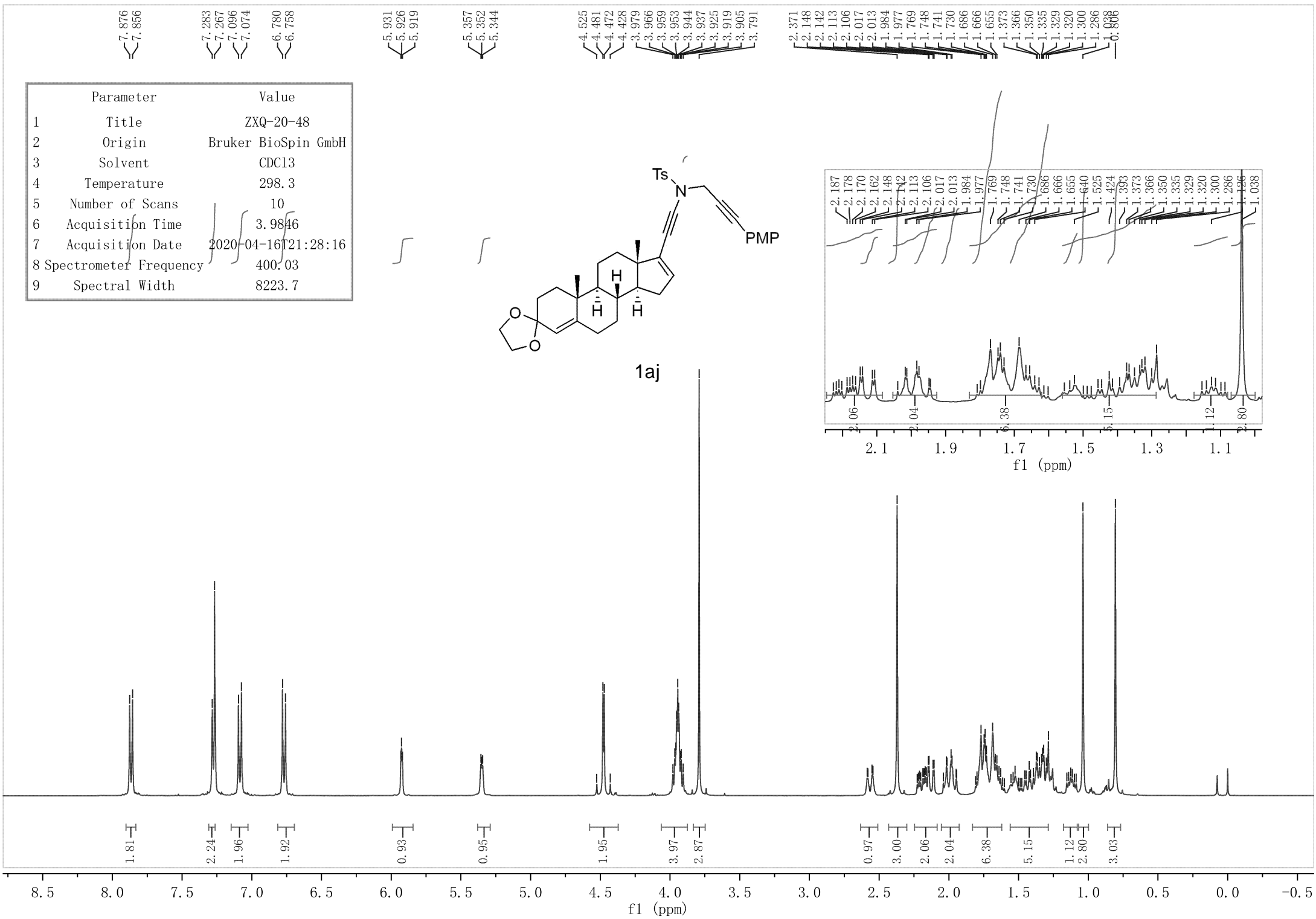
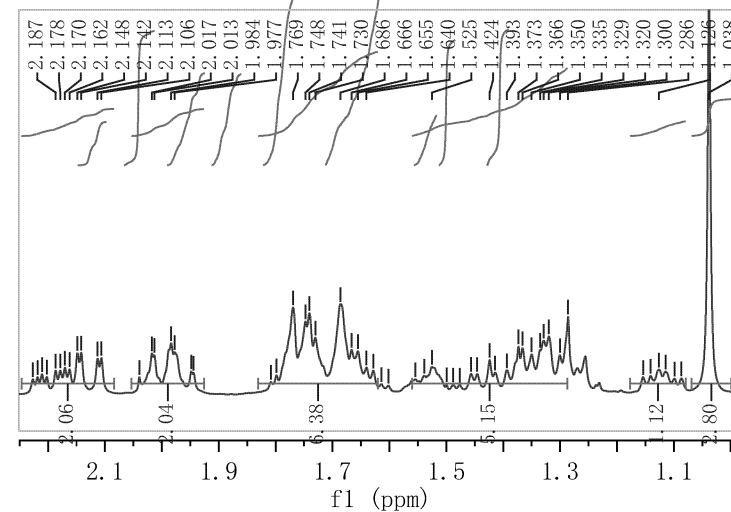
55.23  
44.43  
43.08  
37.11  
34.50  
31.79  
29.36  
27.50  
26.17  
21.56  
21.07  
16.04



Parameter	Value
1 Title	ZXQ-20-48
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.3
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-16T21:28:16
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

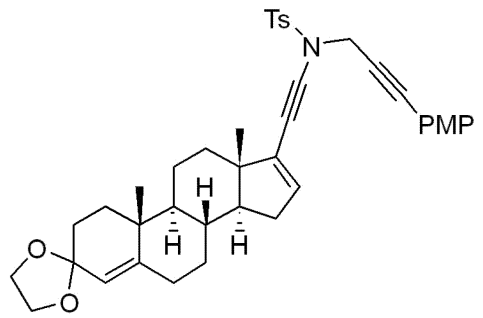


1aj

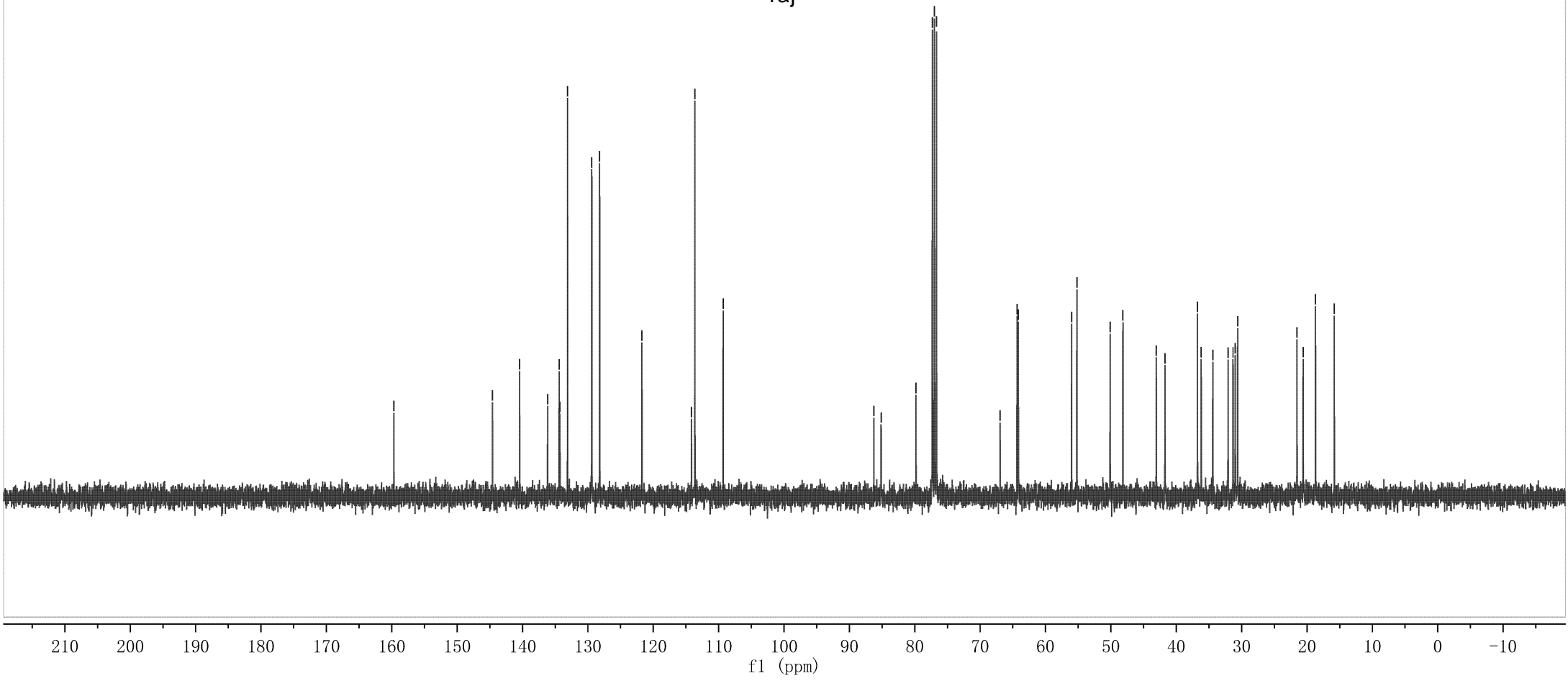


Parameter	Value
1 Title	ZXQ-20-48-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	38
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-16T21:31:23
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

- 144.59
- 140.43
- 136.15
- 134.40
- 134.28
- 133.10
- 129.40
- 128.20
- 121.73
- 114.15
- 113.64
- 109.32
- 86.26
- 85.15
- 79.81
- 77.32
- 77.00
- 76.68
- 66.94
- 64.35
- 64.16
- 56.01
- 55.20
- 50.12
- 48.16
- 43.05
- 41.72
- 36.76
- 36.18
- 32.07
- 31.32
- 30.98
- 29.64
- 29.53
- 20.60
- 18.71
- 15.82



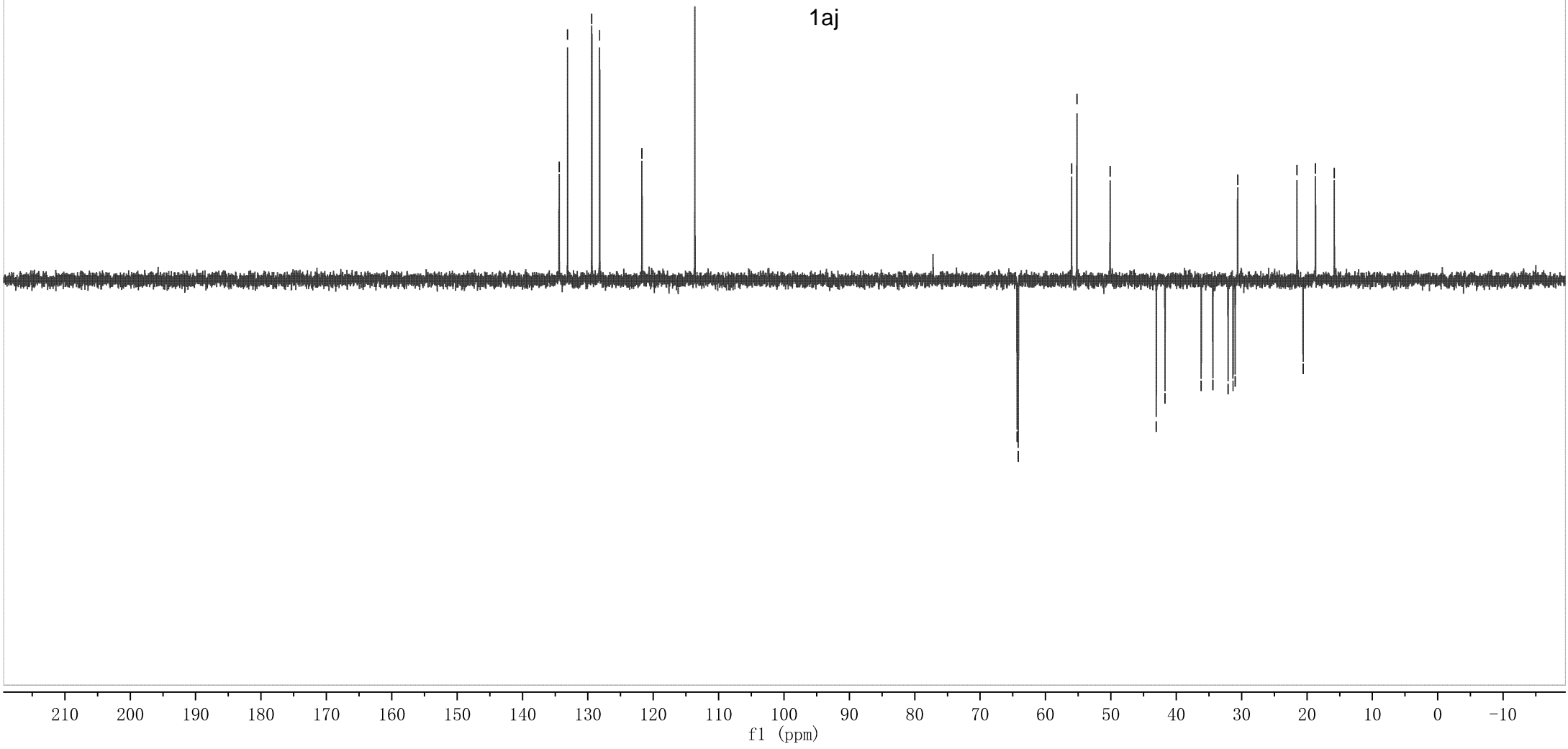
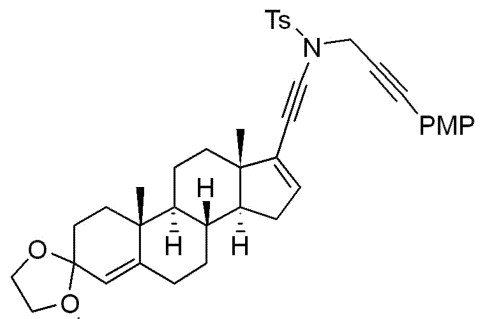
1aj





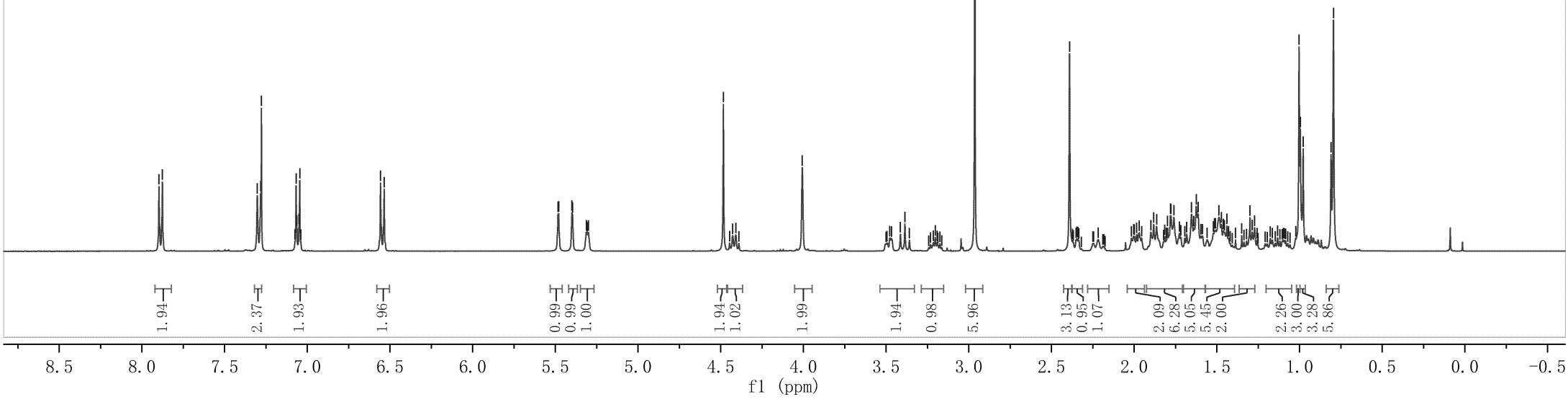
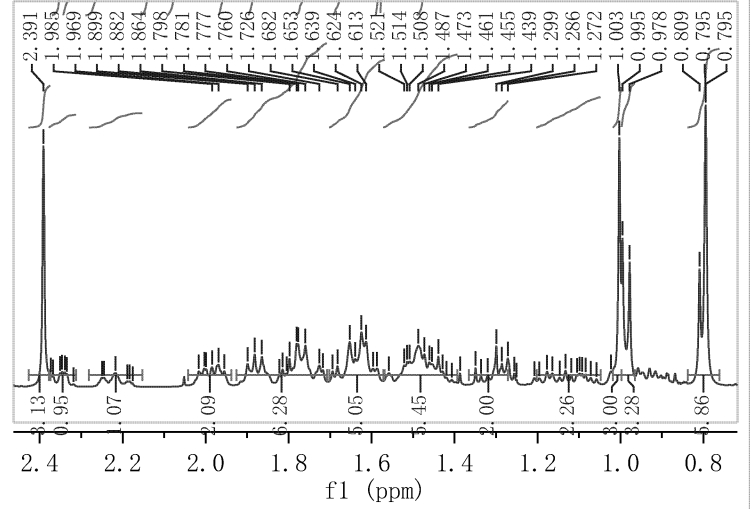
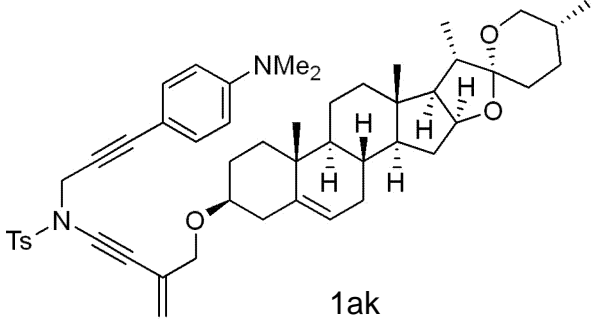
Parameter	Value
1 Title	ZXQ-20-48-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.8
5 Number of Scans	16
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-16T21:33:58
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

134.39  
 133.10  
 129.40  
 128.20  
 121.73  
 113.63  
 64.35  
 64.16  
 56.00  
 55.20  
 50.12  
 43.05  
 41.72  
 36.18  
 34.41  
 32.07  
 31.31  
 30.98  
 30.61  
 21.53  
 20.60  
 18.71  
 15.82

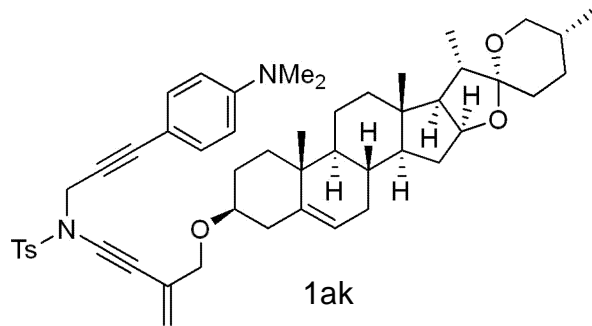


7.897  
7.876  
7.803  
7.282  
7.277  
7.075  
7.068  
7.063  
7.051  
7.046  
7.039  
6.557  
6.535  
5.484  
5.480  
5.400  
5.396  
5.313  
5.308  
5.300  
4.484  
4.446  
4.428  
4.409  
4.007  
3.478  
3.467  
3.413  
3.386  
3.359  
3.359  
3.214  
3.203  
3.192  
2.391  
2.373  
2.368  
2.351  
2.346  
2.339  
2.335  
2.217  
2.017  
2.003  
1.999  
1.985  
1.969  
1.955  
1.899  
1.882  
1.864  
1.823  
1.815  
1.805  
1.798  
1.781  
1.777  
1.760  
1.726  
1.717  
1.694  
1.682  
1.653  
1.639  
1.624  
1.613  
1.597  
1.587  
1.558  
1.521  
1.514  
1.508  
1.487  
1.473  
1.461  
1.455  
1.439  
1.429  
1.387  
1.349  
1.336  
1.320  
1.299  
1.286  
1.272  
1.256  
1.177  
1.164  
1.133  
1.119  
1.105  
1.098  
1.092  
1.084  
1.023  
1.003  
0.995  
0.978  
0.809  
0.795  
0.795

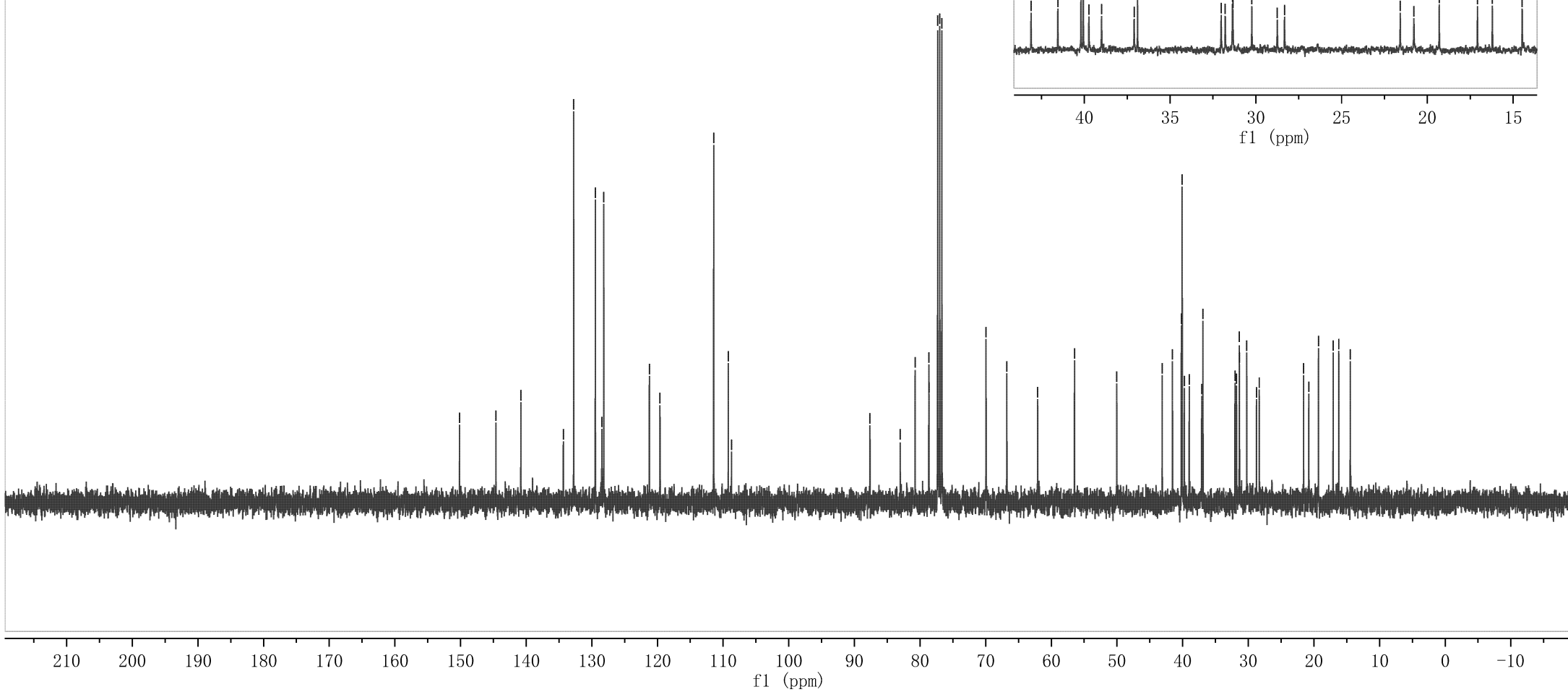
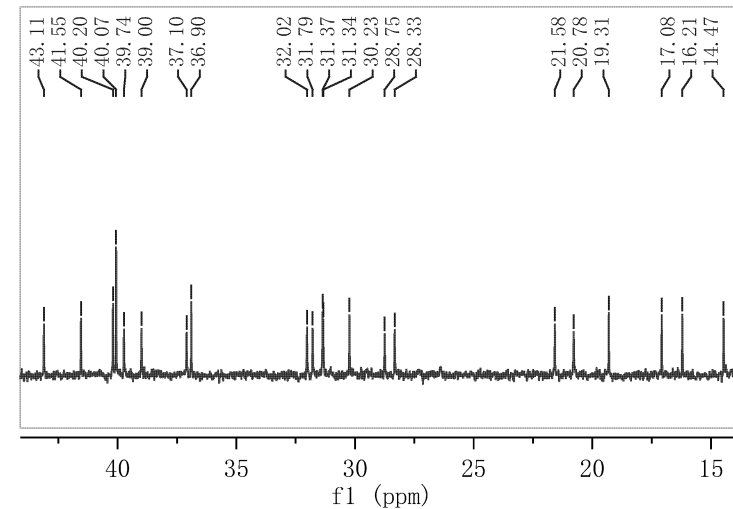
Parameter	Value
1 Title	ZXQ-20-138
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.8
5 Number of Scans	11
6 Acquisition Time	3.9846
7 Acquisition Date	2020-05-06T13:50:11
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



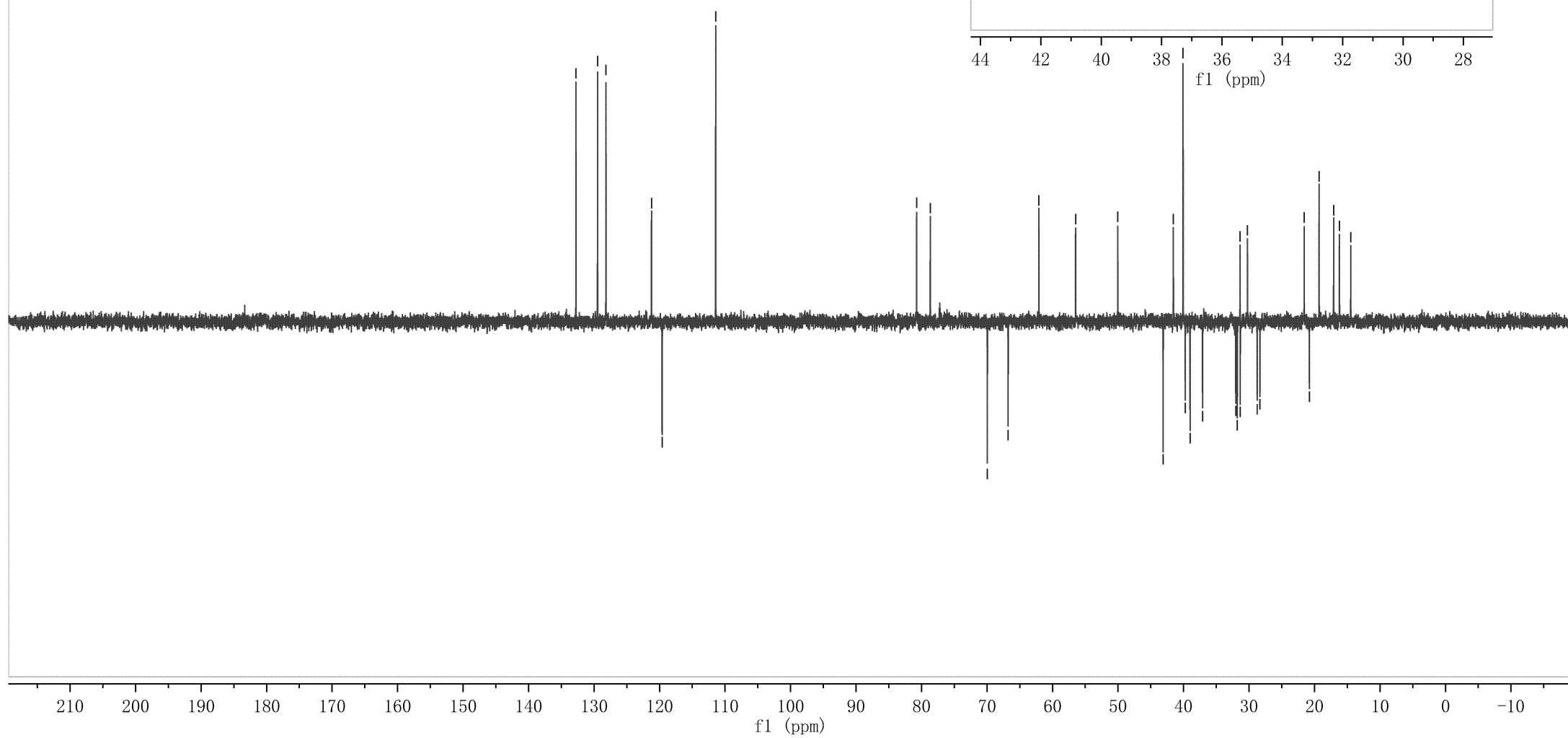
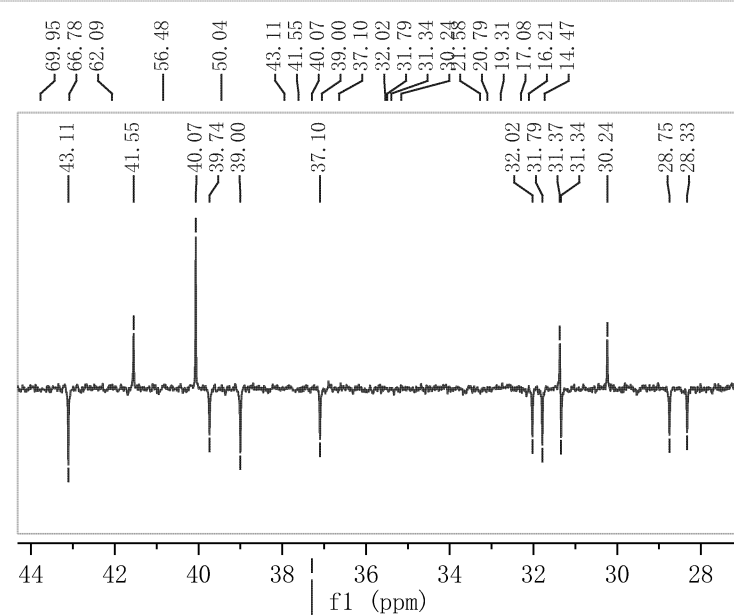
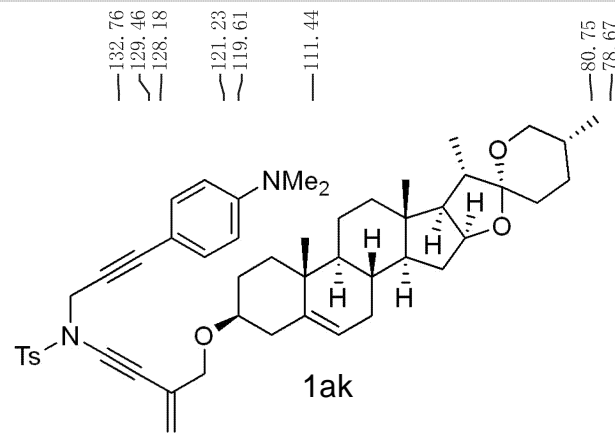
Parameter	Value
1 Title	ZXQ-20-138-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.1
5 Number of Scans	34
6 Acquisition Time	1.3631
7 Acquisition Date	2020-05-06T13:53:22
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



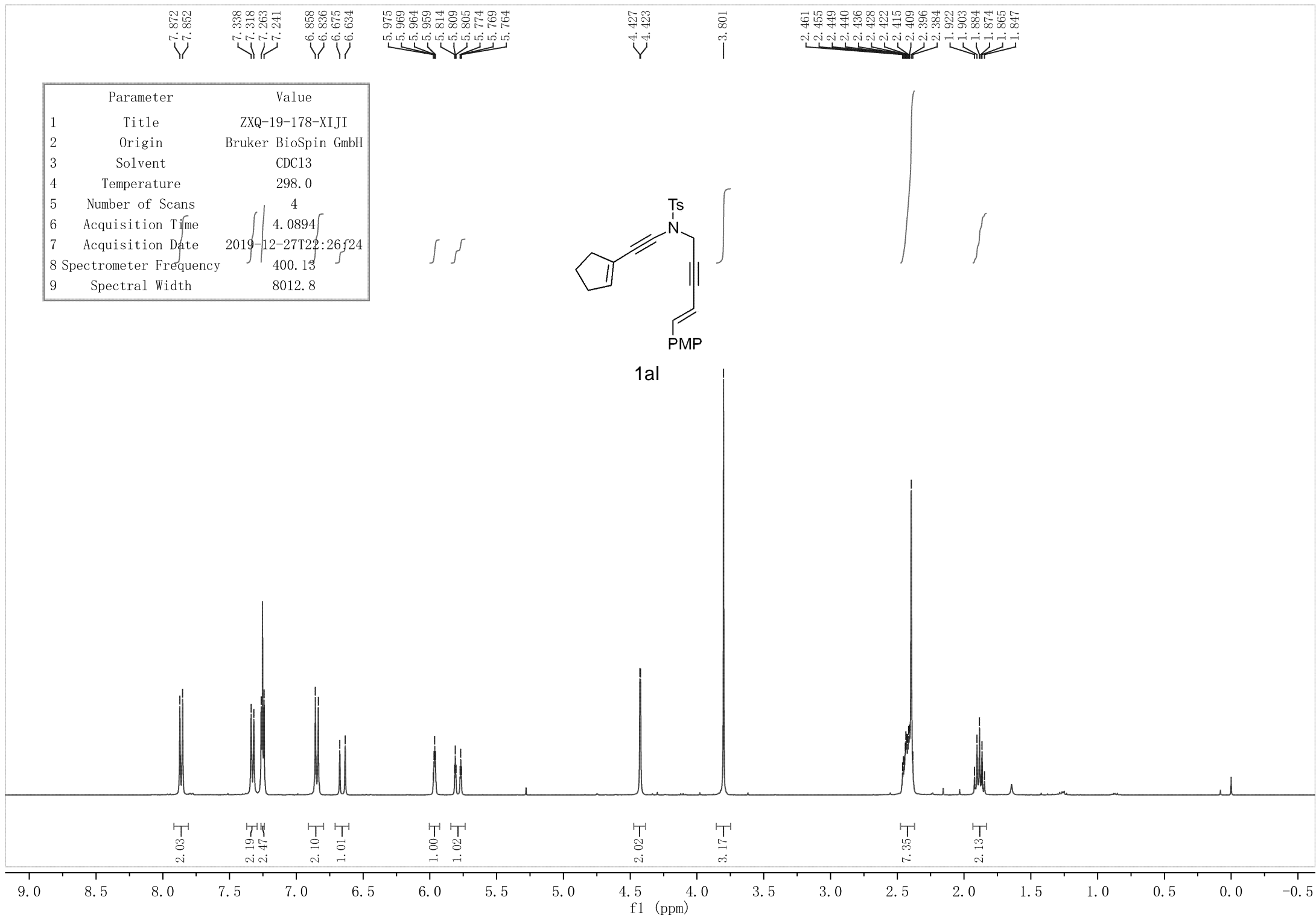
150.15 144.61 140.81 134.34 132.76 129.46 128.48 128.18 121.23 119.62 111.43 109.20 108.71 87.63 83.02 80.75 78.67 78.63 77.32 77.00 76.68 69.95 66.78 62.08 56.47 50.04 43.11 41.55 40.20 40.07 39.00 36.90 31.37 31.34 30.58 21.58 20.78 19.31 17.08 16.21 14.47



Parameter	Value
1 Title	ZXQ-20-138-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.6
5 Number of Scans	18
6 Acquisition Time	1.3631
7 Acquisition Date	2020-05-06T13:55:42
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

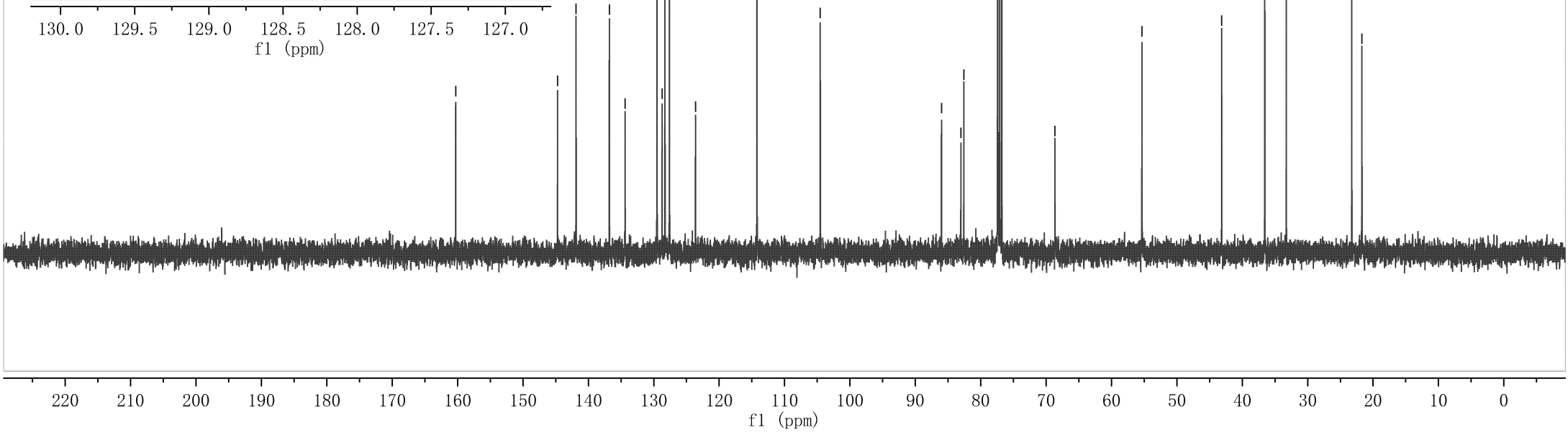
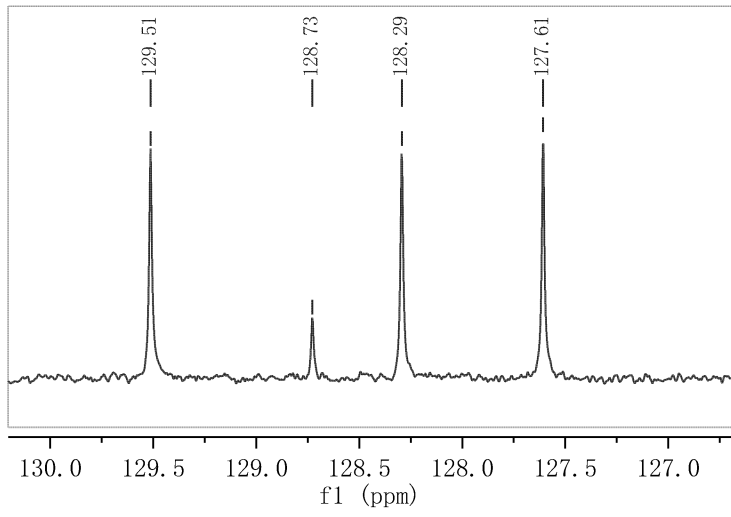
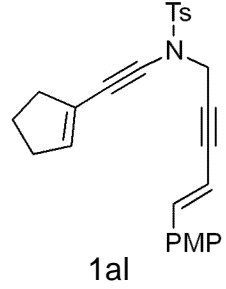


Parameter	Value
1 Title	ZXQ-19-178-XIJI
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-27T22:26:24
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

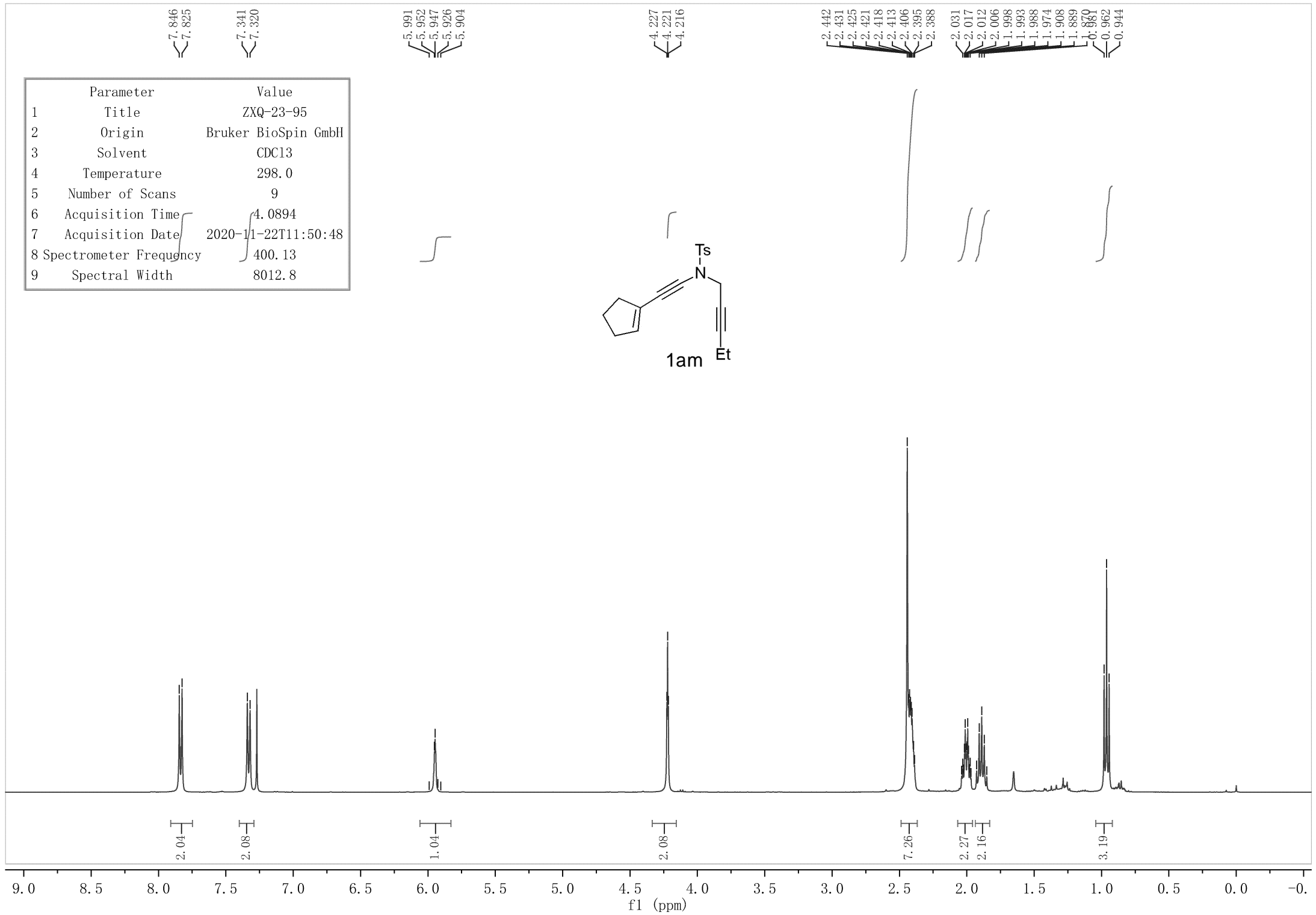
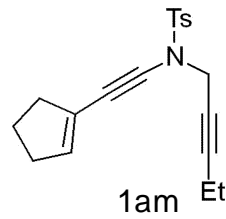


Parameter	Value
1 Title	ZXQ-19-178-XIJI-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	15
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-27T22:27:20
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

160.29 — 144.71 — 141.88 — 136.80 — 134.38 — 129.51 — 128.73 — 128.29 — 127.61 — 123.62 — 114.22 — 104.54 — 86.01 — 83.04 — 82.58 — 77.42 — 77.10 — 76.79 — 68.65 — 55.35 — 43.15 — 36.56 — 33.27 — 23.25 — 21.70

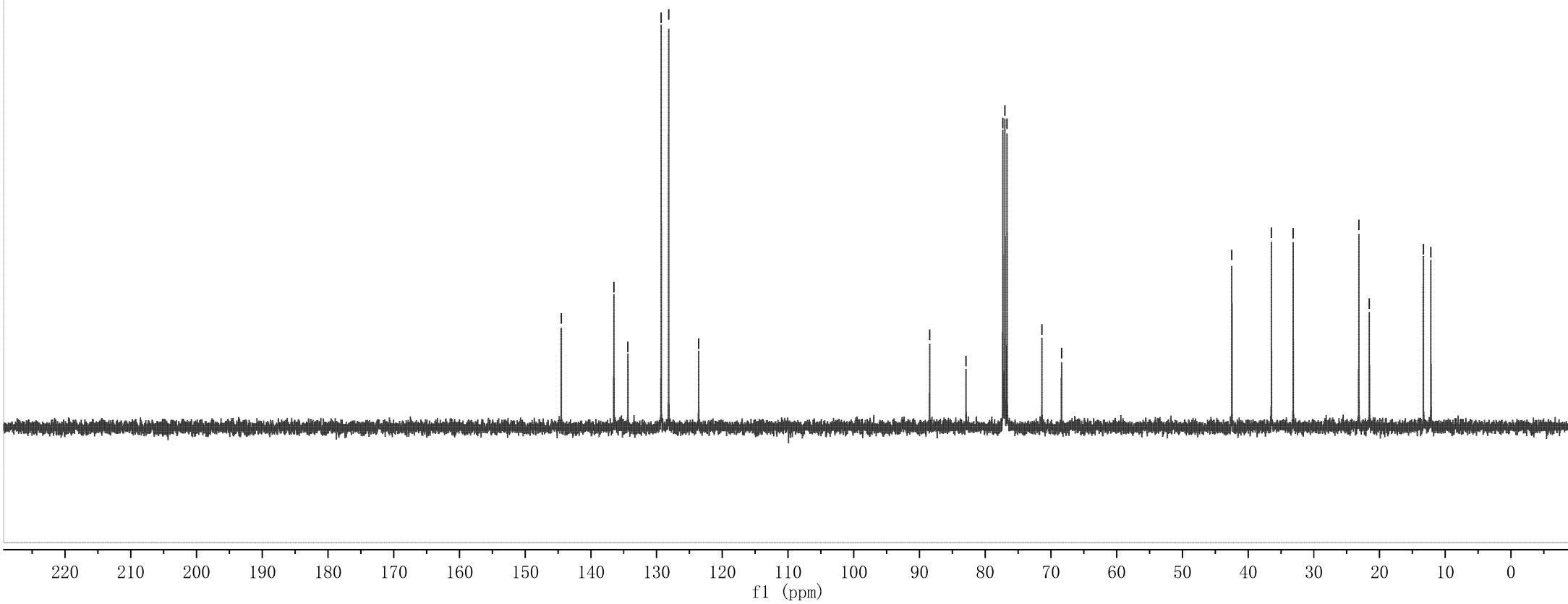
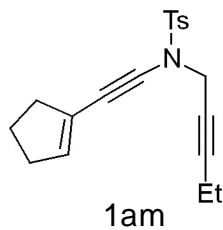


Parameter	Value
1 Title	ZXQ-23-95
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2020-11-22T11:50:48
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-23-95-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	30
6 Acquisition Time	1.3631
7 Acquisition Date	2020-11-22T11:52:07
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.51 136.50 134.37 129.30 128.16 123.60 88.46 82.92 77.32 77.00 76.68 71.37 68.39 42.47 36.46 33.14 23.15 21.56 13.34 12.19





Parameter	Value
1 Title	ZXQ-23-96
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2020-11-22T11:56:44
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

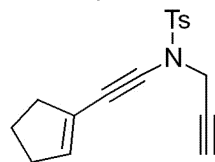
7.842  
7.822

7.349  
7.328

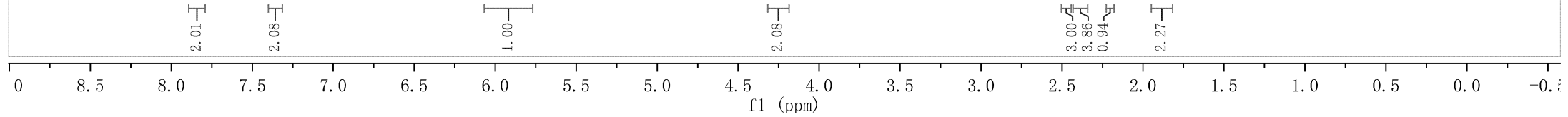
6.011  
6.000  
5.965  
5.960  
5.923  
5.918

4.268  
4.262

2.447  
2.429  
2.423  
2.415  
2.410  
2.404  
2.386  
2.201  
2.195  
2.189  
1.925  
1.906  
1.887  
1.868  
1.850

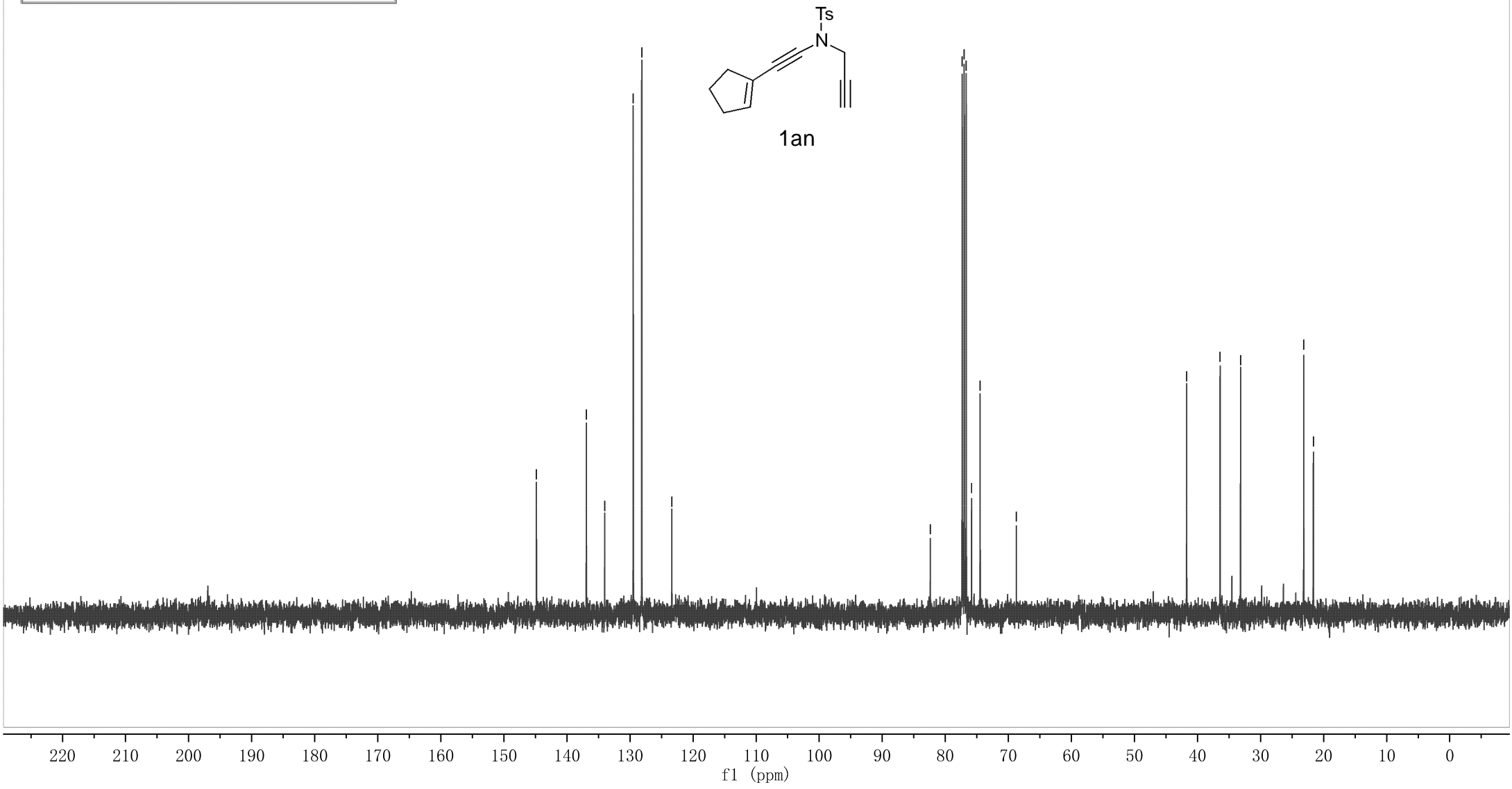
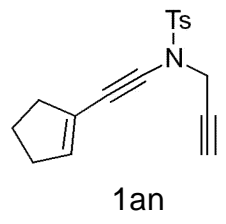


1an

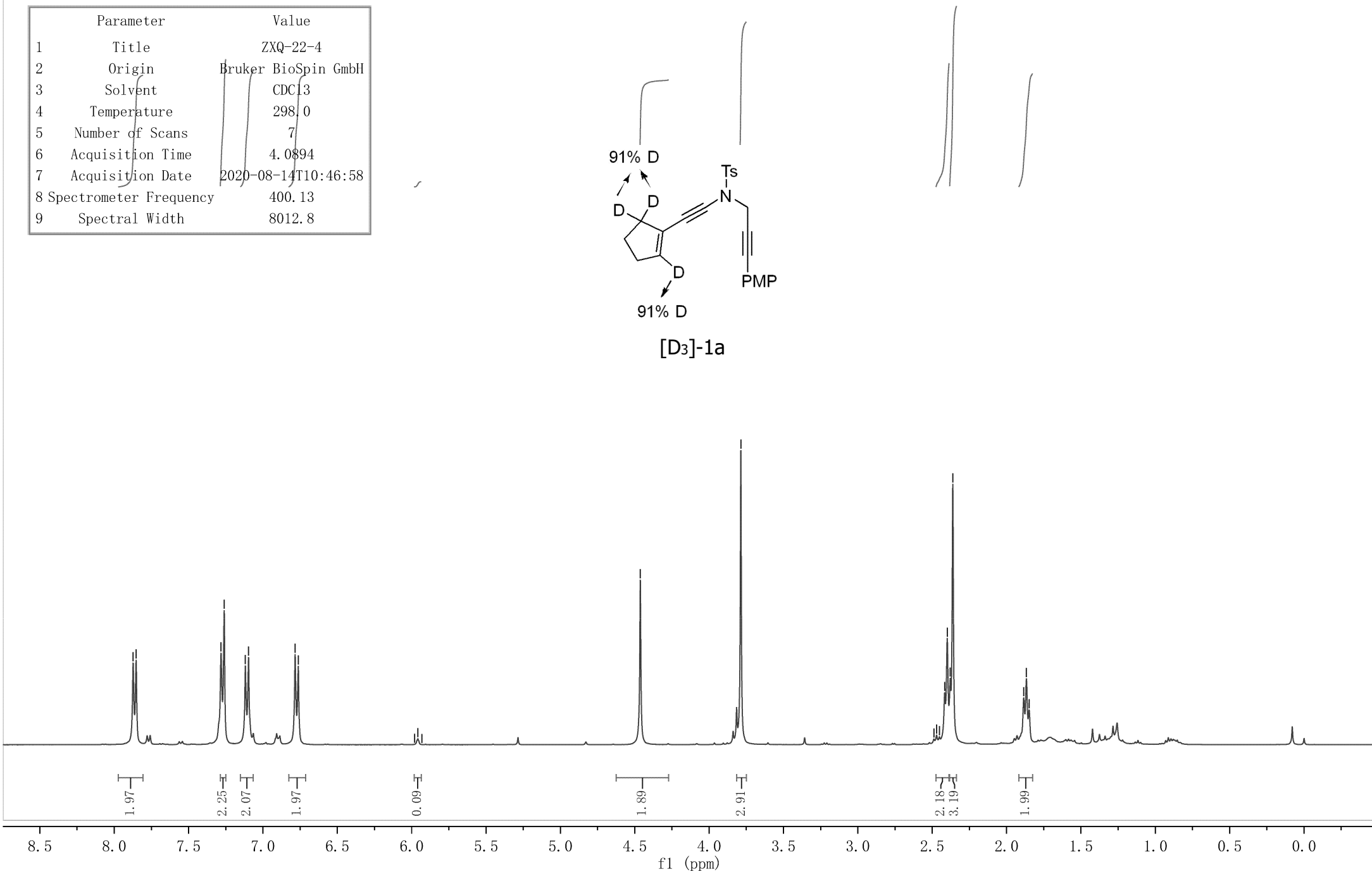
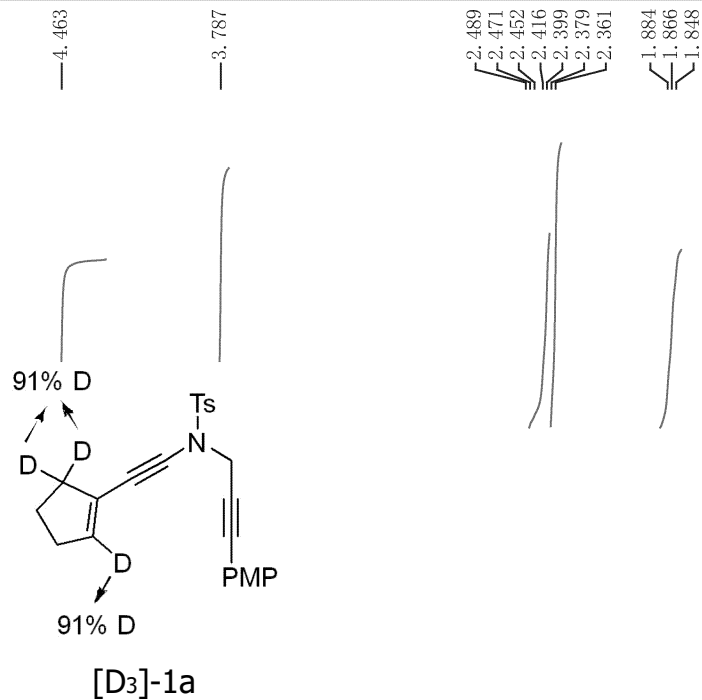


Parameter	Value
1 Title	ZXQ-23-96-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	23
6 Acquisition Time	1.3631
7 Acquisition Date	2020-11-22T11:58:20
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.84  
 136.93  
 134.01  
 129.49  
 128.14  
 123.37  
 82.37  
 77.32  
 77.00  
 76.68  
 74.48  
 68.74  
 41.72  
 36.42  
 33.17  
 23.15  
 21.62

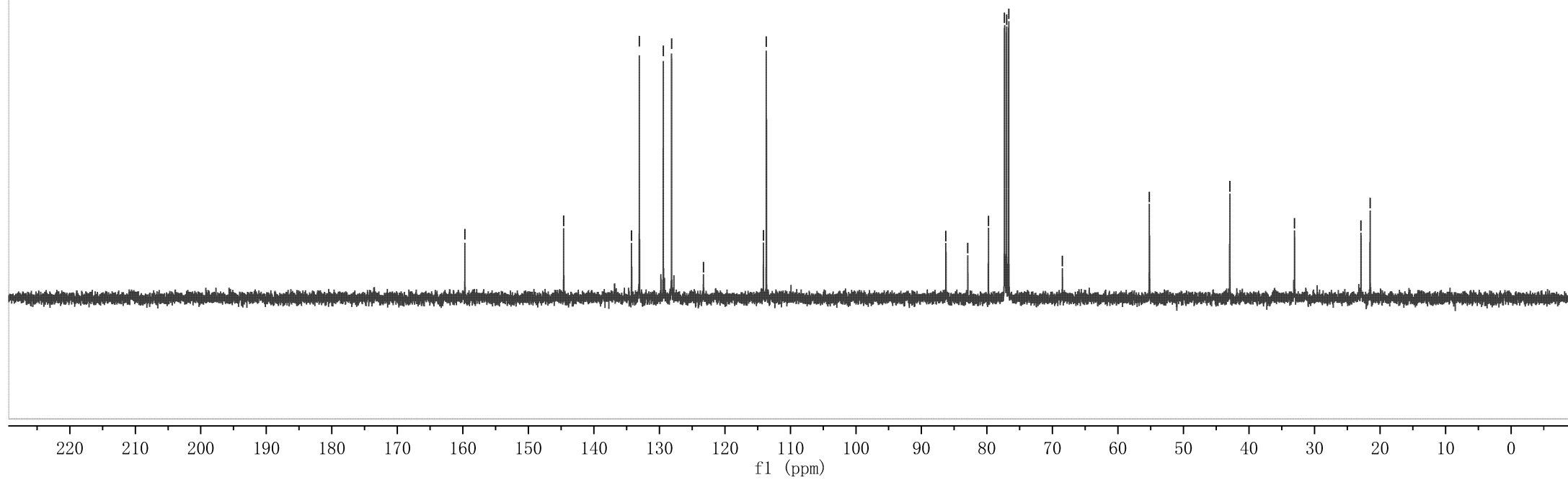
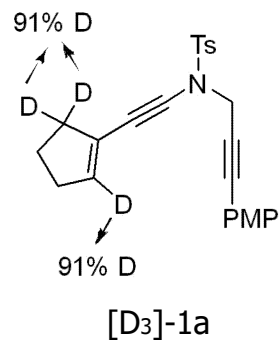


Parameter	Value
1 Title	ZXQ-22-4
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2020-08-14T10:46:58
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-22-4-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	25
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-14T10:48:42
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

159.69 — 144.61 — 134.25 133.06 129.40 128.14 123.27 — 114.11 113.67 — 86.27 82.93 79.77 77.32 77.00 76.68 — 68.49 — 55.21 — 42.93 — 33.05 — 22.90 21.52



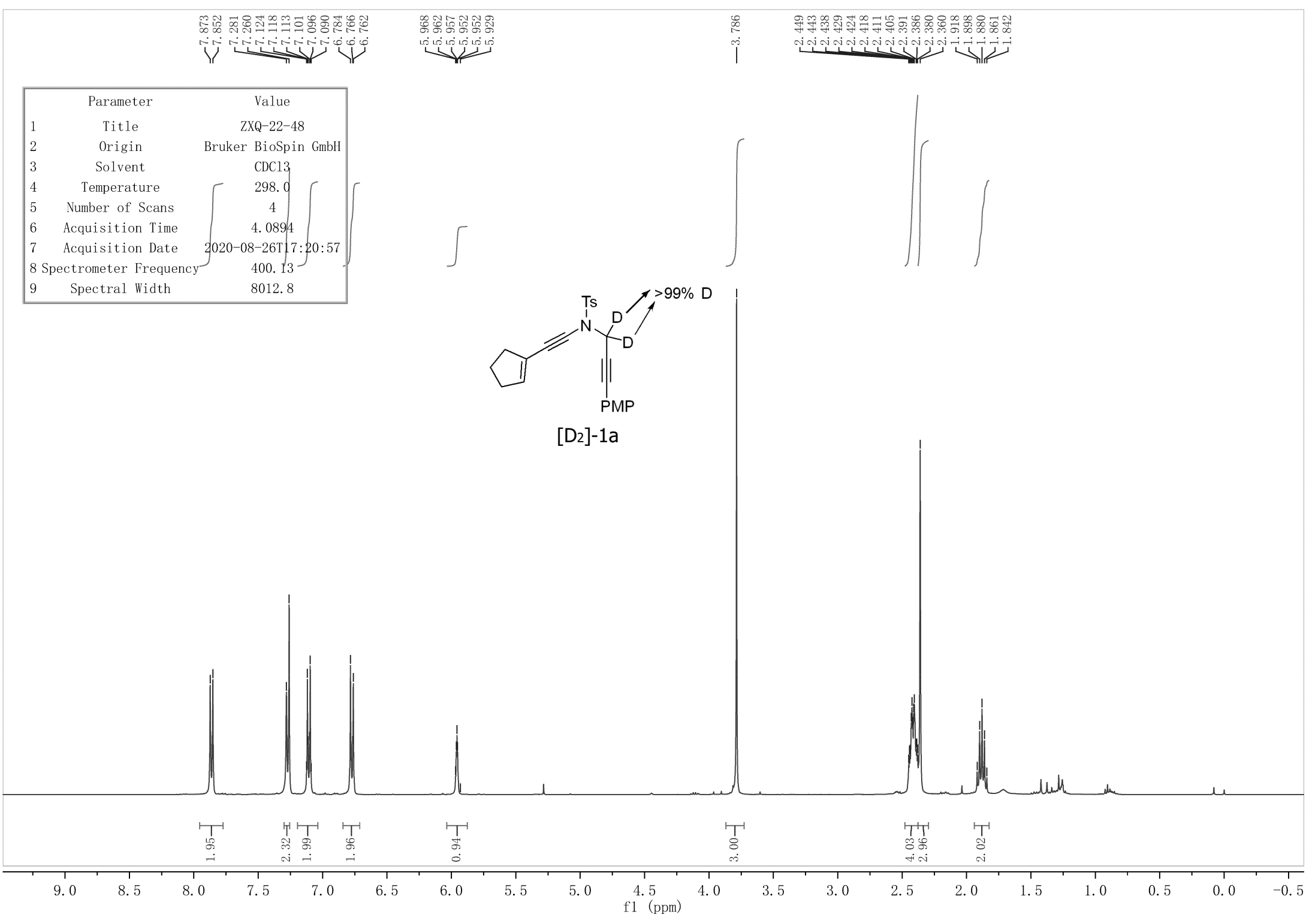
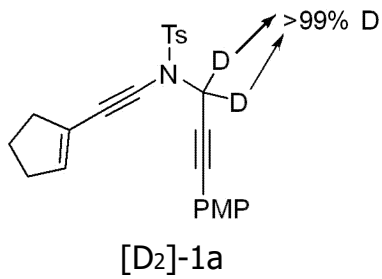
7.873  
7.852  
7.281  
7.124  
7.118  
7.101  
7.096  
6.784  
6.766  
6.762

5.968  
5.962  
5.957  
5.952  
5.929

3.786

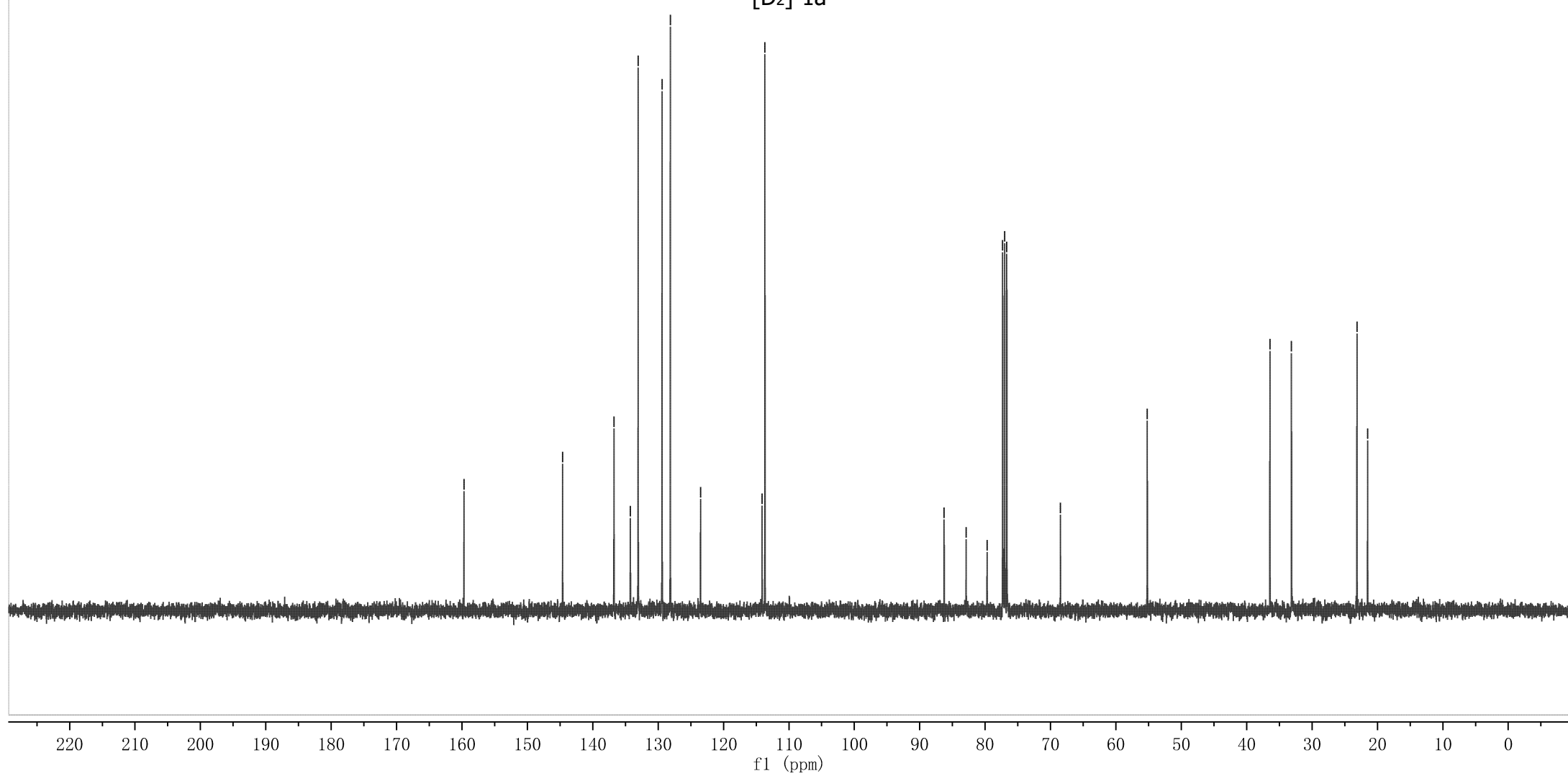
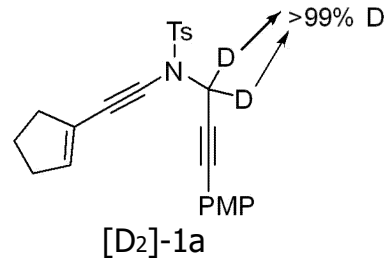
2.449  
2.443  
2.438  
2.429  
2.424  
2.418  
2.411  
2.405  
2.391  
2.386  
2.380  
2.360  
1.918  
1.898  
1.880  
1.861  
1.842

Parameter	Value
1 Title	ZXQ-22-48
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2020-08-26T17:20:57
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-22-48-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	41
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-26T17:22:14
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

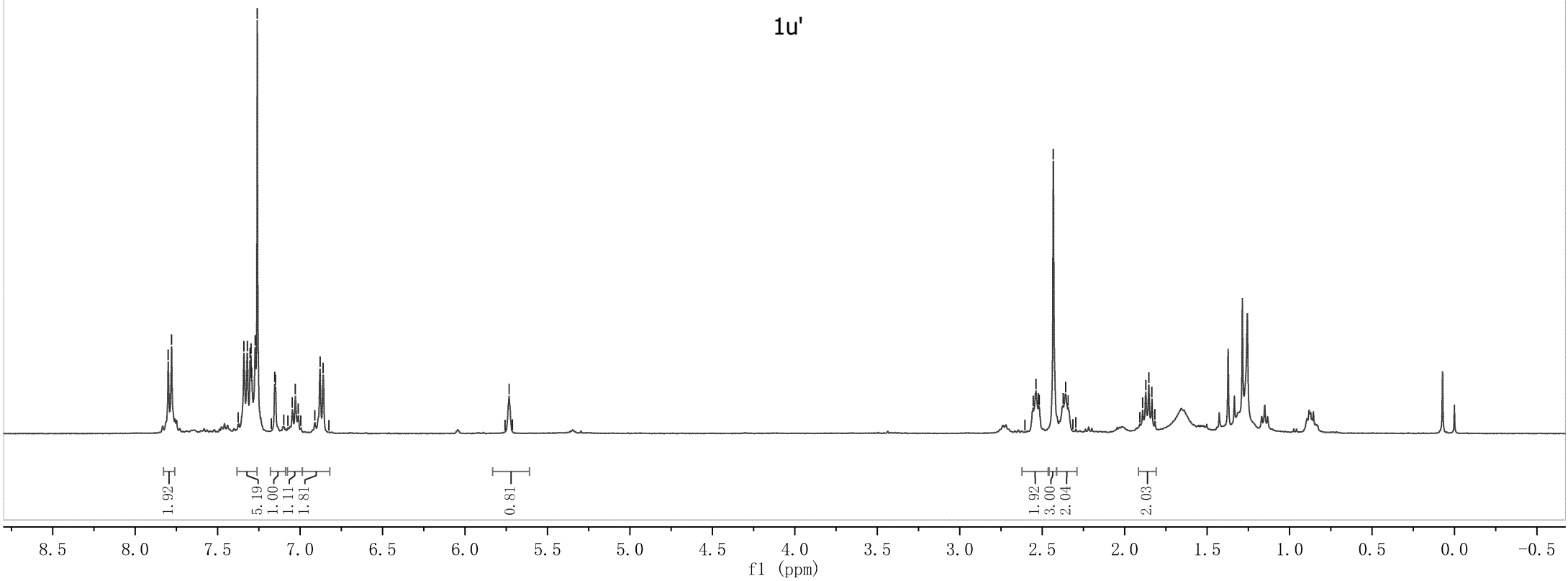
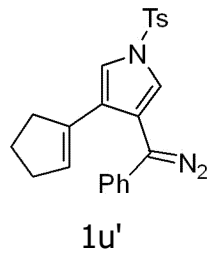
159.69 — 144.61 — 136.75 134.25 133.06 129.40 128.14 123.52 — 114.10 113.67 — 86.27 82.90 79.70 77.32 77.00 76.68 — 68.48 — 55.20 — 36.45 33.15 — 23.14 21.51



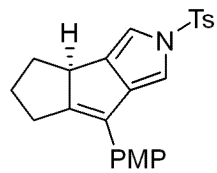
7.800  
7.779  
7.376  
7.340  
7.320  
7.303  
7.297  
7.293  
7.272  
7.259  
7.154  
7.149  
7.099  
7.074  
7.047  
7.028  
7.010  
6.995  
6.910  
6.878  
6.869  
5.732  
5.713

2.604  
2.555  
2.537  
2.522  
2.517  
2.432  
2.373  
2.357  
2.342  
2.314  
2.295  
1.907  
1.891  
1.872  
1.853  
1.834  
1.816

Parameter	Value
1 Title	ZXQ-22-37
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2020-08-24T22:01:29
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-168
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-31T15:36:09
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

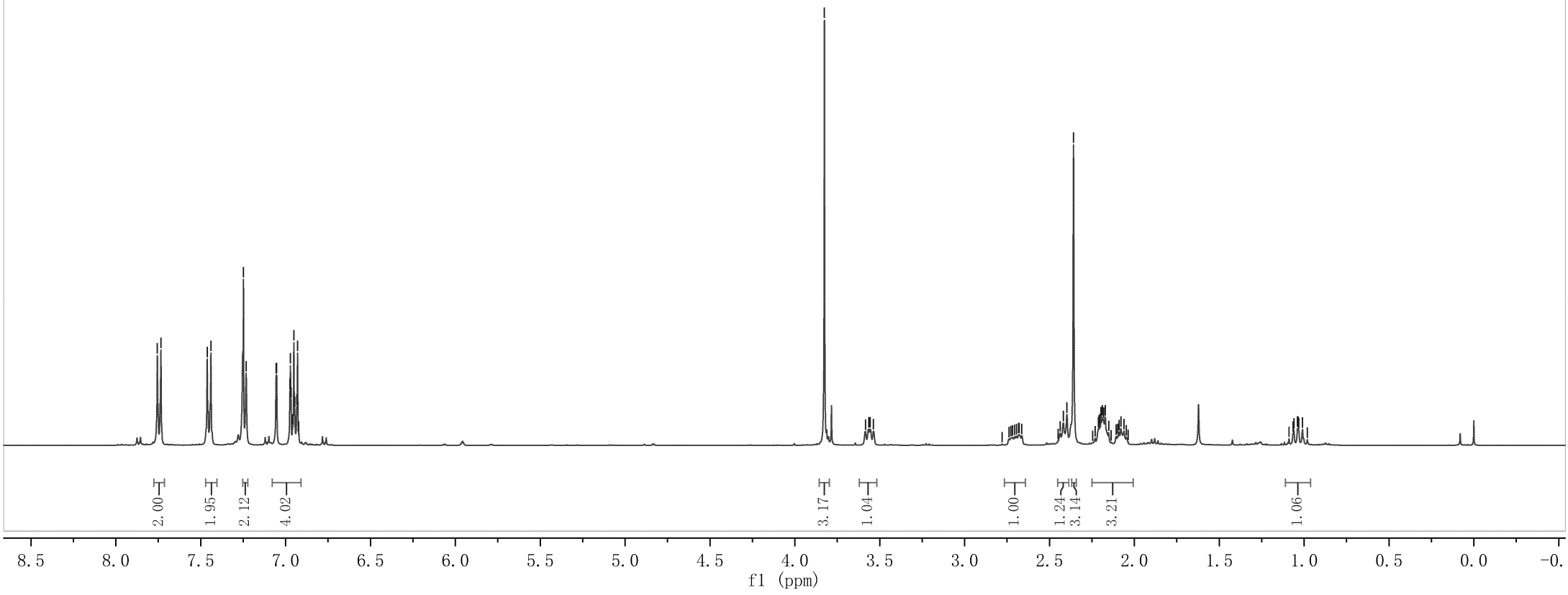


2a

7.755  
7.734  
7.462  
7.440  
7.248  
7.232  
7.056  
7.053  
6.971  
6.968  
6.958  
6.951  
6.946  
6.934  
6.929  
6.922

3.826  
3.584  
3.565  
3.556  
3.537

2.738  
2.727  
2.718  
2.706  
2.695  
2.682  
2.678  
2.663  
2.418  
2.397  
2.358  
2.212  
2.208  
2.203  
2.196  
2.189  
2.181  
2.171  
2.079  
1.889  
1.066  
1.060  
1.039  
1.036  
1.031  
1.009  
0.981





Parameter	Value
1 Title	ZXQ-19-168-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	23
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-31T15:37:42
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.66  
157.77

144.40  
141.50

136.47  
134.92  
129.78  
128.41  
127.42  
127.32  
126.66

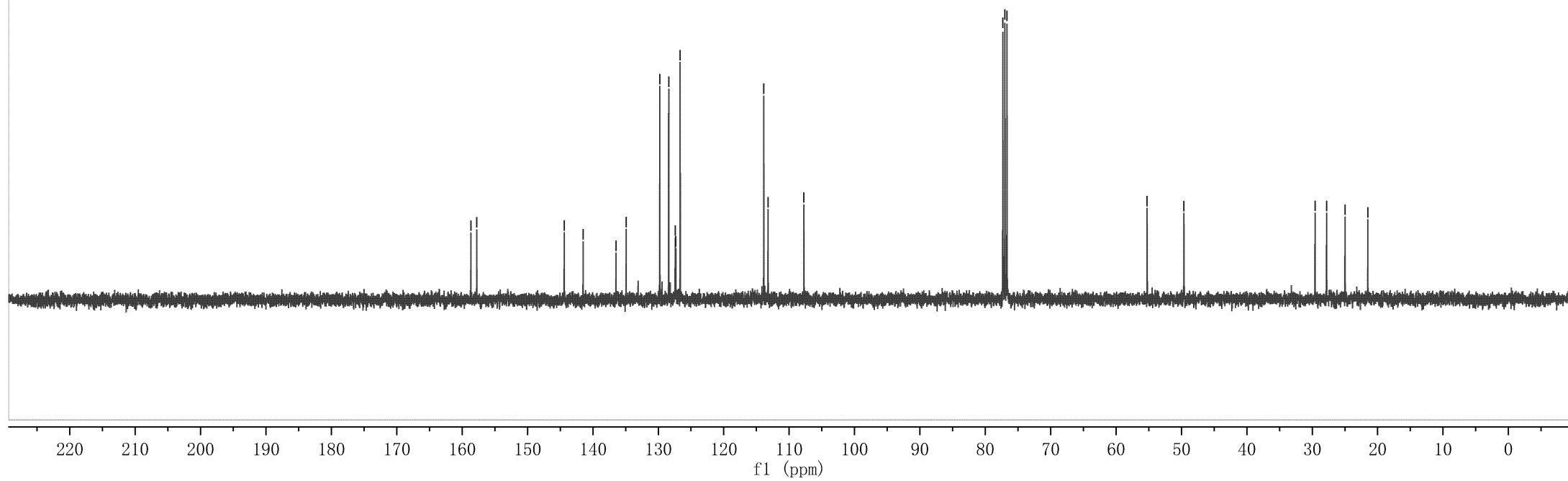
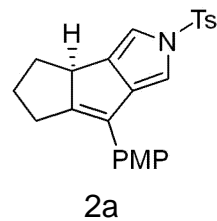
113.87  
113.22  
107.75

77.32  
77.00  
76.68

55.26

49.63

29.57  
27.81  
24.99  
21.50



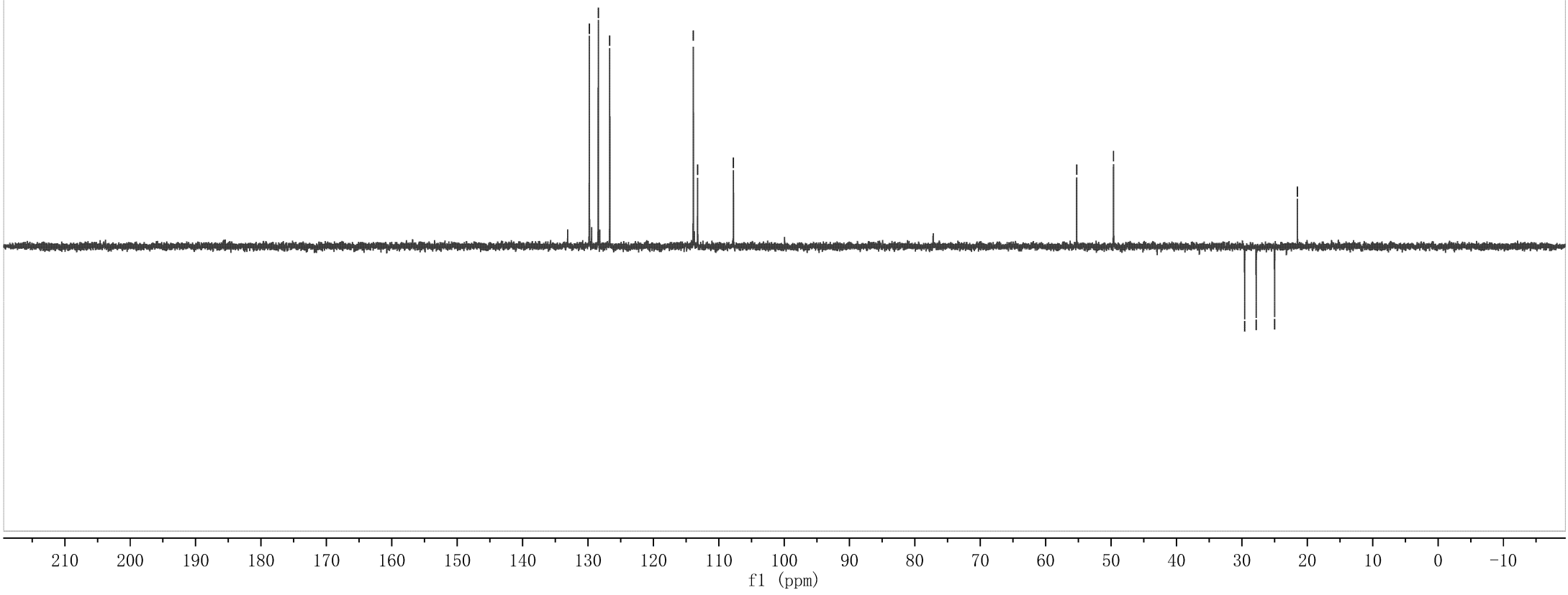
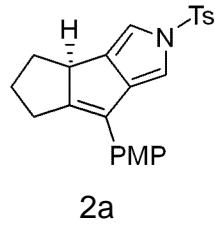
Parameter	Value
1 Title	ZXQ-19-168-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	18
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-31T15:39:28
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

129.79  
128.42  
126.67

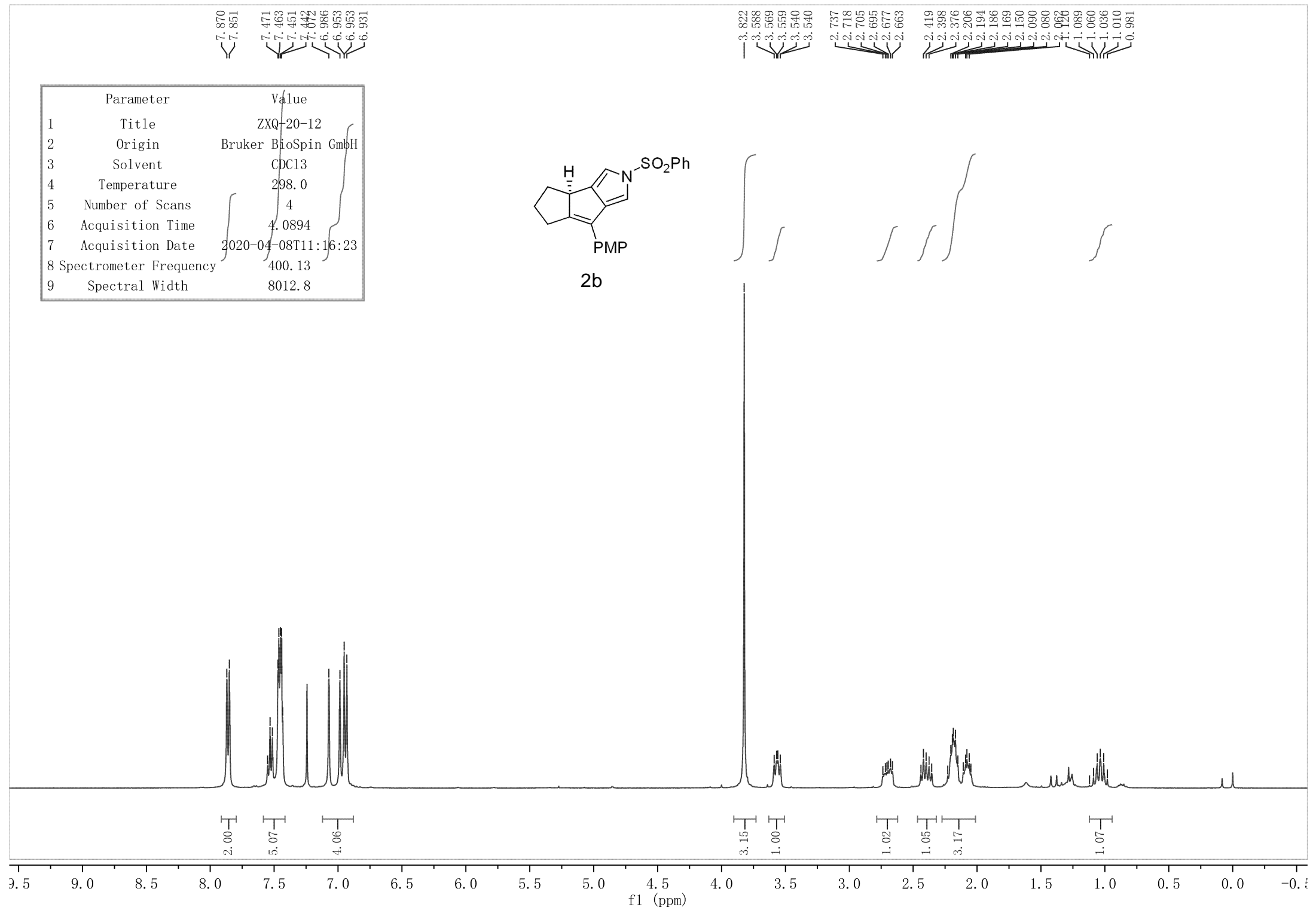
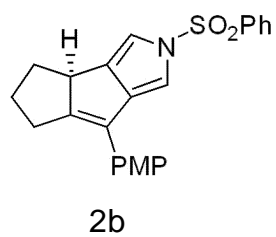
113.88  
113.23  
107.76

55.27  
49.63

29.58  
27.82  
25.00  
21.51



Parameter	Value
1 Title	ZXQ-20-12
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2020-04-08T11:16:23
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.870  
7.851  
7.471  
7.463  
7.451  
7.442  
7.442  
6.986  
6.953  
6.953  
6.931

3.822  
3.588  
3.569  
3.559  
3.540  
3.540  
2.737  
2.718  
2.705  
2.695  
2.677  
2.663  
2.419  
2.398  
2.376  
2.206  
2.194  
2.186  
2.169  
2.150  
2.090  
2.080  
2.062  
2.062  
1.089  
1.060  
1.036  
1.010  
0.981

Parameter	Value
1 Title	ZXQ-20-12-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	24
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-08T11:17:27
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.68  
157.92

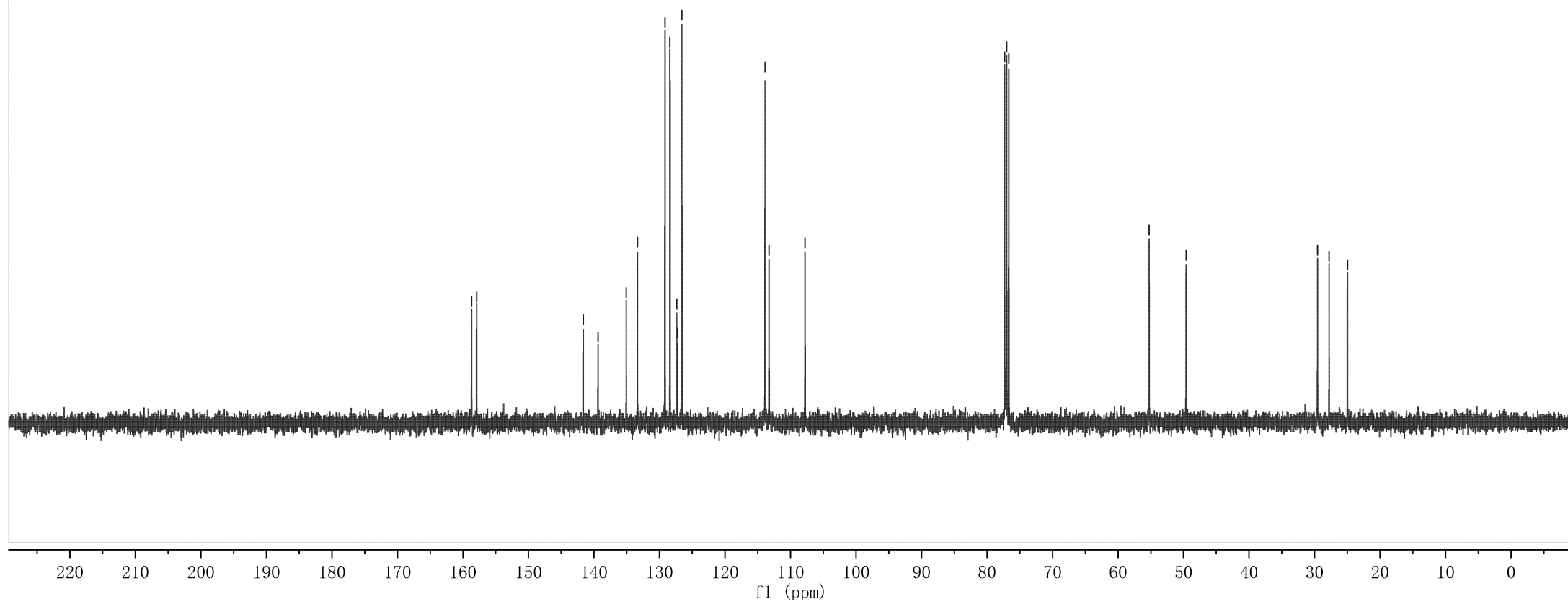
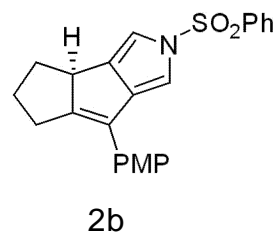
141.65  
139.38  
135.08  
133.36  
129.17  
128.41  
127.36  
127.28  
126.58

113.89  
113.28  
107.78

77.32  
77.00  
76.68

55.25  
49.61

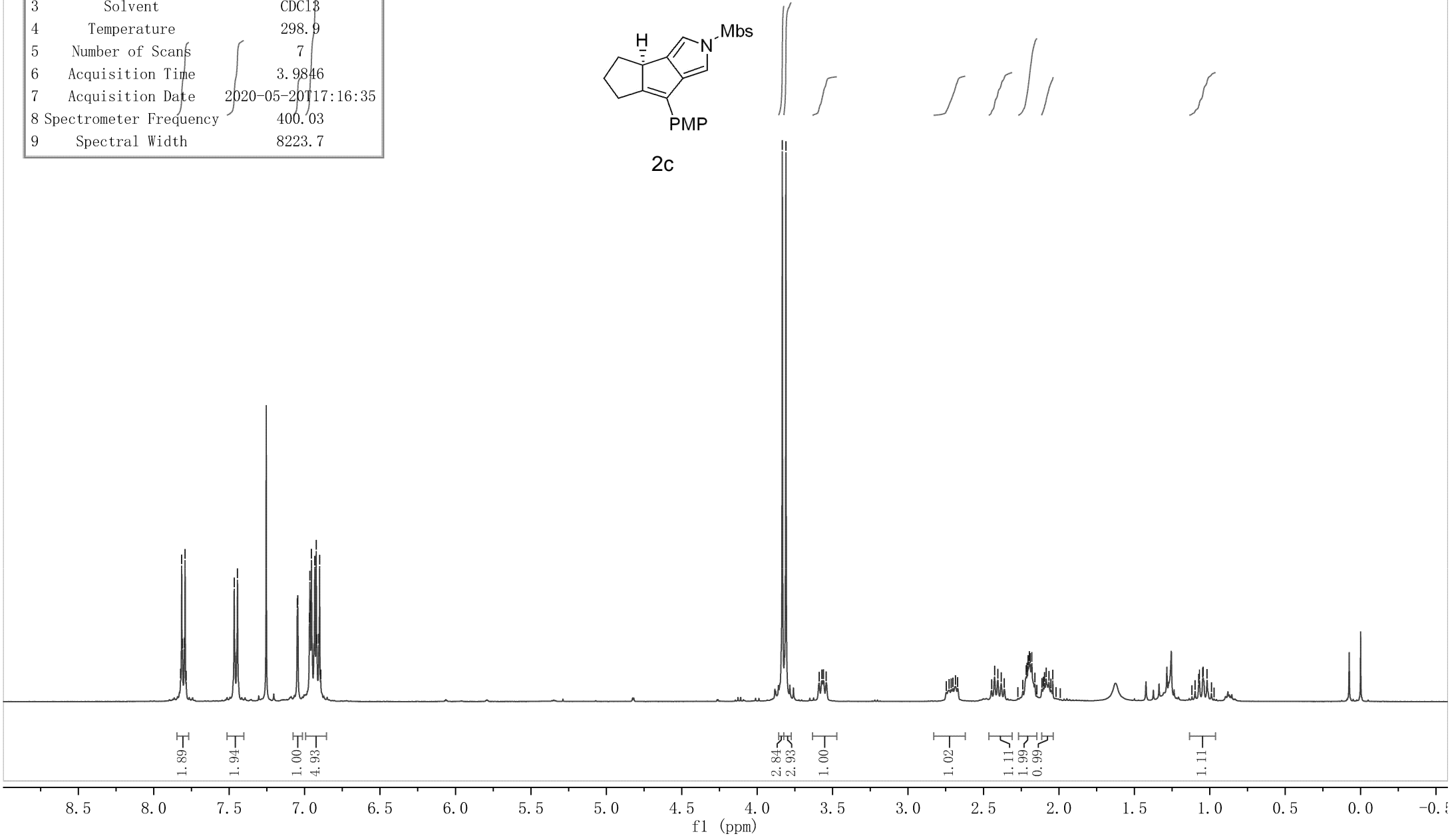
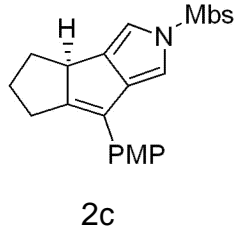
29.55  
27.79  
24.99



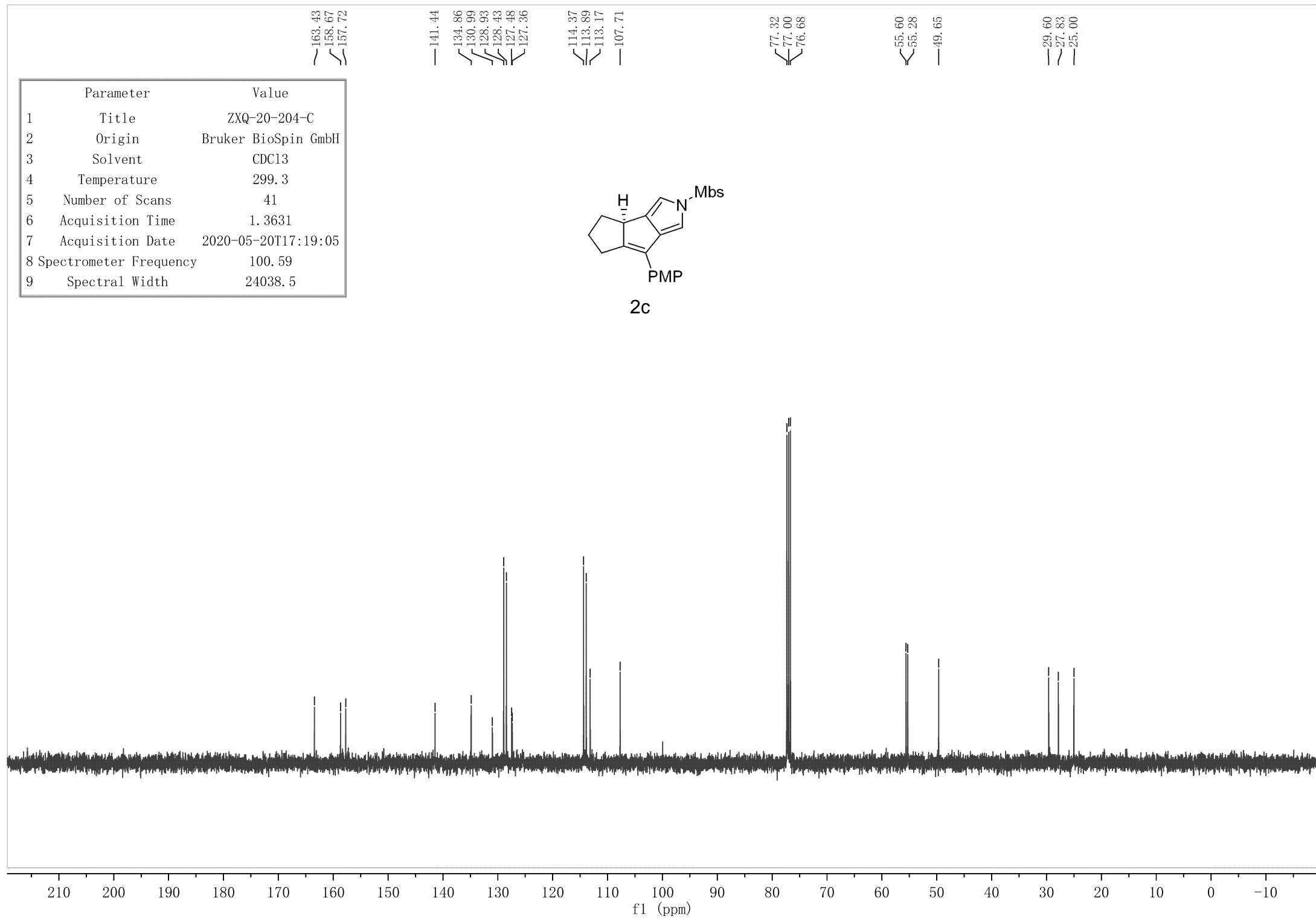
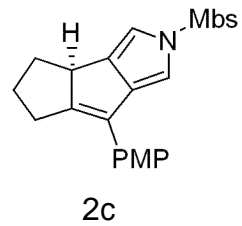
7.822  
7.815  
7.810  
7.797  
7.792  
7.785  
7.467  
7.445  
7.048  
7.045  
6.968  
6.965  
6.962  
6.955  
6.933  
6.923  
6.918  
6.906  
6.901  
6.893

3.833  
3.810  
3.590  
3.570  
3.561  
3.543  
2.746  
2.728  
2.715  
2.703  
2.686  
2.671  
2.426  
2.405  
2.217  
2.211  
2.204  
2.196  
2.190  
2.180  
2.085  
2.066  
1.118  
1.097  
1.074  
1.068  
1.047  
1.044  
1.018  
0.989  
0.972

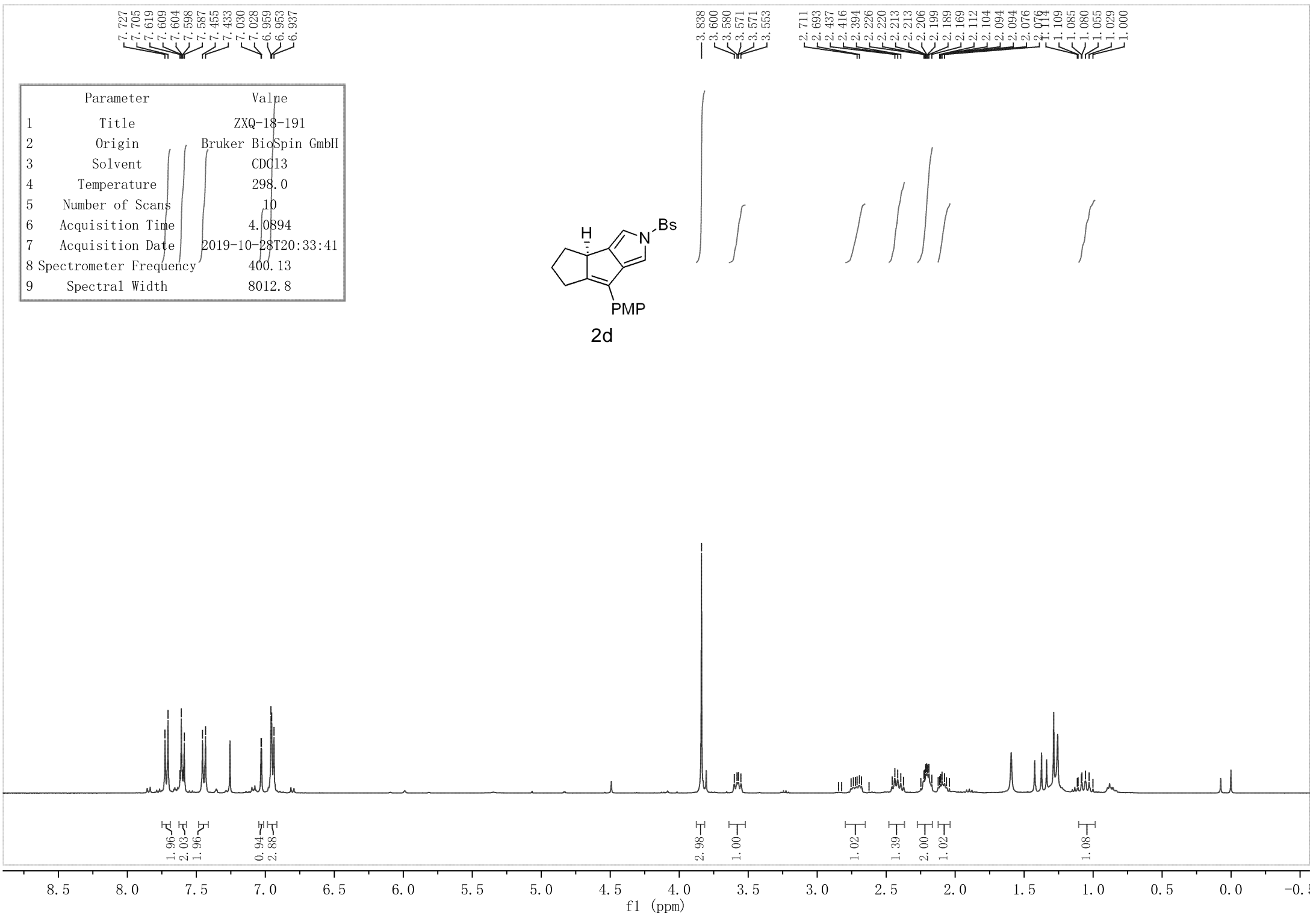
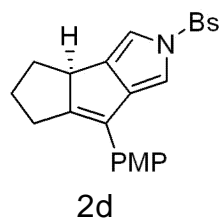
Parameter	Value
1 Title	ZXQ-20-204
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.9
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-05-20T17:16:35
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-20-204-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.3
5 Number of Scans	41
6 Acquisition Time	1.3631
7 Acquisition Date	2020-05-20T17:19:05
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

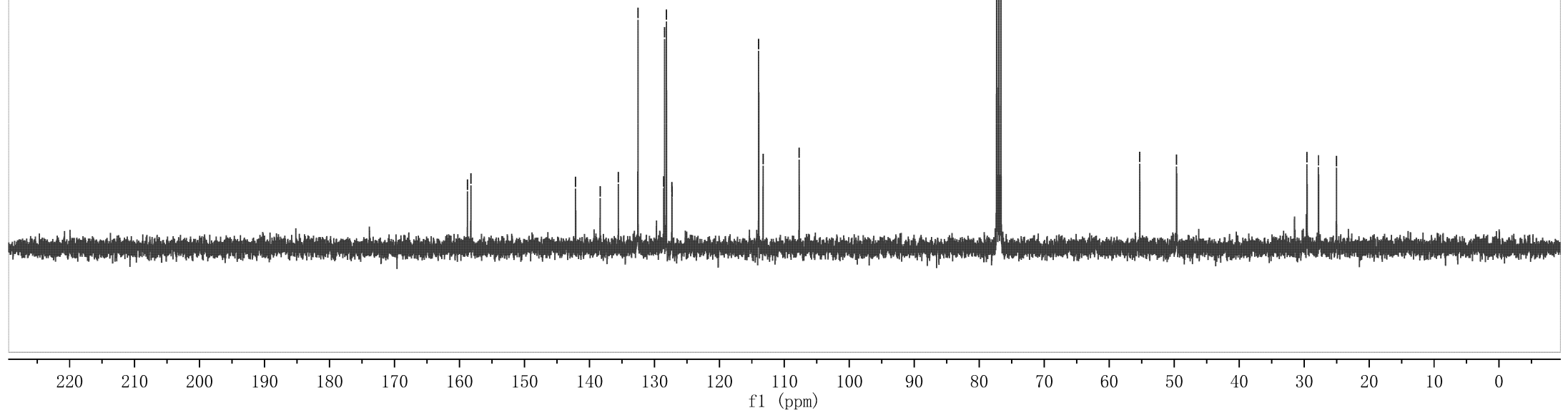
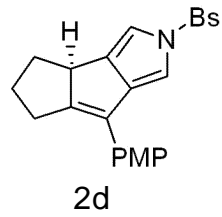


Parameter	Value
1 Title	ZXQ-18-191
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2019-10-28T20:33:41
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



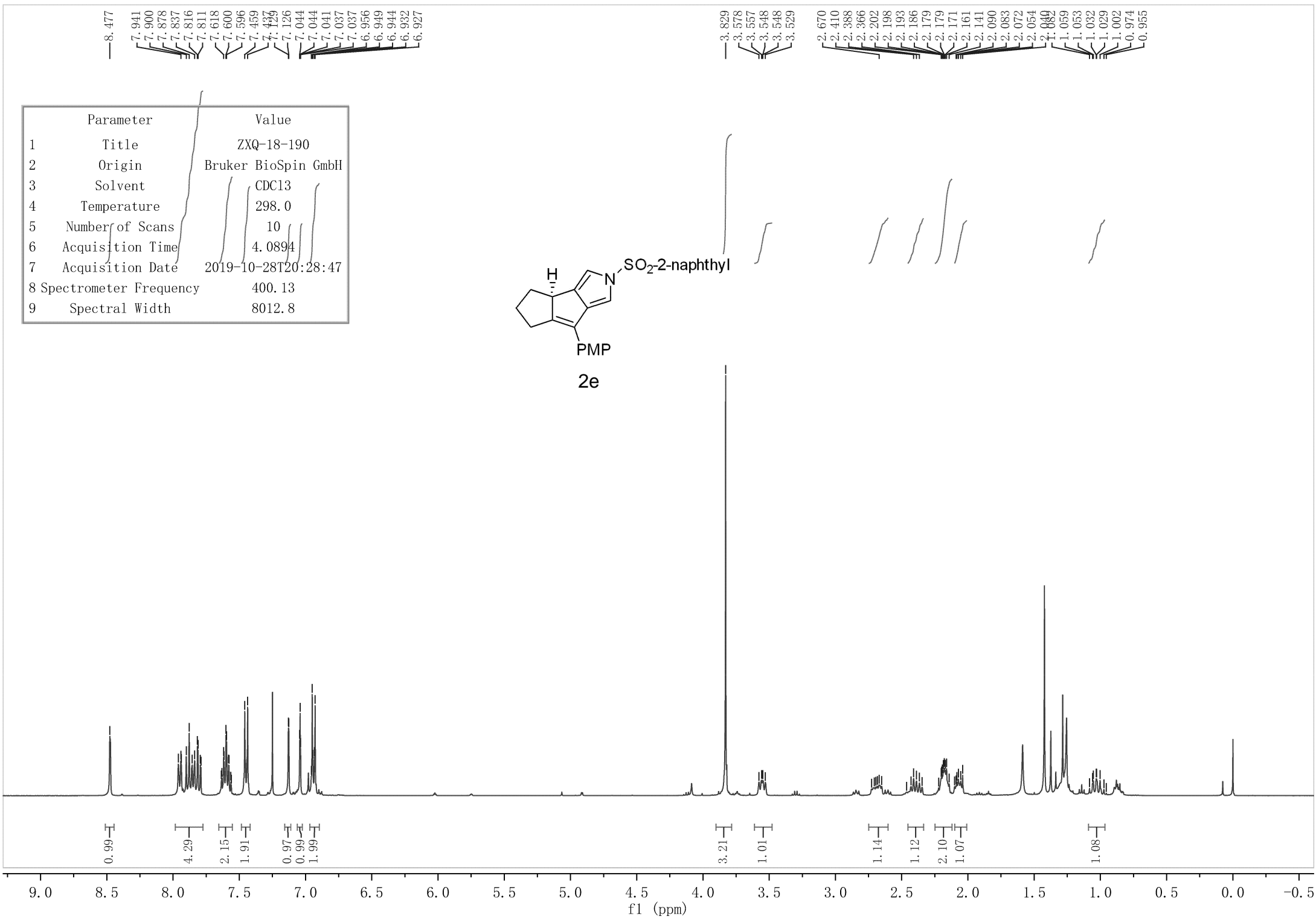
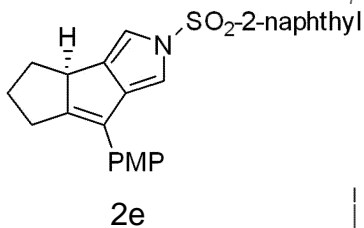
Parameter	Value
1 Title	ZXQ-18-191-C-
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	102
6 Acquisition Time	1.3631
7 Acquisition Date	2019-10-28T20:37:15
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.77  
 156.24  
 142.13  
 138.34  
 135.55  
 132.53  
 128.57  
 128.44  
 128.14  
 127.31  
 127.27  
 113.95  
 113.27  
 107.72  
 77.32  
 77.00  
 76.68  
 55.30  
 49.63  
 29.56  
 27.79  
 25.02



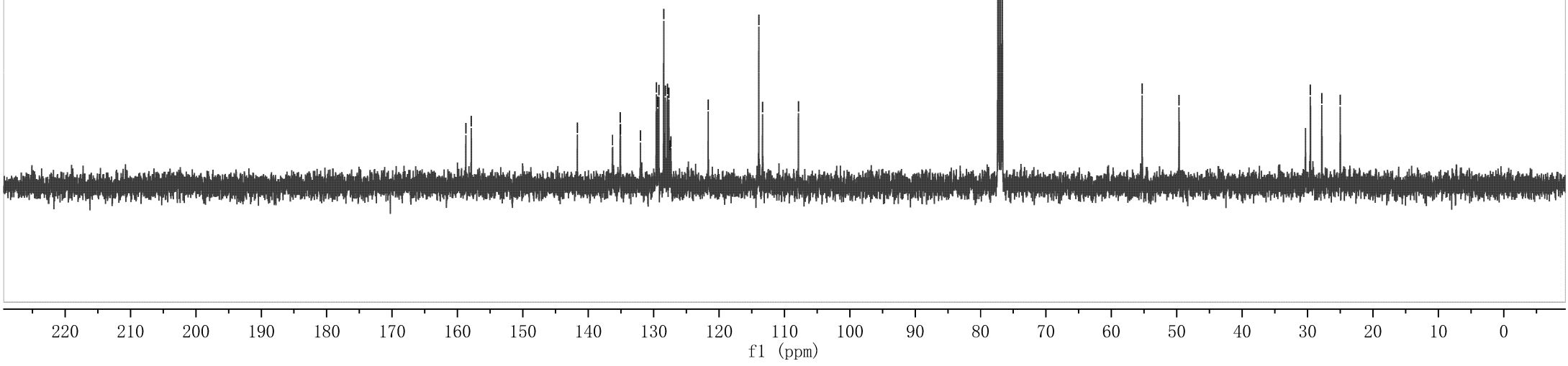
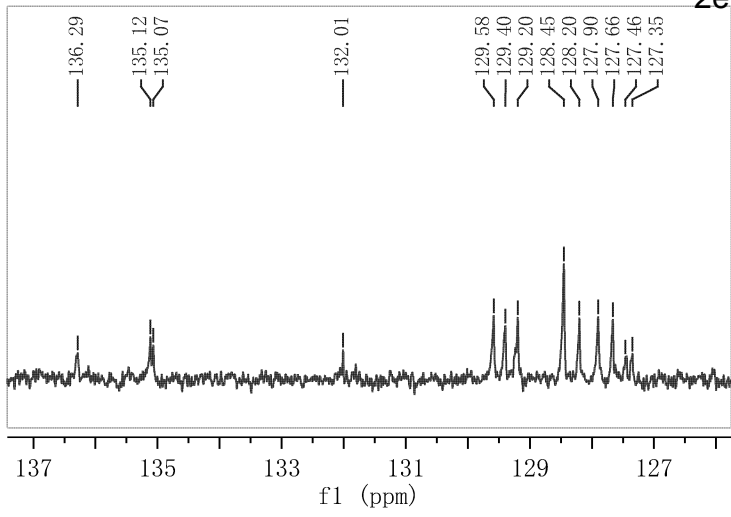
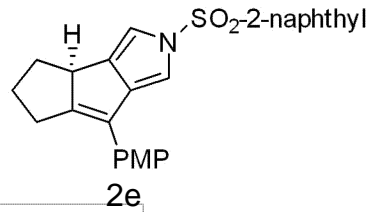


Parameter	Value
1 Title	ZXQ-18-190
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2019-10-28T20:28:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-18-190-C-
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	131
6 Acquisition Time	1.3631
7 Acquisition Date	2019-10-28T20:44:02
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.71 157.88 141.66 129.58 129.40 129.20 128.45 128.20 127.90 127.66 121.65 113.91 113.33 107.85 77.32 77.00 76.68 55.30 49.64 29.57 27.81 24.99



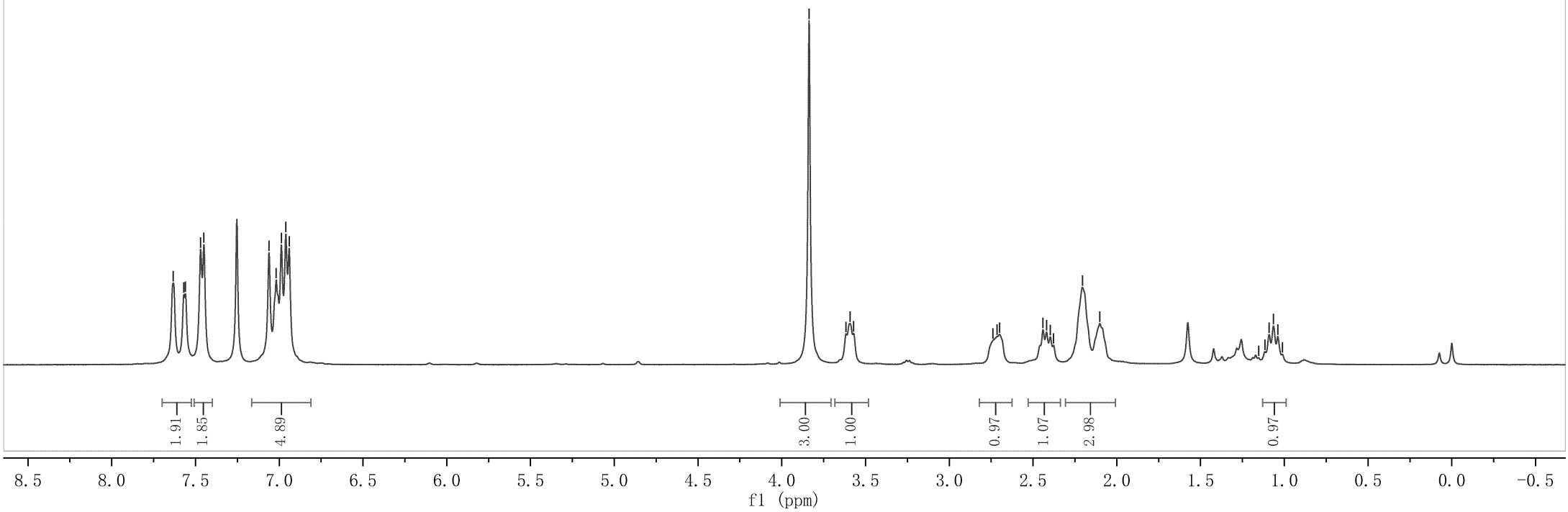
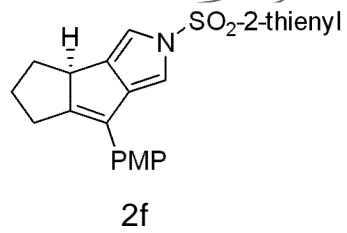
7.633  
7.569  
7.560  
7.469  
7.450  
7.061  
7.018  
6.987  
6.961  
6.941

3.837  
3.617  
3.591  
3.572

2.739  
2.715  
2.700  
2.441  
2.420  
2.420  
2.397  
2.378  
2.205  
2.205  
2.102

1.153  
1.116  
1.090  
1.090  
1.064  
1.039  
1.012

Parameter	Value
1 Title	ZXQ-20-7
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2020-04-04T18:19:54
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-20-7-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	72
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-04T18:21:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.74  
158.20

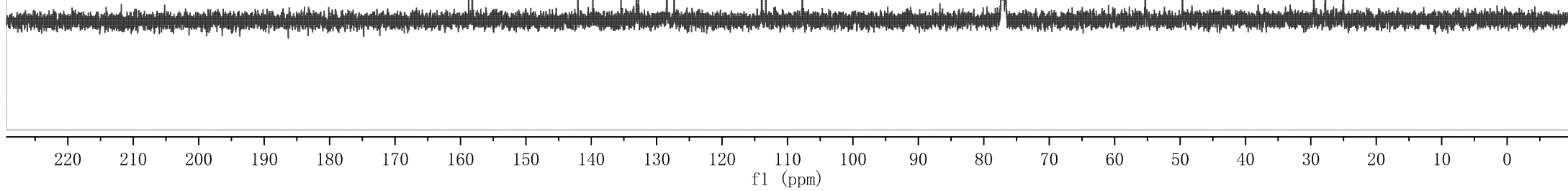
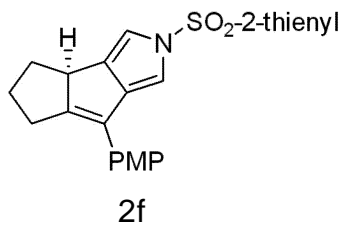
142.03  
139.77  
135.45  
133.06  
132.77  
128.45  
127.33

113.93  
113.33  
107.75

77.32  
77.00  
76.68

55.30  
49.63

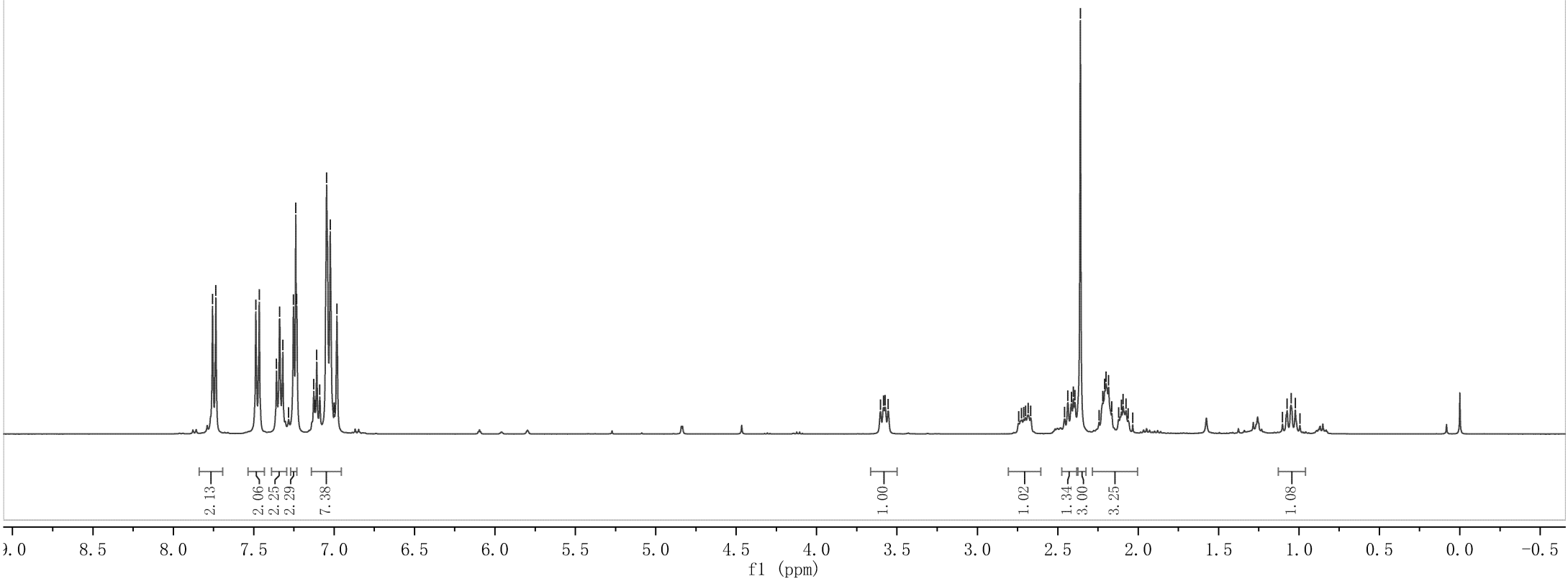
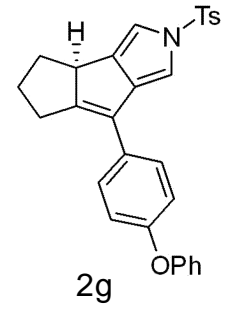
29.55  
27.81  
25.05



7.756  
7.735  
7.487  
7.465  
7.359  
7.359  
7.339  
7.339  
7.319  
7.283  
7.253  
7.239  
7.233  
7.233  
7.233  
7.127  
7.118  
7.108  
7.090  
7.047  
7.024  
7.000  
6.983

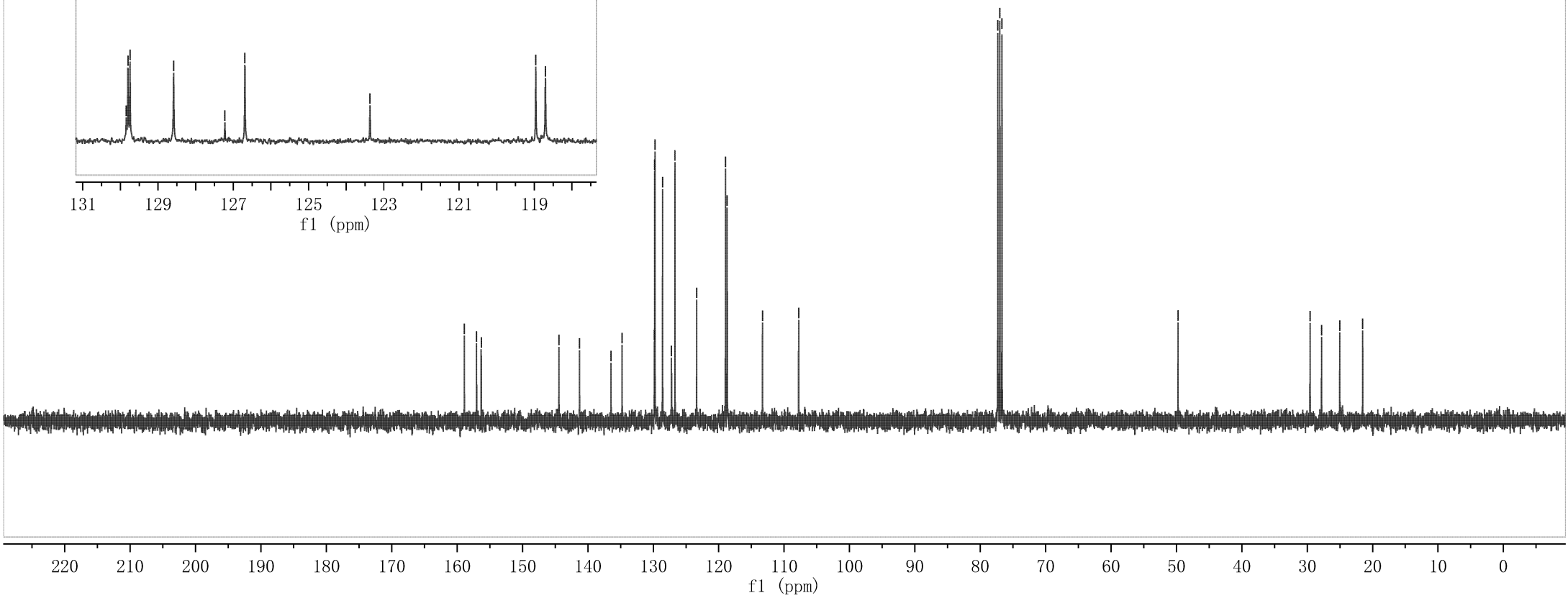
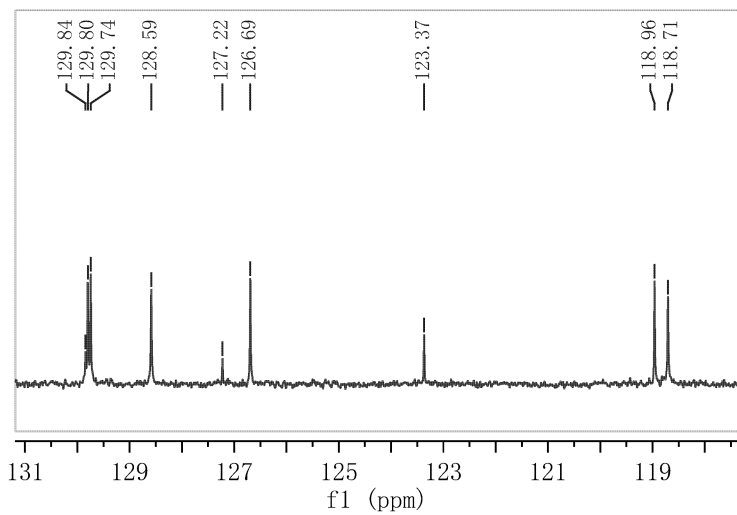
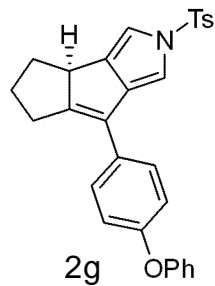
3.603  
3.583  
3.574  
3.555  
2.743  
2.726  
2.711  
2.701  
2.684  
2.668  
2.437  
2.416  
2.403  
2.394  
2.360  
2.221  
2.208  
2.200  
2.184  
2.164  
2.104  
2.094  
2.076  
1.074  
1.049  
1.023  
0.994

Parameter	Value
1 Title	ZXQ-19-69
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-03T16:33:17
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

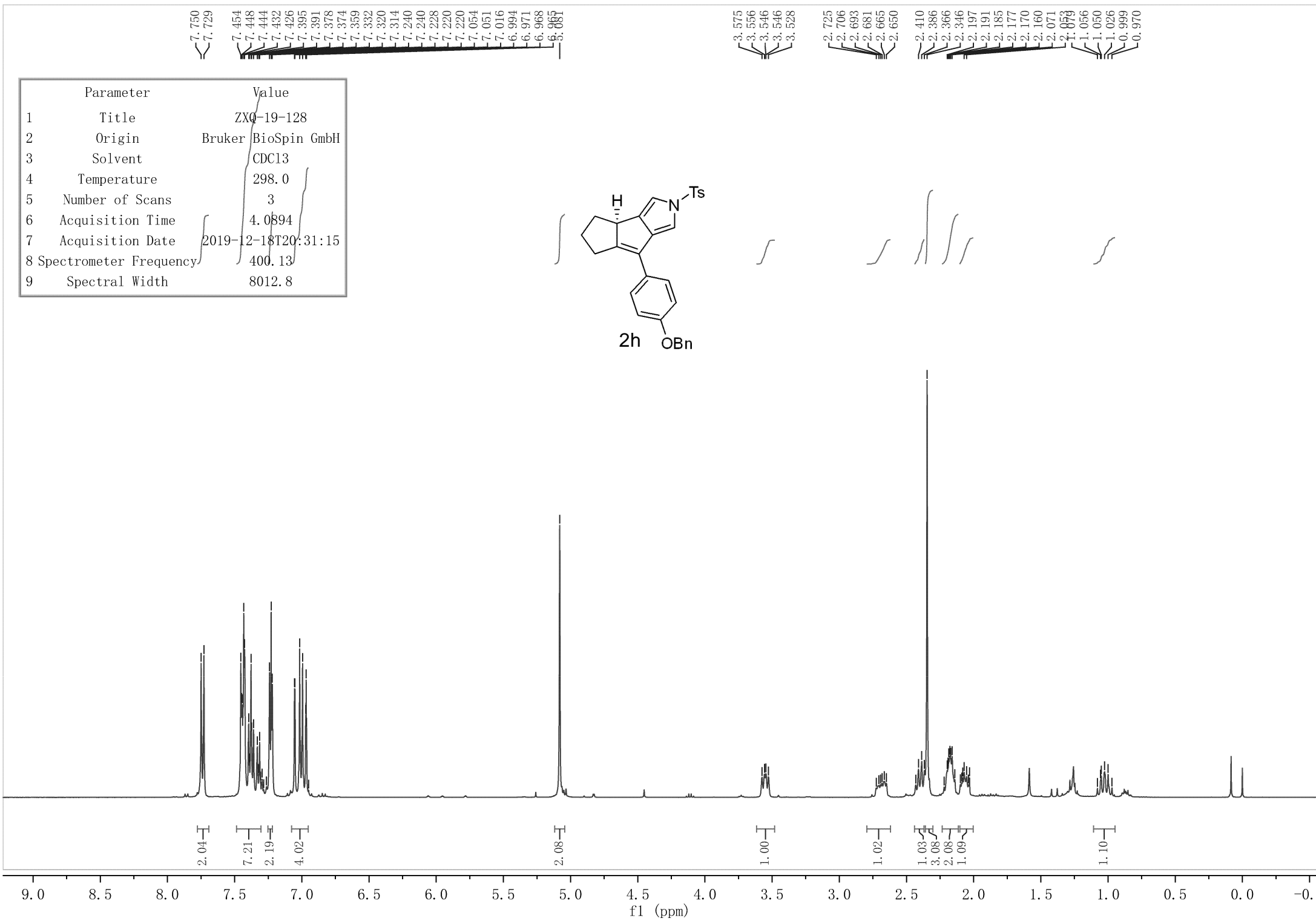
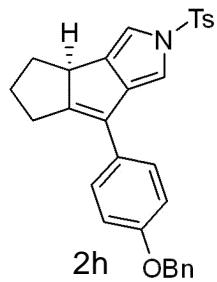


Parameter	Value
1 Title	ZXQ-19-69-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	18
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-03T16:34:42
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.90 157.03 156.31 144.43 141.29 136.47 134.77 129.80 129.74 129.74 128.59 126.69 123.37 118.96 118.71 113.30 107.77 77.32 77.00 76.68 49.76 29.57 27.81 25.03 21.52

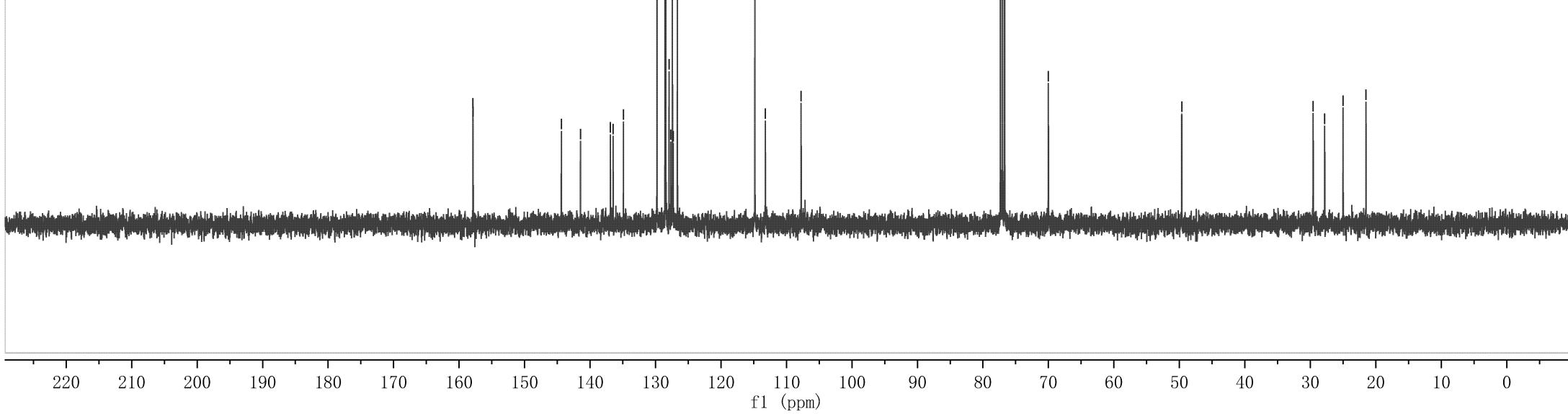
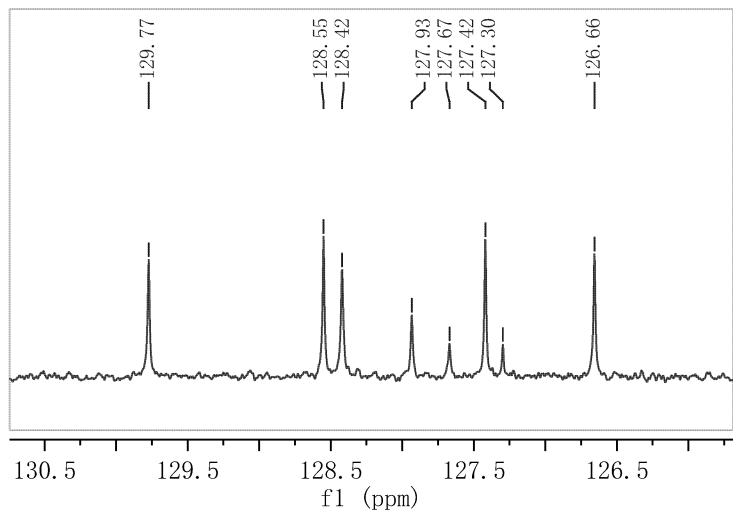
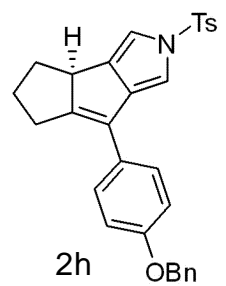


Parameter	Value
1 Title	ZXQ-19-128
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	3
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-18T20:31:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



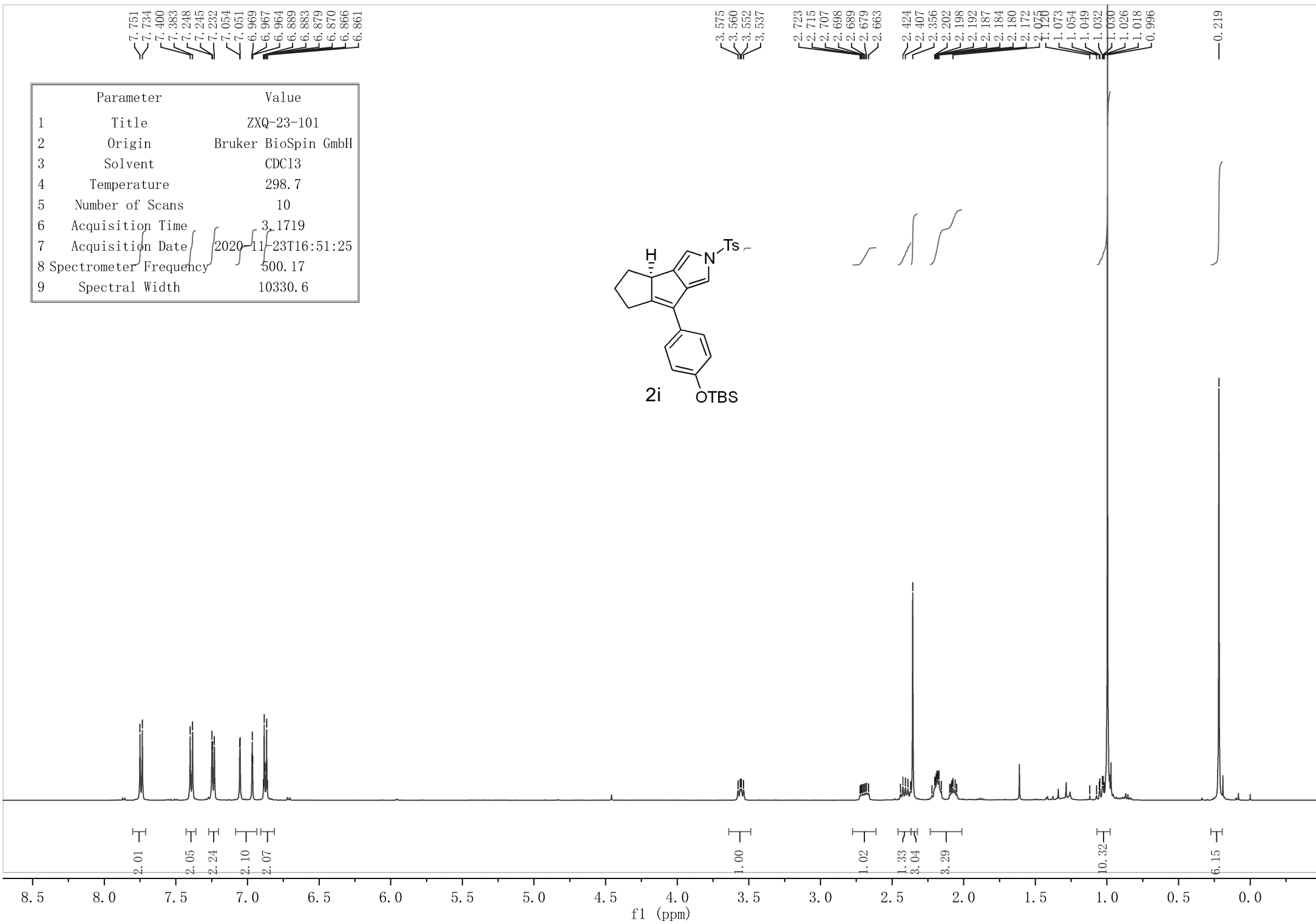
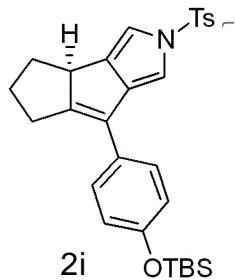
Parameter	Value
1 Title	ZXQ-19-128-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	15
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-18T20:32:13
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

157.88  
157.86  
144.38  
141.46  
136.89  
136.47  
134.90  
129.77  
128.55  
128.42  
127.93  
127.67  
127.42  
126.66  
113.22  
107.76  
77.32  
77.00  
76.68  
70.00  
49.64  
29.57  
27.81  
25.00  
21.50



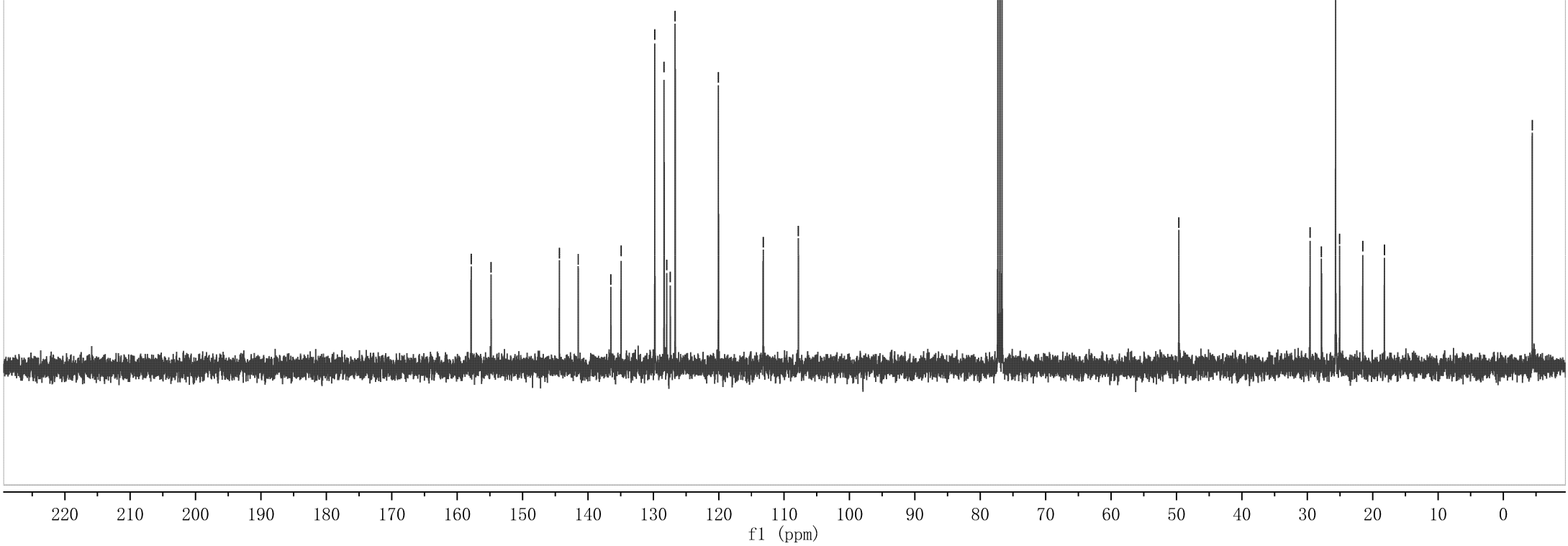
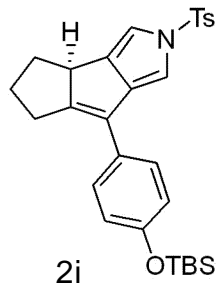


Parameter	Value
1 Title	ZXQ-23-101
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.7
5 Number of Scans	10
6 Acquisition Time	3_1719
7 Acquisition Date	2020-11-23T16:51:25
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6

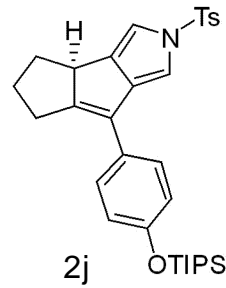


Parameter	Value
1 Title	ZXQ-23-101-1-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	21
6 Acquisition Time	1.3631
7 Acquisition Date	2020-11-26T14:16:13
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

157.87 154.81 144.37 141.49 136.50 134.93 129.78 128.35 127.95 127.41 126.66 120.05 113.20 107.82 77.32 77.00 76.68 49.64 29.58 27.83 25.66 25.05 21.51 18.20 -4.41



Parameter	Value
1 Title	ZXQ-19-20
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-18T16:05:46
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.754  
7.733  
7.394  
7.373  
7.258  
7.253  
7.238  
7.052  
7.049  
6.967  
6.964  
6.961  
6.931  
6.924  
6.919  
6.907  
6.902  
6.895

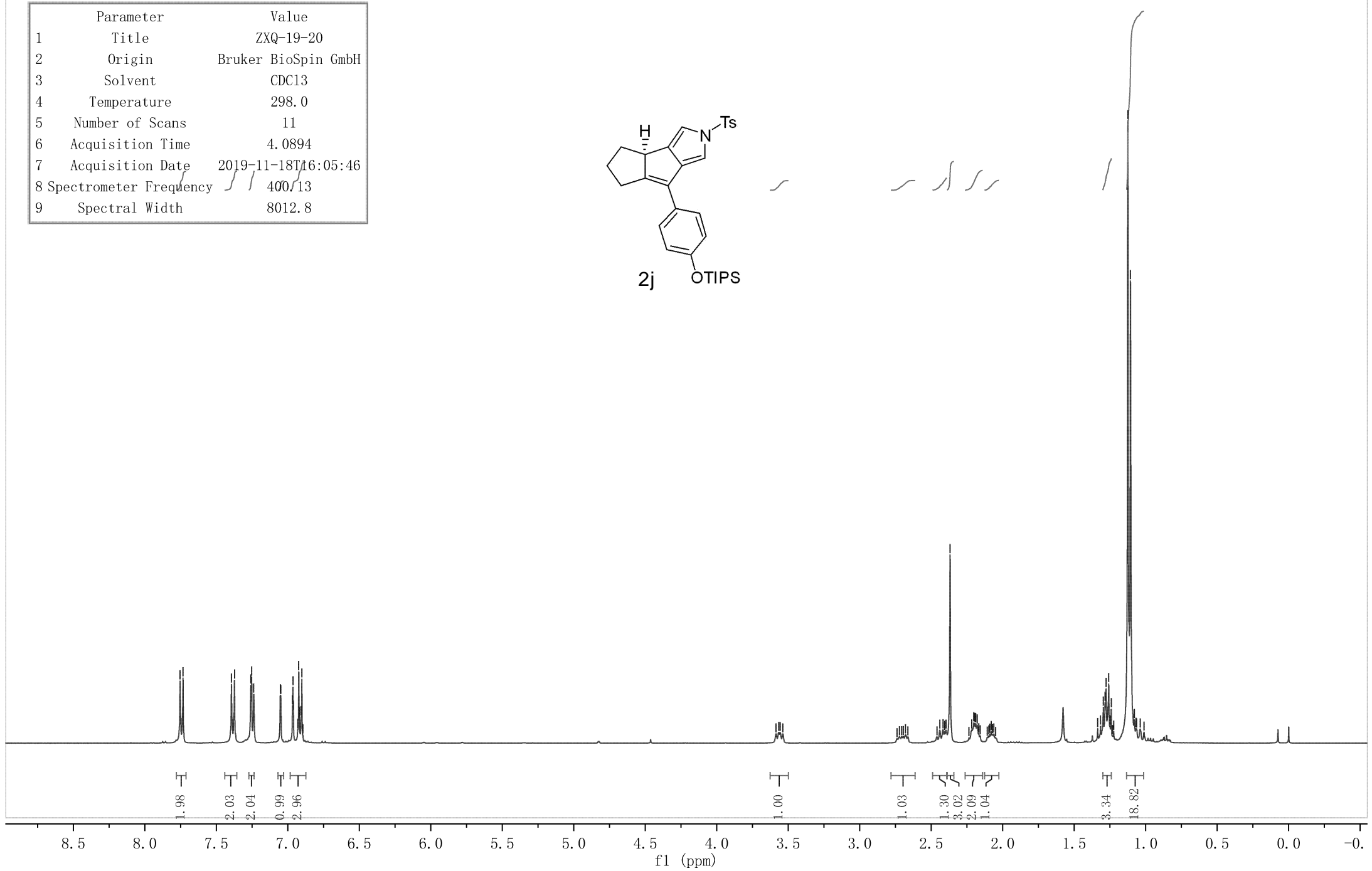
3.586  
3.586  
3.566  
3.557  
3.538

2.739  
2.722  
2.707  
2.695  
2.679  
2.663

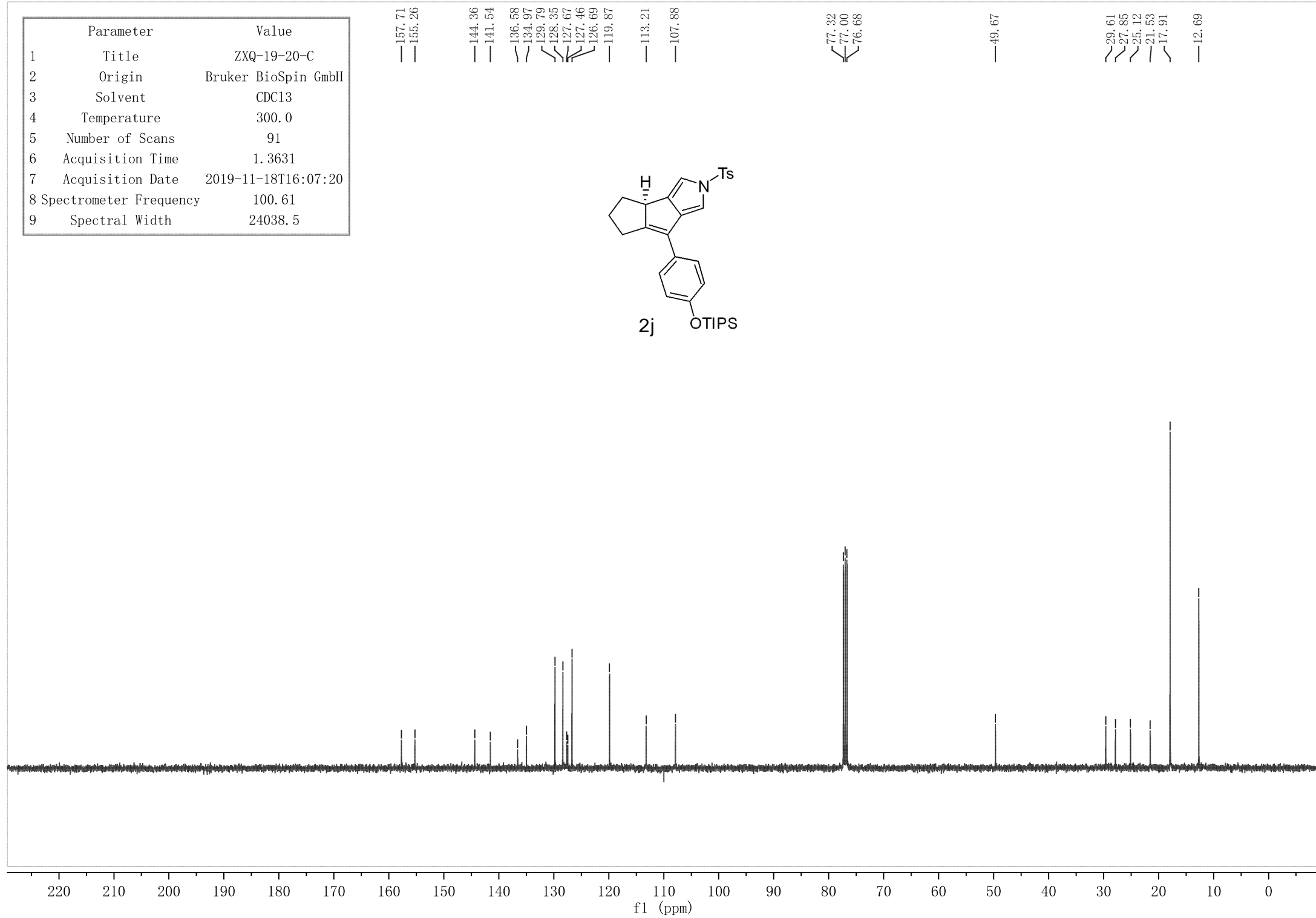
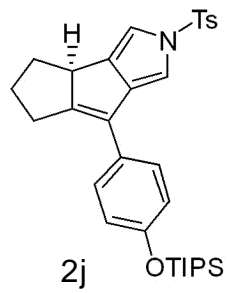
2.440  
2.418  
2.368  
2.217  
2.202  
2.195  
2.189

1.336  
1.316  
1.296  
1.284  
1.278  
1.278  
1.259

1.241  
1.232  
1.224  
1.124  
1.107  
1.080  
1.068  
1.063  
1.038  
1.012



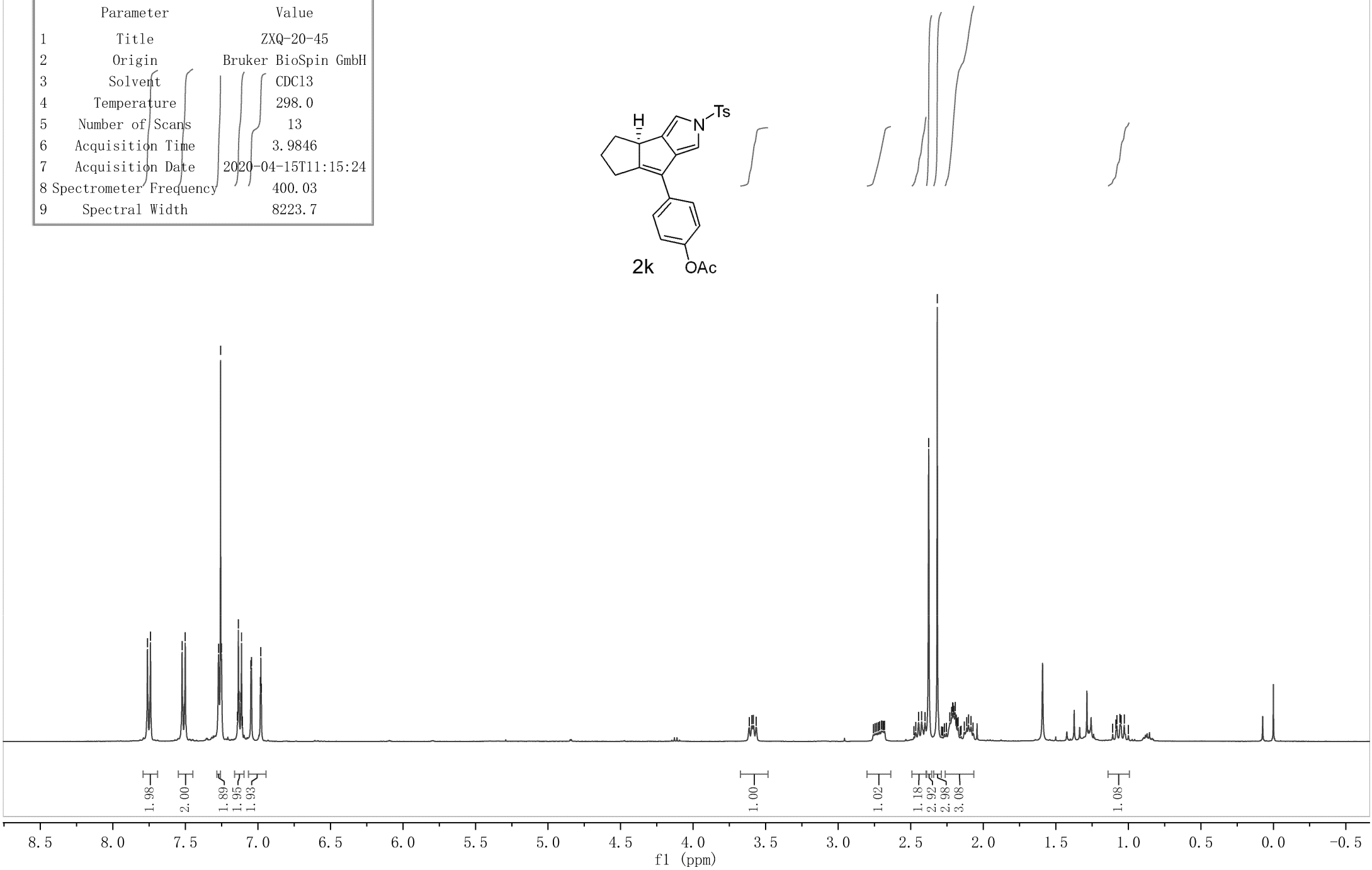
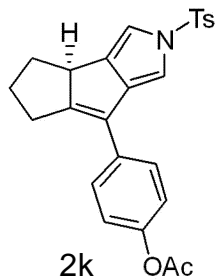
Parameter	Value
1 Title	ZXQ-19-20-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	91
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-18T16:07:20
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



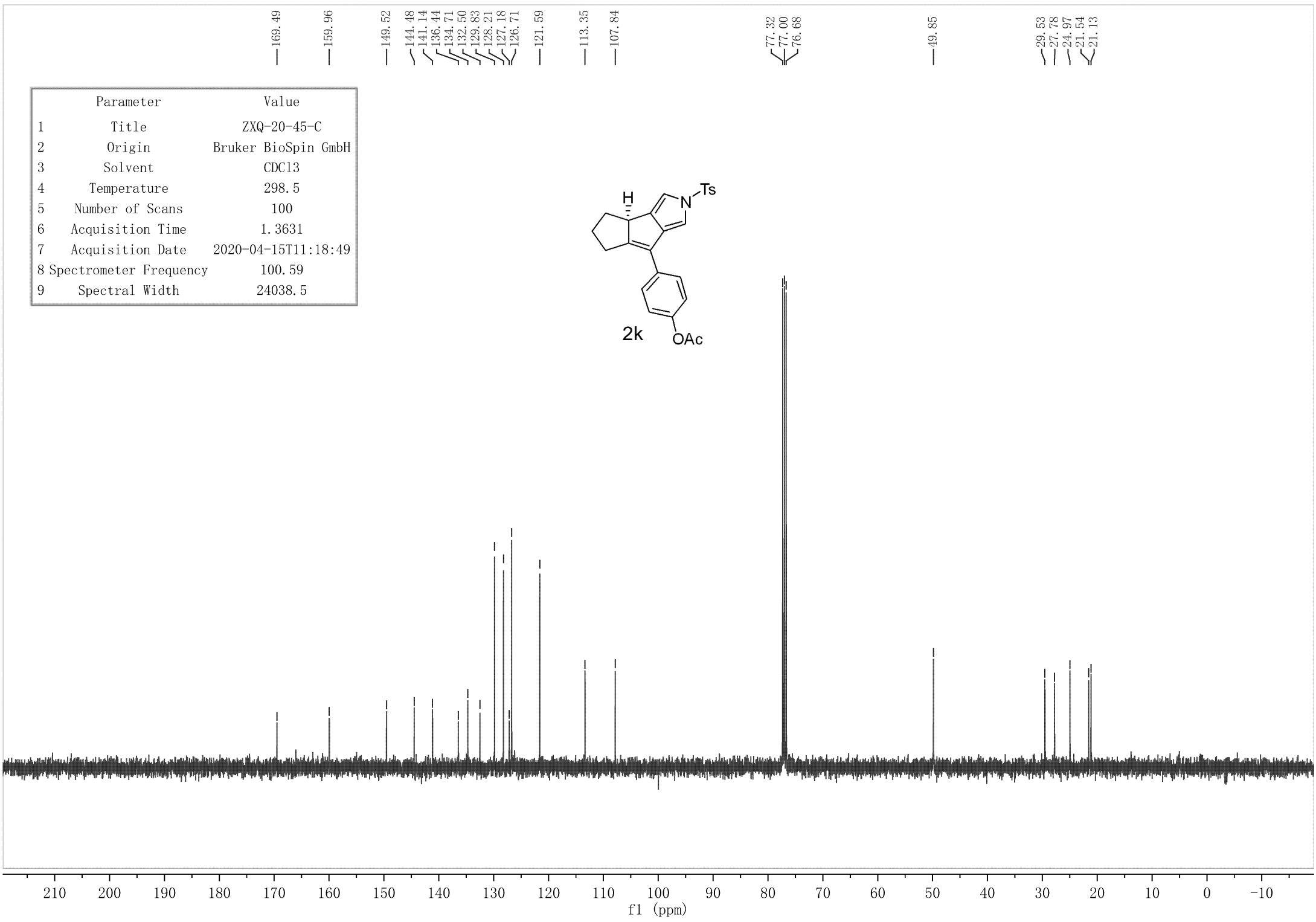
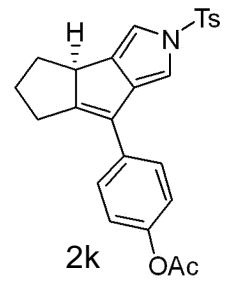
7.762  
7.741  
7.523  
7.501  
7.271  
7.258  
7.251  
7.141  
7.135  
7.130  
7.118  
7.113  
7.107  
7.048  
7.045  
6.983  
6.980  
6.976

3.613  
3.594  
3.585  
3.566  
2.746  
2.735  
2.724  
2.714  
2.701  
2.692  
2.686  
2.681  
2.445  
2.424  
2.402  
2.376  
2.317  
2.230  
2.218  
2.212  
2.208  
2.202  
2.193  
2.188  
2.186  
1.085  
1.079  
1.058  
1.050  
1.028  
0.999

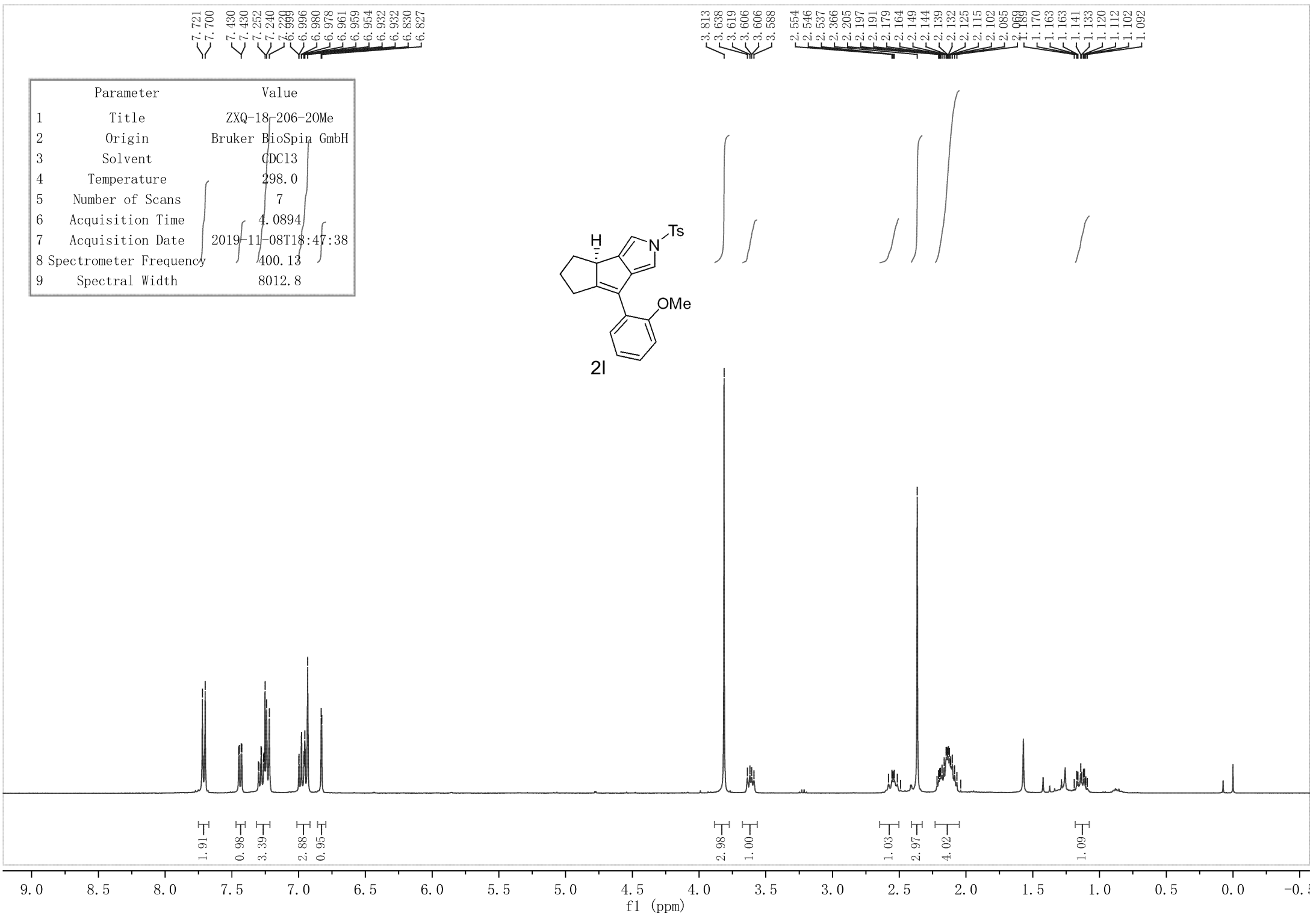
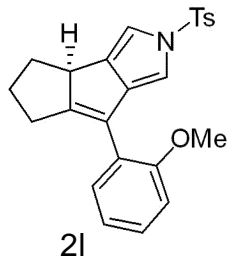
Parameter	Value
1 Title	ZXQ-20-45
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-15T11:15:24
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-20-45-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	100
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-15T11:18:49
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

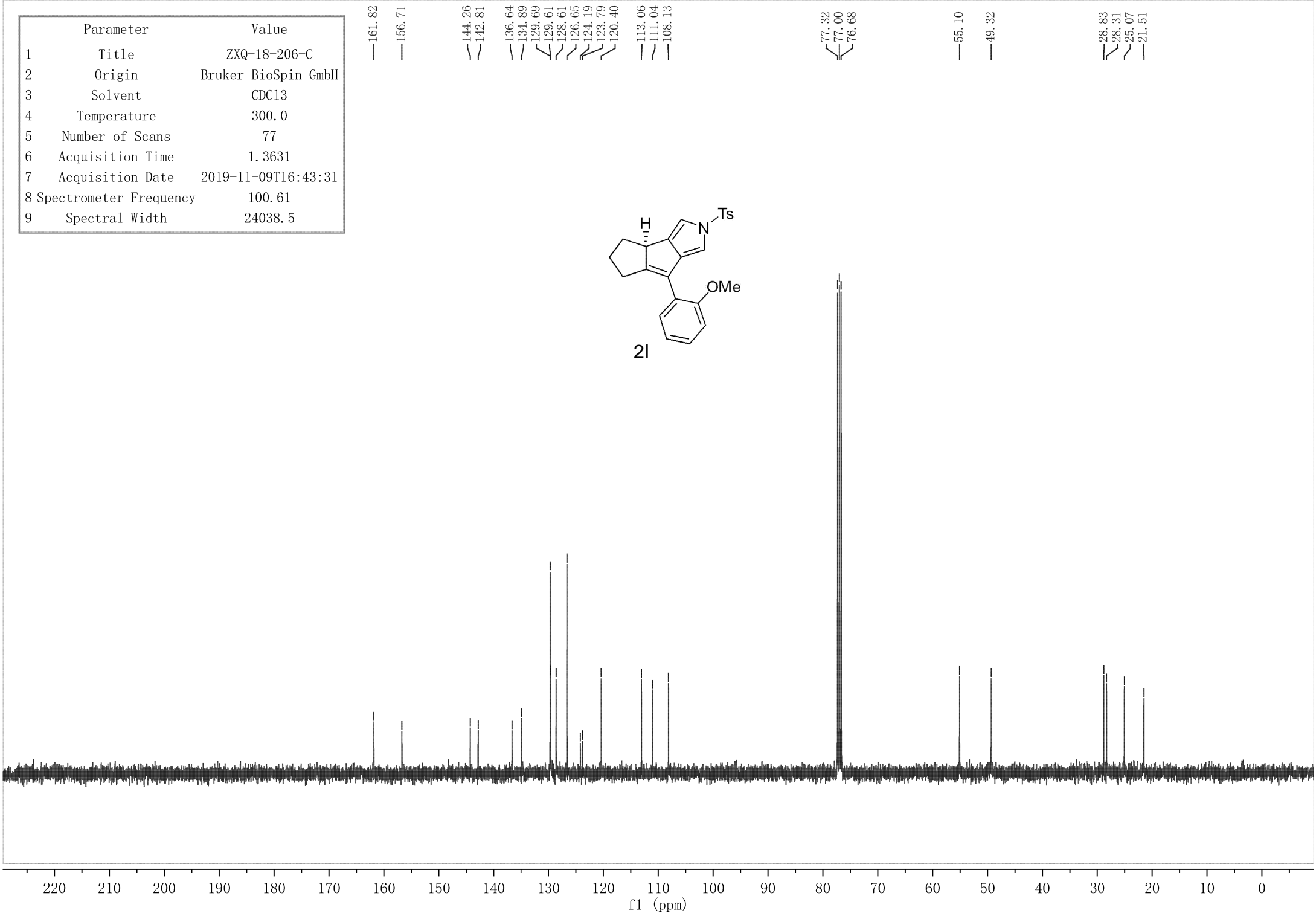
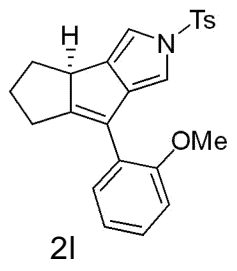


Parameter	Value
1 Title	ZXQ-18-206-20Me
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-08T18:47:38
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-18-206-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	77
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-09T16:43:31
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

161.82 — 156.71 —  
 144.26 142.81  
 136.64 134.89 129.69 128.61 126.65 124.19 123.79 120.40  
 113.06 111.04 108.13  
 77.32 77.00 76.68  
 55.10 49.32  
 28.83 28.31 25.07 21.51





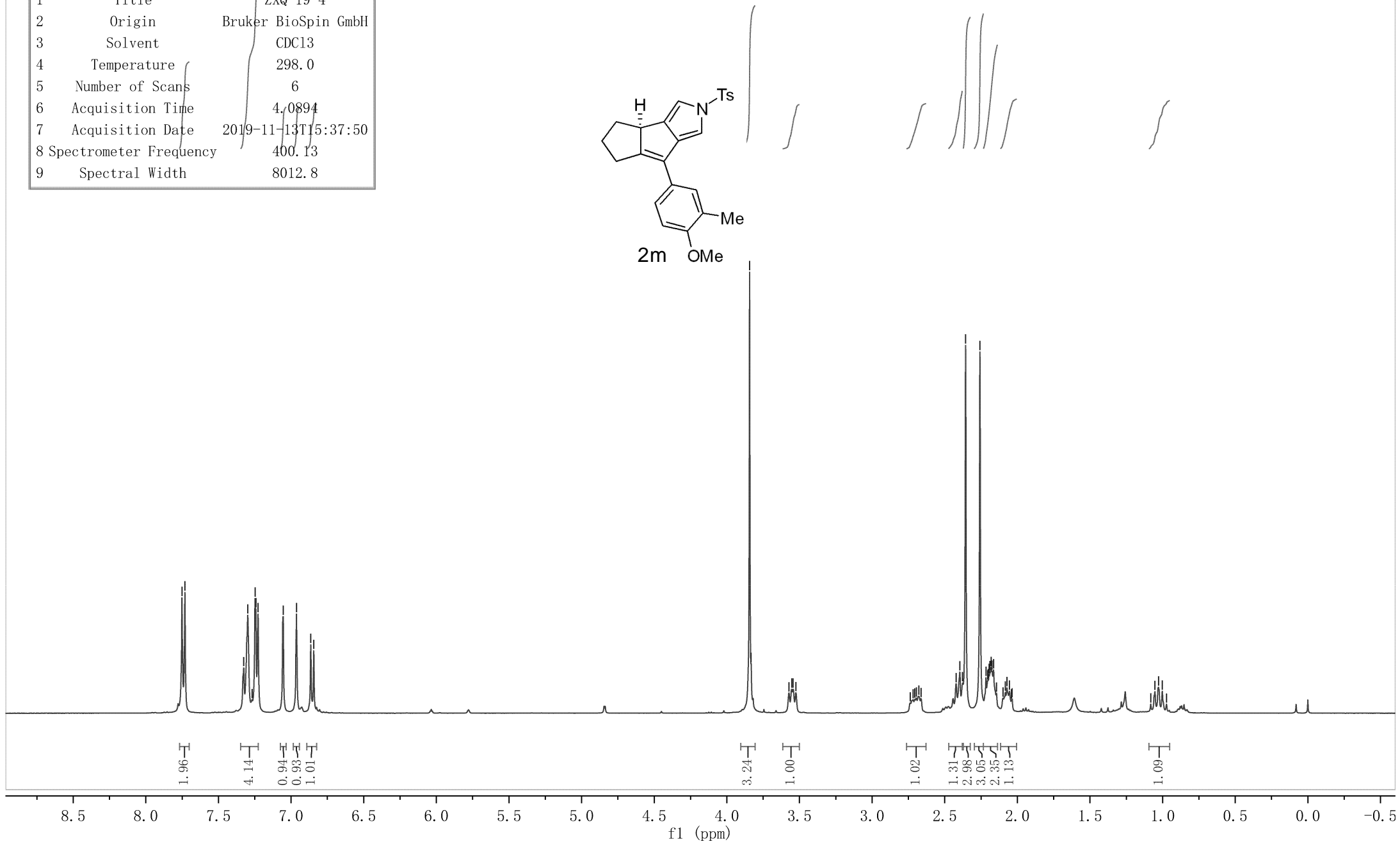
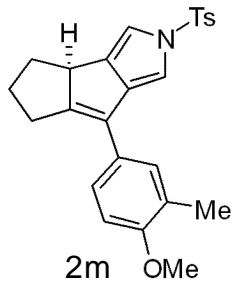
Parameter	Value
1 Title	ZXQ-19-4
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-13T15:37:50
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

7.751  
7.731  
7.326  
7.298  
7.269  
7.248  
7.242  
7.228  
7.054  
7.054  
6.963  
6.865  
6.844

3.843  
3.833  
3.572  
3.553  
3.544  
3.525  
3.525

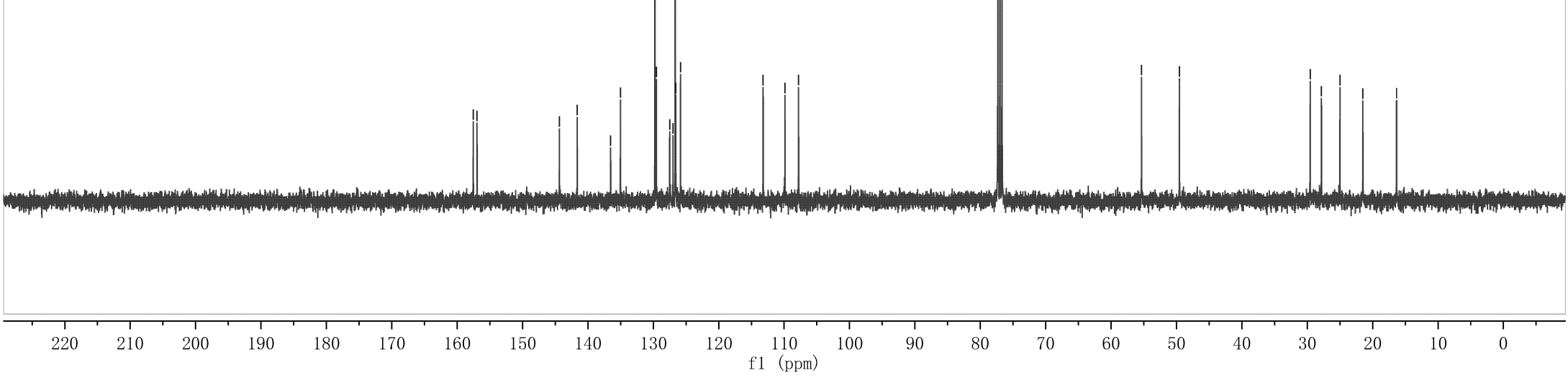
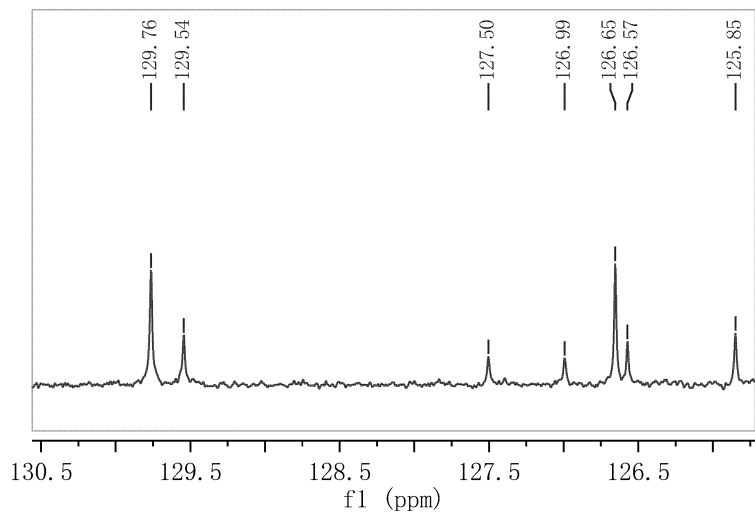
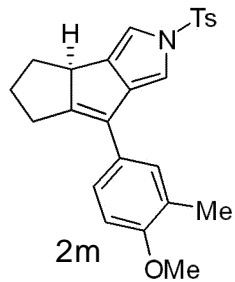
2.737  
2.718  
2.706  
2.696  
2.679  
2.663

2.396  
2.396  
2.377  
2.356  
2.258  
2.216  
2.204  
2.201  
2.195  
2.188  
2.181  
2.174  
2.164  
2.164  
1.053  
1.029  
1.002  
0.973

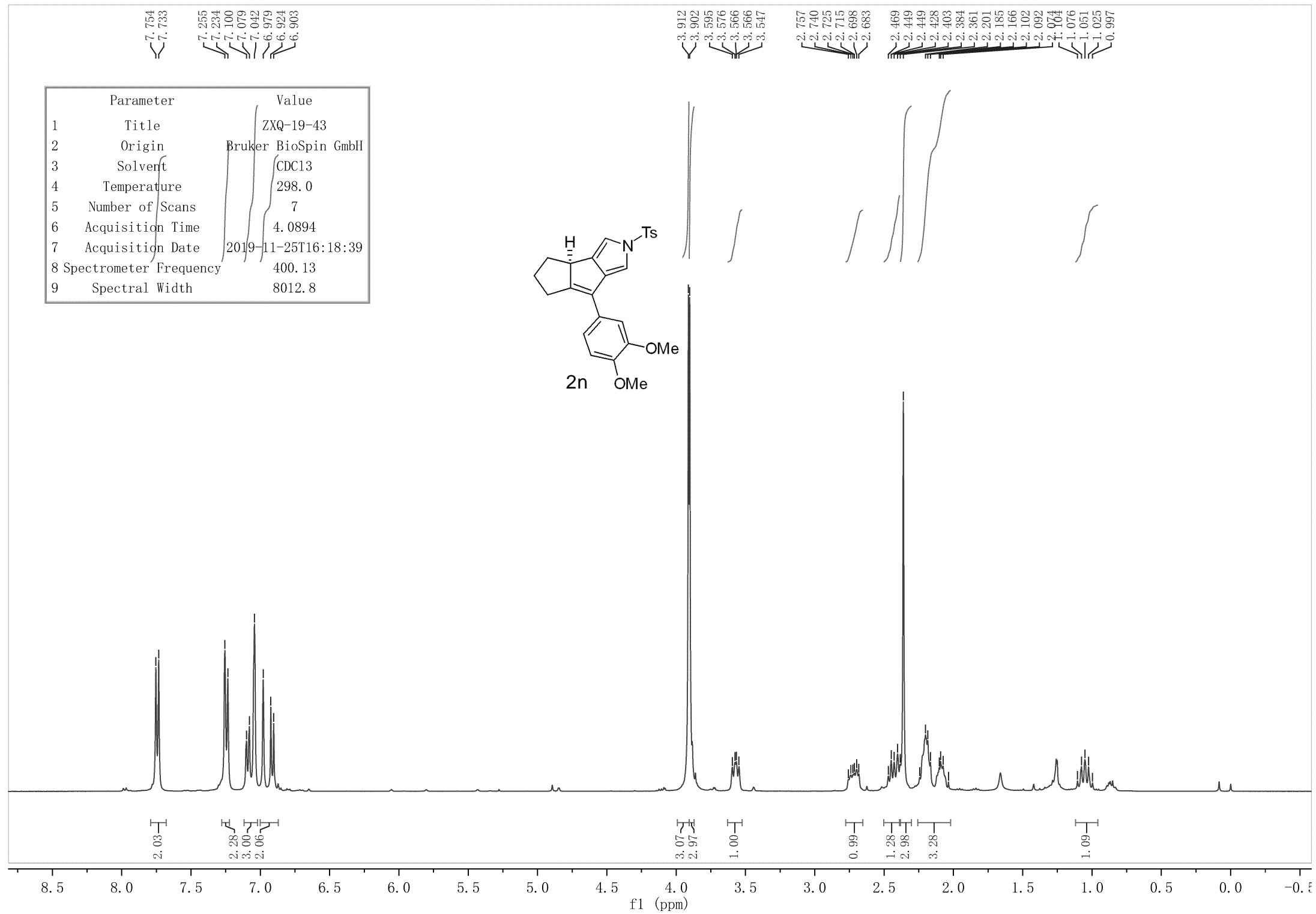
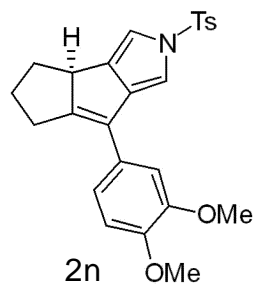


Parameter	Value
1 Title	ZXQ-19-4-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	71
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-13T15:39:34
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

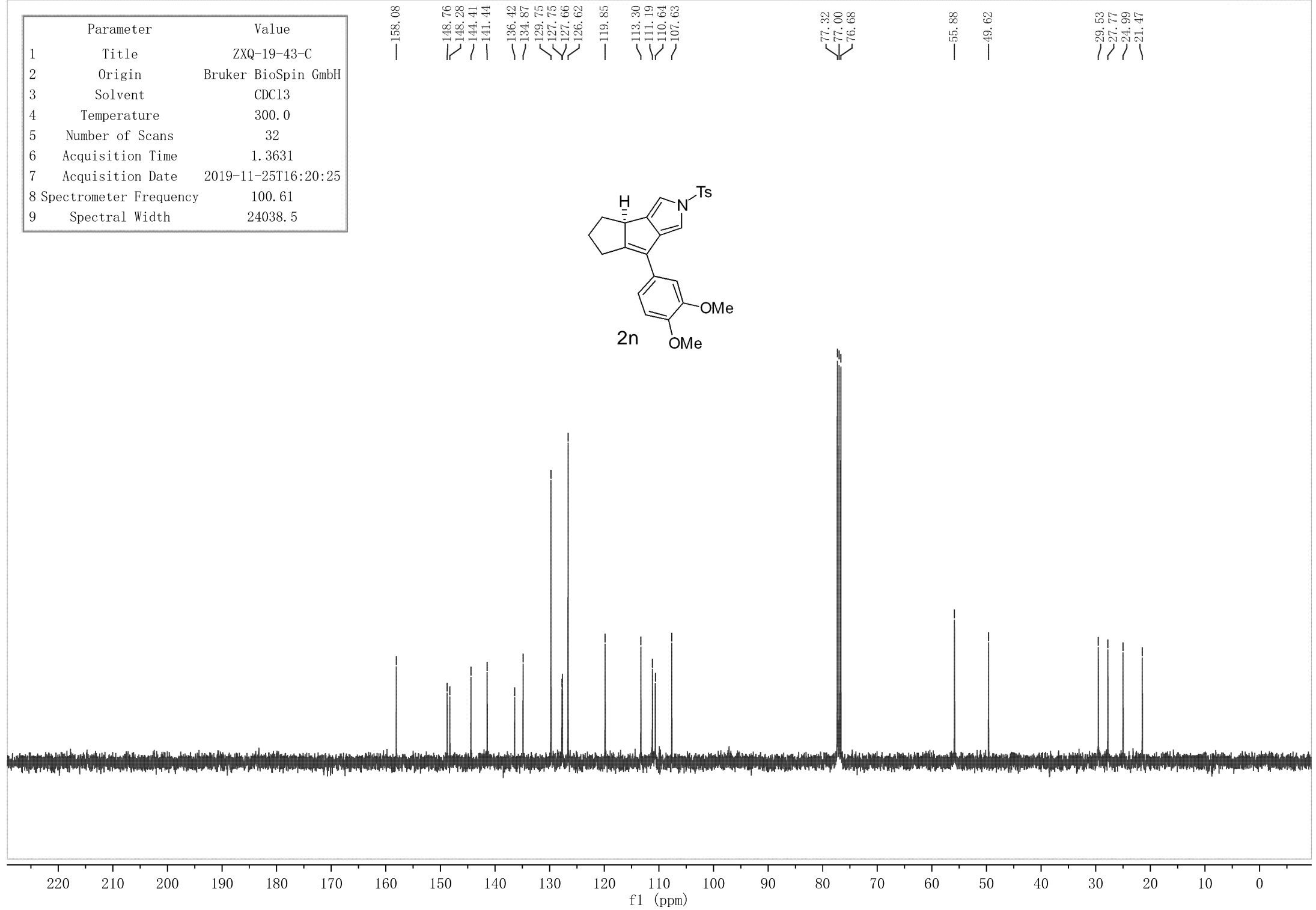
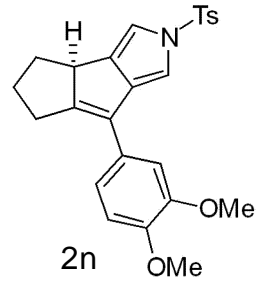
157.53 156.96 144.36 141.64 136.53 135.03 129.76 129.54 127.50 126.99 126.65 126.57 125.85 113.21 109.87 107.79 77.32 77.00 76.68 55.34 49.55 29.55 27.83 25.00 21.49 16.34



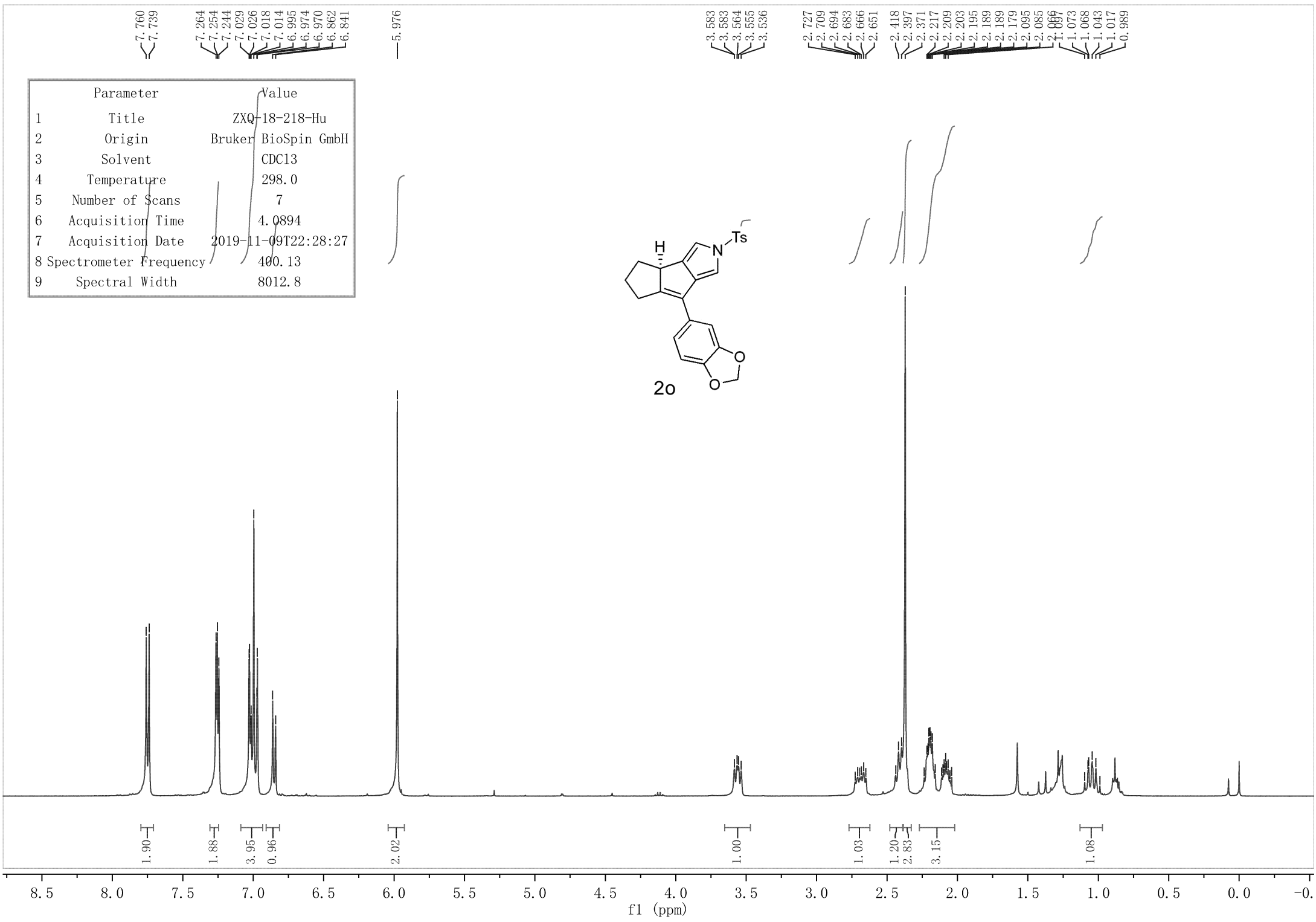
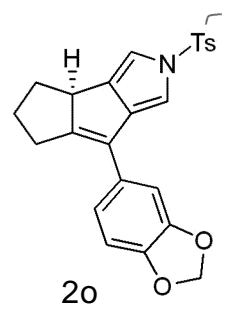
Parameter	Value
1 Title	ZXQ-19-43
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-25T16:18:39
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



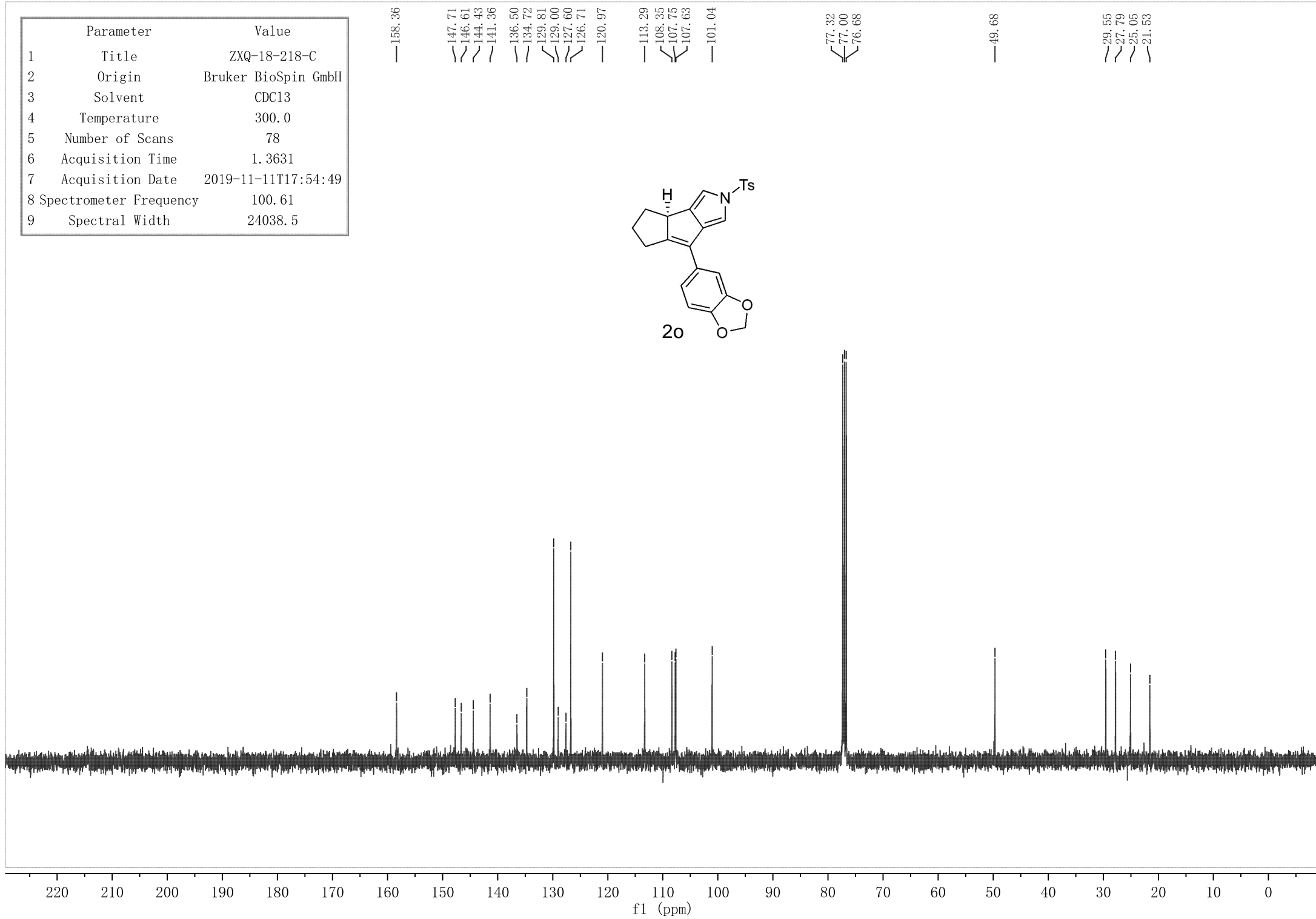
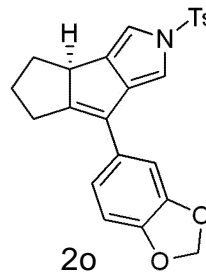
Parameter	Value
1 Title	ZXQ-19-43-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	32
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-25T16:20:25
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



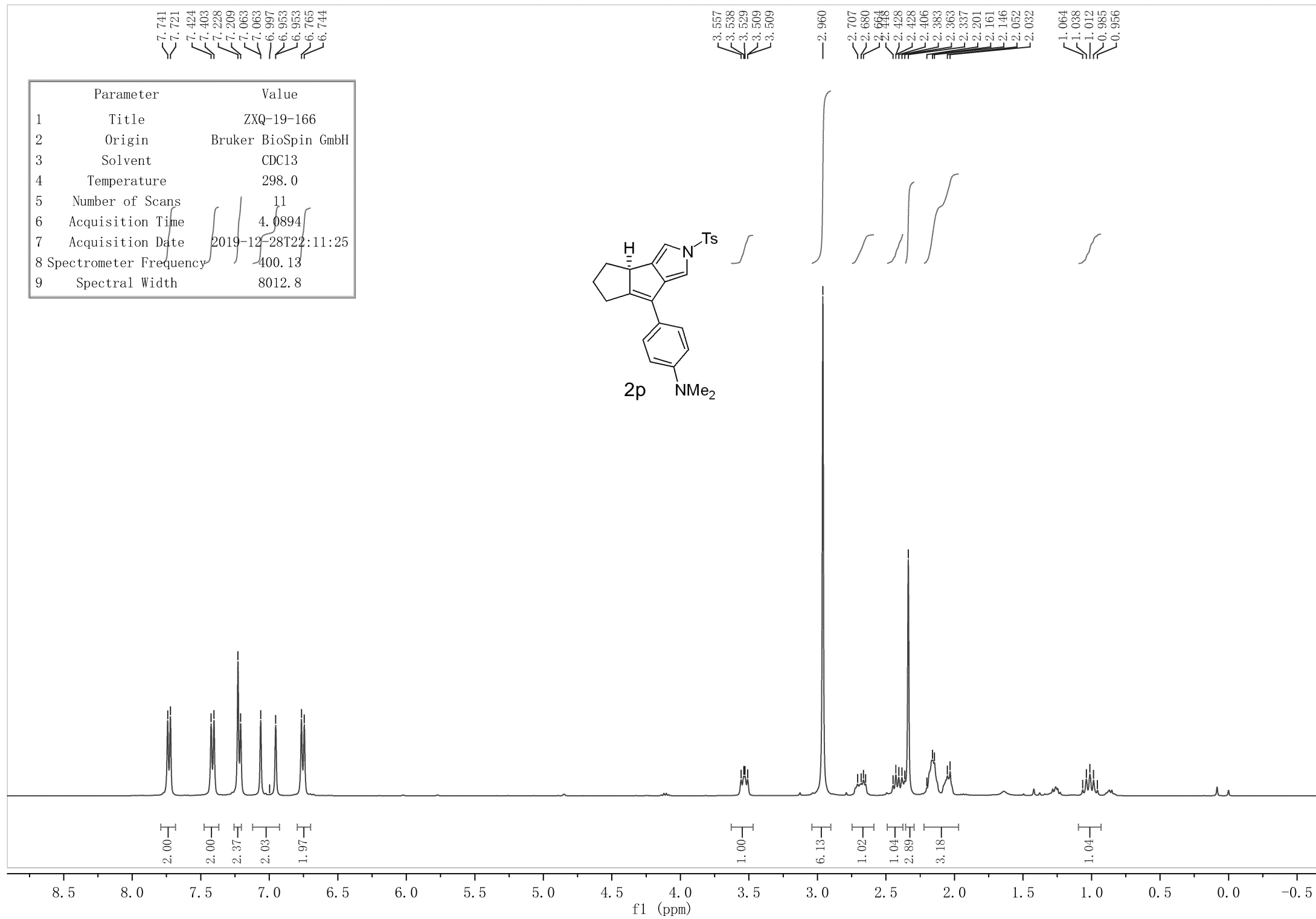
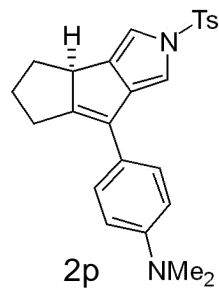
Parameter	Value
1 Title	ZXQ-18-218-Hu
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-09T22:28:27
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



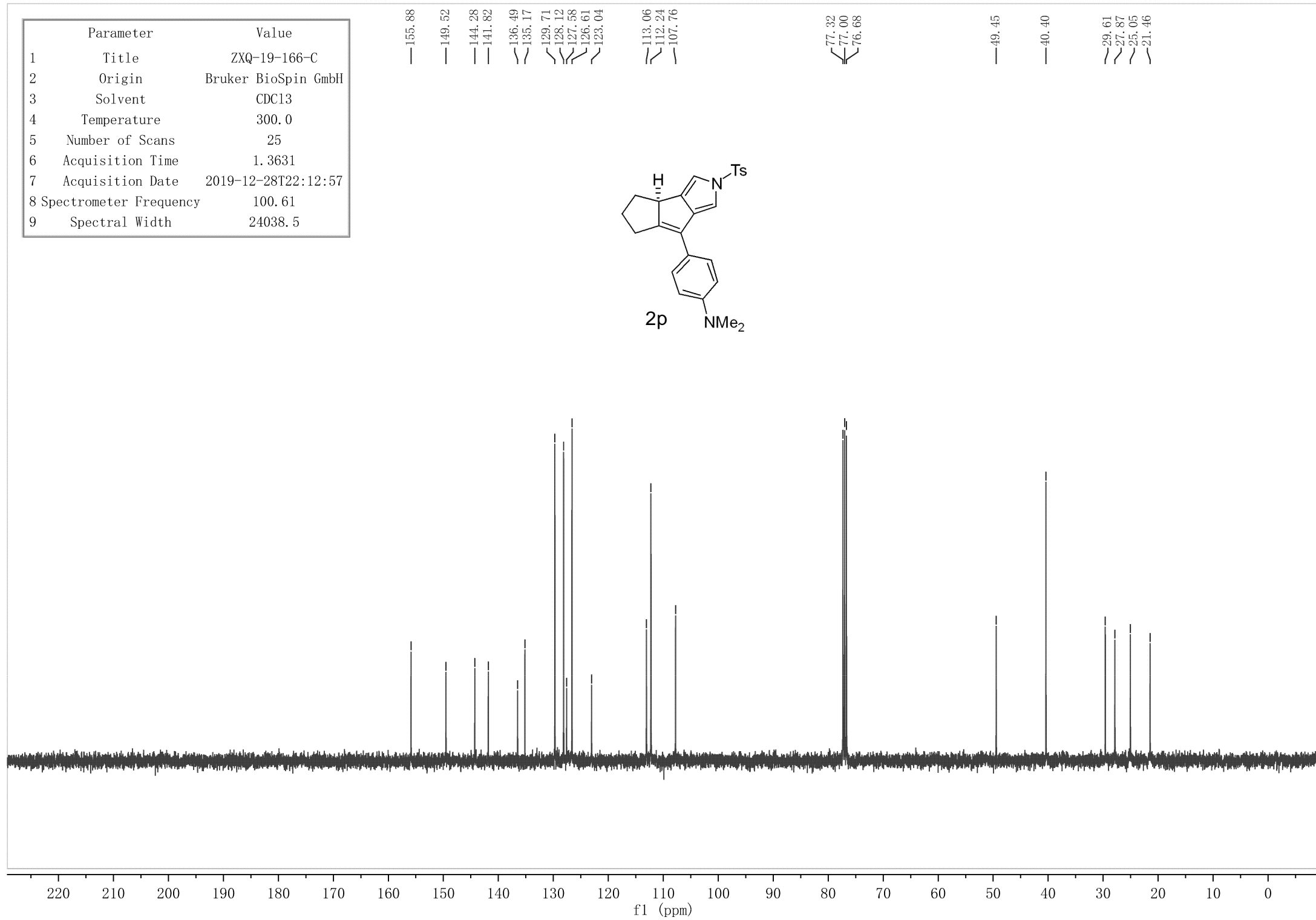
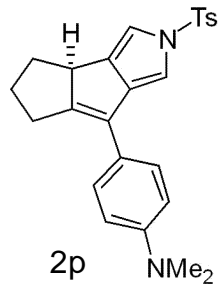
Parameter	Value
1 Title	ZXQ-18-218-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	78
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-11T17:54:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-19-166
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-28T22:11:25
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-166-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	25
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-28T22:12:57
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



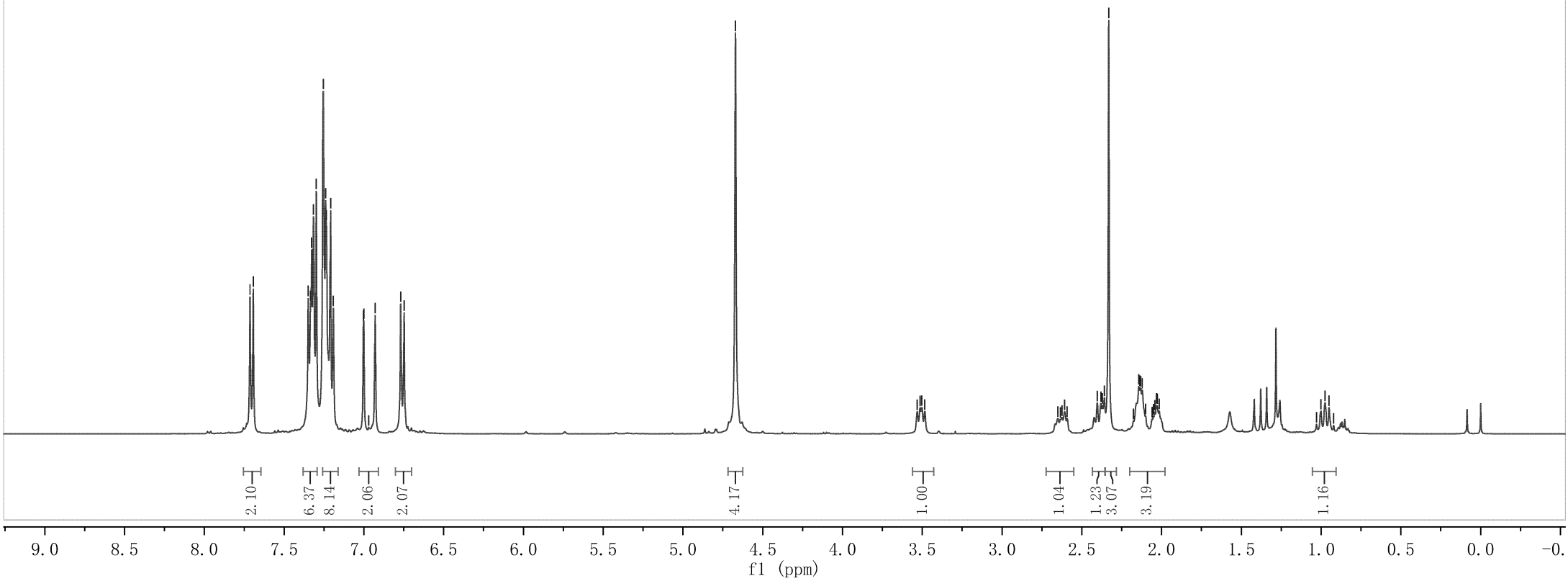
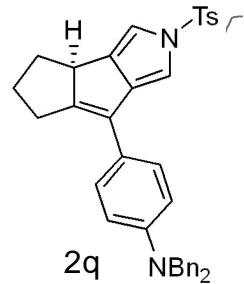


Parameter	Value
1 Title	ZXQ-21-47
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2020-06-19T17:10:24
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

7.714  
7.693  
7.349  
7.334  
7.327  
7.316  
7.298  
7.255  
7.240  
7.236  
7.208  
7.191  
7.003  
7.000  
6.970  
6.929  
6.769  
6.747

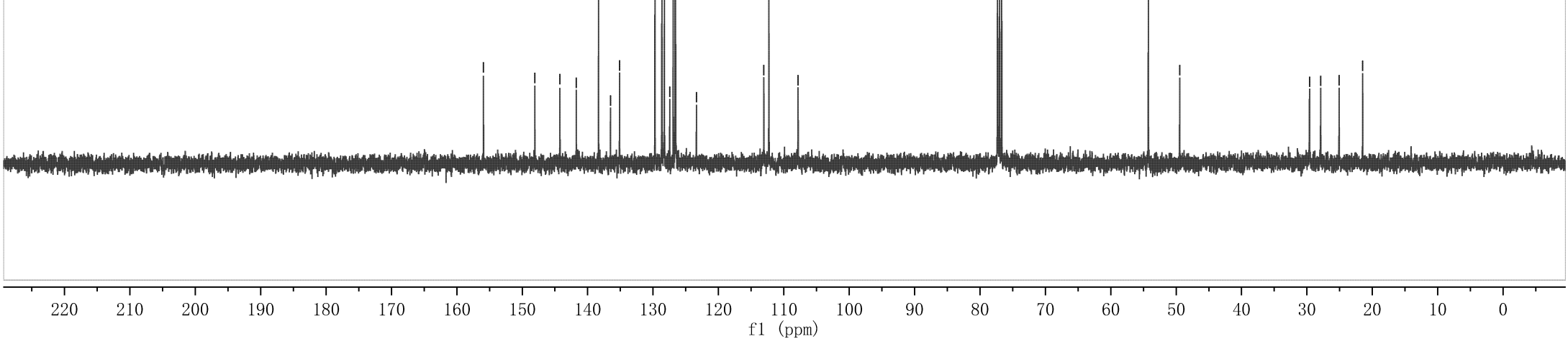
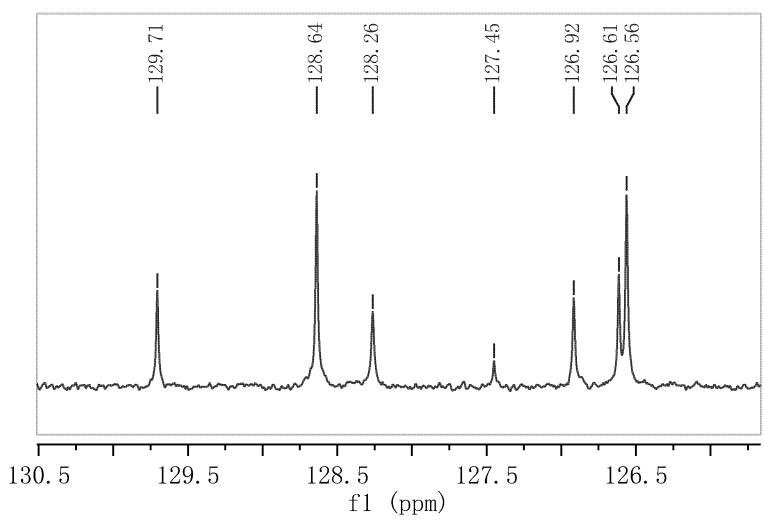
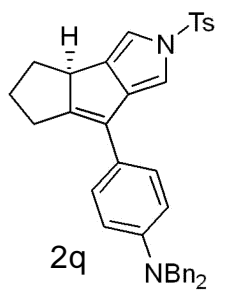
4.671

3.532  
3.513  
3.503  
3.484  
2.650  
2.634  
2.624  
2.608  
2.592  
2.403  
2.381  
2.372  
2.359  
2.331  
2.143  
2.137  
2.130  
2.121  
2.100  
2.060  
2.050  
2.043  
2.033  
2.027  
2.019  
1.001  
0.975  
0.950  
0.921



Parameter	Value
1 Title	ZXQ-21-47-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	23
6 Acquisition Time	1.3631
7 Acquisition Date	2020-06-19T17:11:36
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

155.93 148.08 144.24 141.74 138.34 136.51 135.12 129.71 128.64 128.26 127.45 126.92 126.61 126.56 123.36 113.06 112.28 107.81 77.32 77.00 76.68 54.26 49.46 29.60 27.90 25.08 21.48



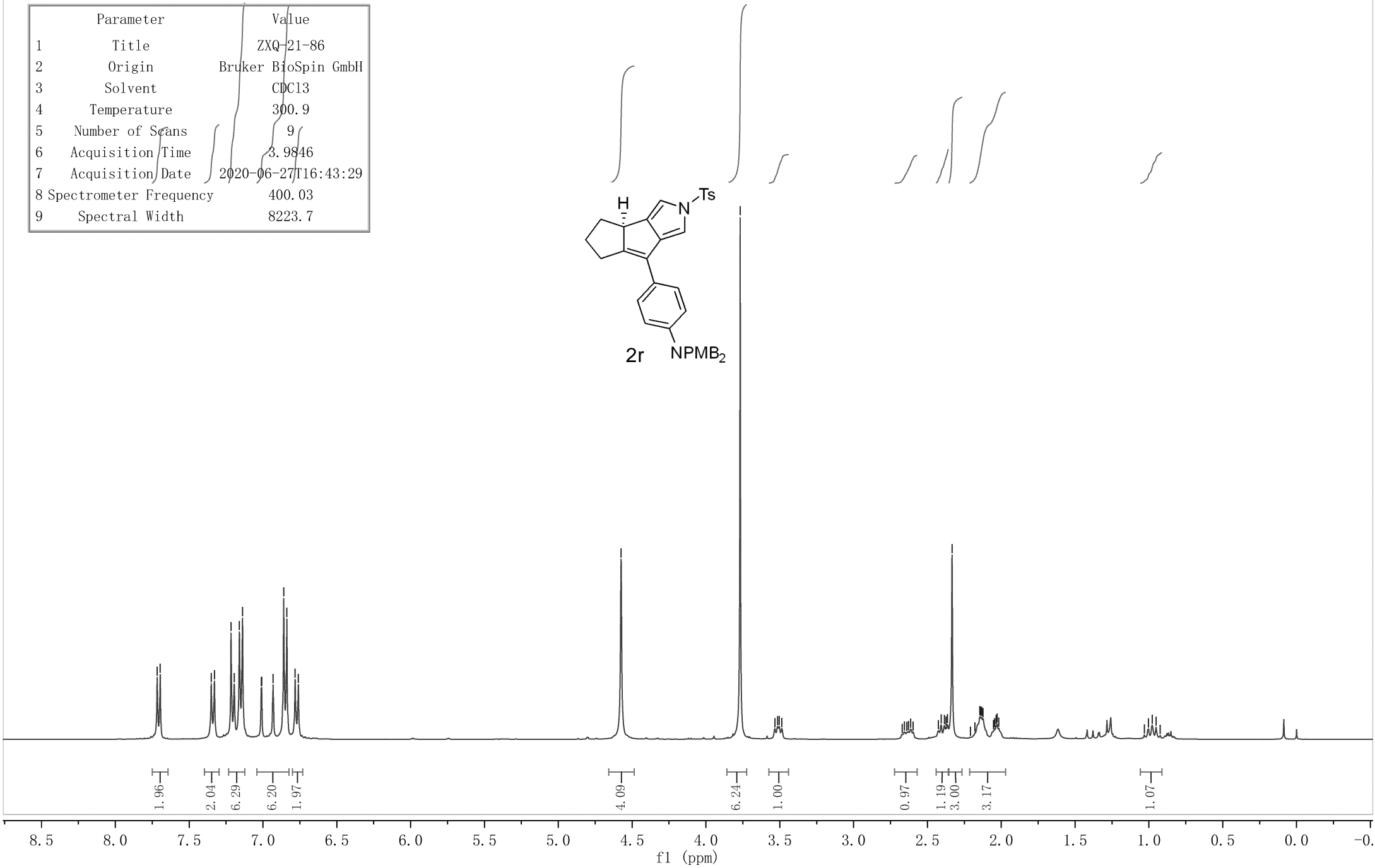
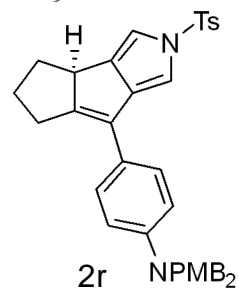
Parameter	Value
1 Title	ZXQ-21-86
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.9
5 Number of Scans	9
6 Acquisition Time	3.9846
7 Acquisition Date	2020-06-27T16:43:29
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

7.717  
7.696  
7.350  
7.328  
7.216  
7.195  
7.160  
7.139  
7.011  
7.009  
6.931  
6.860  
6.838  
6.782  
6.760

4.575

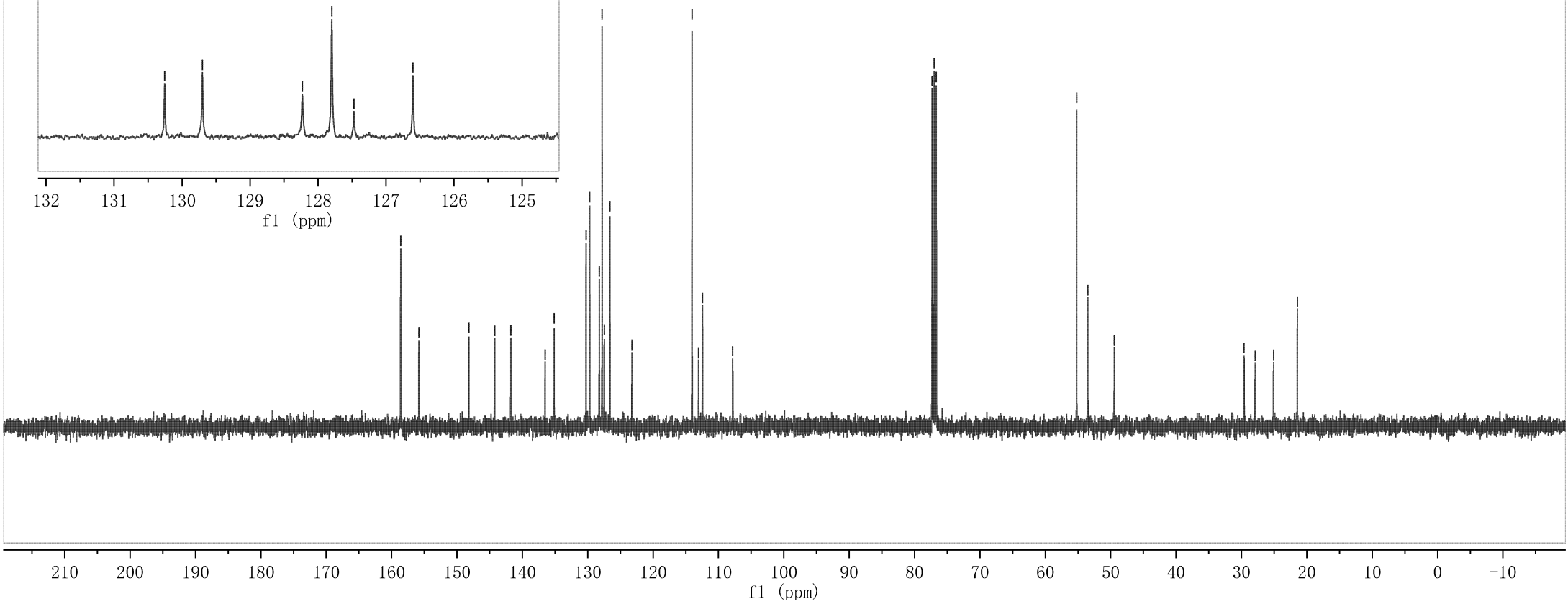
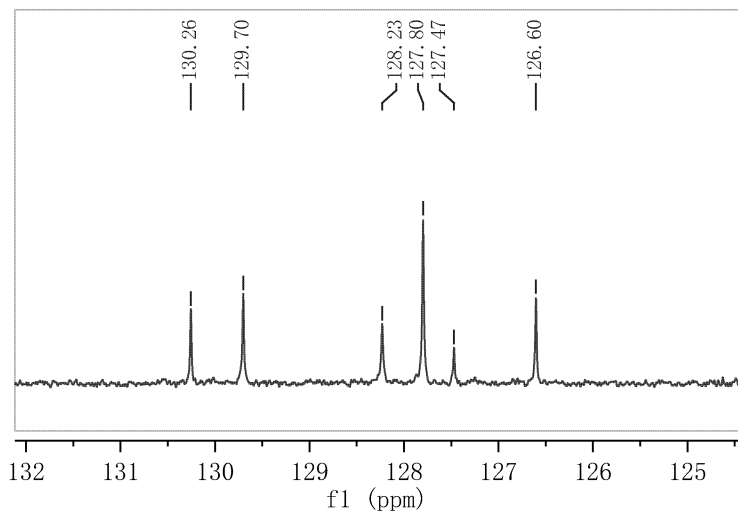
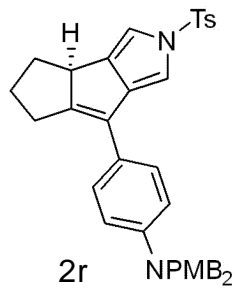
3.768  
3.533  
3.515  
3.504  
3.486

2.671  
2.656  
2.639  
2.628  
2.613  
2.597  
2.425  
2.407  
2.386  
2.375  
2.364  
2.333  
2.178  
2.145  
2.139  
2.132  
2.123  
2.052  
2.044  
2.034  
2.027  
2.016  
1.003  
0.978  
0.951  
0.924



Parameter	Value
1 Title	ZXQ-21-86-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	301.0
5 Number of Scans	54
6 Acquisition Time	1.3631
7 Acquisition Date	2020-06-27T16:44:59
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

158.61 155.83 148.19 144.24 141.76 136.52 135.14 130.26 129.70 128.23 127.80 127.47 126.60 123.24 114.04 113.05 112.43 107.82 77.32 77.00 76.68 55.21 53.52 49.45 29.60 27.90 25.09 21.46

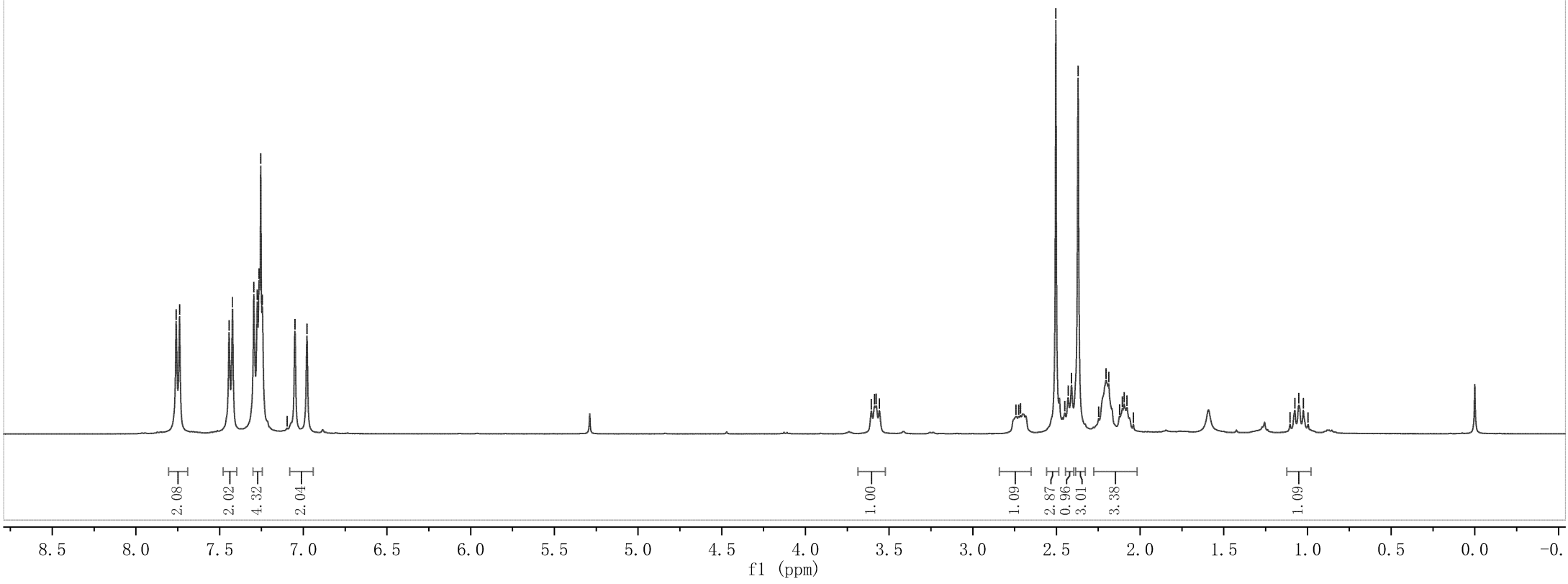
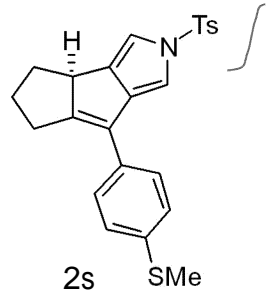


7.760  
7.739  
7.444  
7.423  
7.296  
7.275  
7.264  
7.255  
7.245  
7.097  
7.050  
6.978

3.606  
3.606  
3.587  
3.577  
3.558

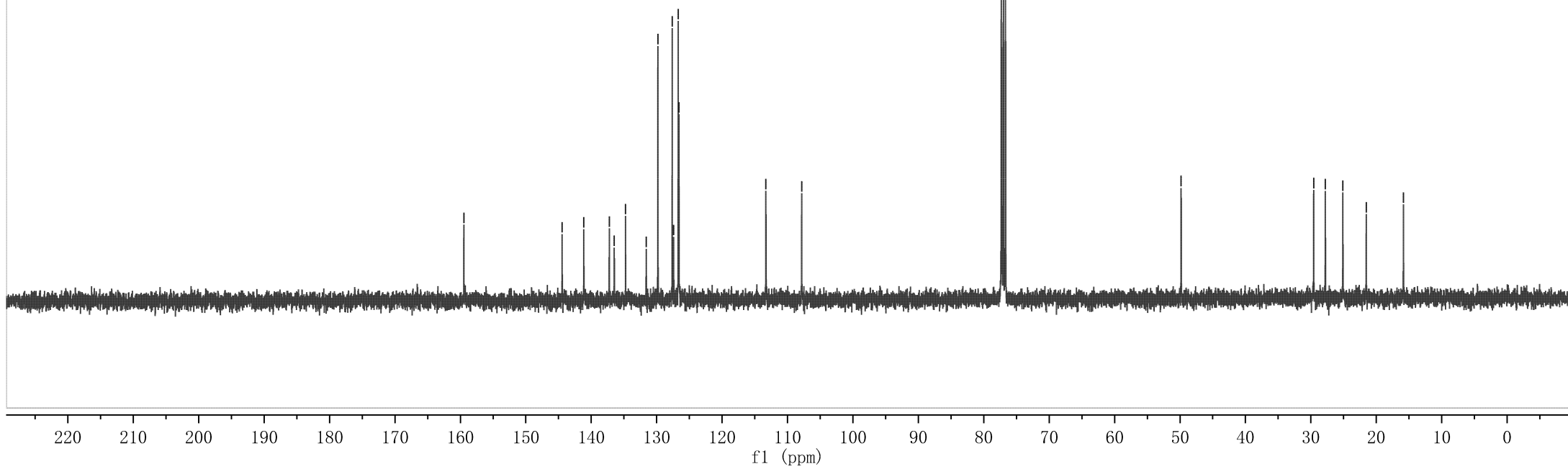
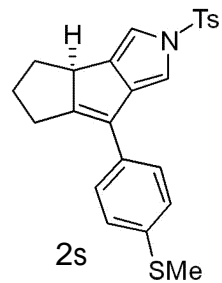
2.742  
2.725  
2.715  
2.504  
2.450  
2.430  
2.410  
2.371  
2.247  
2.204  
2.188  
2.123  
2.106  
2.095  
2.078  
2.041  
1.104  
1.076  
1.051  
1.025  
0.997

Parameter	Value
1 Title	ZXQ-19-40-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-28T16:17:28
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-40-2-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	109
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-28T16:19:11
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

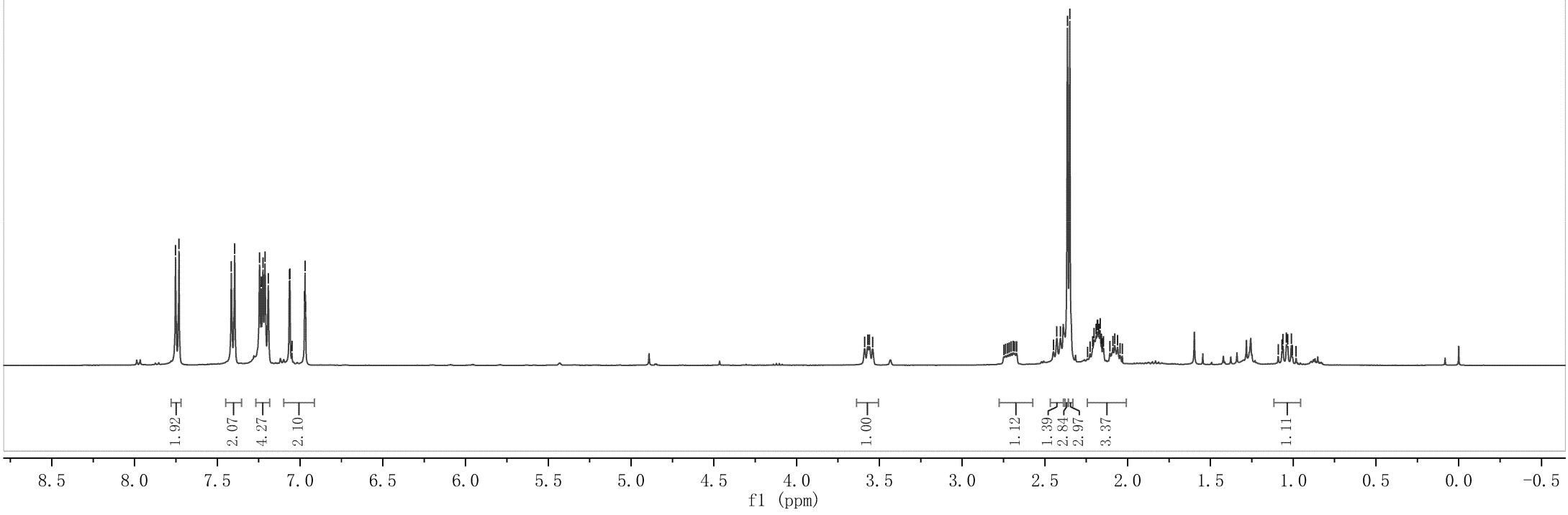
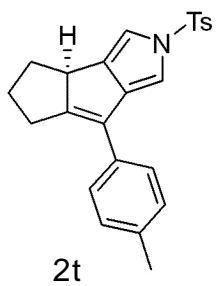
159.47  
 144.45  
 141.13  
 137.24  
 136.48  
 134.76  
 131.60  
 129.81  
 127.62  
 127.41  
 126.70  
 126.59  
 113.30  
 107.83  
 77.32  
 77.00  
 76.68  
 49.83  
 29.57  
 27.79  
 25.11  
 21.53  
 15.85



7.752  
7.731  
7.415  
7.395  
7.244  
7.234  
7.224  
7.212  
7.192  
7.064  
7.061  
7.049  
6.973  
6.970  
6.966

3.589  
3.570  
3.560  
3.541  
3.541  
2.747  
2.737  
2.725  
2.715  
2.704  
2.692  
2.682  
2.671  
2.428  
2.406  
2.364  
2.350  
2.203  
2.190  
2.184  
2.180  
2.174  
2.166  
2.068  
2.068  
1.062  
1.041  
1.033  
1.011  
1.011  
1.005  
1.005  
0.983

Parameter	Value
1 Title	ZXQ-18-229
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-07T16:40:22
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-18-229-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	12
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-07T16:43:39
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

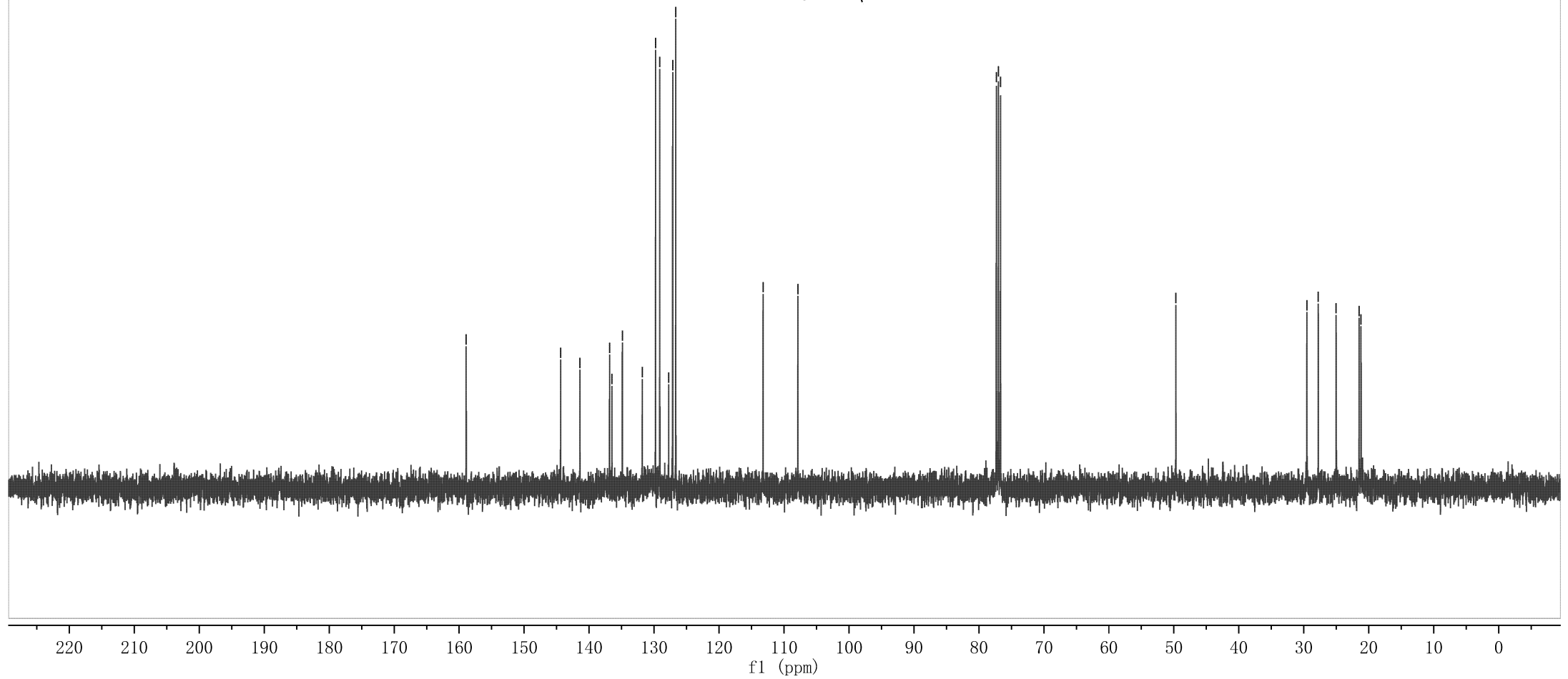
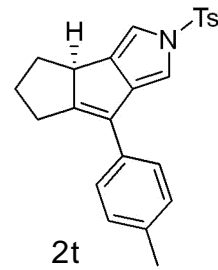
158.91  
 144.38  
 141.41  
 136.85  
 136.48  
 134.88  
 131.81  
 129.77  
 129.12  
 127.75  
 127.13  
 126.66

113.22  
 107.86

77.32  
 77.00  
 76.68

49.69

29.53  
 27.77  
 25.02  
 21.49  
 21.19

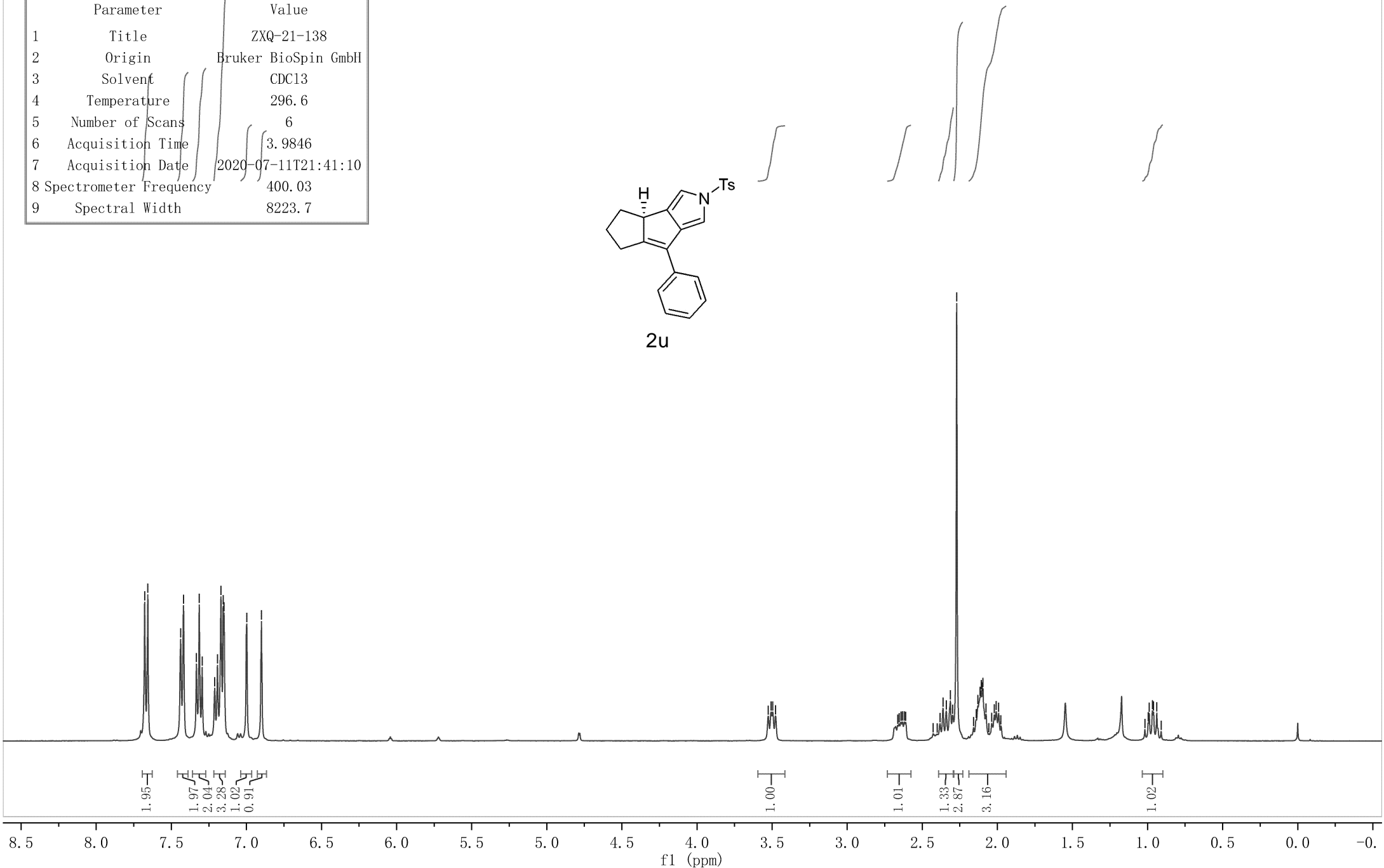
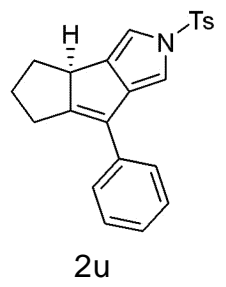




7.678  
7.657  
7.438  
7.419  
7.333  
7.314  
7.295  
7.211  
7.193  
7.170  
7.155  
7.149  
6.998  
6.900

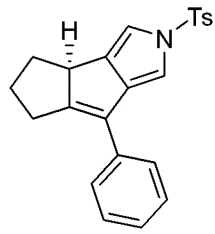
3.525  
3.506  
3.496  
3.477  
2.654  
2.642  
2.633  
2.620  
2.611  
2.382  
2.362  
2.340  
2.313  
2.298  
2.271  
2.140  
2.130  
2.116  
2.107  
2.101  
2.096  
2.076  
2.038  
2.020  
2.008  
1.982  
1.018  
0.996  
0.989  
0.968  
0.960  
0.939  
0.910

Parameter	Value
1 Title	ZXQ-21-138
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	296.6
5 Number of Scans	6
6 Acquisition Time	3.9846
7 Acquisition Date	2020-07-11T21:41:10
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

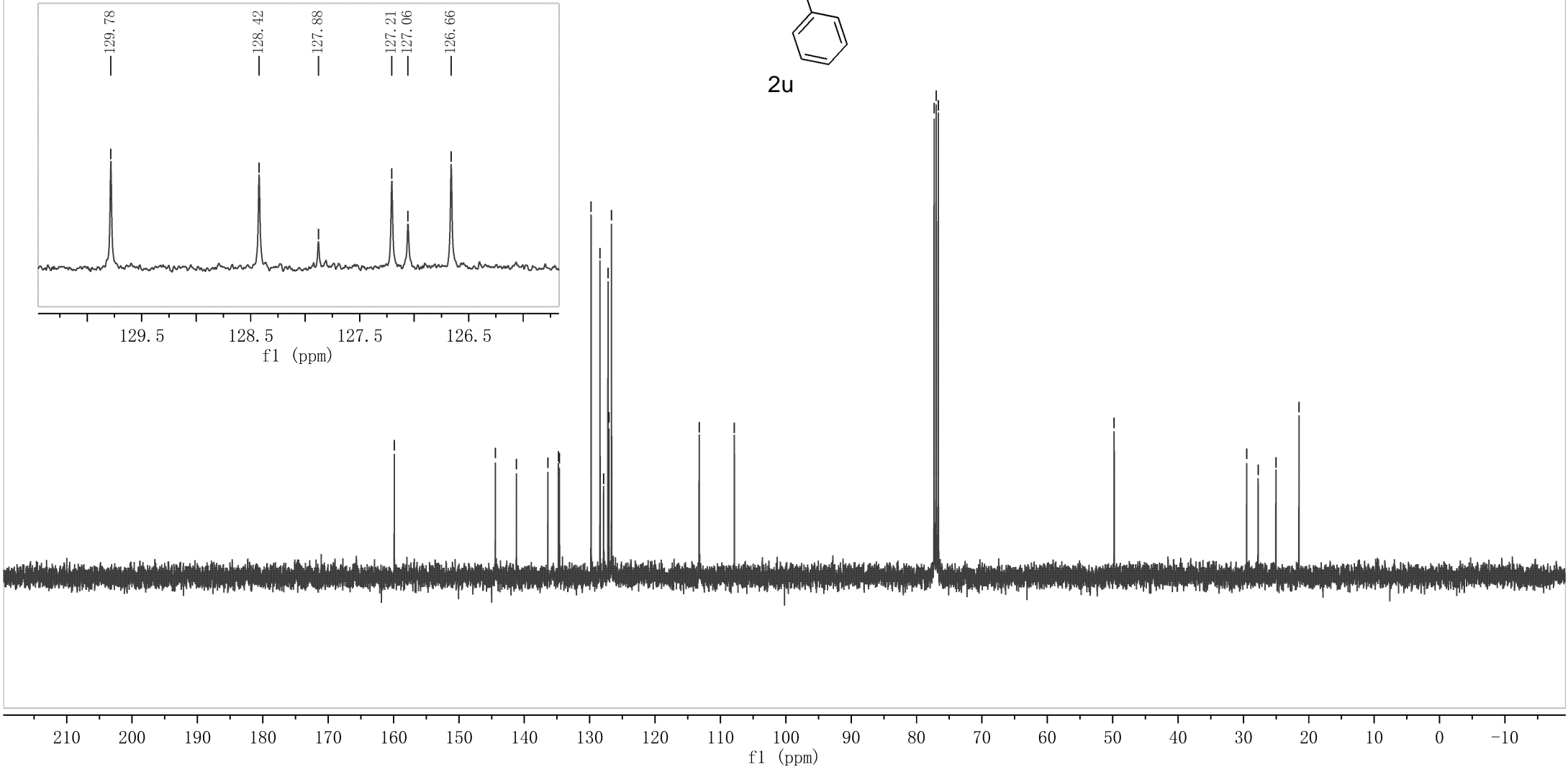
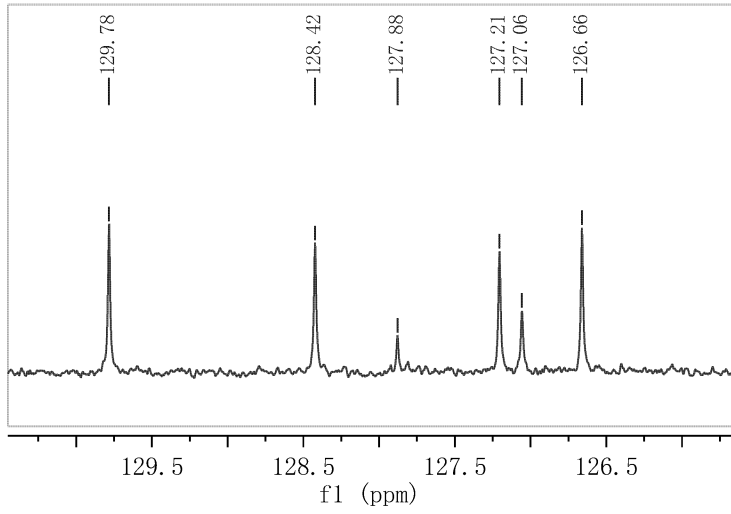


Parameter	Value
1 Title	ZXQ-21-138-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	296.7
5 Number of Scans	24
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-11T21:43:53
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

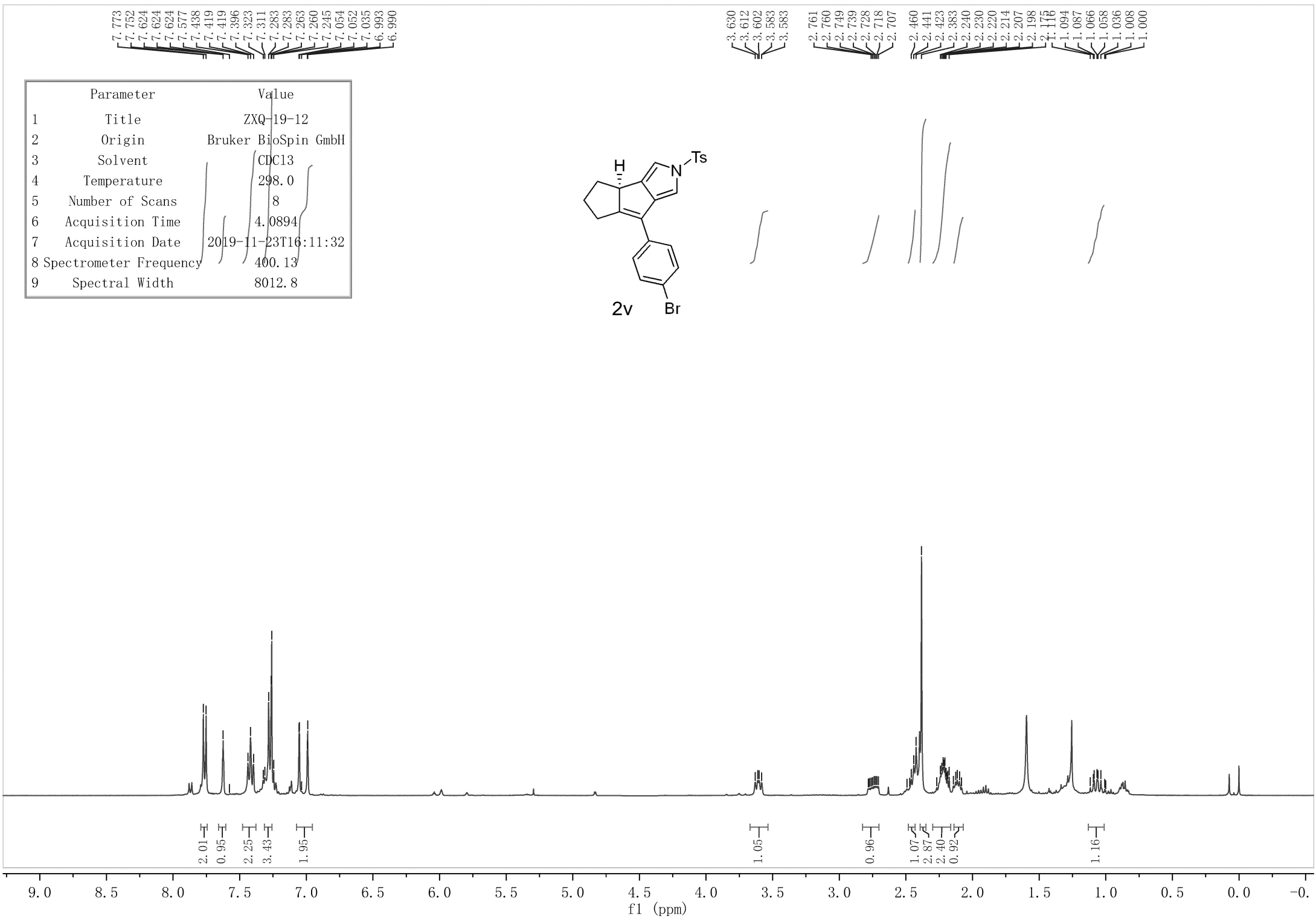
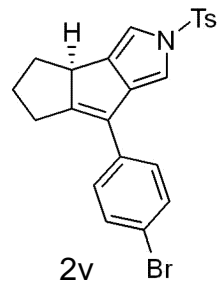
159.89  
 144.43  
 141.22  
 136.40  
 134.79  
 134.62  
 129.78  
 128.42  
 127.88  
 127.21  
 127.06  
 126.66  
 113.25  
 107.87  
 77.32  
 77.00  
 76.68  
 49.77  
 29.50  
 27.75  
 25.03  
 21.50



2u



Parameter	Value
1 Title	ZXQ-19-12
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-23T16:11:32
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.773  
7.752  
7.624  
7.624  
7.577  
7.438  
7.419  
7.419  
7.396  
7.323  
7.311  
7.283  
7.283  
7.263  
7.260  
7.245  
7.054  
7.052  
7.035  
6.993  
6.990

3.630  
3.612  
3.602  
3.583  
3.583  
2.761  
2.760  
2.749  
2.739  
2.728  
2.718  
2.707  
2.460  
2.441  
2.423  
2.383  
2.240  
2.230  
2.220  
2.214  
2.207  
2.198  
1.116  
1.094  
1.087  
1.066  
1.058  
1.036  
1.008  
1.000

Parameter	Value
1 Title	ZXQ-19-12-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	154
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-23T16:13:11
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

161.41

144.55

140.67

136.84

134.50

130.08

130.01

129.98

129.87

126.76

125.80

122.66

113.46

107.83

77.32

77.00

76.68

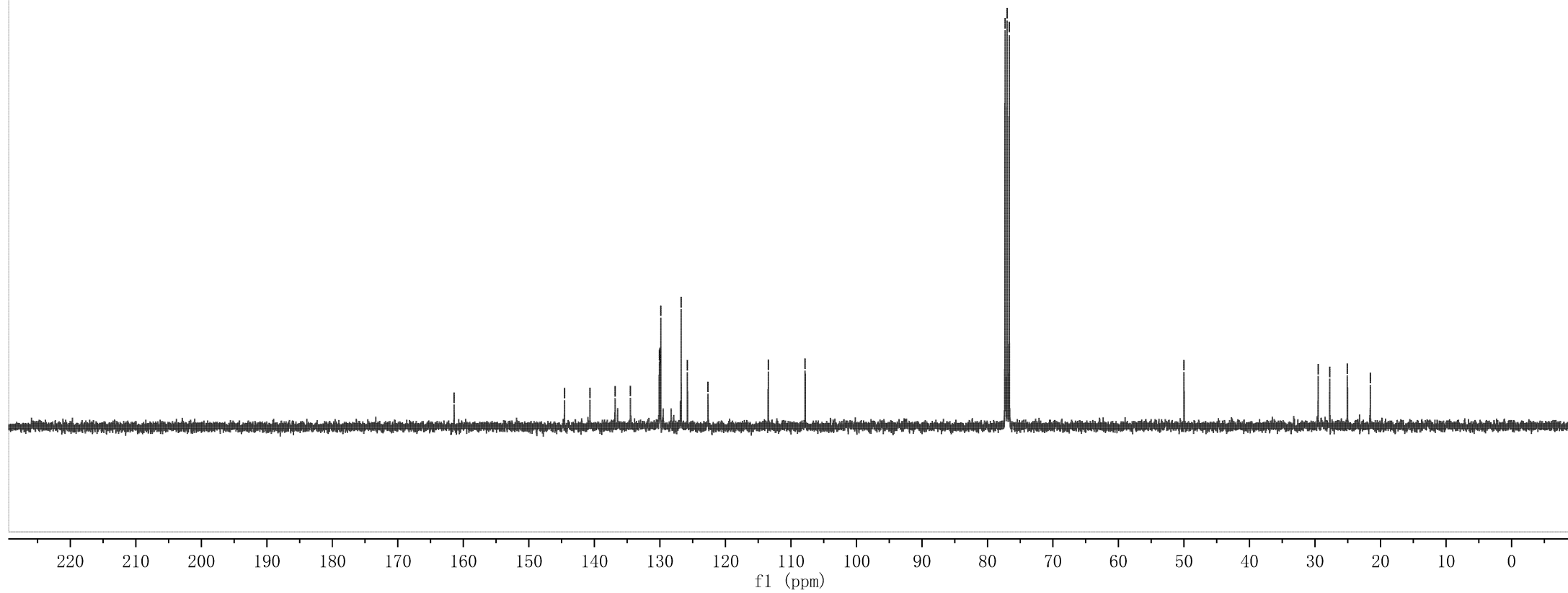
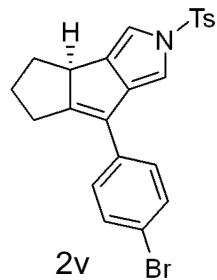
50.00

29.52

27.76

25.06

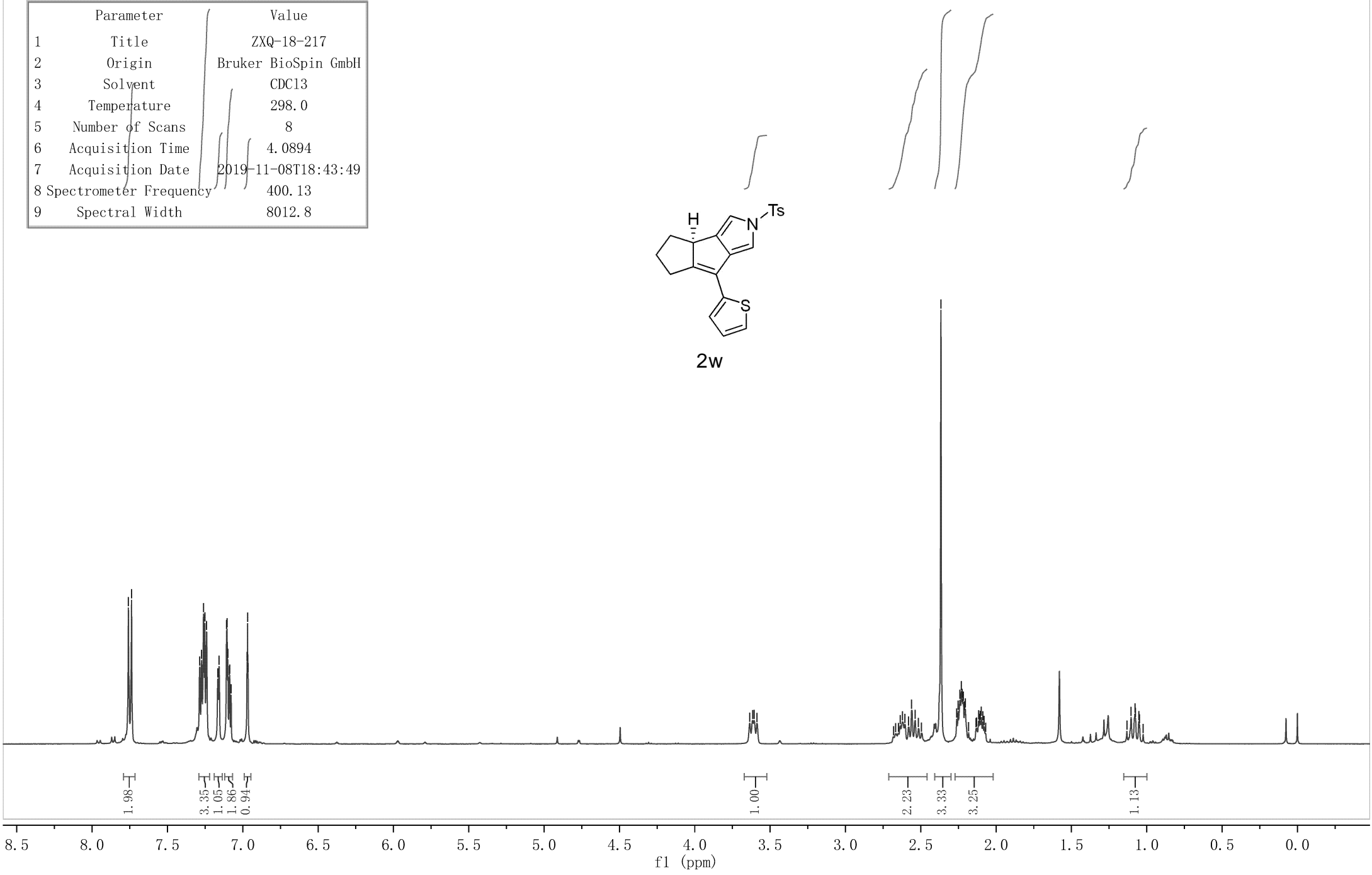
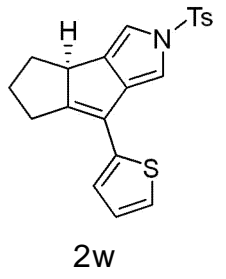
21.55



7.759  
7.738  
7.286  
7.274  
7.260  
7.251  
7.240  
7.166  
7.157  
7.108  
7.099  
7.090  
7.086  
7.077  
6.971  
6.968  
6.965  
6.965

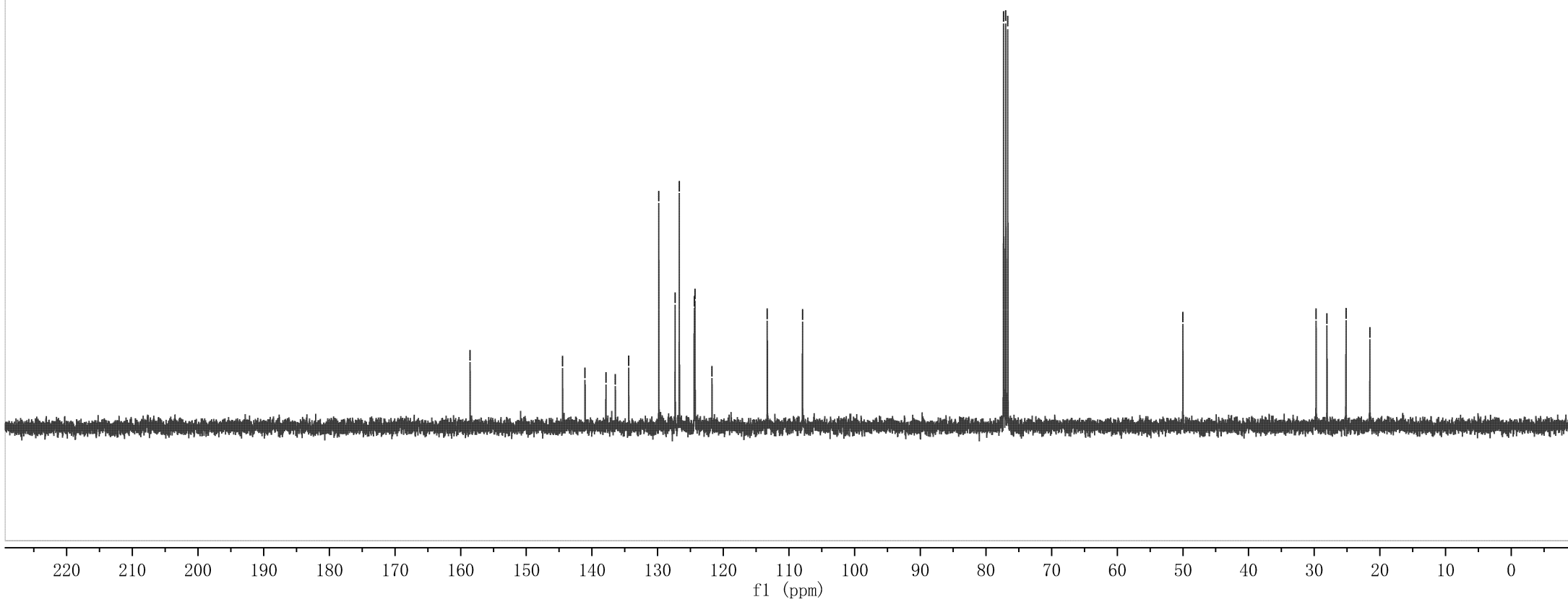
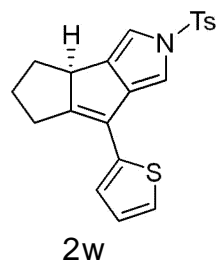
3.635  
3.616  
3.606  
3.606  
3.587  
2.636  
2.622  
2.605  
2.561  
2.537  
2.366  
2.261  
2.252  
2.240  
2.231  
2.225  
2.220  
2.217  
2.210  
2.204  
2.116  
2.110  
2.106  
2.098  
2.087  
1.132  
1.104  
1.078  
1.075  
1.053  
1.048  
1.024

Parameter	Value
1 Title	ZXQ-18-217
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-08T18:43:49
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-18-217-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	55
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-09T16:49:02
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.56  
 144.48  
 141.05  
 137.88  
 136.44  
 134.41  
 129.82  
 127.34  
 126.70  
 124.42  
 124.31  
 121.72  
 113.30  
 107.94  
 77.32  
 77.00  
 76.68  
 50.01  
 29.71  
 28.07  
 25.16  
 21.53

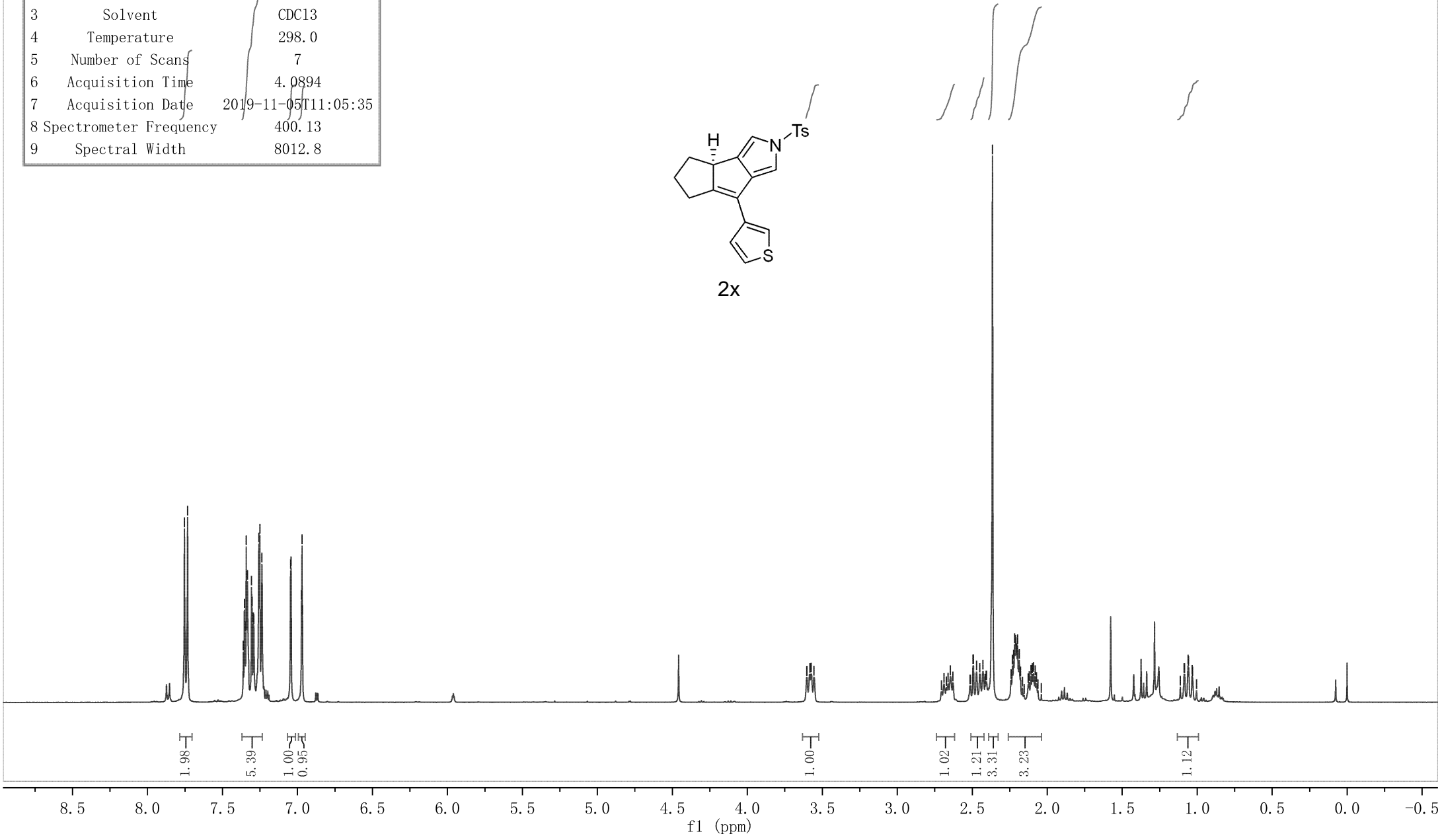
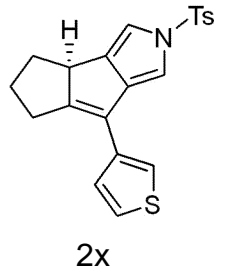


7.754  
7.733  
7.361  
7.354  
7.349  
7.342  
7.334  
7.306  
7.303  
7.294  
7.291  
7.257  
7.251  
7.237  
7.046  
7.043  
6.973  
6.970  
6.966  
6.966

3.604  
3.602  
3.583  
3.574  
3.556

2.645  
2.495  
2.492  
2.471  
2.451  
2.428  
2.365  
2.232  
2.225  
2.218  
2.212  
2.208  
2.204  
2.198  
2.187  
2.109  
2.100  
2.094  
1.112  
1.112  
1.087  
1.084  
1.061  
1.057  
1.034  
1.034  
1.031  
1.005

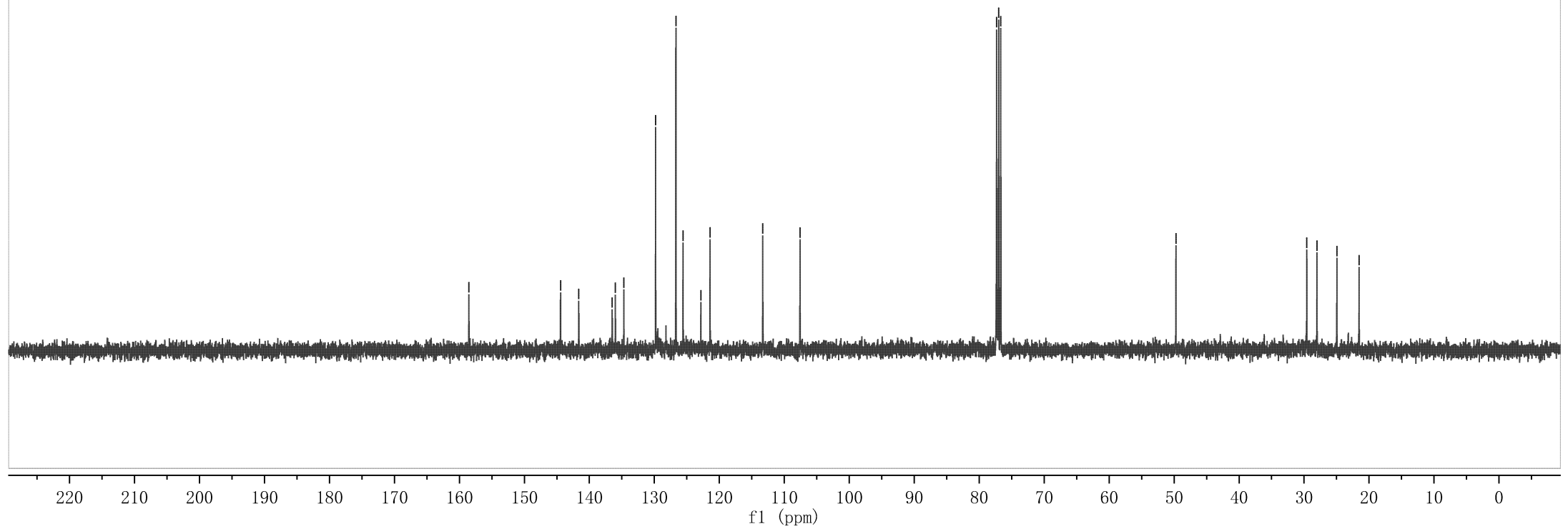
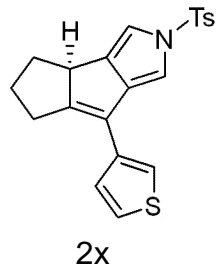
Parameter	Value
1 Title	ZXQ-18-213
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-05T11:05:35
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5  
f1 (ppm)

Parameter	Value
1 Title	ZXQ-18-213-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	74
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-05T17:42:14
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.54  
 144.43  
 141.62  
 136.48  
 135.99  
 134.69  
 129.80  
 126.68  
 125.58  
 122.84  
 121.42  
 113.31  
 107.57  
 77.32  
 77.00  
 76.68  
 49.72  
 29.58  
 28.01  
 24.94  
 21.52





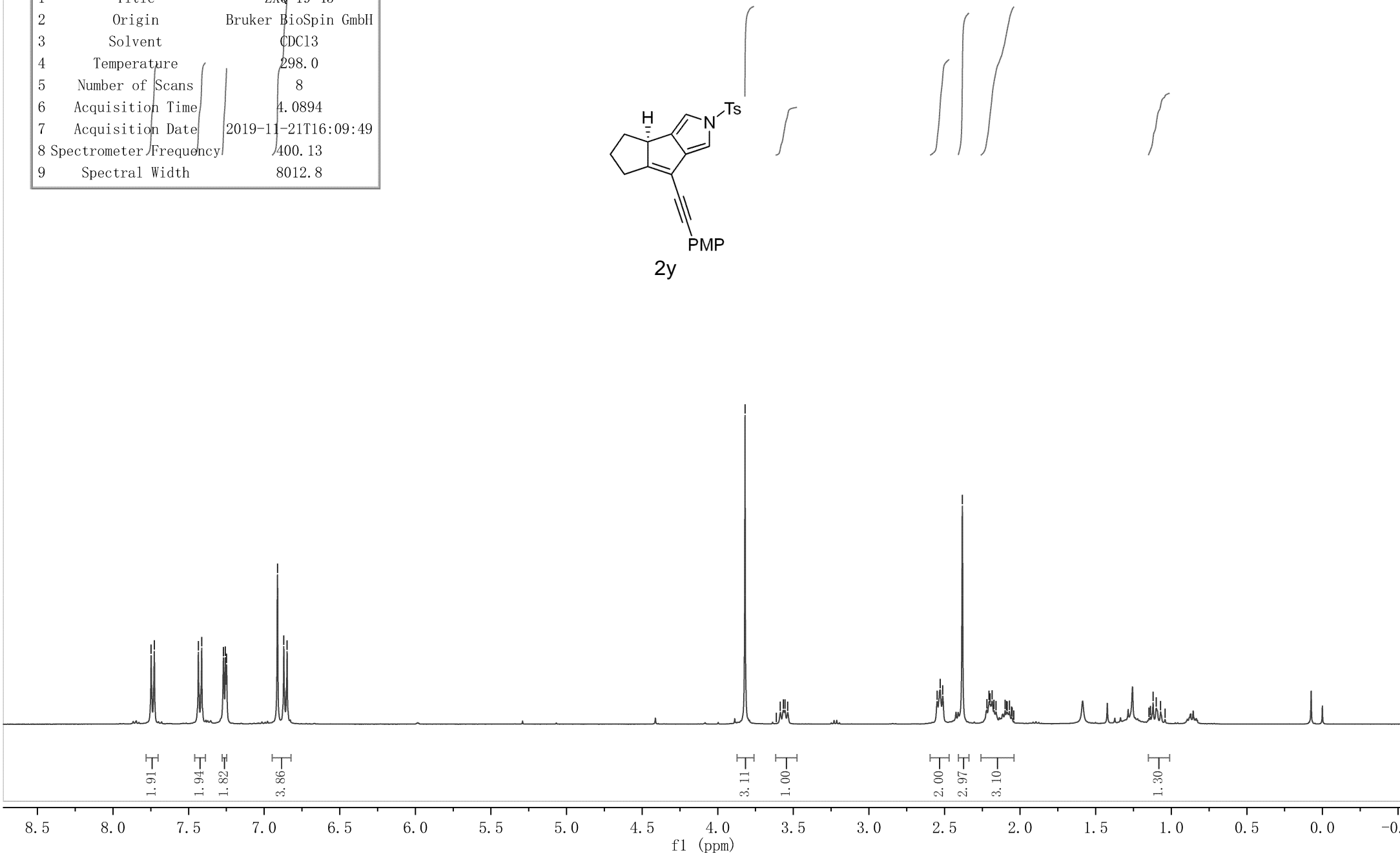
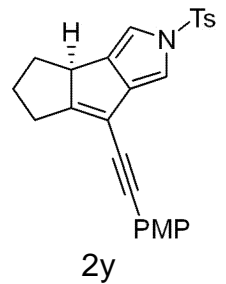
7.748  
7.727  
7.435  
7.413  
7.269  
7.257  
7.249  
6.912  
6.870  
6.848

3.819  
3.613  
3.586  
3.566  
3.555  
3.537

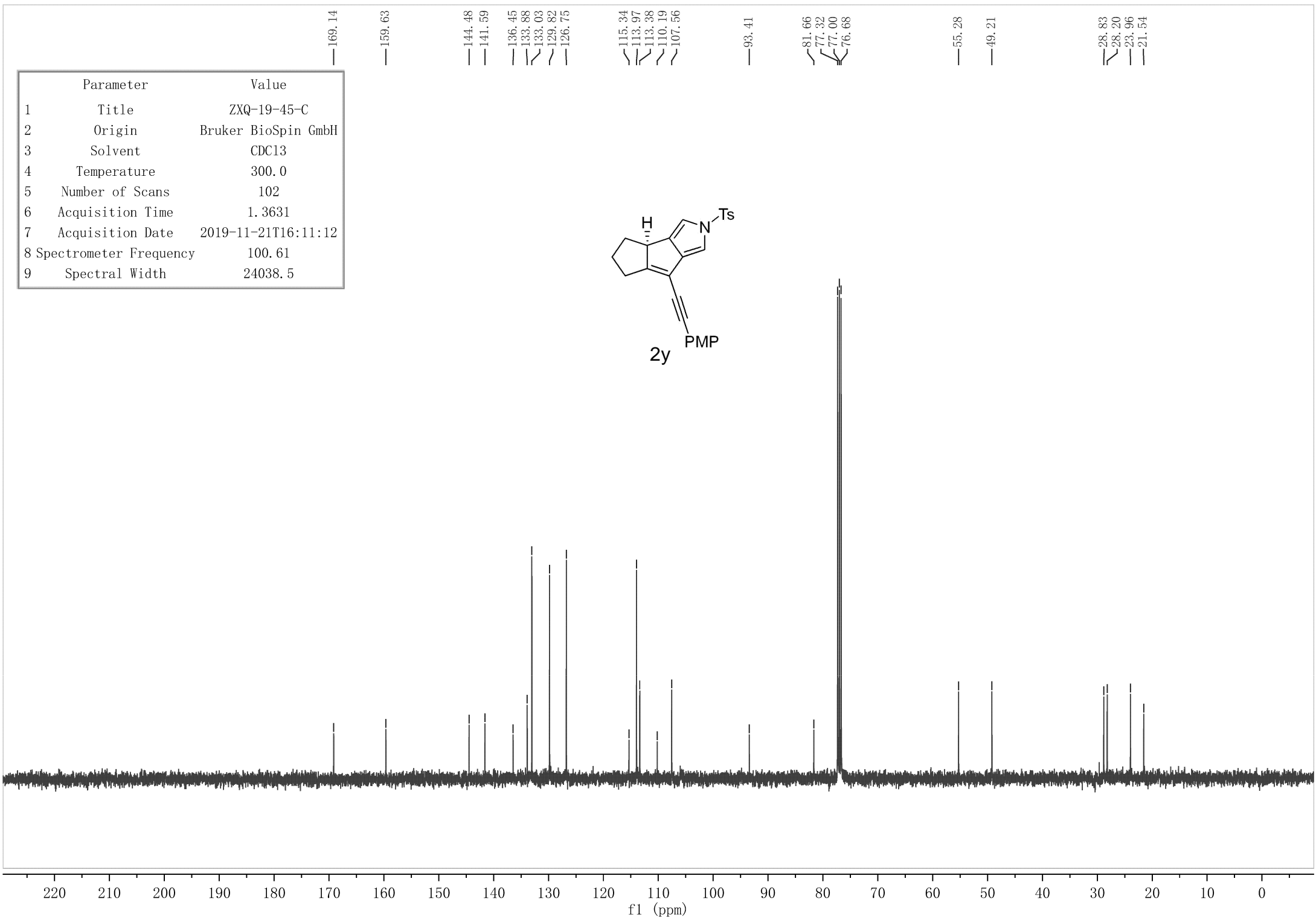
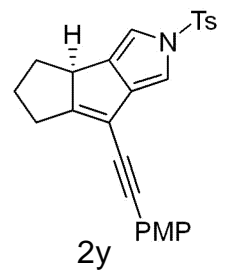
2.548  
2.528  
2.512  
2.382  
2.220  
2.205  
2.199  
2.185  
2.173  
2.159  
2.099  
2.090  
2.085  
2.071  
2.057  
2.052  
2.042

1.148  
1.138  
1.120  
1.099  
1.070  
1.041

Parameter	Value
1 Title	ZXQ-19-45
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2019-11-21T16:09:49
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

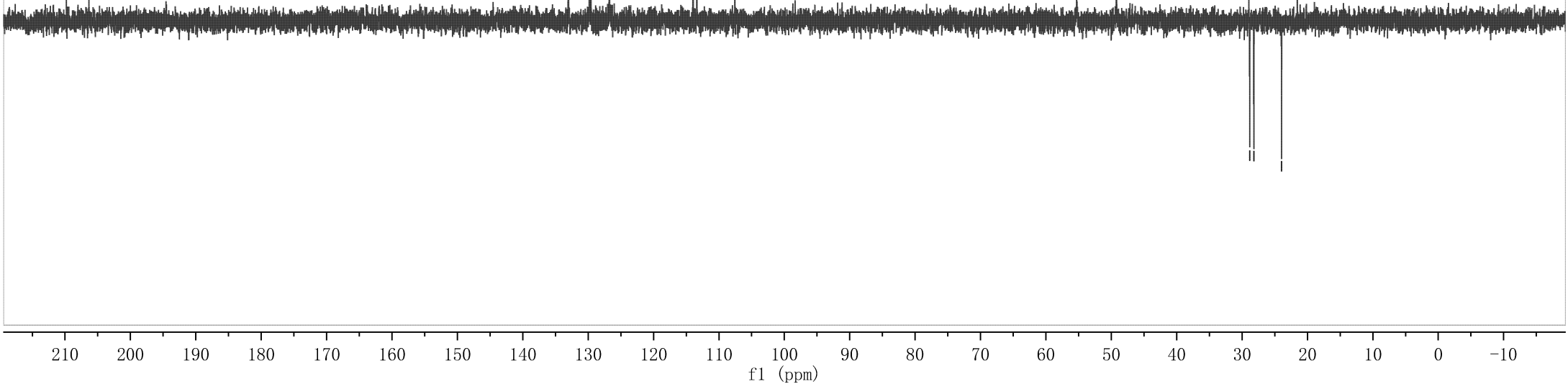
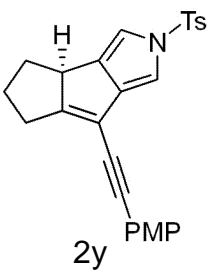


Parameter	Value
1 Title	ZXQ-19-45-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	102
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-21T16:11:12
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-19-45-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	27
6 Acquisition Time	1.3631
7 Acquisition Date	2019-11-21T16:17:40
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

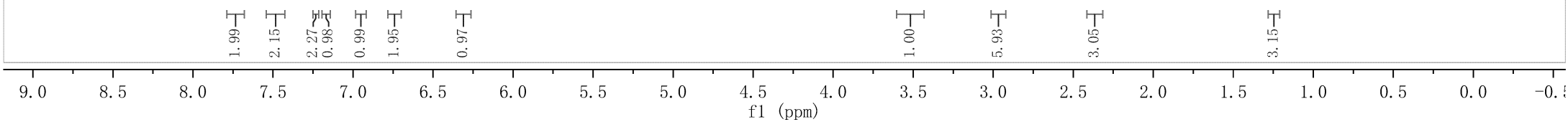
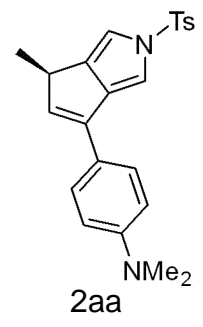
133.03  
 129.82  
 126.75  
 113.97  
 113.38  
 107.56  
 55.28  
 49.21  
 28.83  
 28.21  
 23.96  
 21.54



7.752  
7.731  
7.500  
7.478  
7.250  
7.170  
6.965  
6.948  
6.738  
6.726  
6.324  
6.318

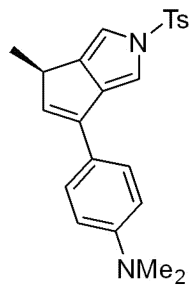
3.528  
3.512  
3.493  
3.491  
3.475  
2.976  
2.365  
1.263  
1.244

Parameter	Value
1 Title	ZXQ-20-43
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.2
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-16T15:23:22
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

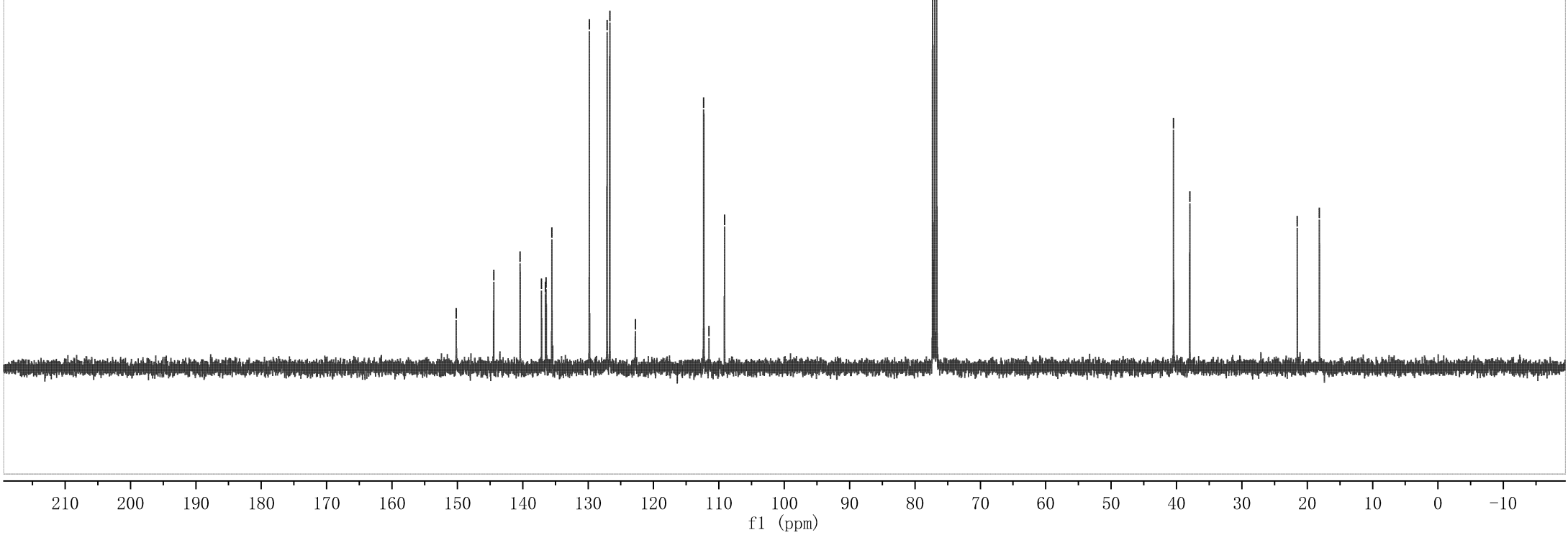


Parameter	Value
1 Title	ZXQ-20-43-C-
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	174
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-16T15:26:21
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

150.17 144.44 140.40 137.12 136.52 136.42 135.55 129.81 127.10 126.69 122.77 112.32 111.52 109.13 77.32 77.00 76.68 40.46 37.97 21.53 18.14



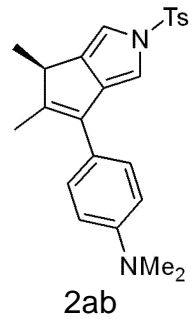
2aa



7.716  
7.696  
7.358  
7.341  
7.336  
7.223  
6.993  
6.922  
6.919  
6.894  
6.891  
6.775  
6.770  
6.752  
6.746  
6.746

3.291  
3.273  
3.255  
3.236  
2.969  
2.342  
2.021  
1.268  
1.249

Parameter	Value
1 Title	ZXQ-20-69
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-22T17:52:41
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



1.97  
1.97  
1.93  
1.92  
2.04

1.00  
5.92  
3.08  
3.07  
3.15

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5  
f1 (ppm)

Parameter	Value
1 Title	ZXQ-20-69
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-22T17:52:41
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

149.46  
145.75  
144.23  
139.59  
138.52  
136.52

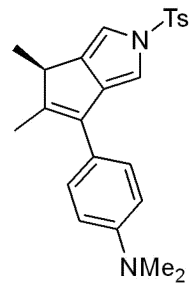
130.35  
129.69  
128.83  
126.62  
123.44

112.28  
112.18  
107.50

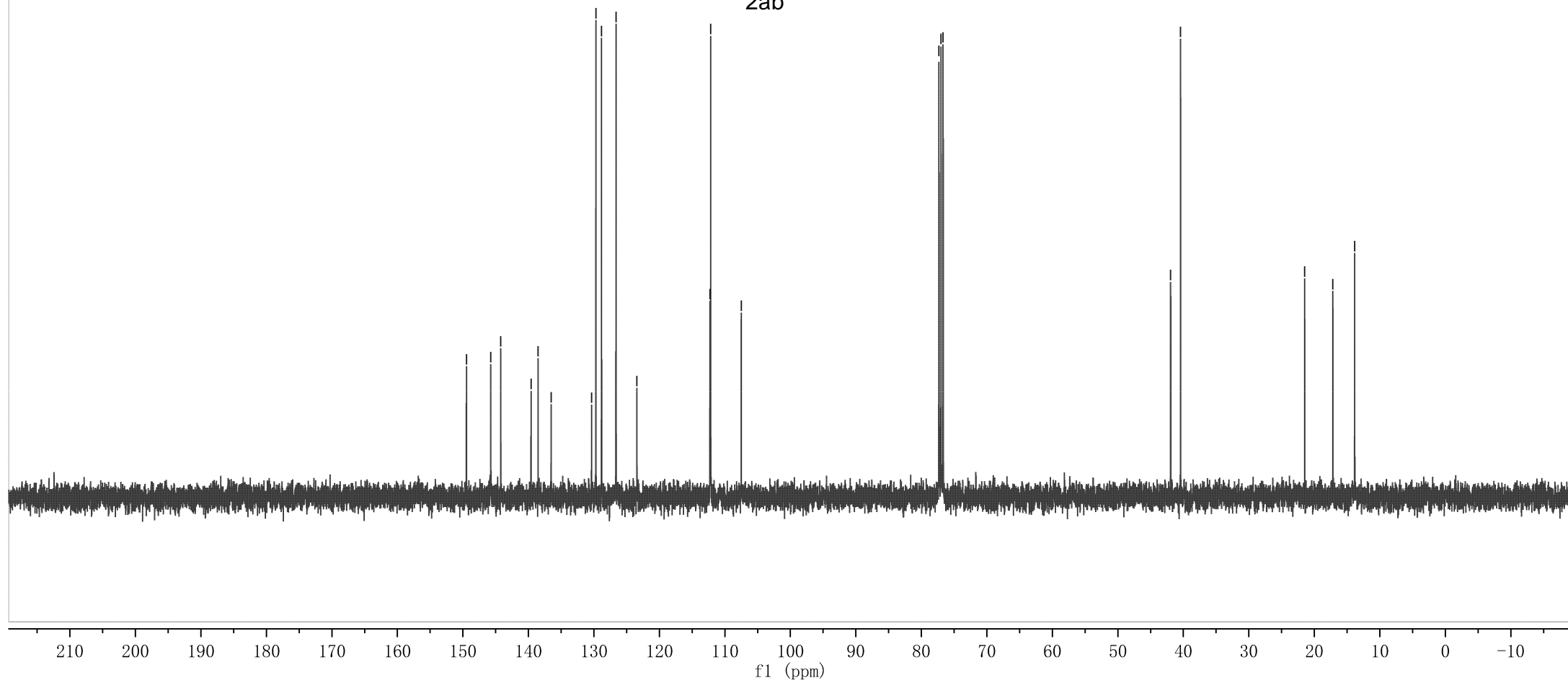
77.32  
77.00  
76.68

41.94  
40.43

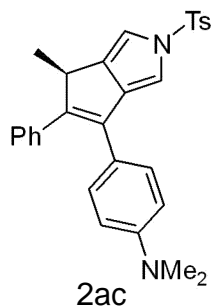
21.47  
17.17  
13.84



2ab



Parameter	Value
1 Title	ZXQ-20-70
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	15
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-22T20:02:00
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



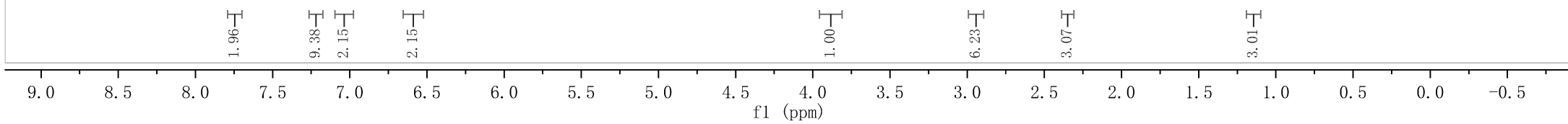
7.752  
7.731  
7.245  
7.229  
7.220  
7.207  
7.202  
7.198  
7.190  
7.058  
6.879  
6.819  
6.591

3.908  
3.892  
3.890  
3.873  
3.871  
3.855

2.927

2.355

1.146  
1.128





Parameter	Value
1 Title	ZXQ-20-70-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.6
5 Number of Scans	25
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-22T20:05:15
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

149.52  
147.67  
144.43

139.42  
138.24  
136.85  
136.61

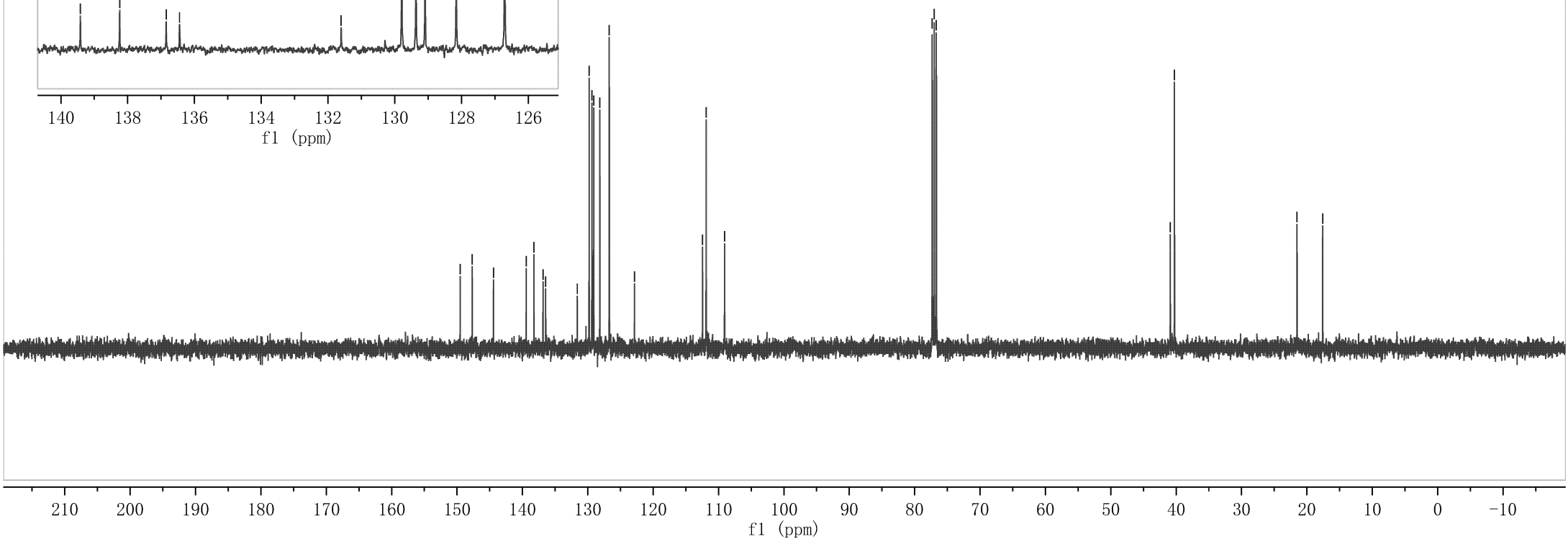
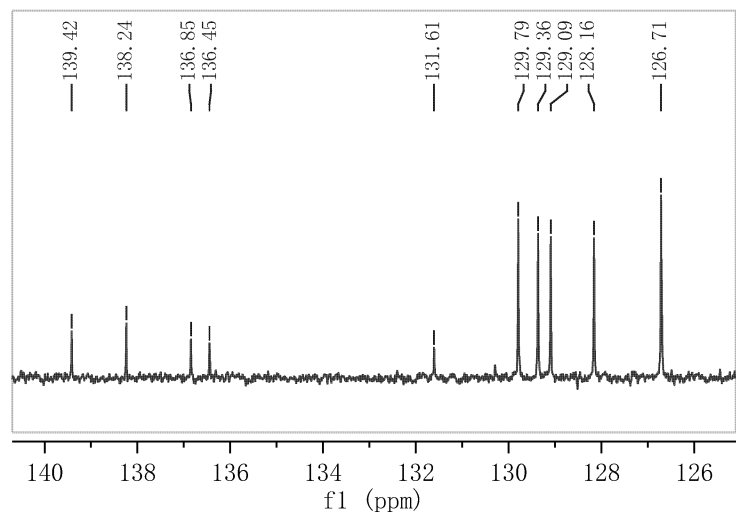
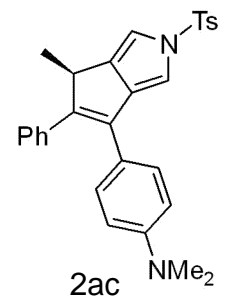
129.79  
129.36  
129.09  
128.16  
126.71  
122.86

112.45  
111.89  
109.07

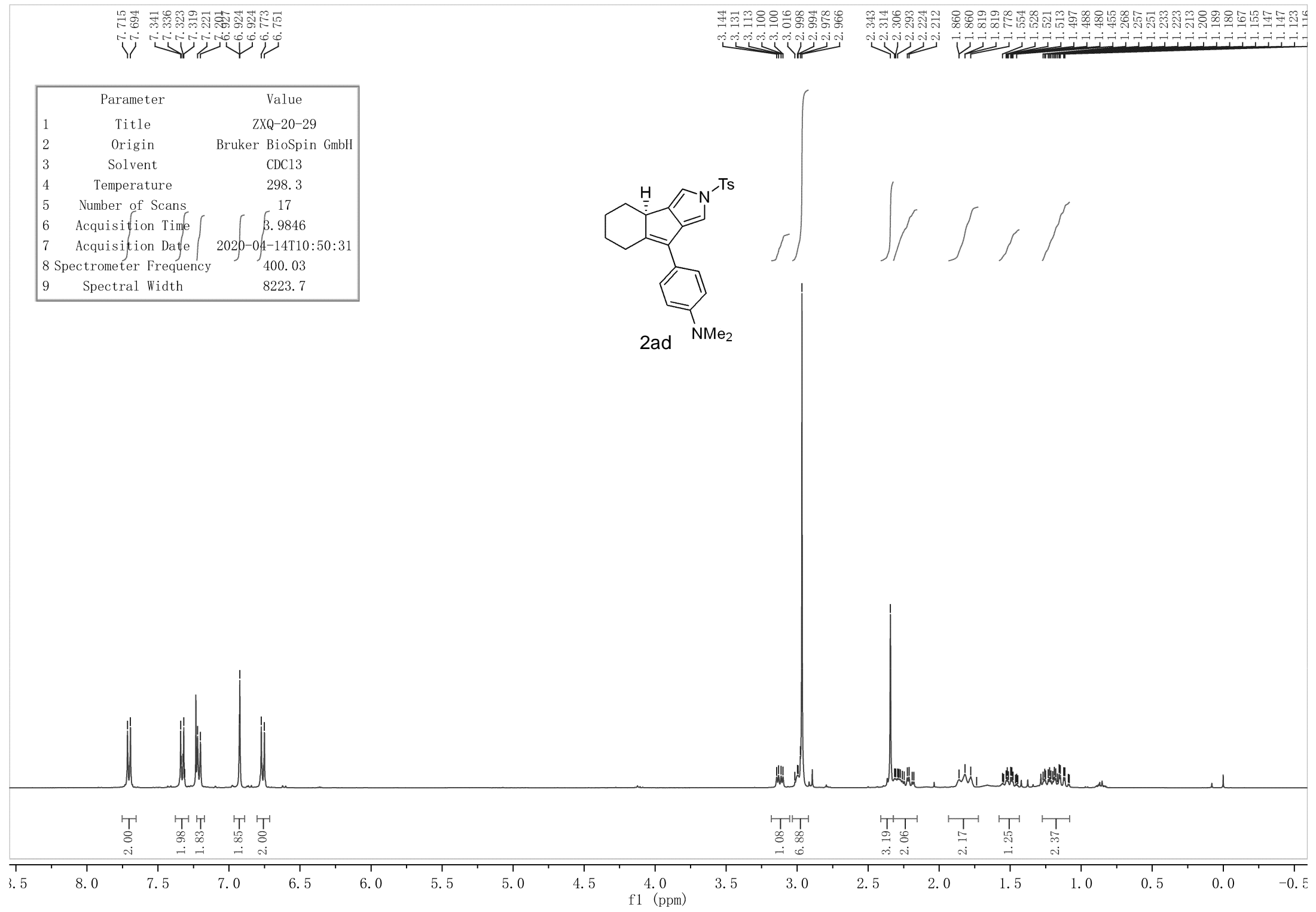
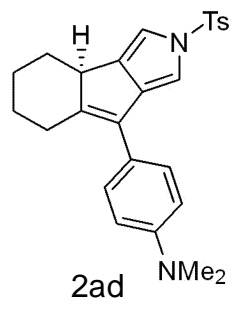
77.32  
77.00  
76.68

40.90  
40.26

21.51  
17.59

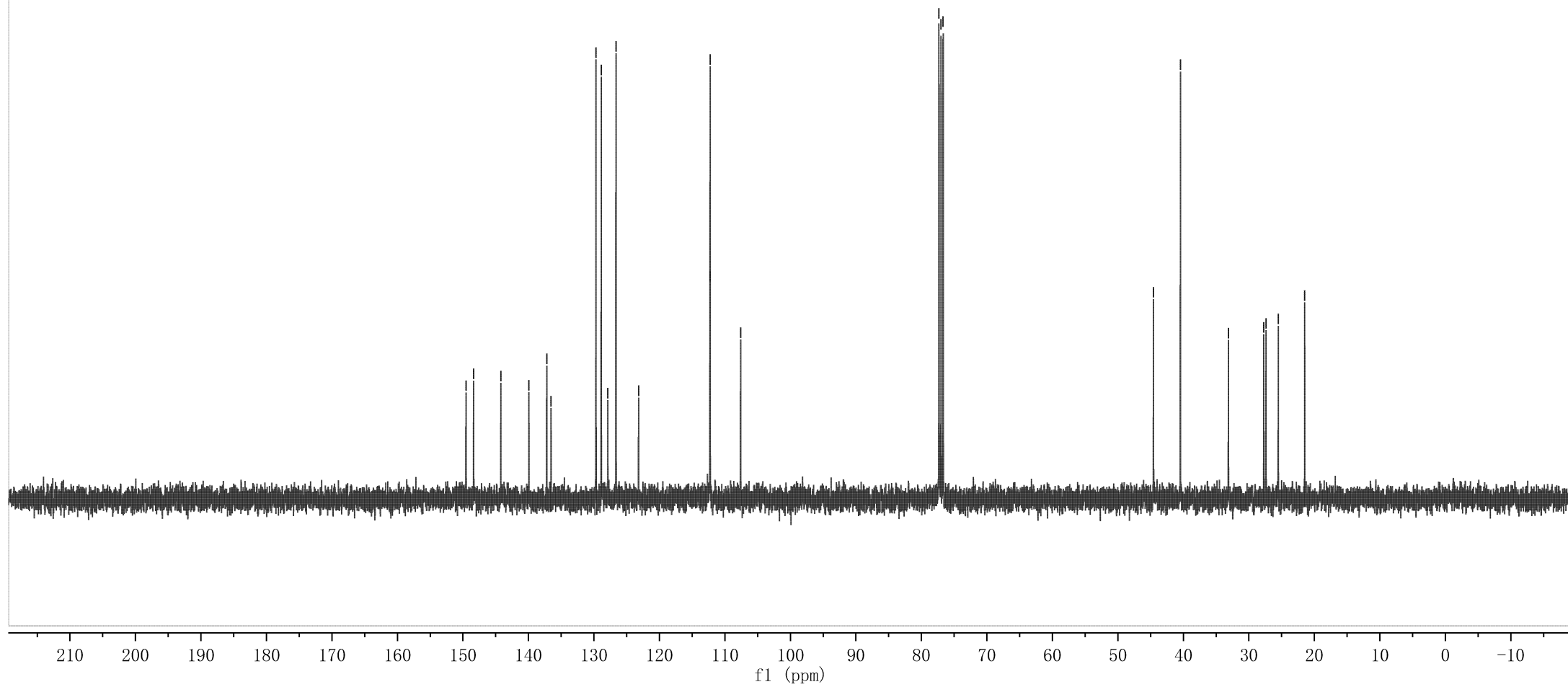
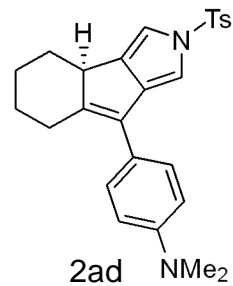


Parameter	Value
1 Title	ZXQ-20-29
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.3
5 Number of Scans	17
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-14T10:50:31
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

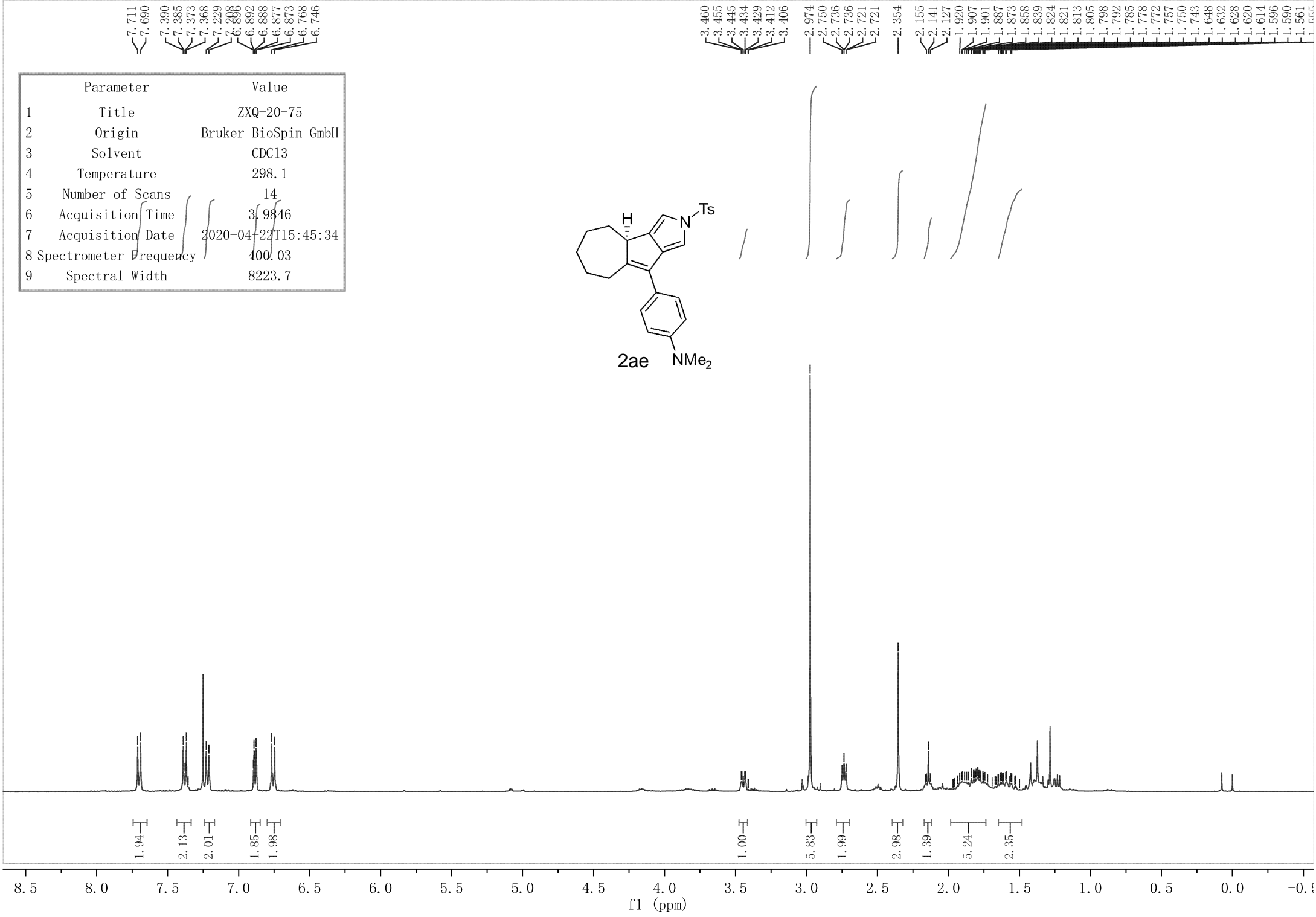
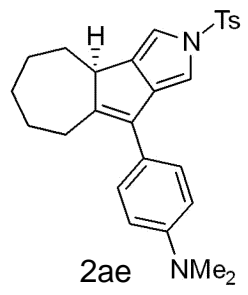


Parameter	Value
1 Title	ZXQ-20-29-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.7
5 Number of Scans	28
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-14T10:53:41
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

149.54  
148.37  
144.22  
139.93  
137.20  
136.55  
129.69  
128.88  
127.89  
126.63  
123.18  
112.29  
112.26  
107.61  
77.32  
77.00  
76.68  
44.57  
40.46  
33.12  
27.72  
27.39  
25.51  
21.48



Parameter	Value
1 Title	ZXQ-20-75
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.1
5 Number of Scans	14
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-22T15:45:34
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-20-75-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	46
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-22T15:48:38
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

151.12  
149.34  
144.20  
139.82  
138.29  
136.56  
129.79  
129.69  
128.73  
126.63  
123.85  
112.13  
107.42

77.32  
77.00  
76.68

47.45

40.44

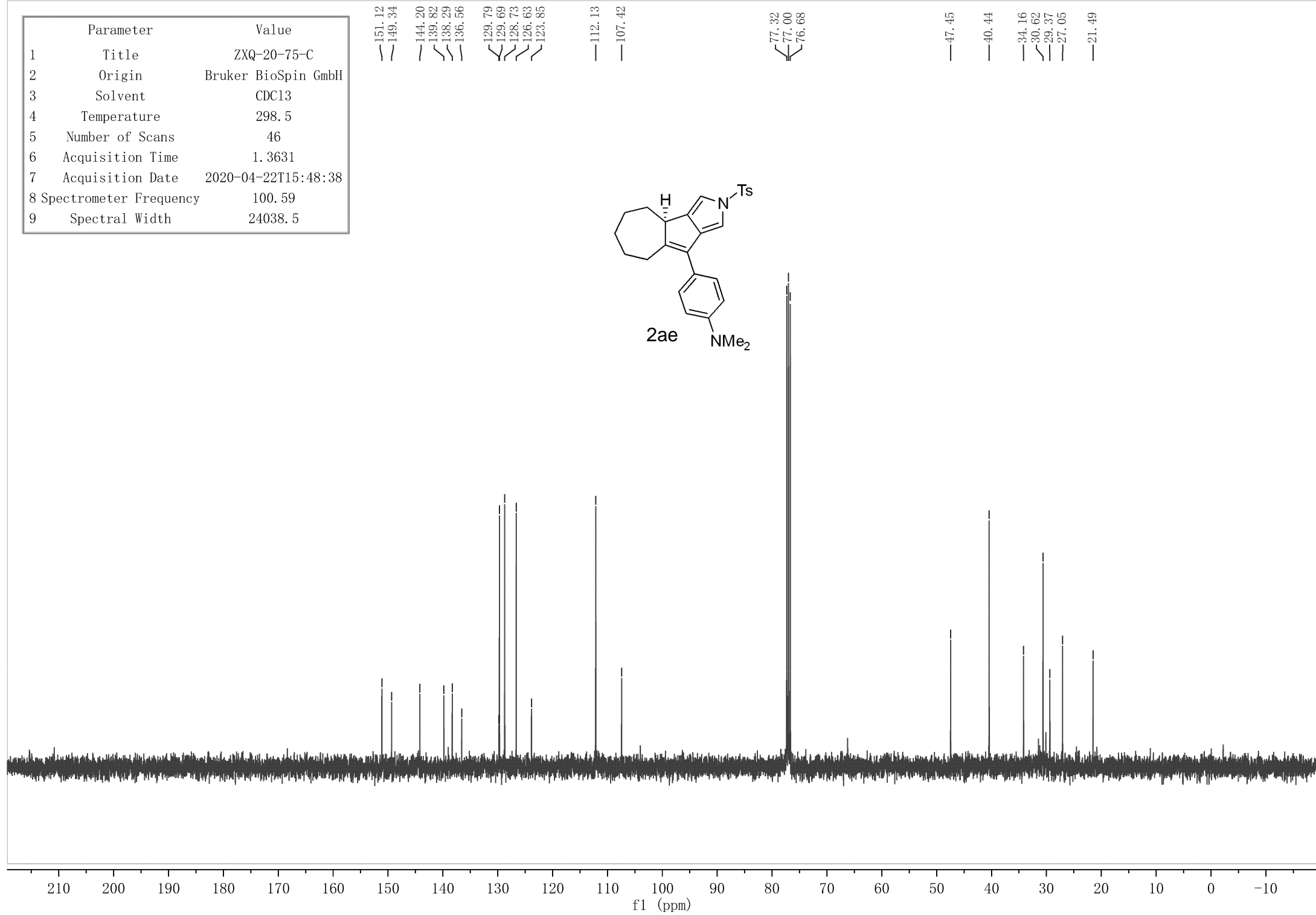
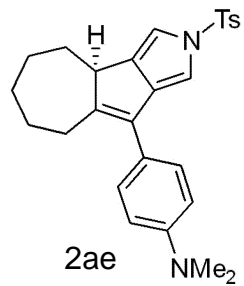
34.16

30.62

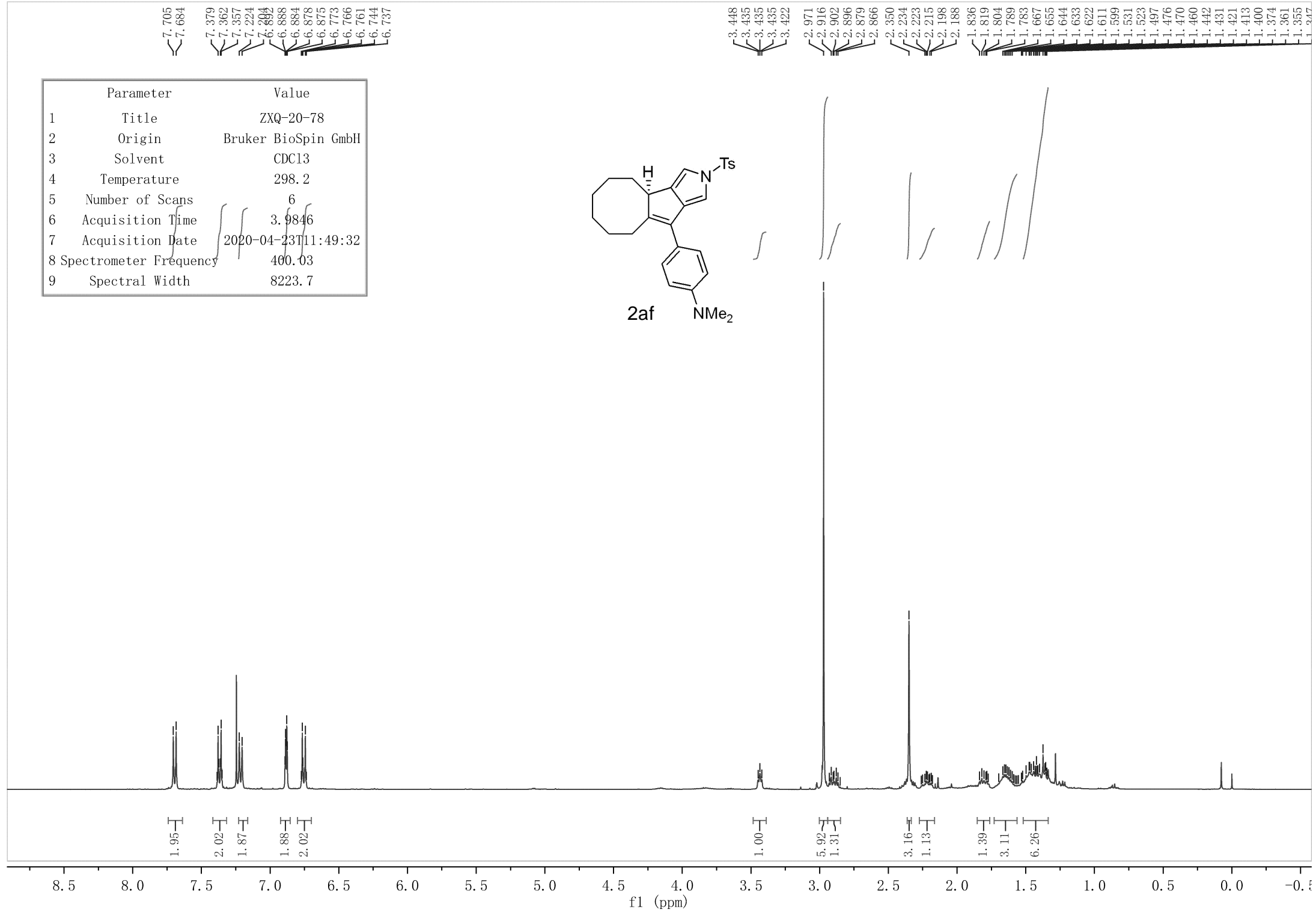
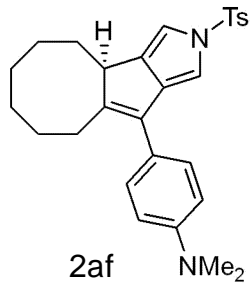
29.37

27.05

21.49

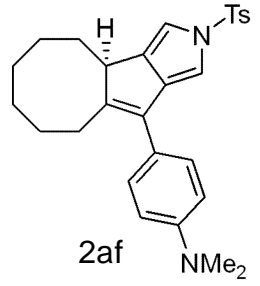


Parameter	Value
1 Title	ZXQ-20-78
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.2
5 Number of Scans	6
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-23T11:49:32
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-20-78-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	32
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-23T11:51:55
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

150.30  
149.40  
144.18  
140.36  
137.03  
136.56  
131.59  
129.65  
128.48  
126.57  
123.98



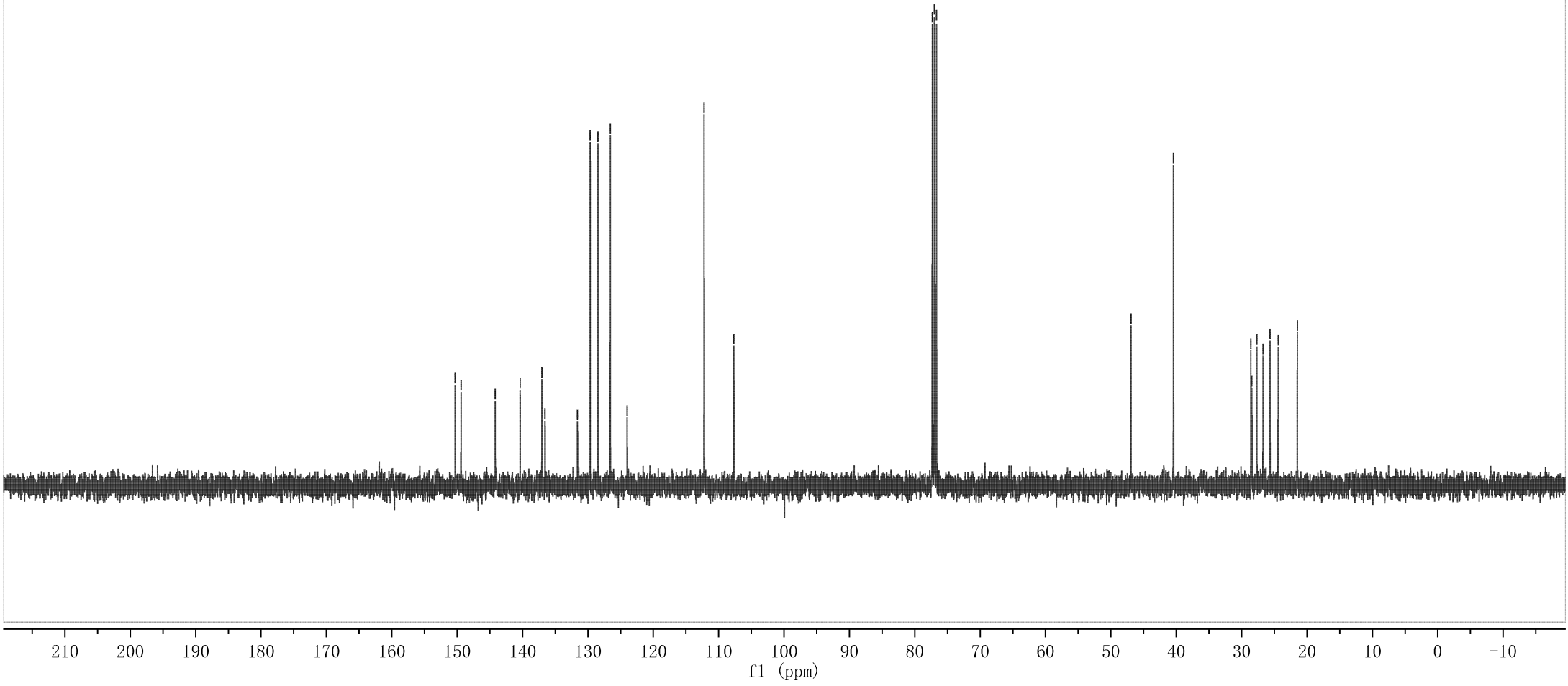
112.22  
107.67

77.32  
77.00  
76.68

46.92

40.42

28.58  
28.44  
27.68  
26.72  
25.66  
24.40  
21.49

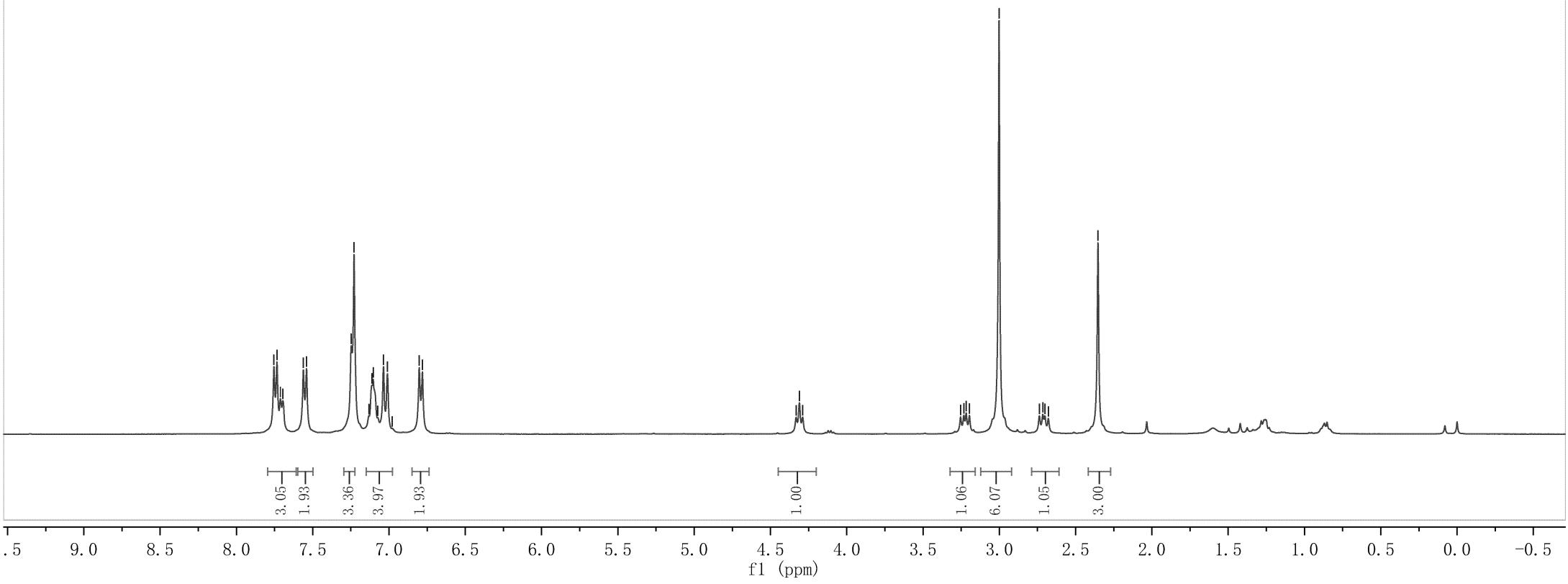
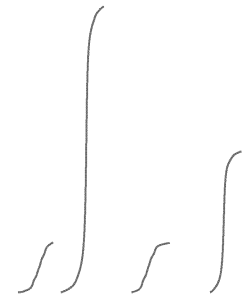
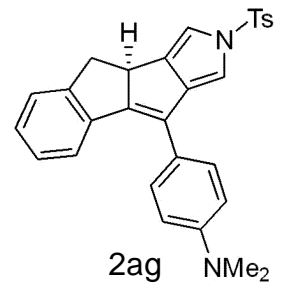


7.754  
7.734  
7.712  
7.696  
7.561  
7.541  
7.247  
7.229  
7.132  
7.111  
7.103  
7.074  
7.036  
7.010  
6.979  
6.802  
6.781

4.332  
4.310  
4.289

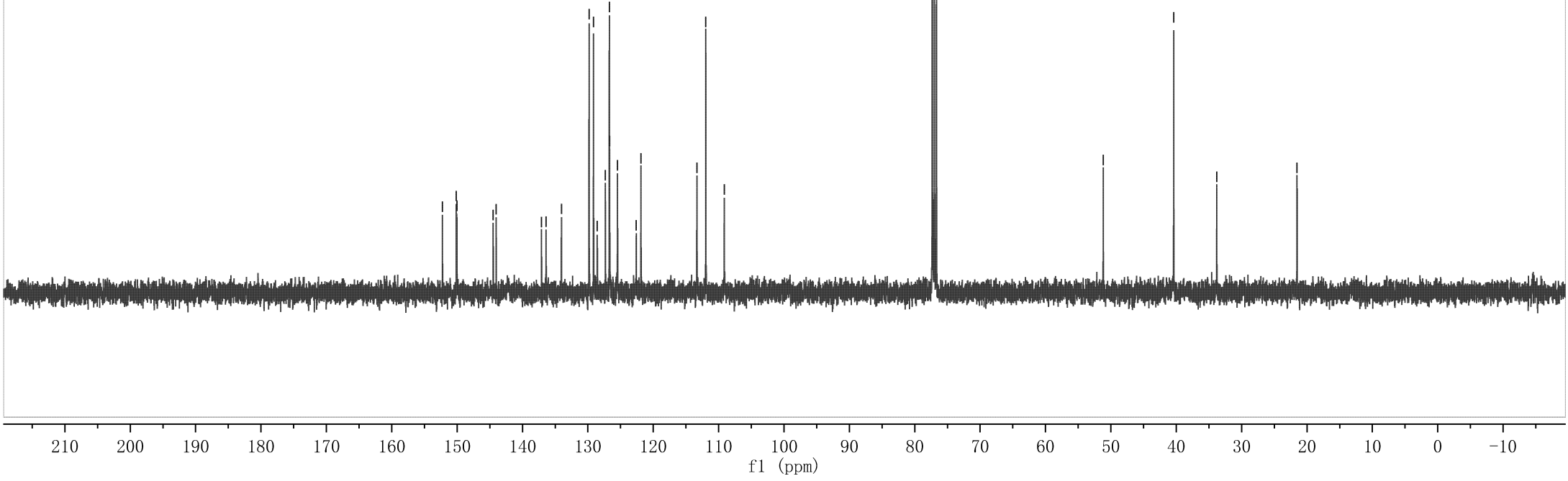
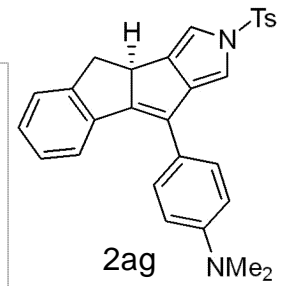
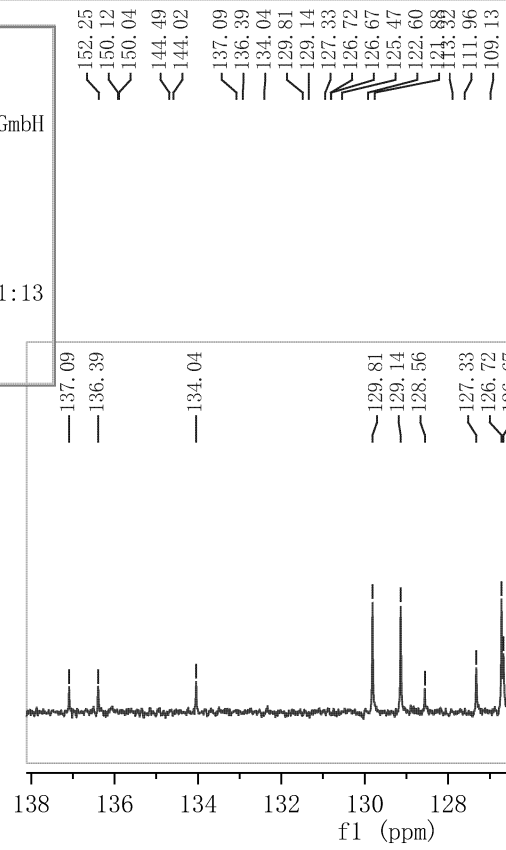
3.254  
3.233  
3.217  
3.196  
3.002  
2.738  
2.715  
2.702  
2.679  
2.353

Parameter	Value
1 Title	ZXQ-20-31
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.4
5 Number of Scans	16
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-14T10:58:54
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

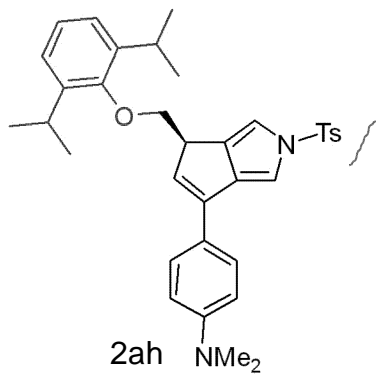




Parameter	Value
1 Title	ZXQ-20-31-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.6
5 Number of Scans	46
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-14T11:01:13
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-21-106
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.9
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2020-07-03T22:13:23
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

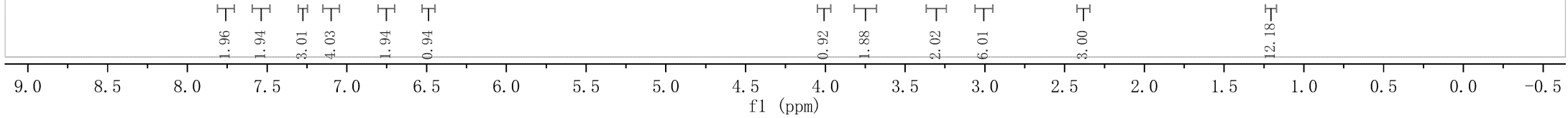


7.776  
7.755  
7.549  
7.527  
7.271  
7.265  
7.262  
7.251  
7.087  
6.745  
6.487  
6.481

4.021  
4.003  
3.985  
3.792  
3.771  
3.753  
3.739  
3.718  
3.697  
3.323  
3.305  
3.288  
2.953

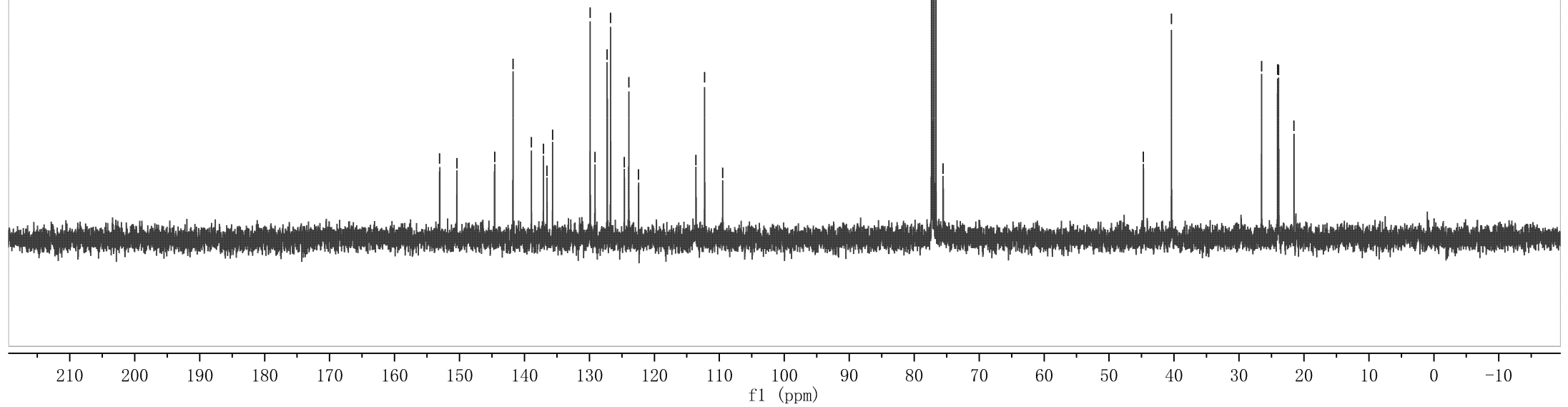
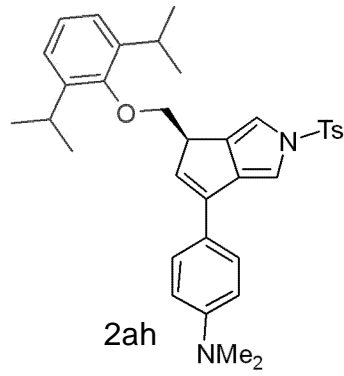
2.377

1.219  
1.203  
1.186



Parameter	Value
1 Title	ZXQ-21-106-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	301.0
5 Number of Scans	98
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-03T22:16:31
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

153.05  
150.40  
144.59  
141.76  
138.94  
137.08  
136.54  
135.66  
129.89  
129.14  
127.26  
126.74  
124.62  
123.94  
122.43  
113.60  
112.26  
109.49  
77.32  
77.00  
76.68  
75.55  
44.71  
40.39  
26.52  
24.06  
23.90  
21.53



Parameter	Value
1 Title	ZXQ-21-106-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	301.5
5 Number of Scans	19
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-03T22:22:47
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

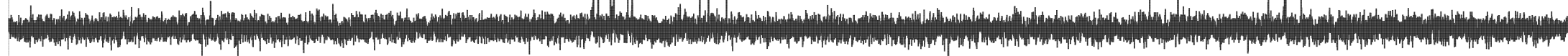
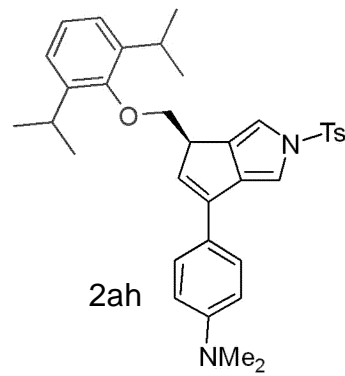
129.89  
129.14  
127.26  
126.74  
124.62  
123.94

113.60  
112.26  
109.49

75.55

44.71  
40.39

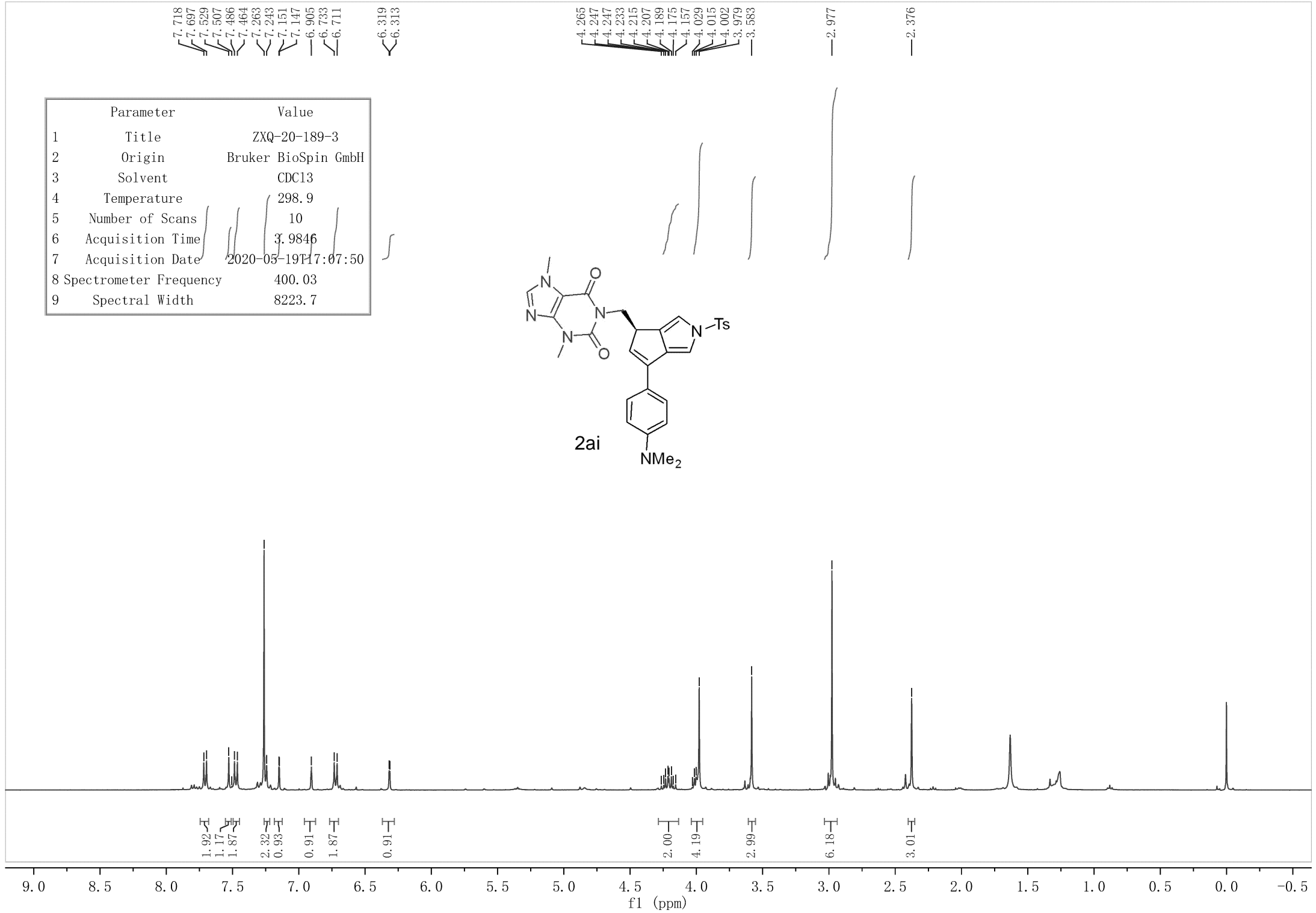
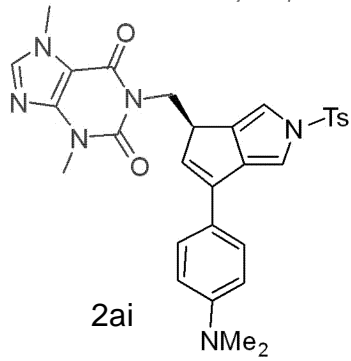
26.52  
24.06  
23.90  
21.53



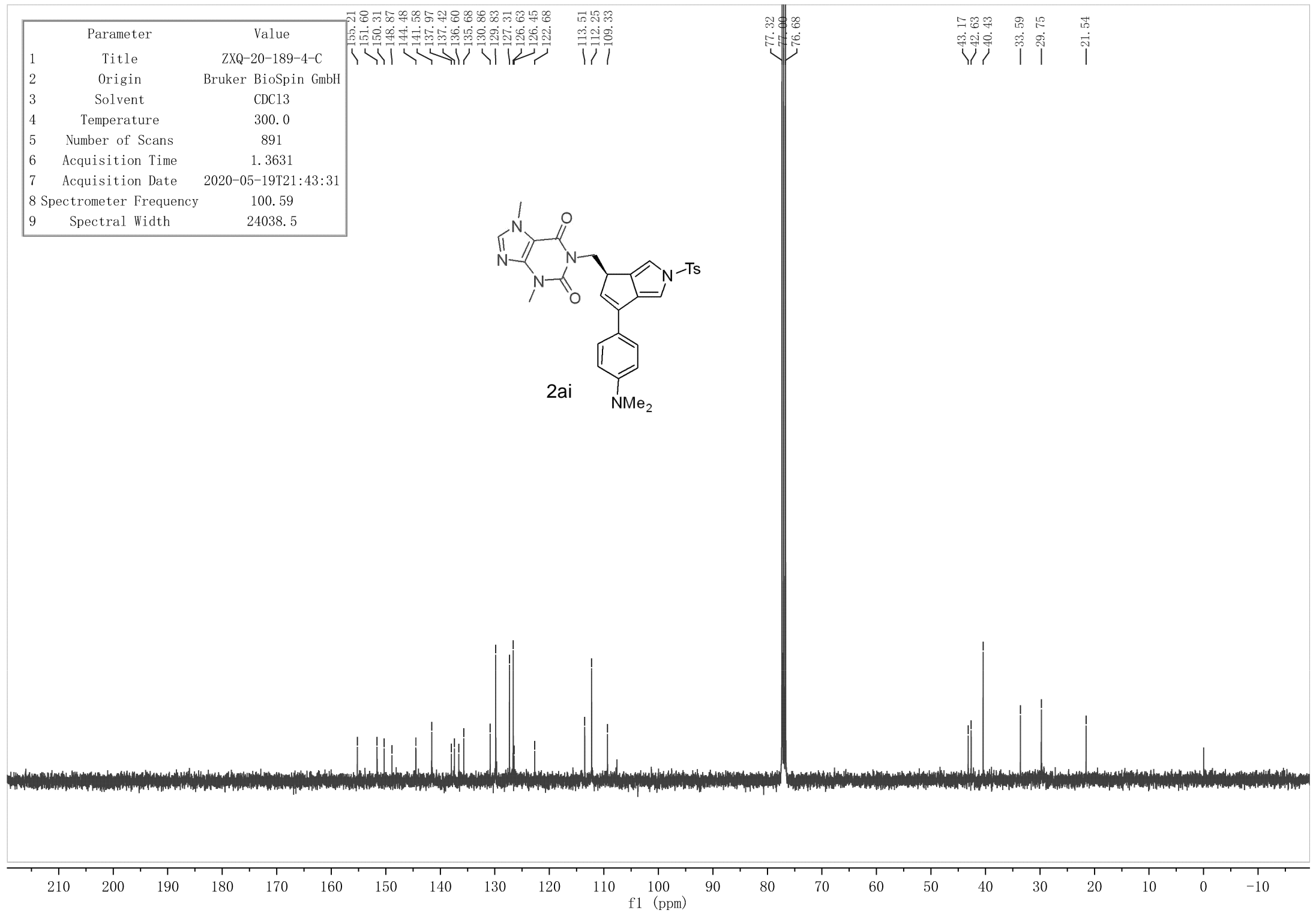
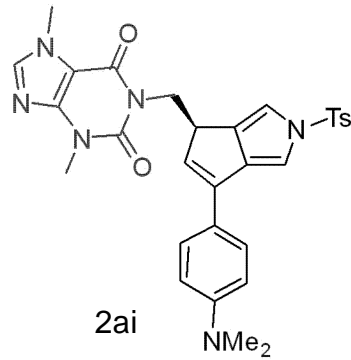
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

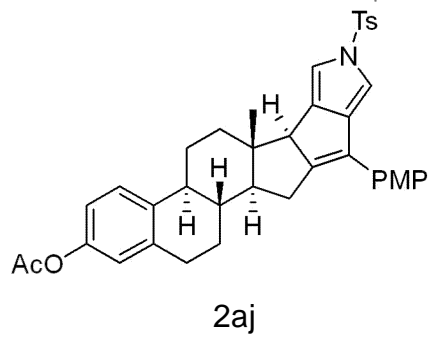
Parameter	Value
1 Title	ZXQ-20-189-3
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.9
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2020-05-19T17:07:50
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-20-189-4-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	891
6 Acquisition Time	1.3631
7 Acquisition Date	2020-05-19T21:43:31
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-19-157-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	16
6 Acquisition Time	4.0894
7 Acquisition Date	2019-12-25T16:37:41
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.746  
7.726  
7.518  
7.496  
7.297  
7.275  
7.261  
7.251  
7.242  
7.214  
7.212  
7.105  
6.980  
6.961  
6.940  
6.857  
6.852  
6.836  
6.831  
6.831  
6.783

3.837

3.465  
3.422  
3.422  
3.382

2.944  
2.926  
2.902  
2.863  
2.862

2.370  
2.370  
2.370  
2.271  
2.087  
2.065  
2.056  
1.941  
1.678  
1.646  
1.522  
1.504  
1.470  
1.438  
1.424

0.288

1.97  
2.07  
2.39  
1.17  
1.09  
3.05  
1.19  
1.16

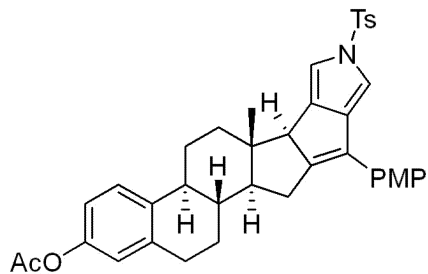
3.14  
1.00  
3.19  
5.09  
3.47  
4.40  
1.38  
2.90

2.89

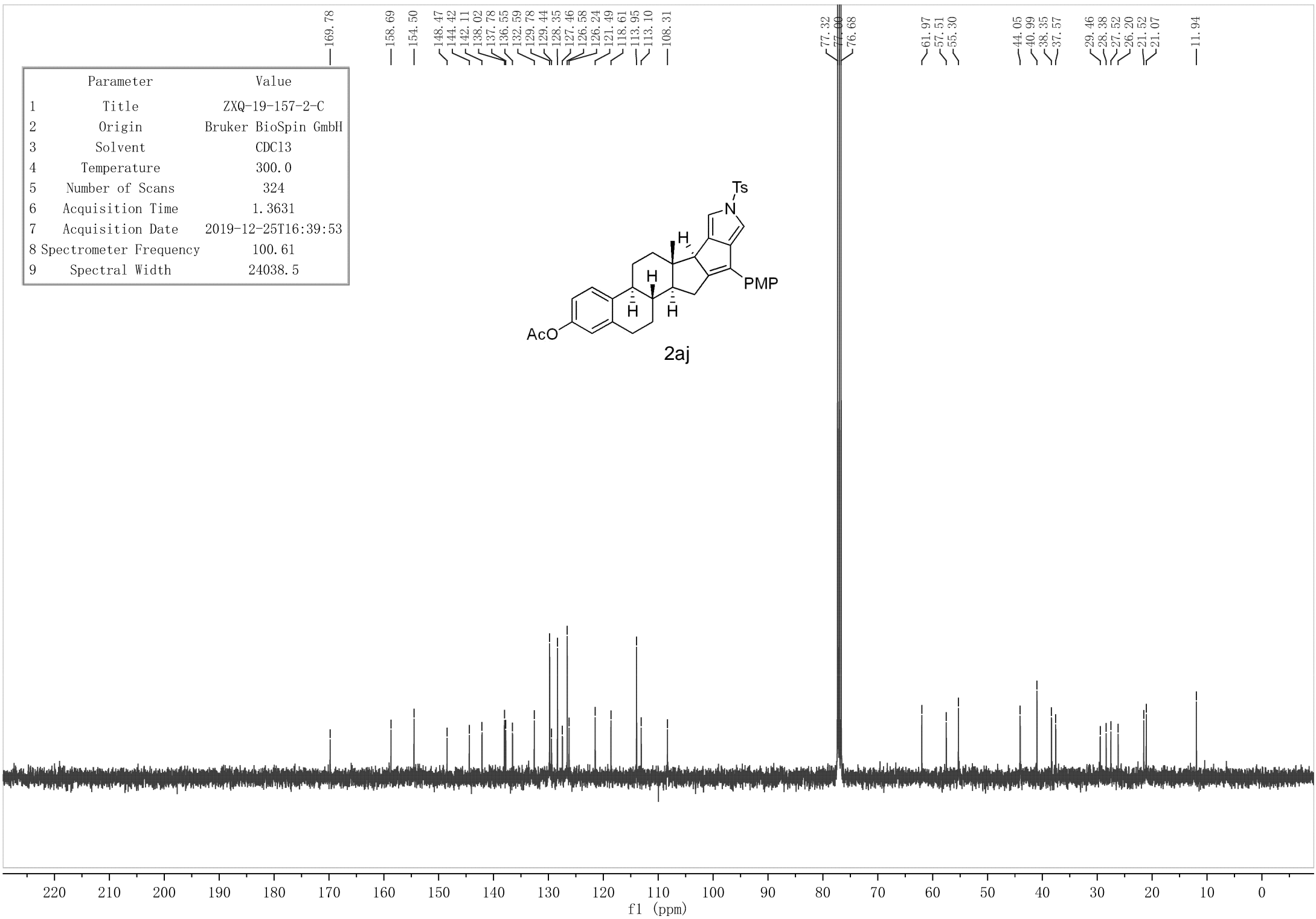
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

Parameter	Value
1 Title	ZXQ-19-157-2-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	324
6 Acquisition Time	1.3631
7 Acquisition Date	2019-12-25T16:39:53
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

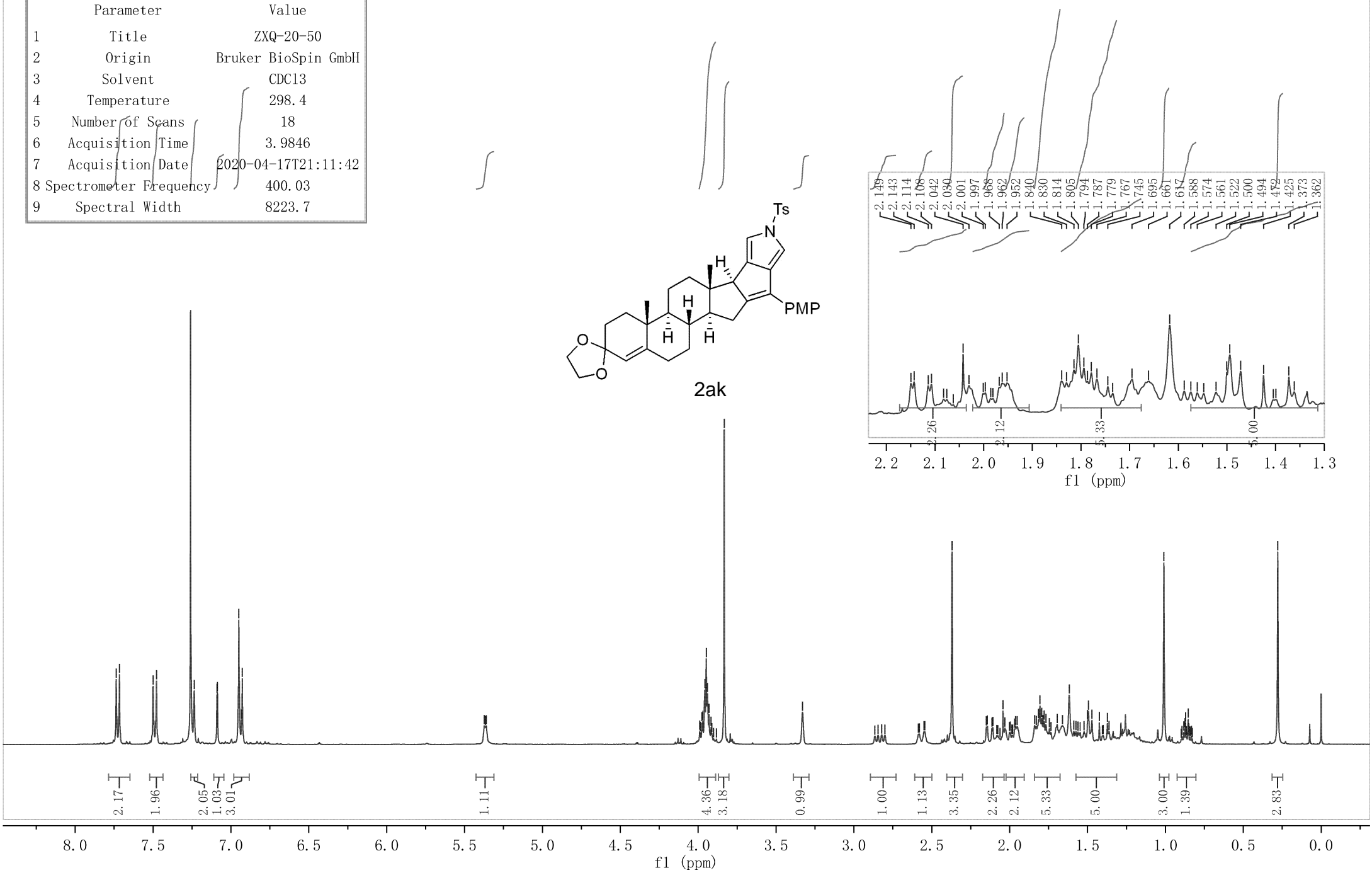
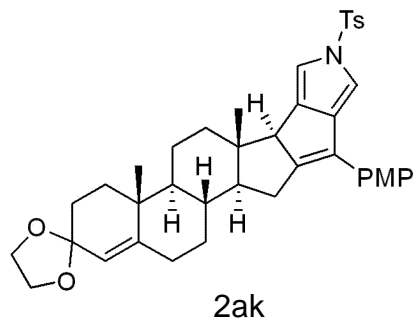


2aj

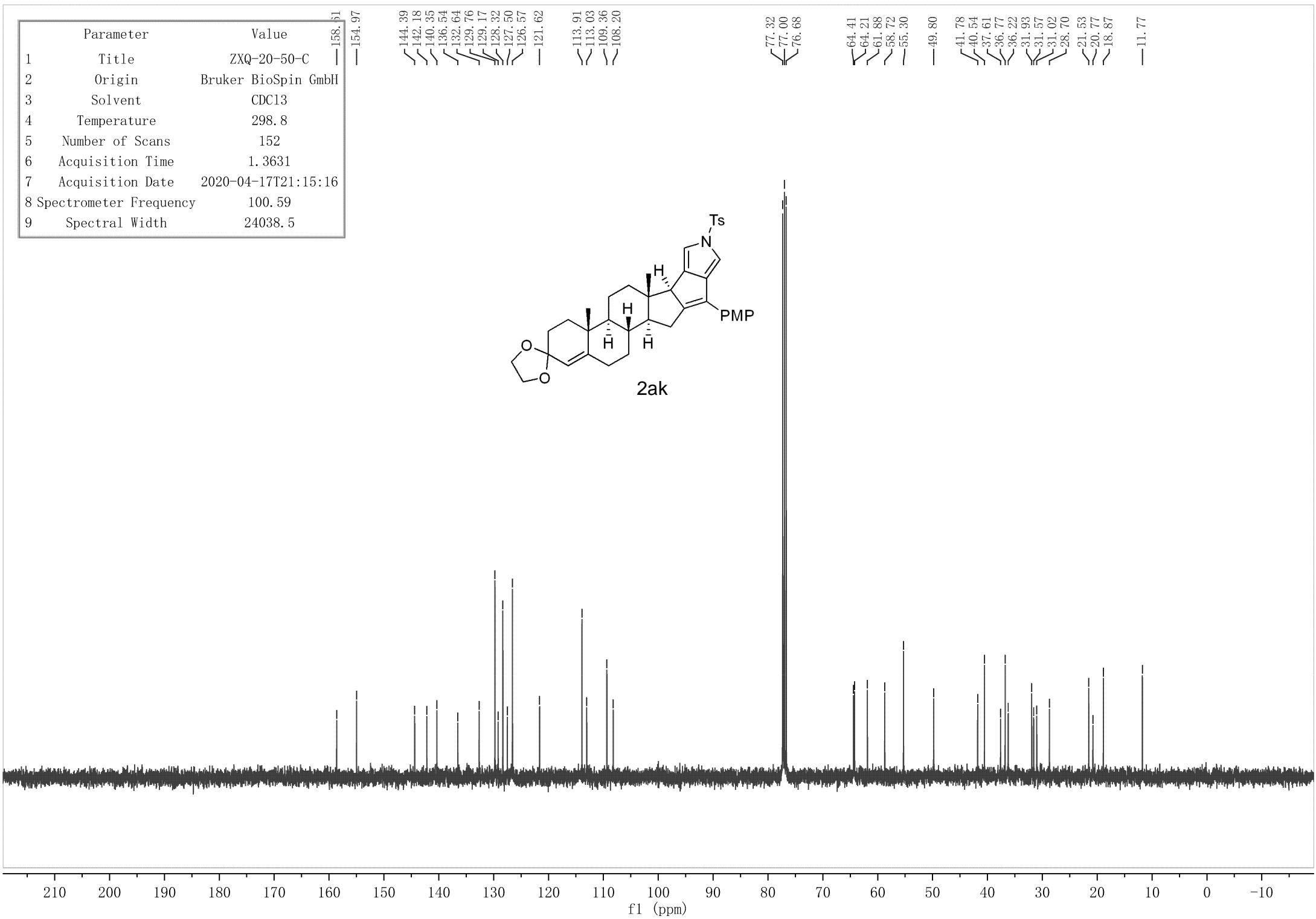
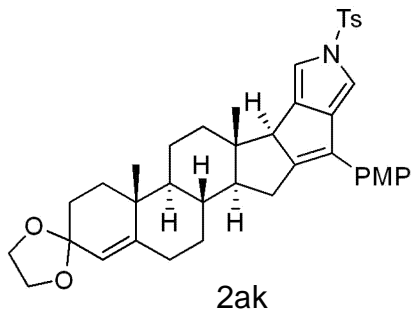




Parameter	Value
1 Title	ZXQ-20-50
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.4
5 Number of Scans	18
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-17T21:11:42
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

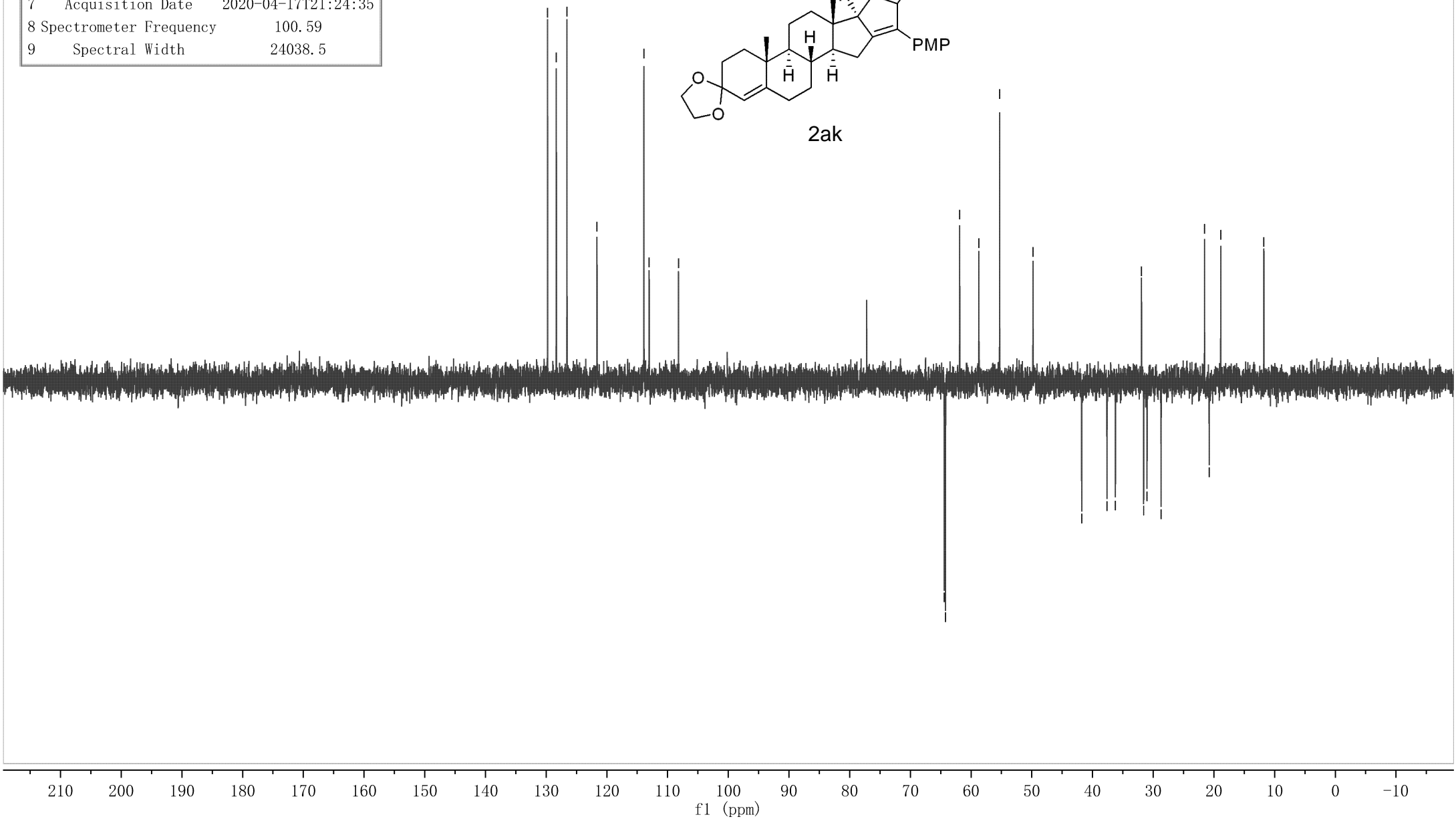
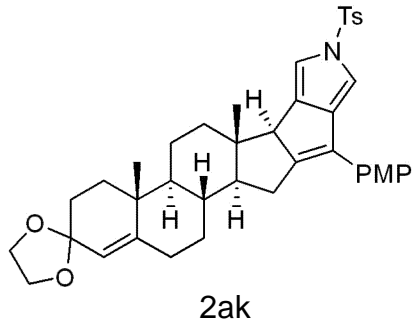


Parameter	Value
1 Title	ZXQ-20-50-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.8
5 Number of Scans	152
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-17T21:15:16
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



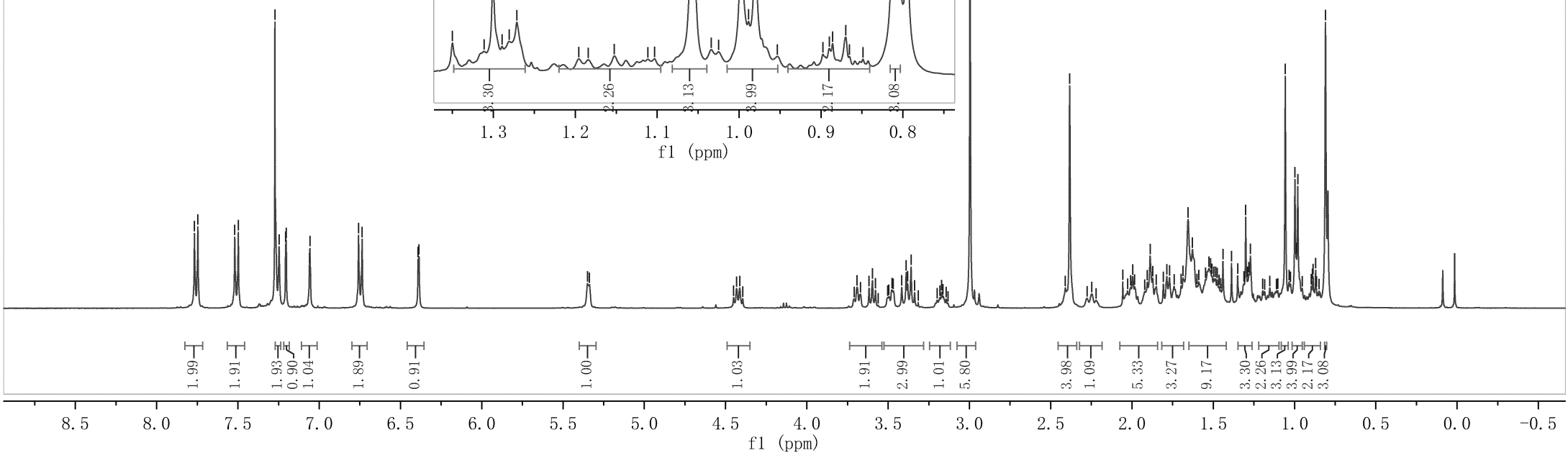
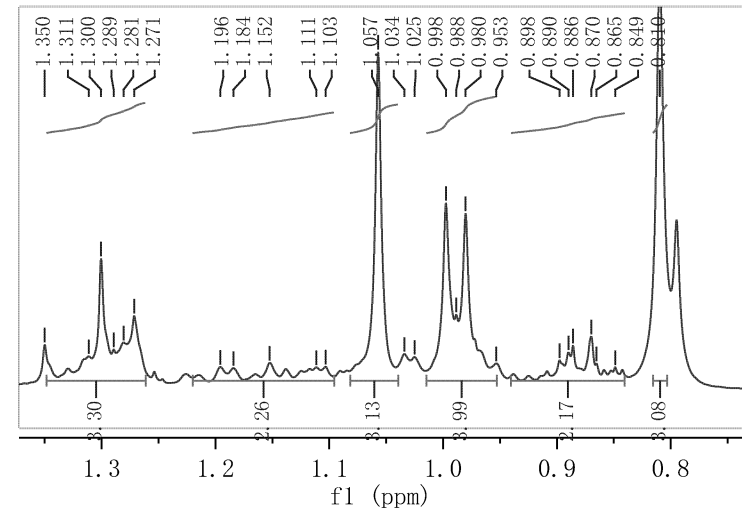
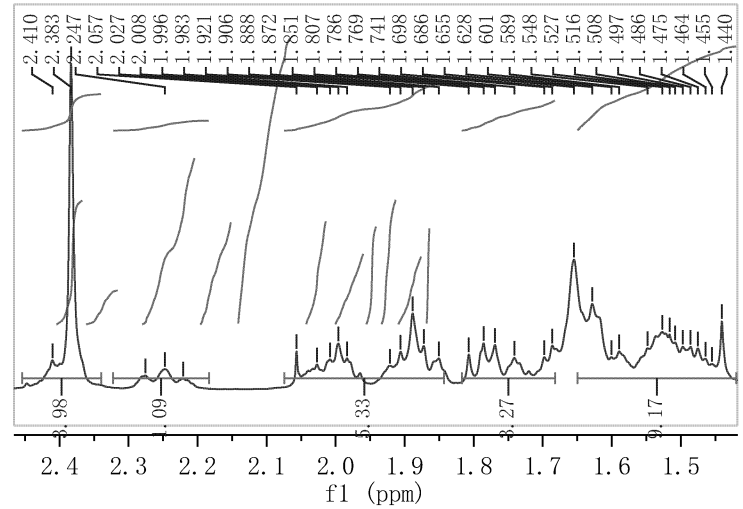
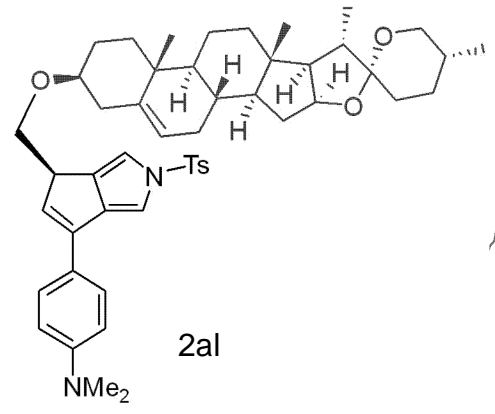
Parameter	Value
1 Title	ZXQ-20-50-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.2
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-17T21:24:35
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

129.76 128.32 126.57 121.63 113.90 113.03 108.20  
 64.41 64.21 61.88 58.71 55.30 49.80 41.78 37.61 36.22 31.93 31.57 31.01 28.70 21.54 20.77 18.87 11.77



7.767  
7.746  
7.520  
7.498  
7.272  
7.247  
7.206  
7.203  
7.060  
7.057  
6.758  
6.736  
6.392  
6.386  
5.350  
5.337  
4.451  
4.432  
4.413  
3.709  
3.691  
3.671  
3.618  
3.596  
3.578  
3.502  
3.496  
3.476  
3.469  
3.416  
3.389  
3.380  
3.359  
3.337  
3.182  
3.171  
3.163  
3.143  
2.996  
2.410  
2.383  
2.276  
2.247  
2.207  
2.057  
2.008  
1.996  
1.983  
1.921  
1.906  
1.888  
1.872  
1.851  
1.807  
1.786  
1.769  
1.741  
1.698  
1.686  
1.655  
1.628  
1.601  
1.589  
1.548  
1.527  
1.516  
1.508  
1.497  
1.486  
1.464  
1.455  
1.440  
1.388  
1.350  
1.311  
1.300  
1.289  
1.281  
1.271  
1.289  
1.281  
1.271  
1.196  
1.184  
1.152  
1.111  
1.103  
1.057  
1.034  
1.025  
0.998  
0.988  
0.980  
0.953  
0.898  
0.890  
0.886  
0.870  
0.865  
0.849  
0.810

Parameter	Value
1 Title	ZXQ-21-13
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.7
5 Number of Scans	9
6 Acquisition Time	3.9846
7 Acquisition Date	2020-06-07T08:29:44
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-21-13-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.8
5 Number of Scans	630
6 Acquisition Time	1.3631
7 Acquisition Date	2020-06-07T08:32:27
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

150.27  
144.47  
140.92  
138.35  
137.16  
136.51  
136.44  
130.05  
129.80  
127.18  
126.71  
122.54  
121.30  
113.49  
112.22  
109.26

80.80  
79.40  
77.32  
77.00  
76.68

69.77  
66.82  
62.08

56.49

50.08

44.70

41.58

40.41

40.24

39.16

37.00

31.41

30.27

28.78

21.55

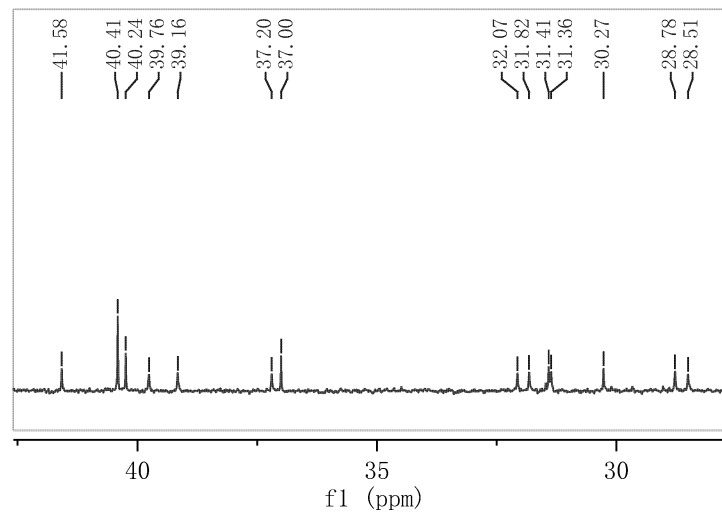
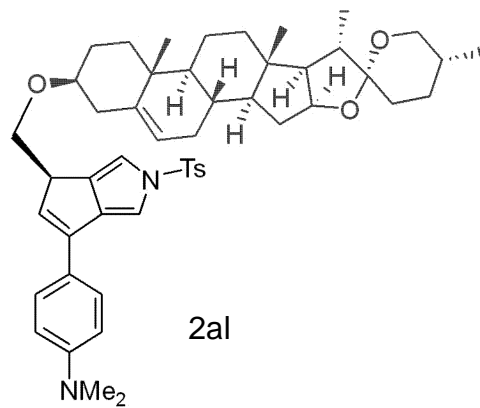
20.83

19.42

17.11

16.26

14.50

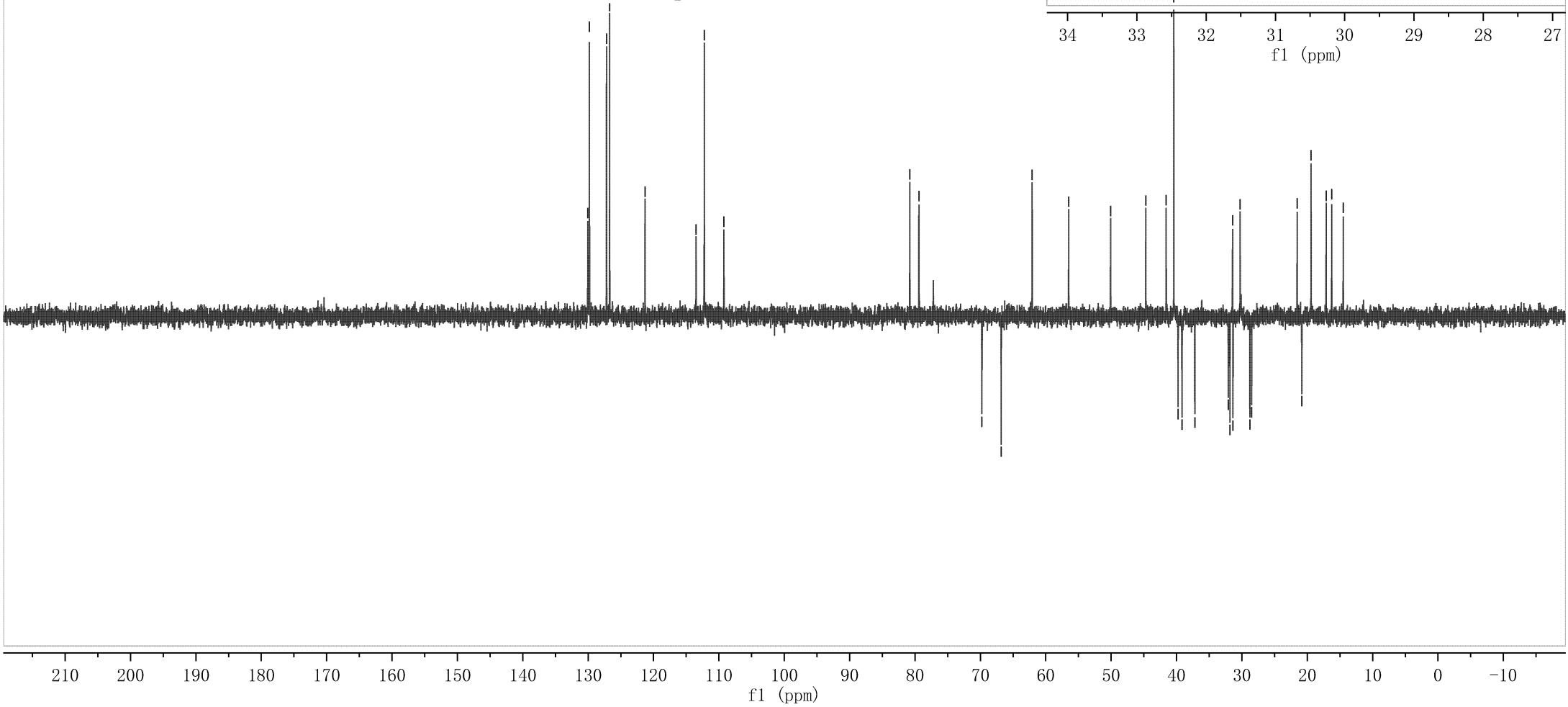
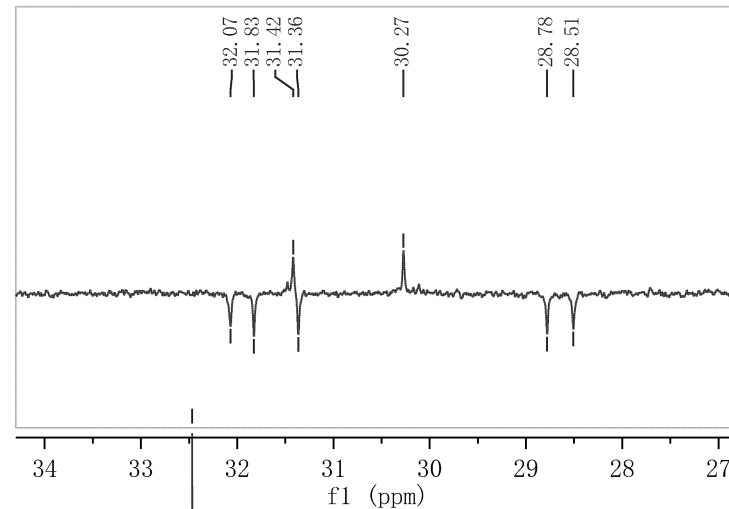
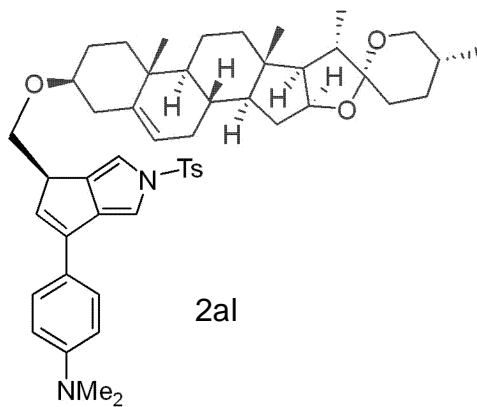


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

Parameter	Value
1 Title	ZXQ-21-13-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.9
5 Number of Scans	80
6 Acquisition Time	1.3631
7 Acquisition Date	2020-06-07T09:08:51
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

130.05 129.81 127.18 126.71 121.30 113.49 112.23 109.23 80.80 79.41 69.77 66.82 62.08 56.50 50.09 44.70 41.58 40.41 39.16 37.20 31.83 31.36 30.27 28.78 28.55 20.84 19.42 17.11 16.26 14.50



7.738  
7.718

7.353  
7.333

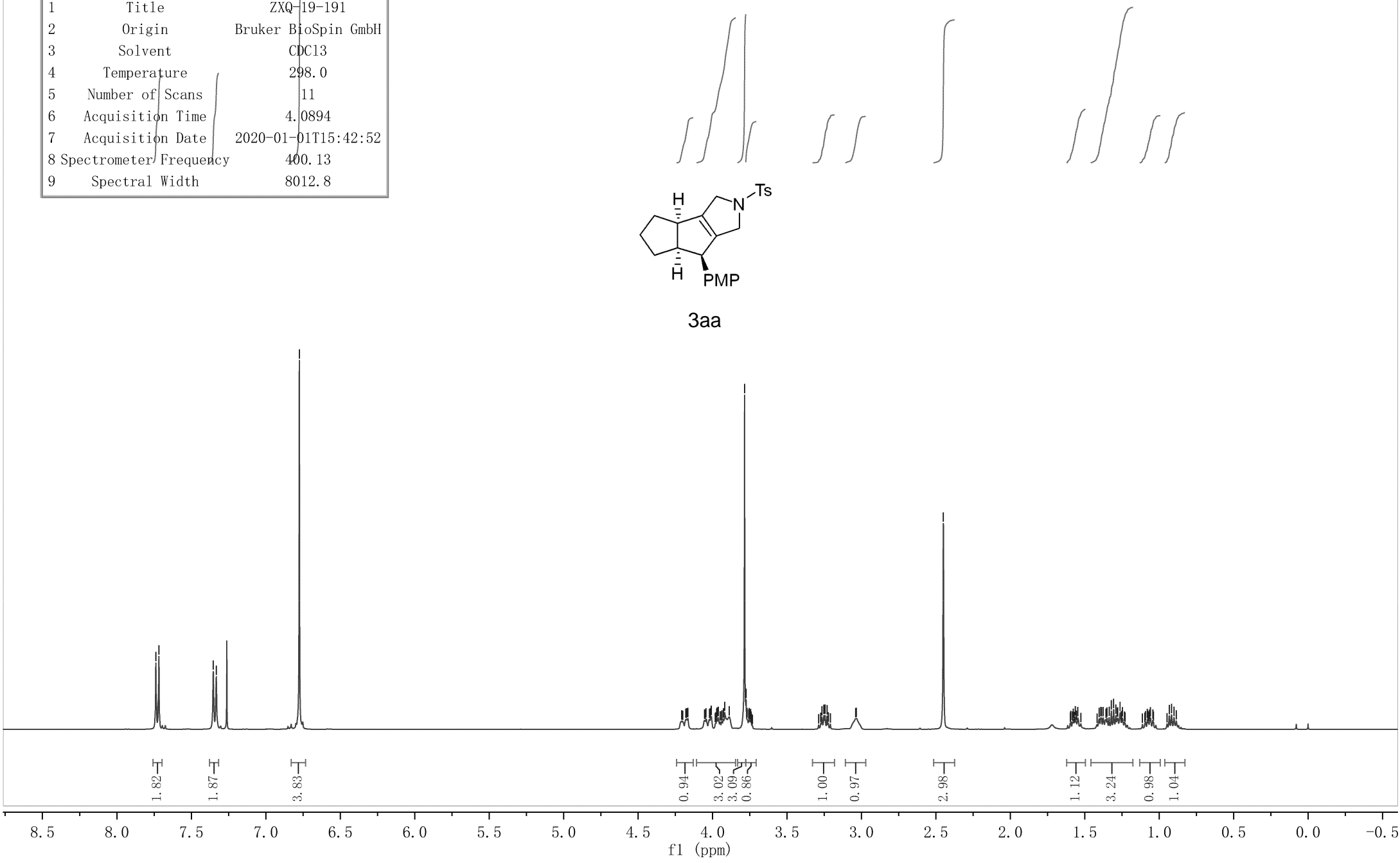
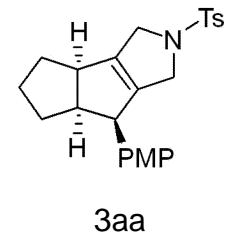
6.775

4.206  
4.200  
4.179  
4.176  
4.173  
4.166  
4.054  
4.049  
4.043  
4.021  
4.015  
4.010  
4.008  
3.981  
3.978  
3.972  
3.969  
3.948  
3.939  
3.936  
3.927  
3.918  
3.887  
3.785  
3.774  
3.768  
3.757  
3.753  
3.749  
3.744  
3.740  
3.736  
3.732

3.273  
3.273  
3.266  
3.252  
3.244  
3.231  
3.222  
3.039  
3.039  
3.034  
3.030

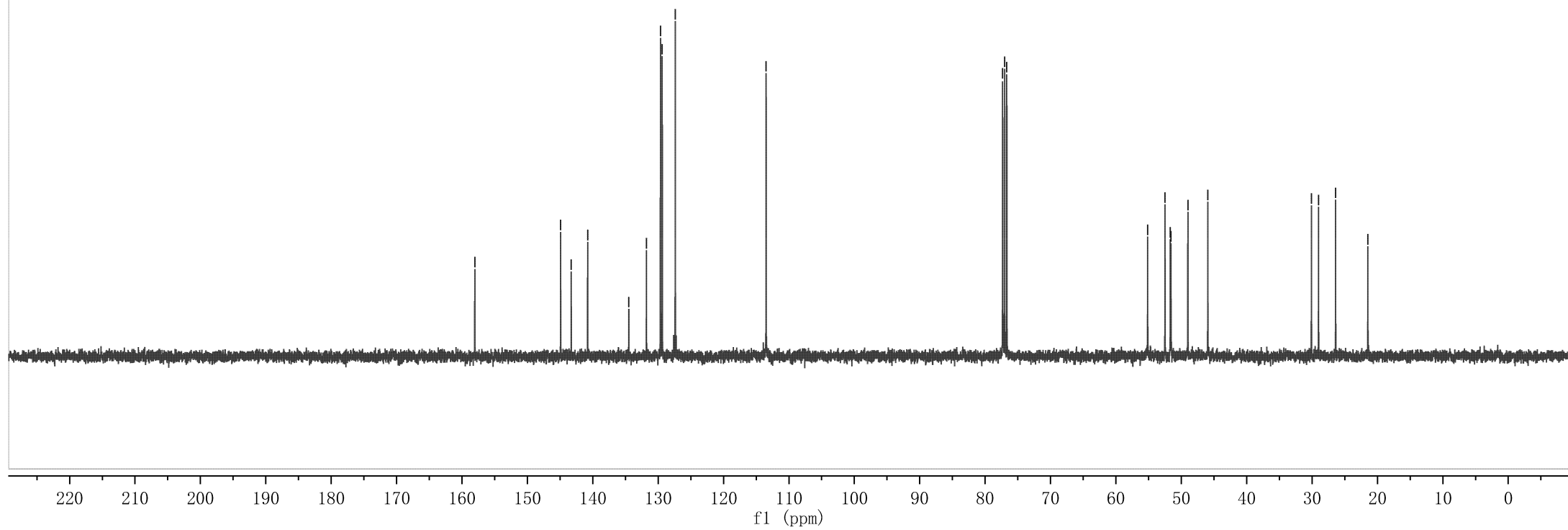
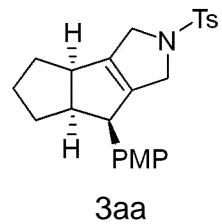
1.593  
1.583  
1.577  
1.563  
1.557  
1.547  
1.403  
1.392  
1.389  
1.376  
1.357  
1.350  
1.336  
1.336  
1.321  
1.306  
1.291  
1.281  
1.279  
1.263  
1.254  
1.248  
1.092  
1.080  
1.076  
1.064  
1.059  
1.043  
0.933  
0.917  
0.901  
0.886

Parameter	Value
1 Title	ZXQ-19-191
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2020-01-01T15:42:52
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-191-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	31
6 Acquisition Time	1.3631
7 Acquisition Date	2020-01-01T15:44:34
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.04  
 144.91  
 143.30  
 140.78  
 134.48  
 131.79  
 129.64  
 129.38  
 127.38  
 113.49  
 77.32  
 77.00  
 76.68  
 55.14  
 52.49  
 51.68  
 51.58  
 48.99  
 45.94  
 30.10  
 29.01  
 26.40  
 21.47





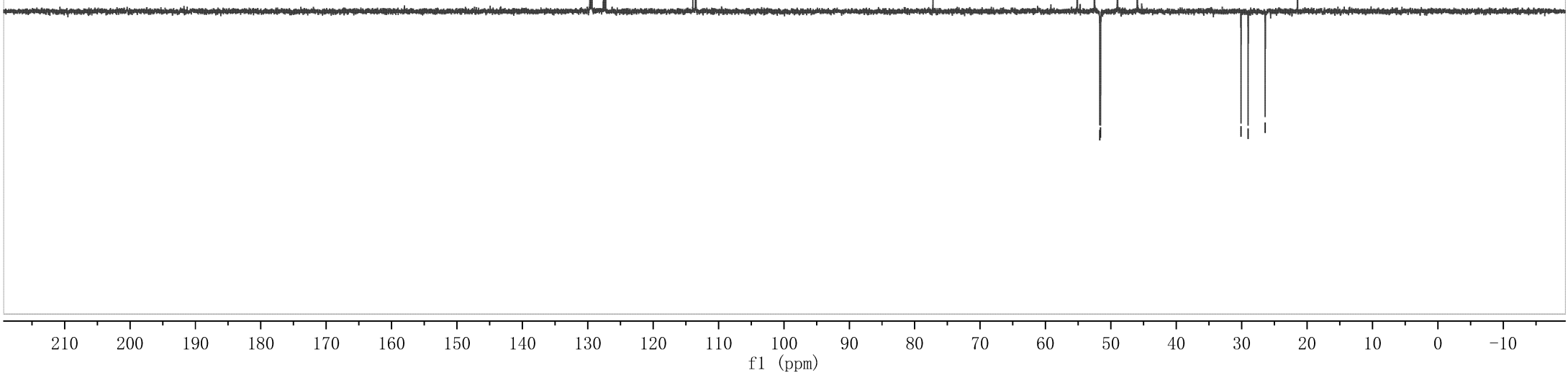
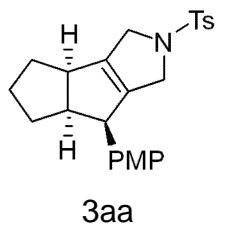
Parameter	Value
1 Title	ZXQ-19-191-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	32
6 Acquisition Time	1.3631
7 Acquisition Date	2020-01-01T15:47:31
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

129.65  
129.38  
127.39

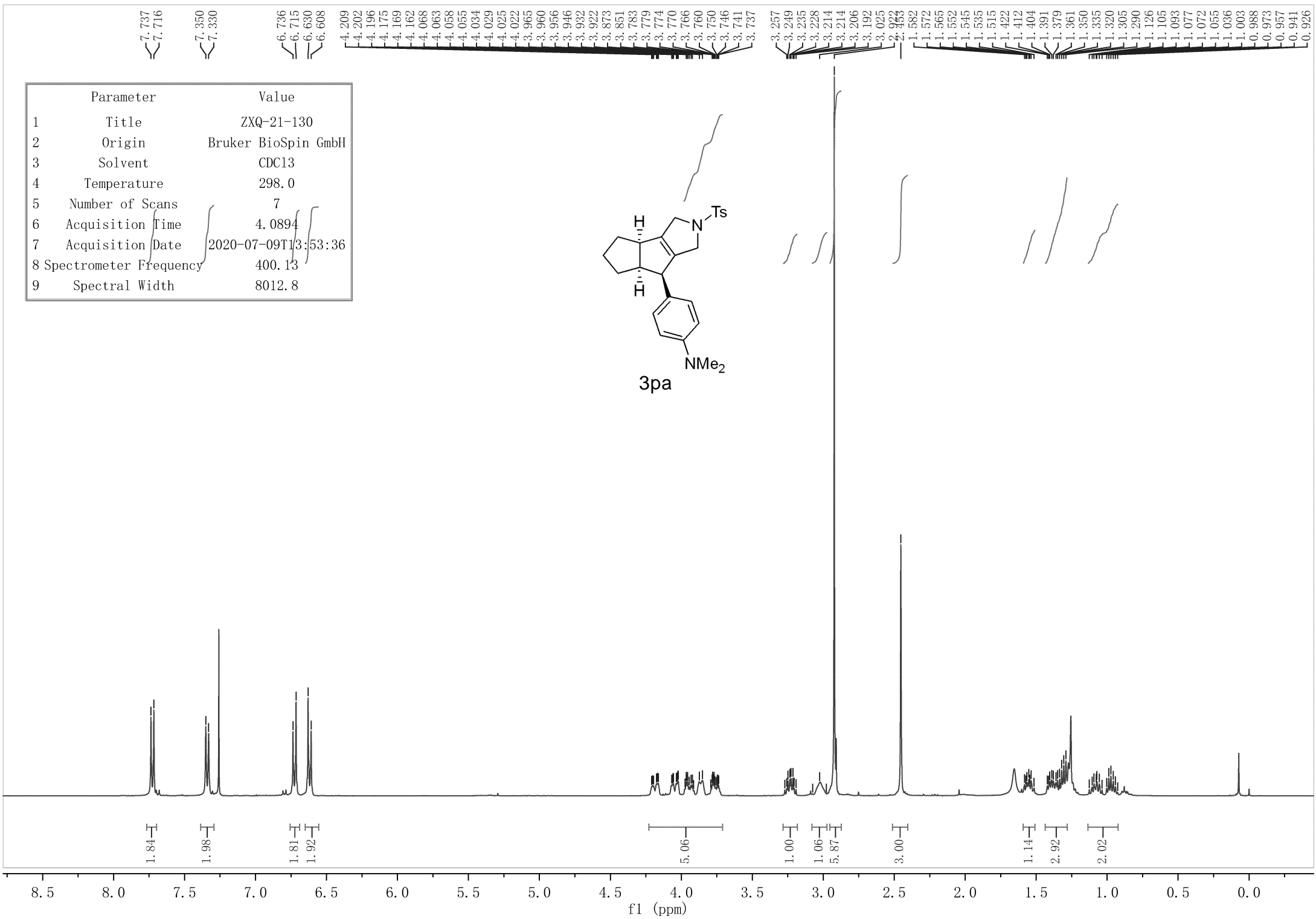
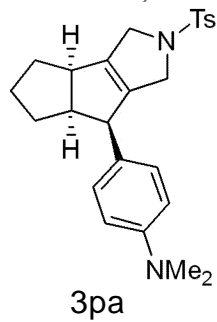
113.50

55.15  
52.50  
51.68  
51.58  
49.00  
45.95

30.10  
29.01  
26.40  
21.47



Parameter	Value
1 Title	ZXQ-21-130
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2020-07-09T13:53:36
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



7.737  
7.716

7.350  
7.330

6.736  
6.715  
6.630  
6.608

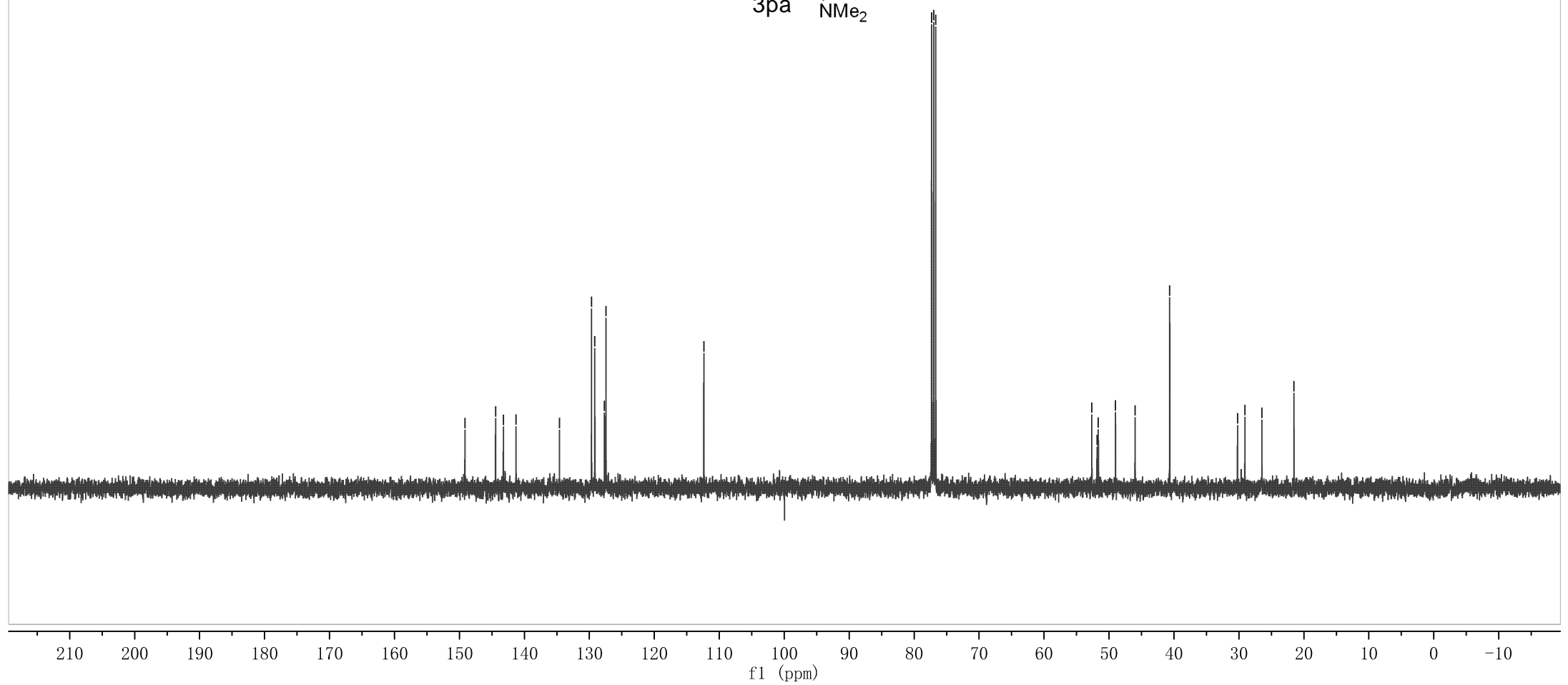
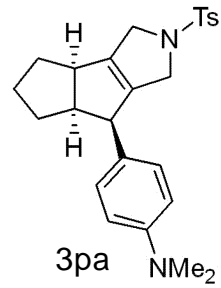
4.209  
4.202  
4.196  
4.175  
4.169  
4.162  
4.068  
4.063  
4.055  
4.034  
4.029  
4.025  
4.022  
3.965  
3.960  
3.956  
3.946  
3.932  
3.922  
3.873  
3.851  
3.783  
3.779  
3.774  
3.770  
3.766  
3.760  
3.750  
3.746  
3.741  
3.737

3.257  
3.249  
3.235  
3.228  
3.214  
3.214  
3.206  
3.192  
3.025  
2.453  
2.452

1.582  
1.572  
1.565  
1.552  
1.545  
1.535  
1.515  
1.422  
1.412  
1.404  
1.391  
1.379  
1.361  
1.350  
1.335  
1.320  
1.305  
1.290  
1.126  
1.105  
1.093  
1.077  
1.072  
1.055  
1.036  
1.003  
0.988  
0.973  
0.957  
0.941  
0.926

Parameter	Value
1 Title	ZXQ-21-130-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.9
5 Number of Scans	64
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-09T16:46:11
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

149.16 144.44 143.24 141.29  
 134.59 129.67 129.16 127.67 127.45  
 112.38  
 77.32 77.00 76.68  
 52.64 51.85 51.65 49.00 45.99 40.65  
 30.22 29.08 26.46 21.52



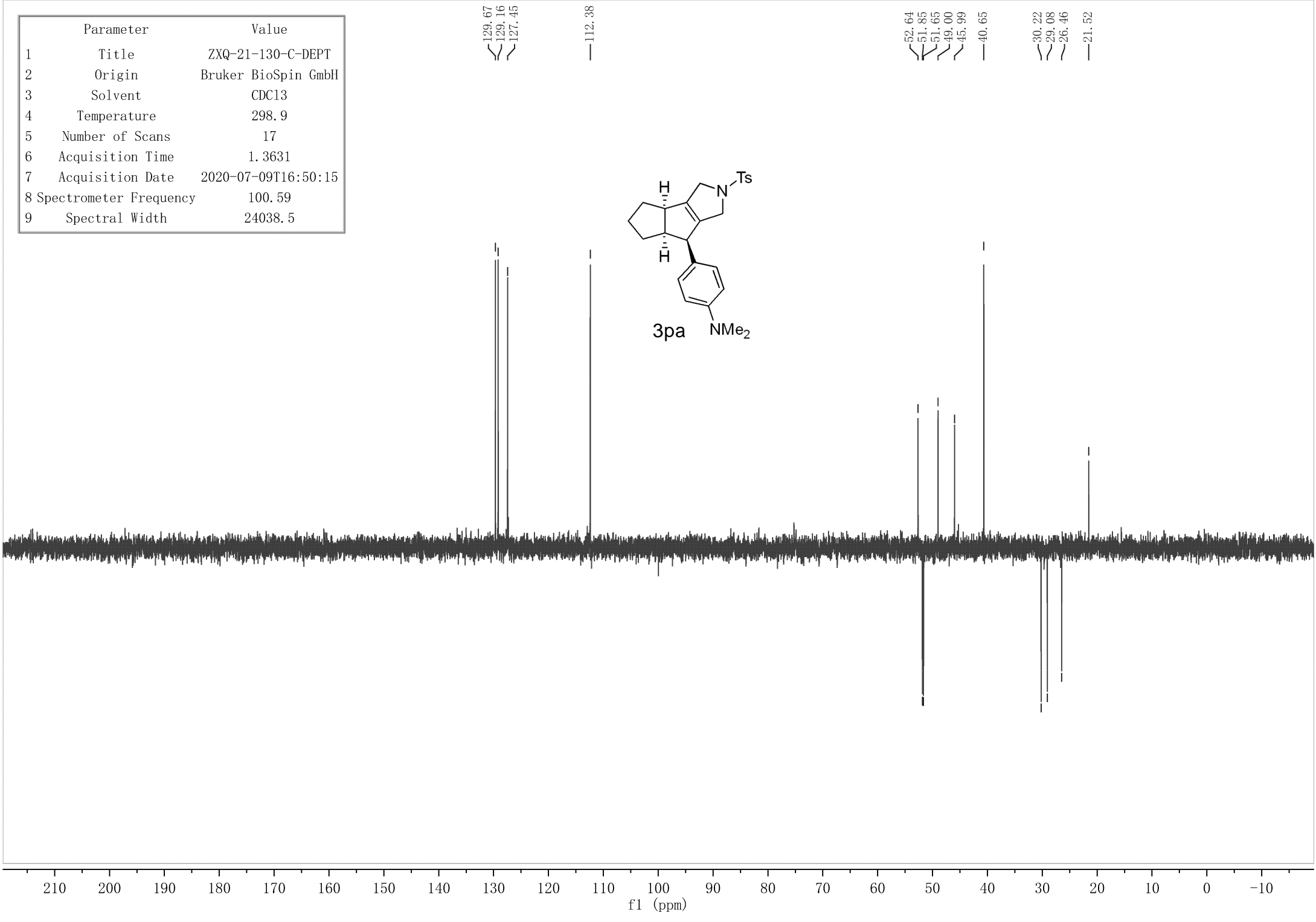
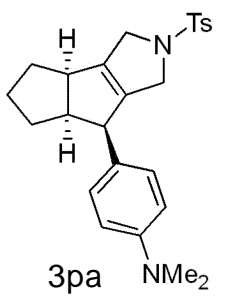
Parameter	Value
1 Title	ZXQ-21-130-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.9
5 Number of Scans	17
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-09T16:50:15
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

129.67  
129.16  
127.45

112.38

52.64  
51.85  
51.65  
49.00  
45.99  
40.65

30.22  
29.08  
26.46  
21.52



7.731  
7.710  
7.281  
7.261  
7.140  
7.119  
6.841  
6.834  
6.829  
6.818  
6.813  
6.787  
6.783  
6.779

4.397  
4.377

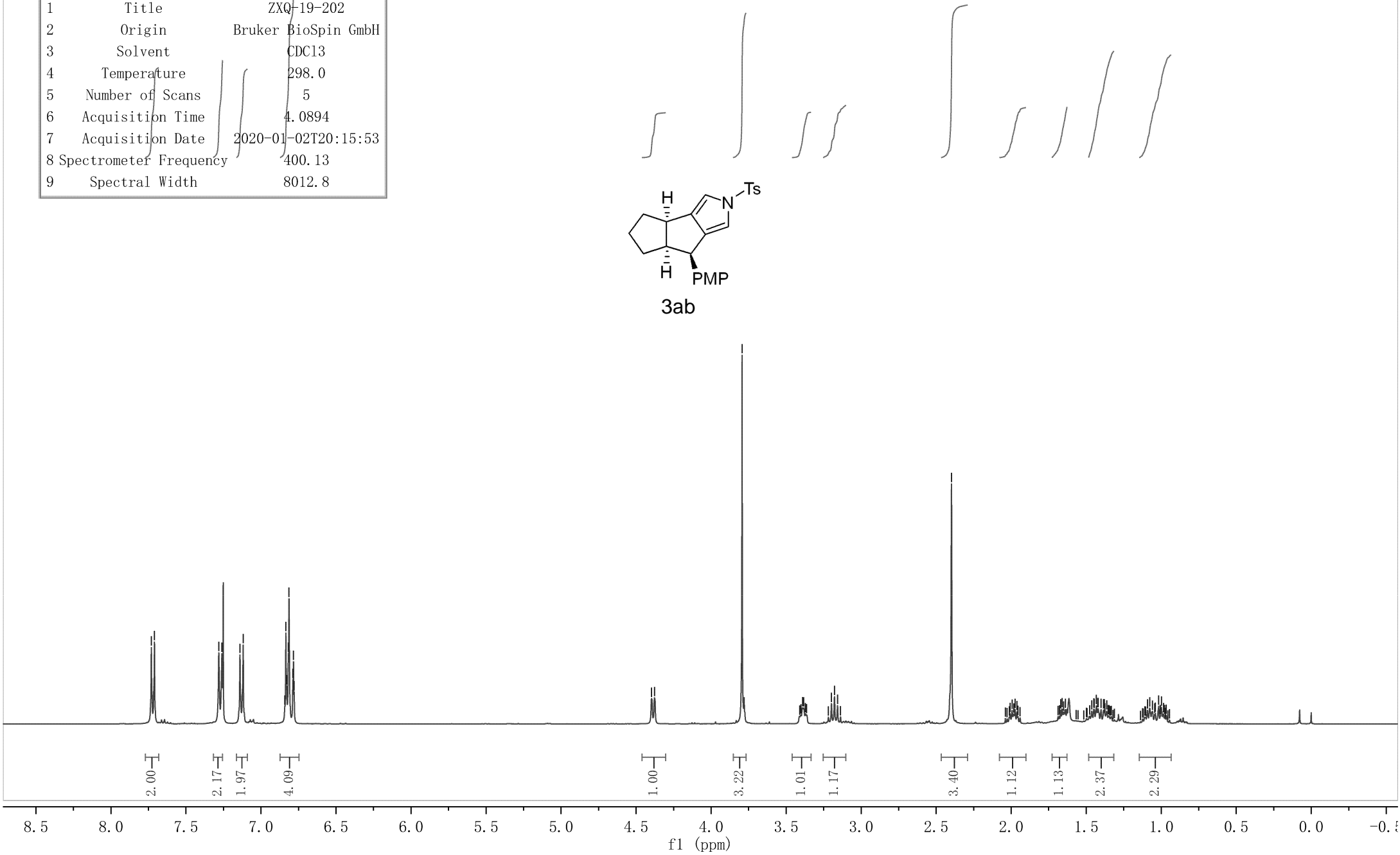
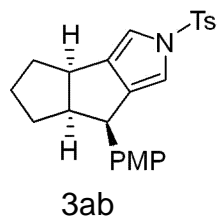
3.793  
3.410  
3.400  
3.391  
3.383  
3.372  
3.372  
3.364  
3.218  
3.198  
3.178  
3.157  
3.137

2.398

2.006  
1.994  
1.982  
1.974  
1.961

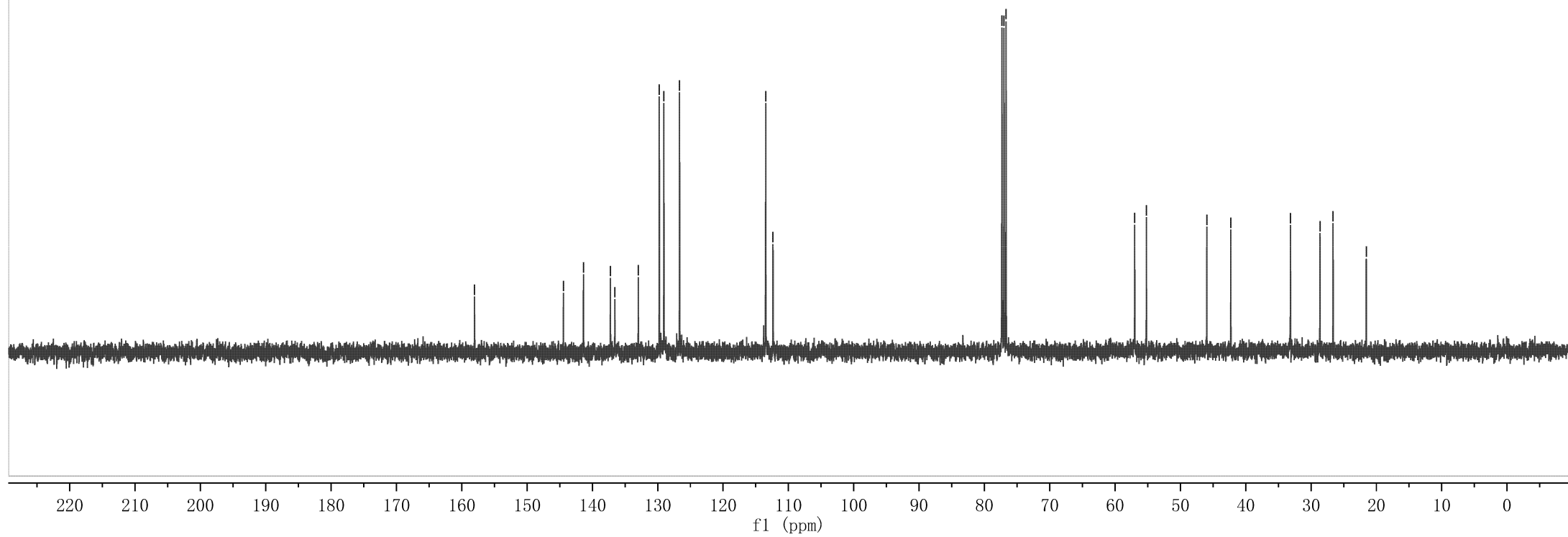
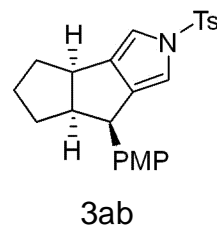
1.669  
1.660  
1.651  
1.638  
1.463  
1.450  
1.446  
1.432  
1.423  
1.420  
1.401  
1.385  
1.382  
1.379  
1.375  
1.363  
1.092  
1.077  
1.059  
1.043  
1.039  
1.017  
0.999  
0.985  
0.967

Parameter	Value
1 Title	ZXQ-19-202
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2020-01-02T20:15:53
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-202-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	37
6 Acquisition Time	1.3631
7 Acquisition Date	2020-01-03T15:48:48
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

158.05  
 144.44  
 141.37  
 137.25  
 136.57  
 132.97  
 129.76  
 129.06  
 126.66  
 113.47  
 112.36  
 77.32  
 77.00  
 76.68  
 56.99  
 55.20  
 45.95  
 42.28  
 33.15  
 28.63  
 26.63  
 21.55



Parameter	Value
1 Title	ZXQ-19-202-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	12
6 Acquisition Time	1.3631
7 Acquisition Date	2020-01-03T15:51:47
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

129.76  
129.07  
126.66

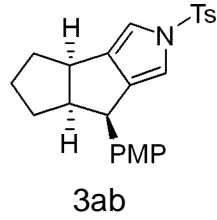
113.47  
112.36

57.00  
55.20

45.96  
42.29

33.15  
28.63  
26.63

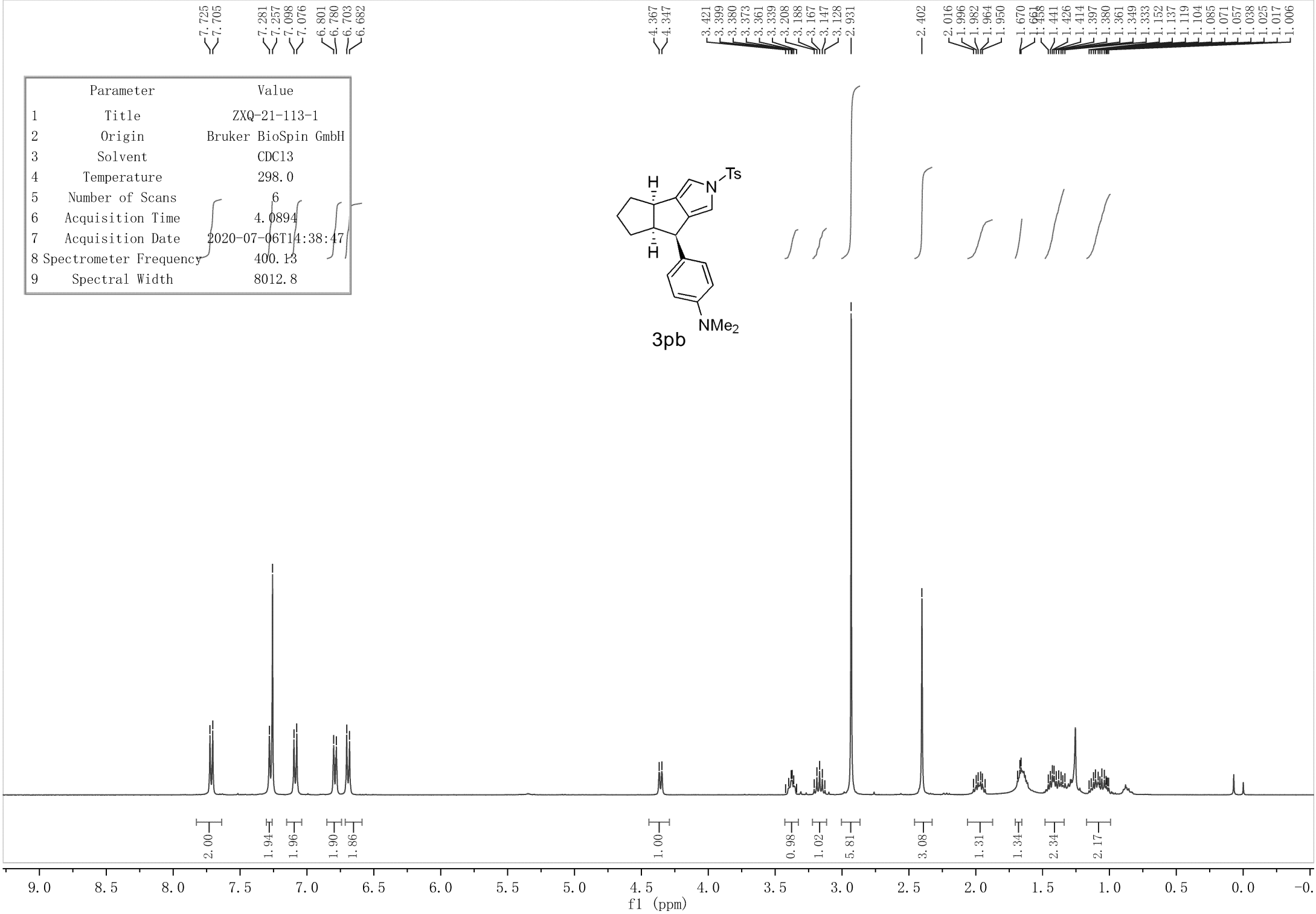
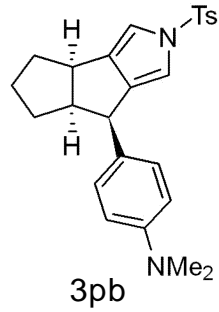
21.55



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)

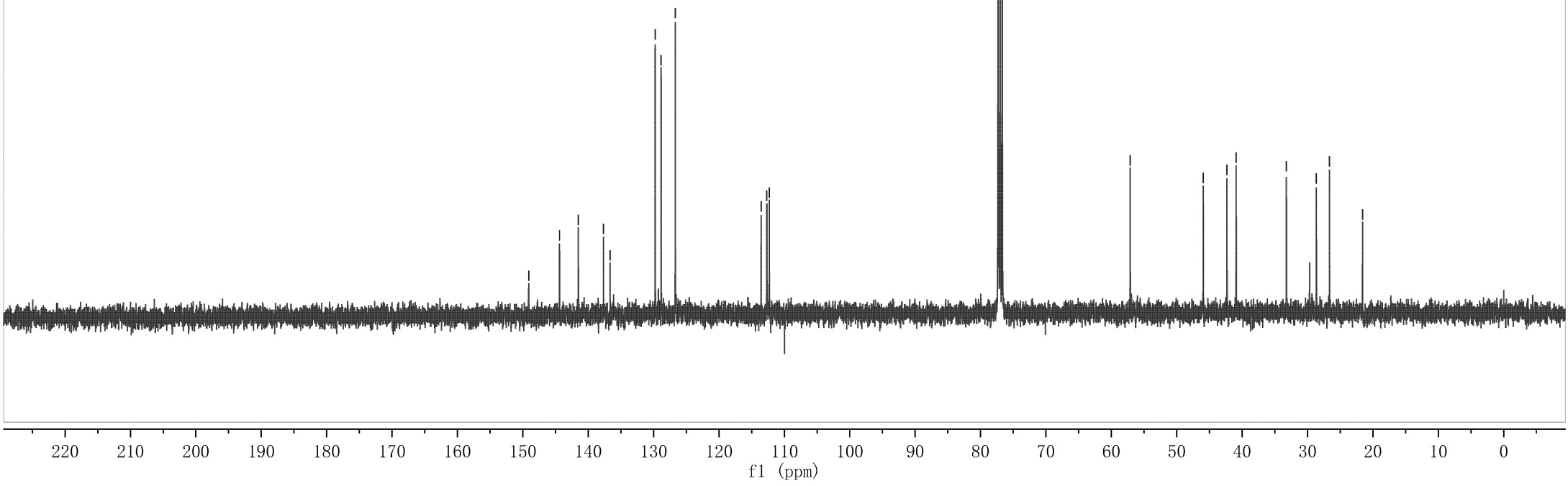
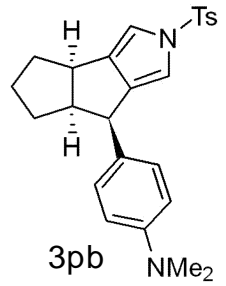
Parameter	Value
1 Title	ZXQ-21-113-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2020-07-06T14:38:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8





Parameter	Value
1 Title	ZXQ-21-113-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	290
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-27T17:02:33
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

149.09 144.38 141.50 137.67 136.65 129.76 128.85 126.68 113.56 112.68 112.31 77.32 77.00 76.68 57.11 45.94 42.32 40.91 33.22 28.65 26.64 21.58



Parameter	Value
1 Title	ZXQ-21-113-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	53
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-27T17:19:24
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

129.76  
128.85  
126.68

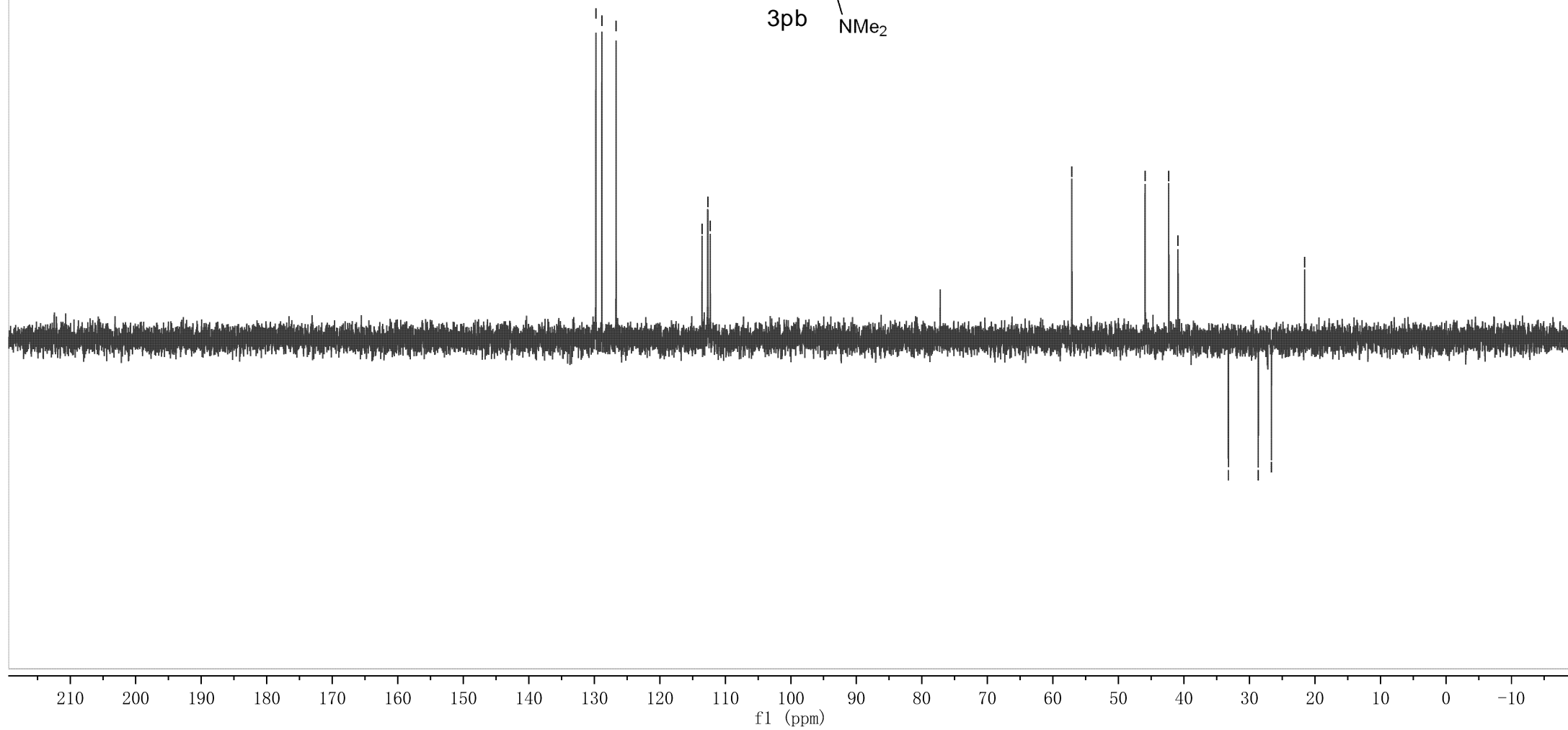
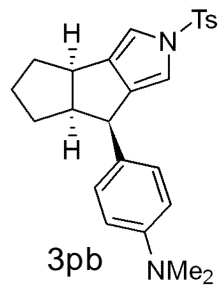
113.55  
112.68  
112.31

57.11

45.93  
42.31  
40.90

33.22  
28.65  
26.64

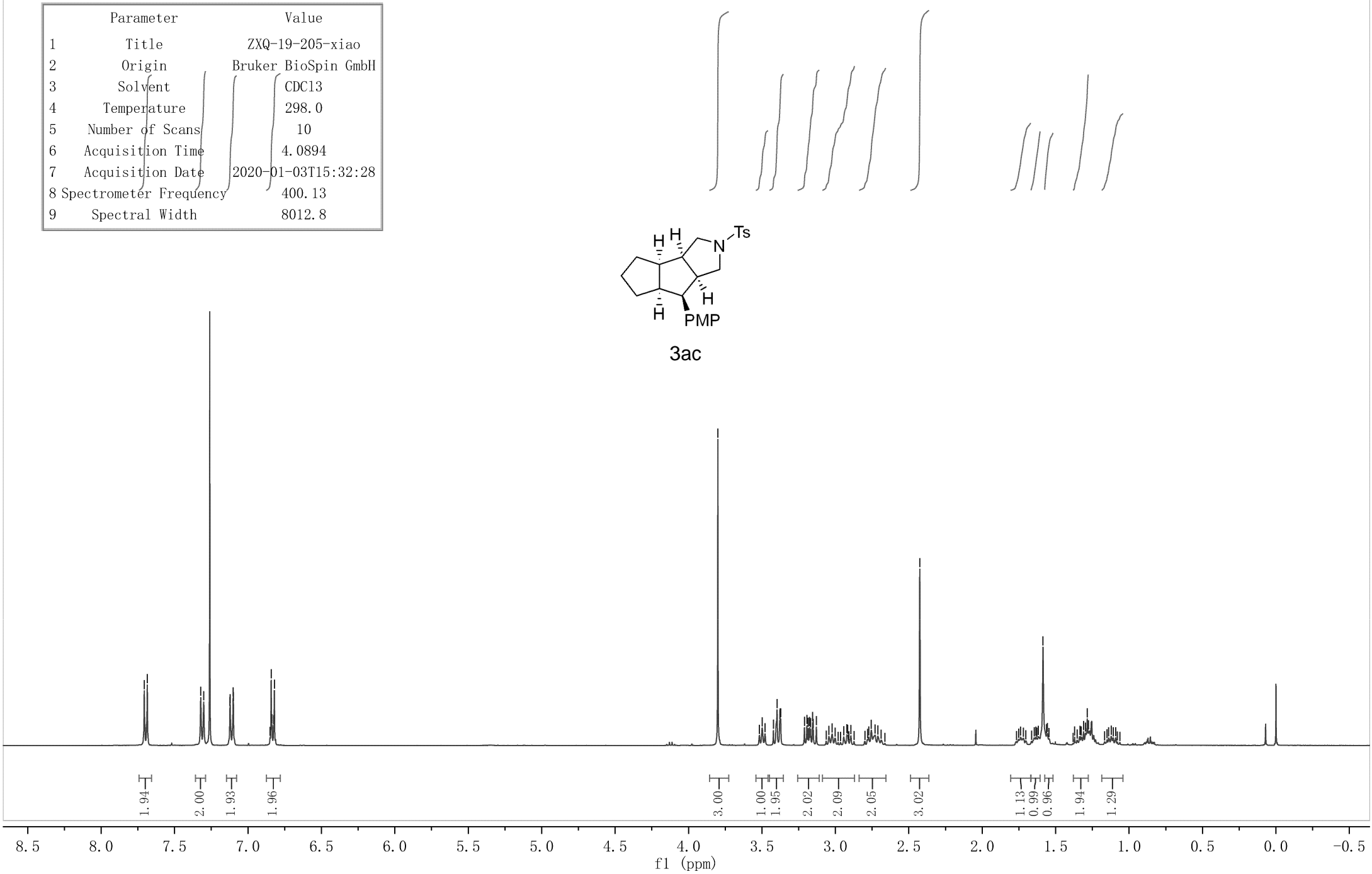
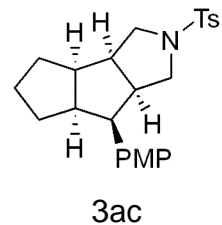
21.58



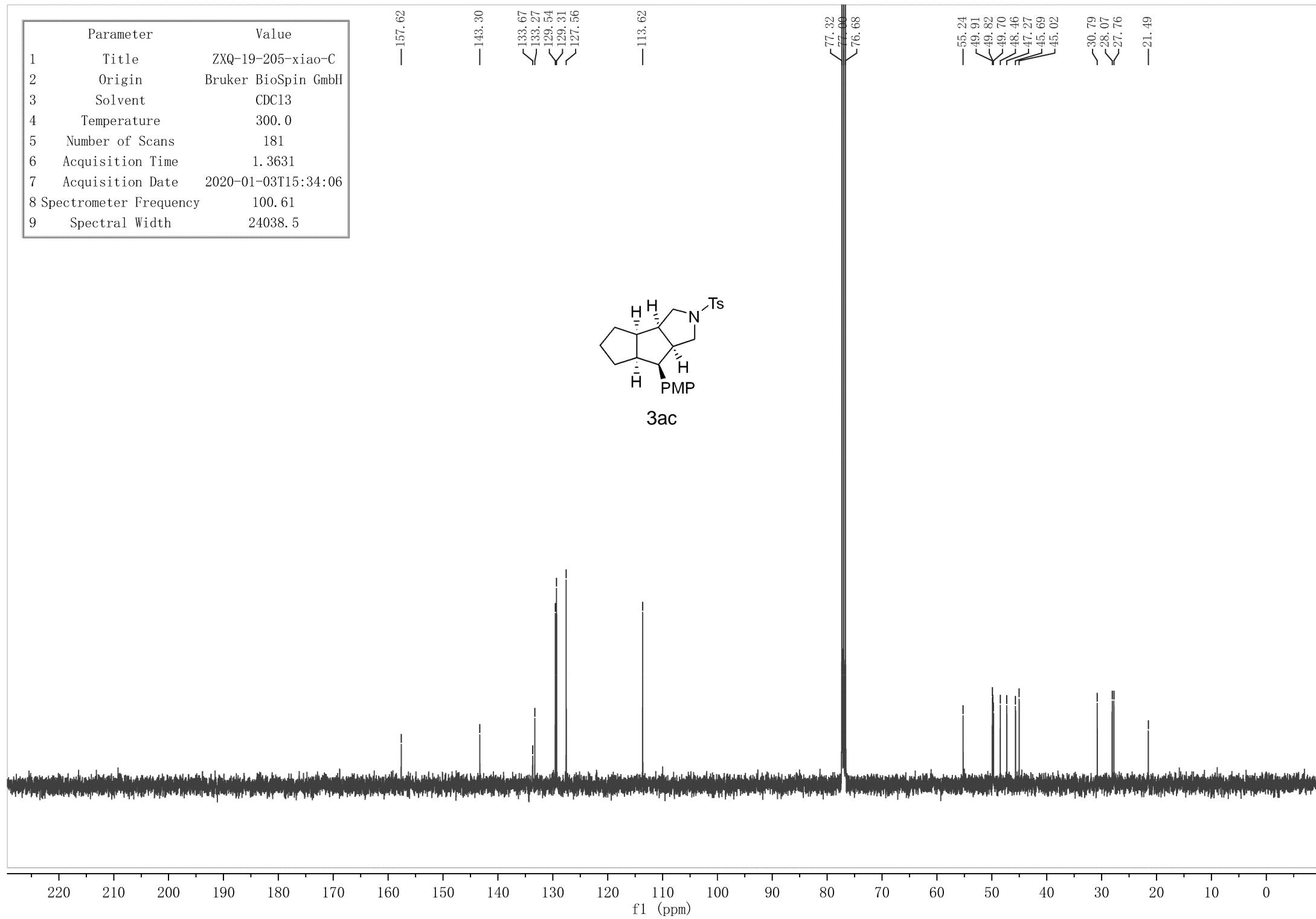
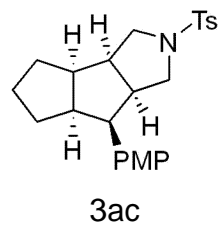
7.706  
7.686  
7.321  
7.302  
7.121  
7.101  
7.099  
6.856  
6.842  
6.837  
6.825  
6.820

3.800  
3.498  
3.397  
3.378  
3.376  
3.372  
3.211  
3.194  
3.186  
3.186  
3.176  
3.169  
3.155  
3.129  
3.129  
1.767  
1.751  
1.738  
1.719  
1.703  
1.663  
1.646  
1.635  
1.628  
1.618  
1.586  
1.561  
1.556  
1.545  
1.381  
1.371  
1.353  
1.333  
1.326  
1.310  
1.297  
1.285  
1.276  
1.167  
1.150  
1.139  
1.122  
1.108  
1.091  
1.080  
1.063

Parameter	Value
1 Title	ZXQ-19-205-xiao
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2020-01-03T15:32:28
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-19-205-xiao-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	181
6 Acquisition Time	1.3631
7 Acquisition Date	2020-01-03T15:34:06
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-19-205-xiao-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	48
6 Acquisition Time	1.3631
7 Acquisition Date	2020-01-03T15:44:59
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

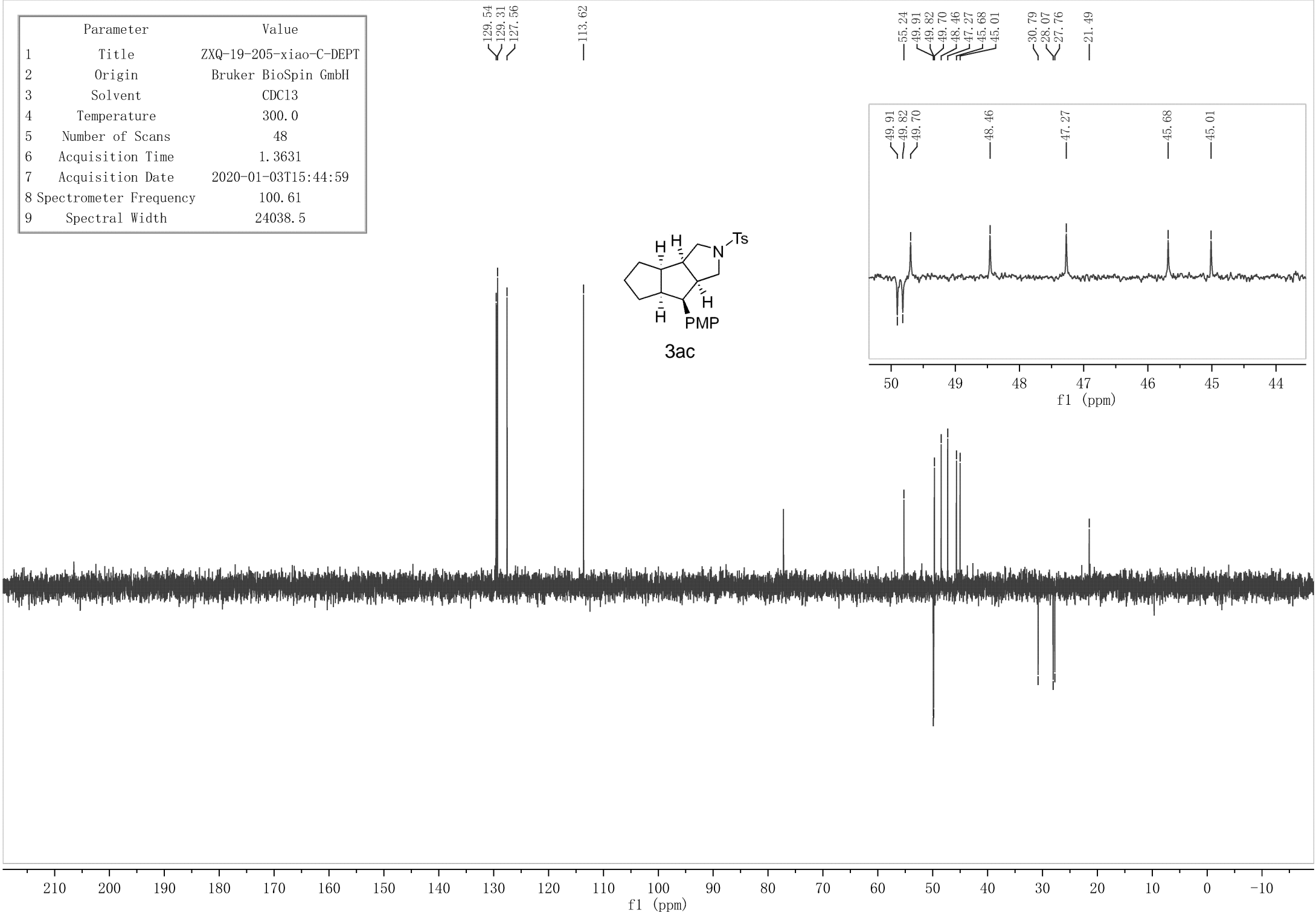
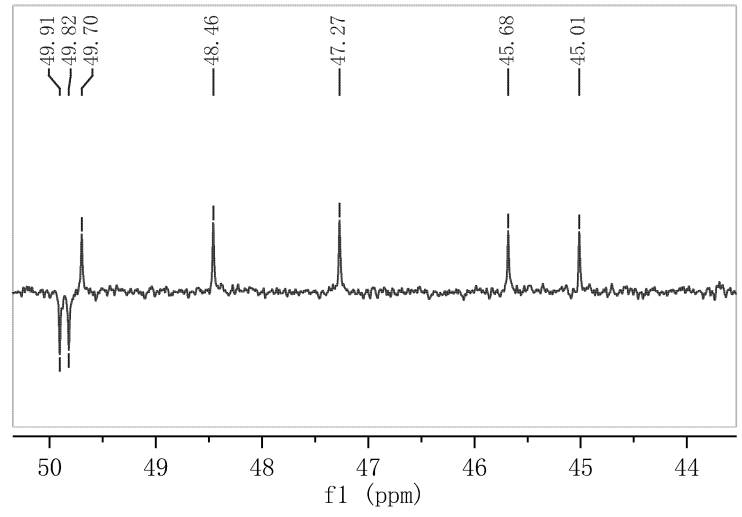
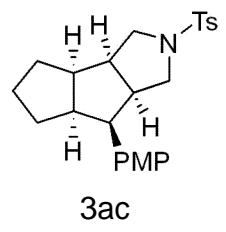
129.54  
129.31  
127.56

113.62

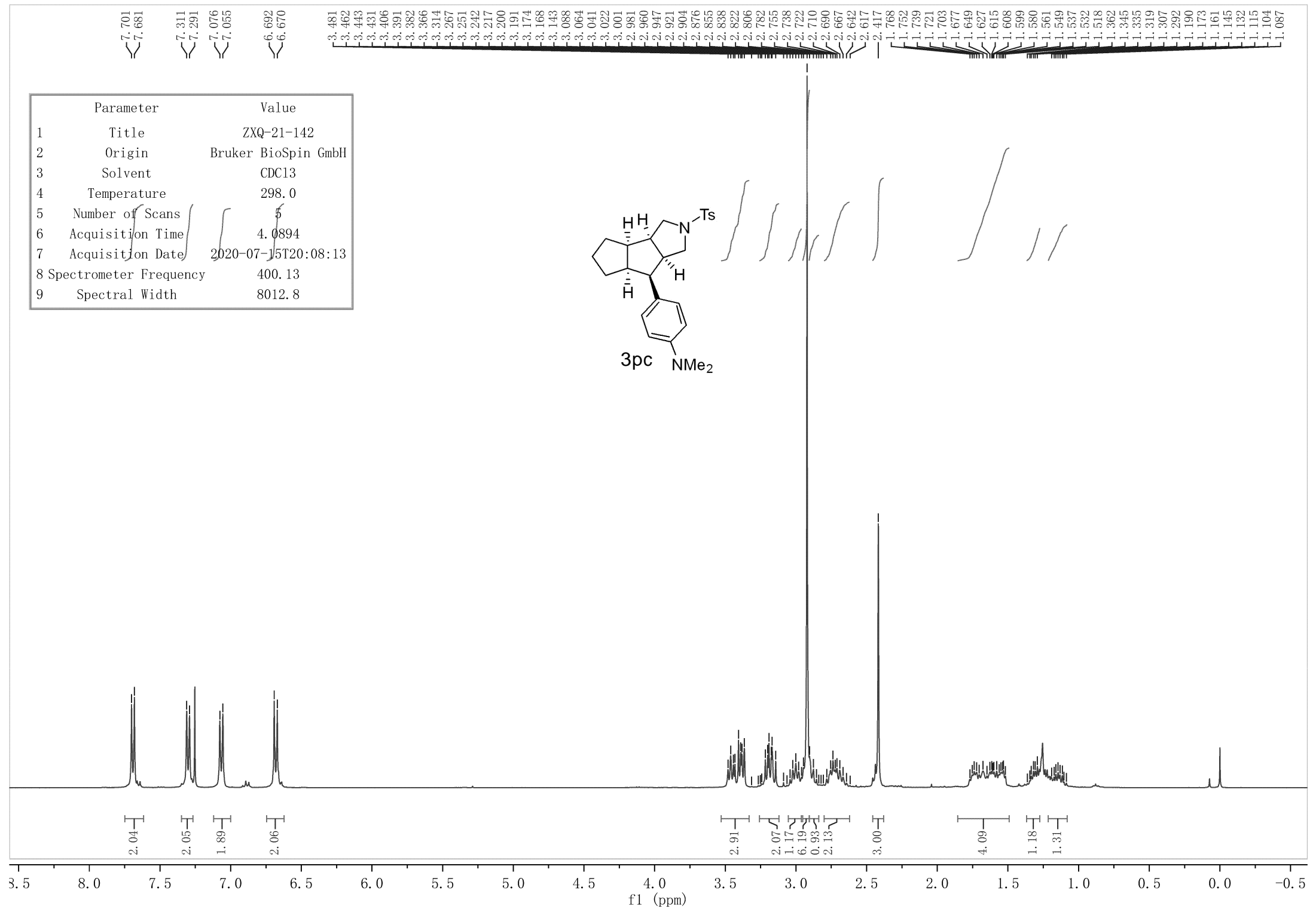
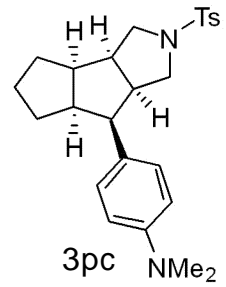
55.24  
49.91  
49.82  
49.70  
48.46  
47.27  
45.68  
45.01

30.79  
28.07  
27.76

21.49

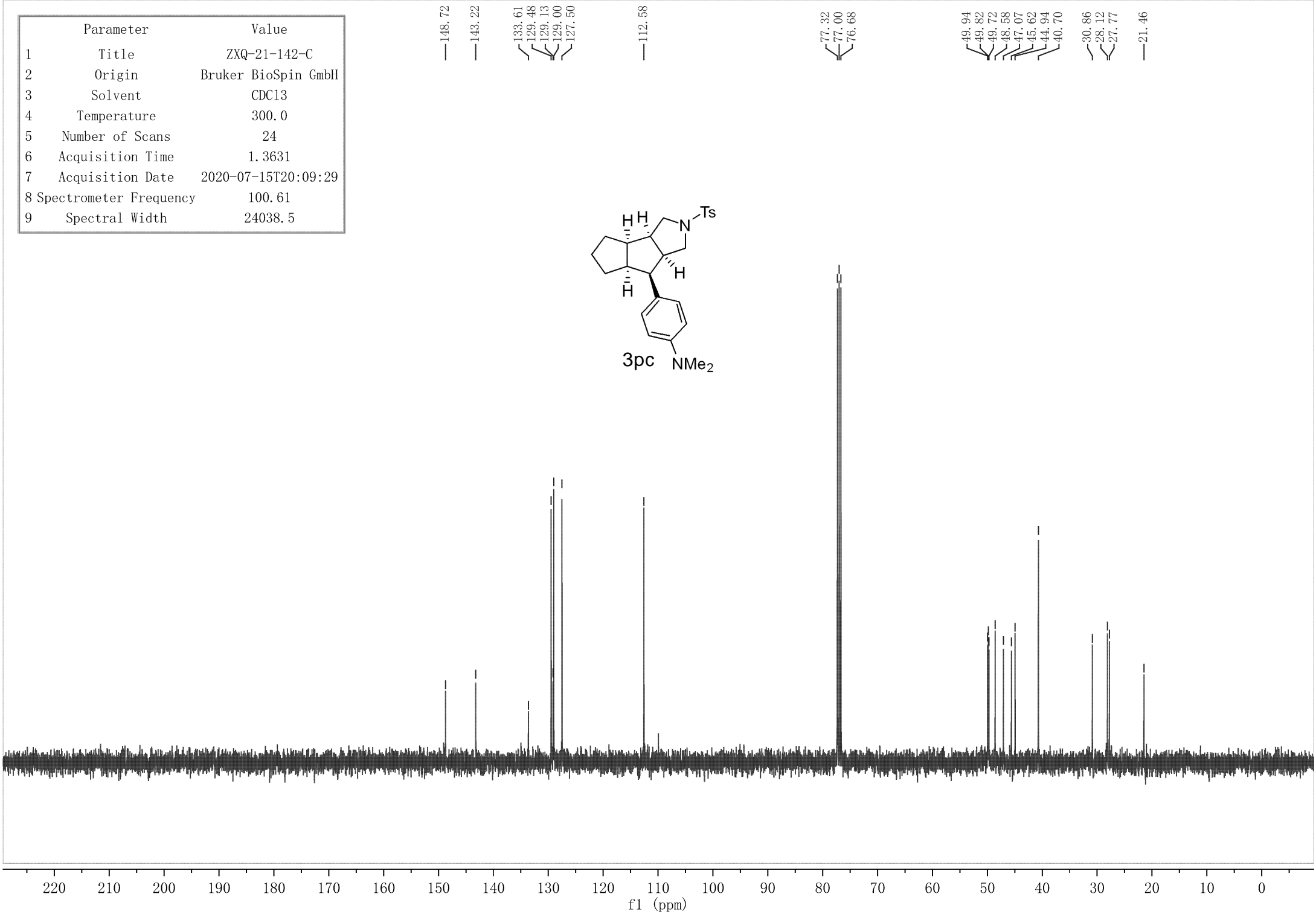
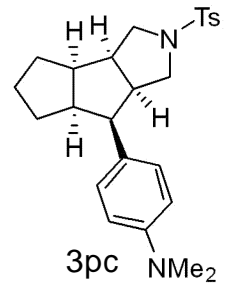


Parameter	Value
1 Title	ZXQ-21-142
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2020-07-15T20:08:13
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-21-142-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	24
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-15T20:09:29
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

— 148.72 — 143.22 — 133.61 — 129.48 — 129.13 — 129.00 — 127.50 — 112.58 — 77.32 — 77.00 — 76.68 — 49.94 — 49.82 — 49.72 — 48.58 — 47.07 — 45.62 — 44.94 — 40.70 — 30.86 — 28.12 — 27.77 — 21.46



Parameter	Value
1 Title	ZXQ-21-142-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	11
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-15T20:11:38
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

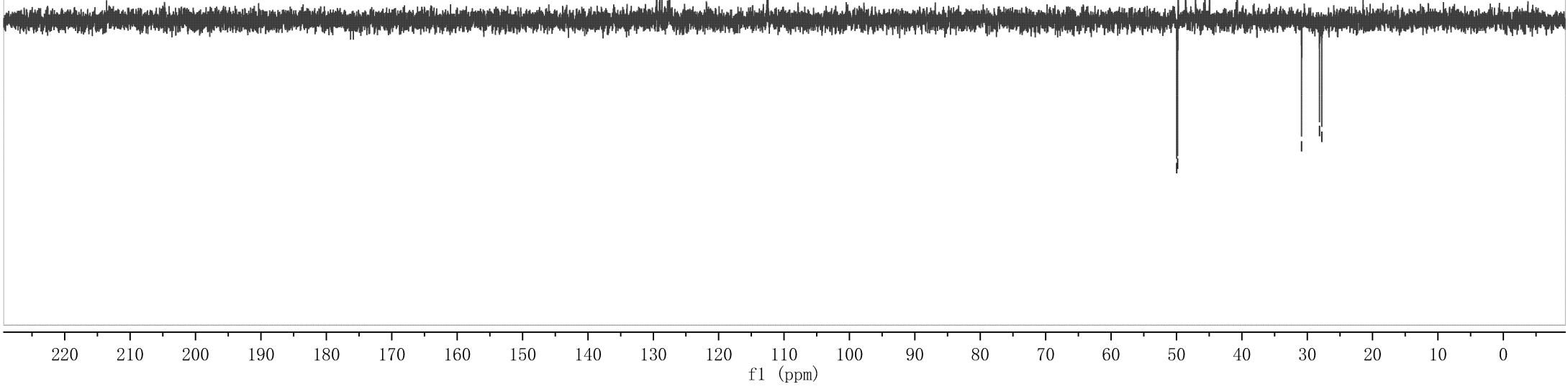
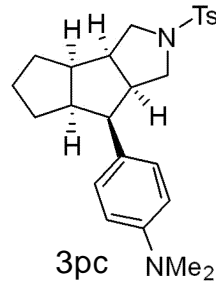
129.49  
129.01  
127.51

112.58

49.95  
49.82  
49.72  
48.59  
47.08  
45.63  
44.95  
40.70

30.86  
28.12  
27.77

21.46





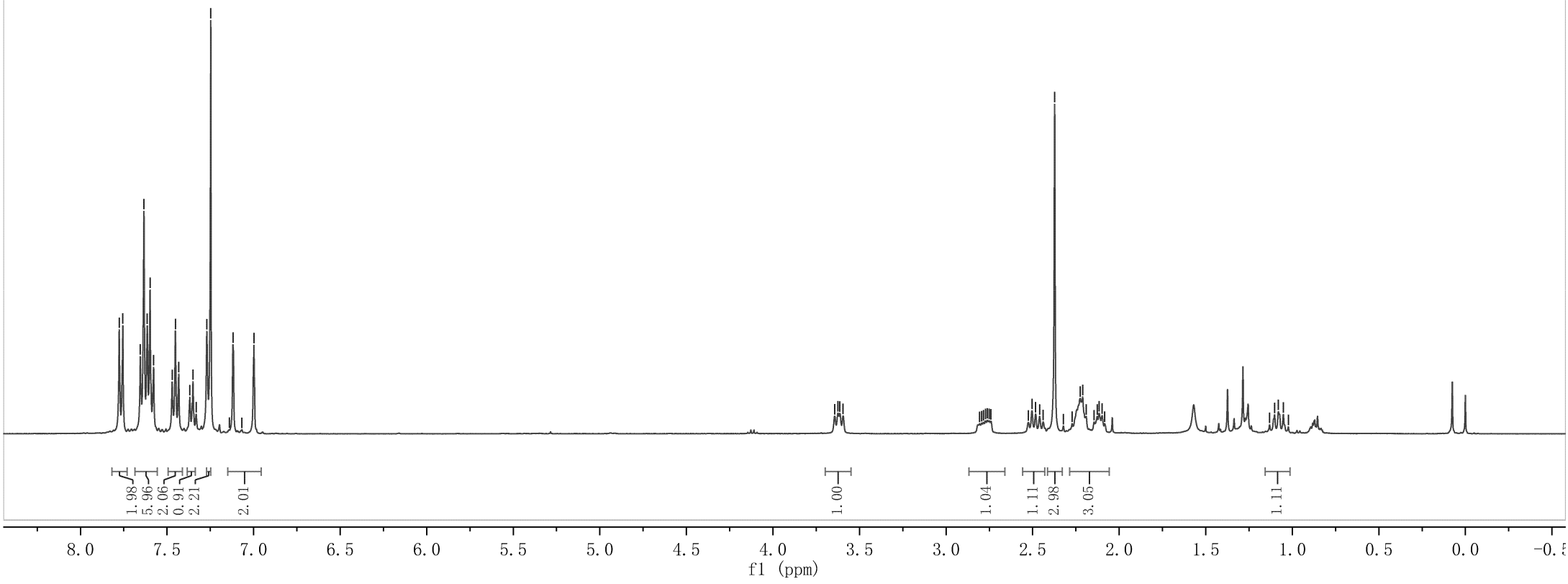
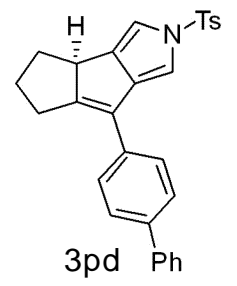
7.776  
7.755  
7.654  
7.633  
7.614  
7.598  
7.577  
7.470  
7.452  
7.432  
7.368  
7.350  
7.332  
7.270  
7.247  
7.140  
7.119  
7.068  
6.998

3.644  
3.624  
3.614  
3.595

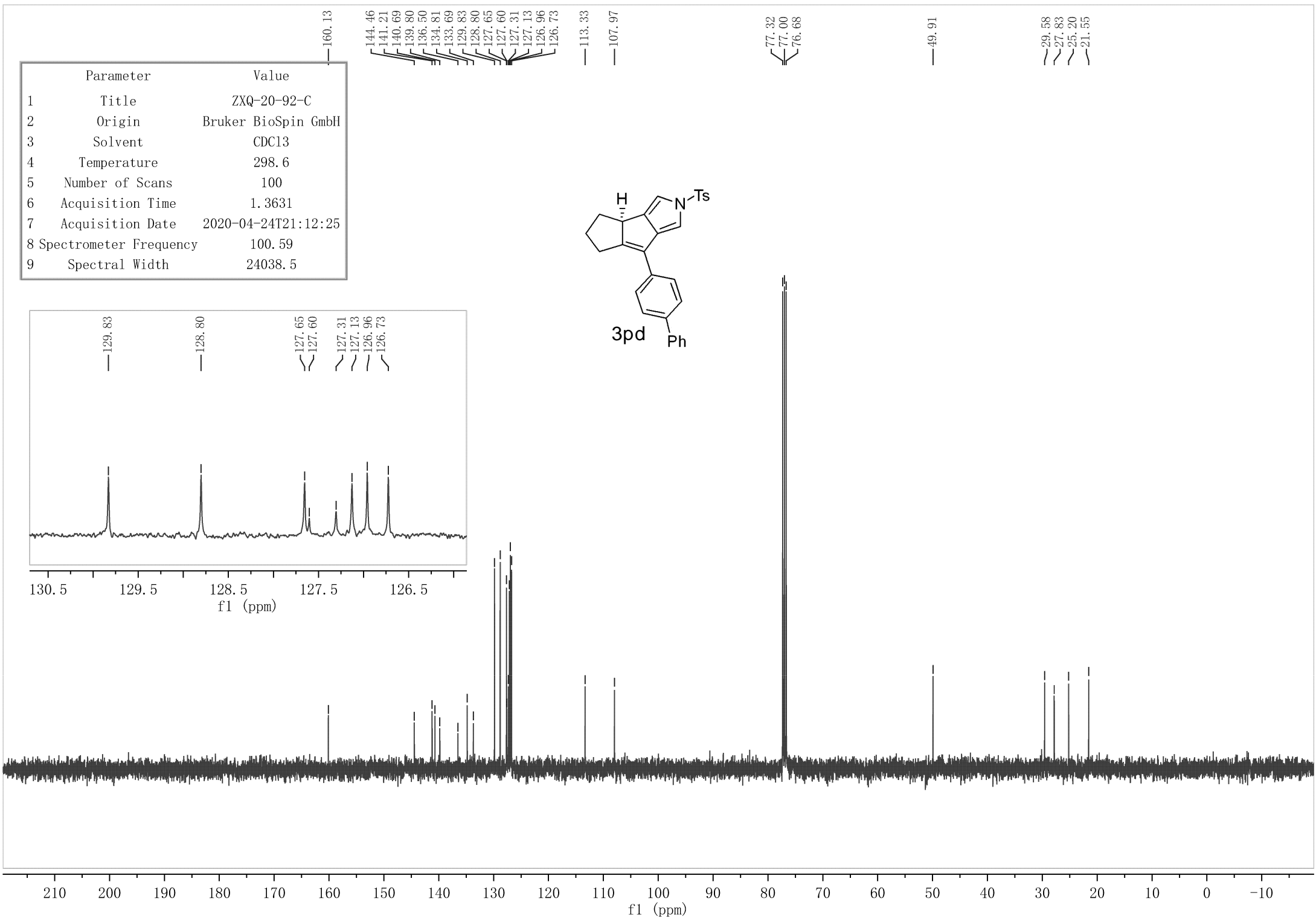
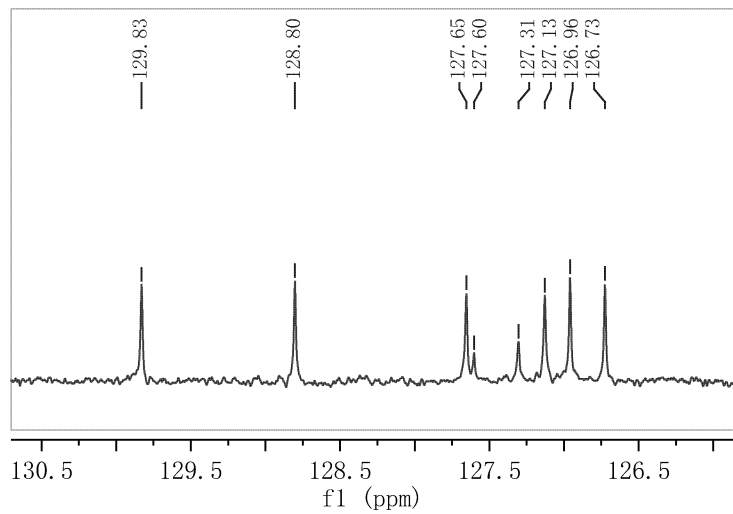
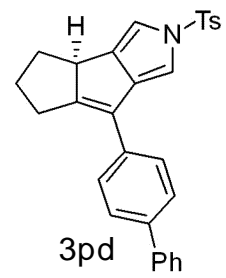
2.807  
2.795  
2.783  
2.772  
2.761  
2.751  
2.741

2.525  
2.504  
2.483  
2.460  
2.439  
2.373  
2.225  
2.211  
2.191  
2.145  
2.127  
2.116  
2.099  
2.084  
1.131  
1.102  
1.081  
1.052  
1.023

Parameter	Value
1 Title	ZXQ-20-92
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.2
5 Number of Scans	5
6 Acquisition Time	3.9846
7 Acquisition Date	2020-04-24T21:10:18
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-20-92-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.6
5 Number of Scans	100
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-24T21:12:25
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-20-92-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.2
5 Number of Scans	43
6 Acquisition Time	1.3631
7 Acquisition Date	2020-04-24T21:18:39
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

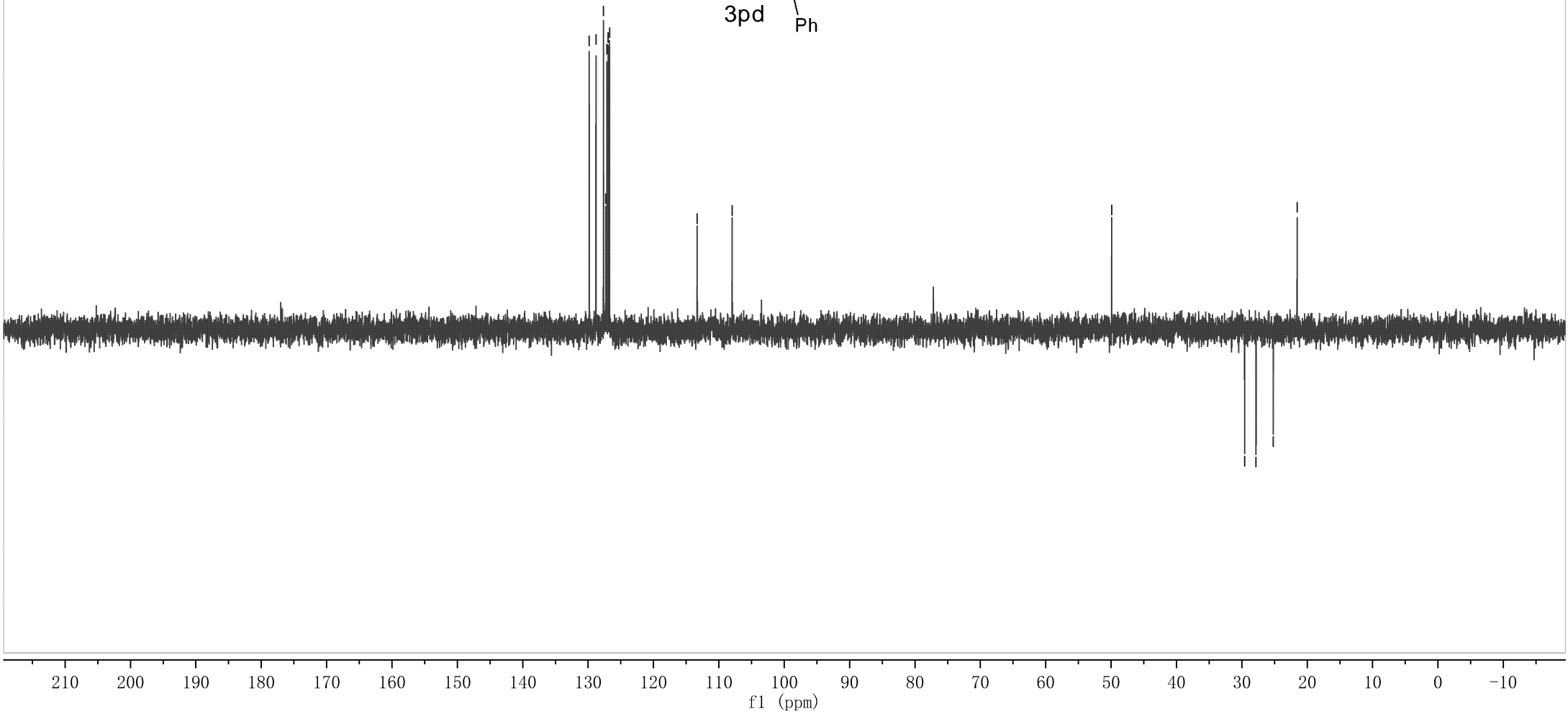
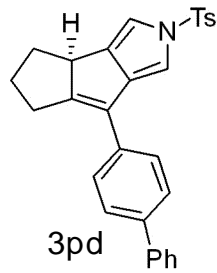
129.83  
128.80  
127.65  
127.30  
127.12  
126.95  
126.72

113.32

107.97

49.91

29.58  
27.83  
25.19  
21.55



7.726  
7.706  
7.280  
7.259  
7.013  
6.993  
6.800  
6.773  
6.632  
6.611

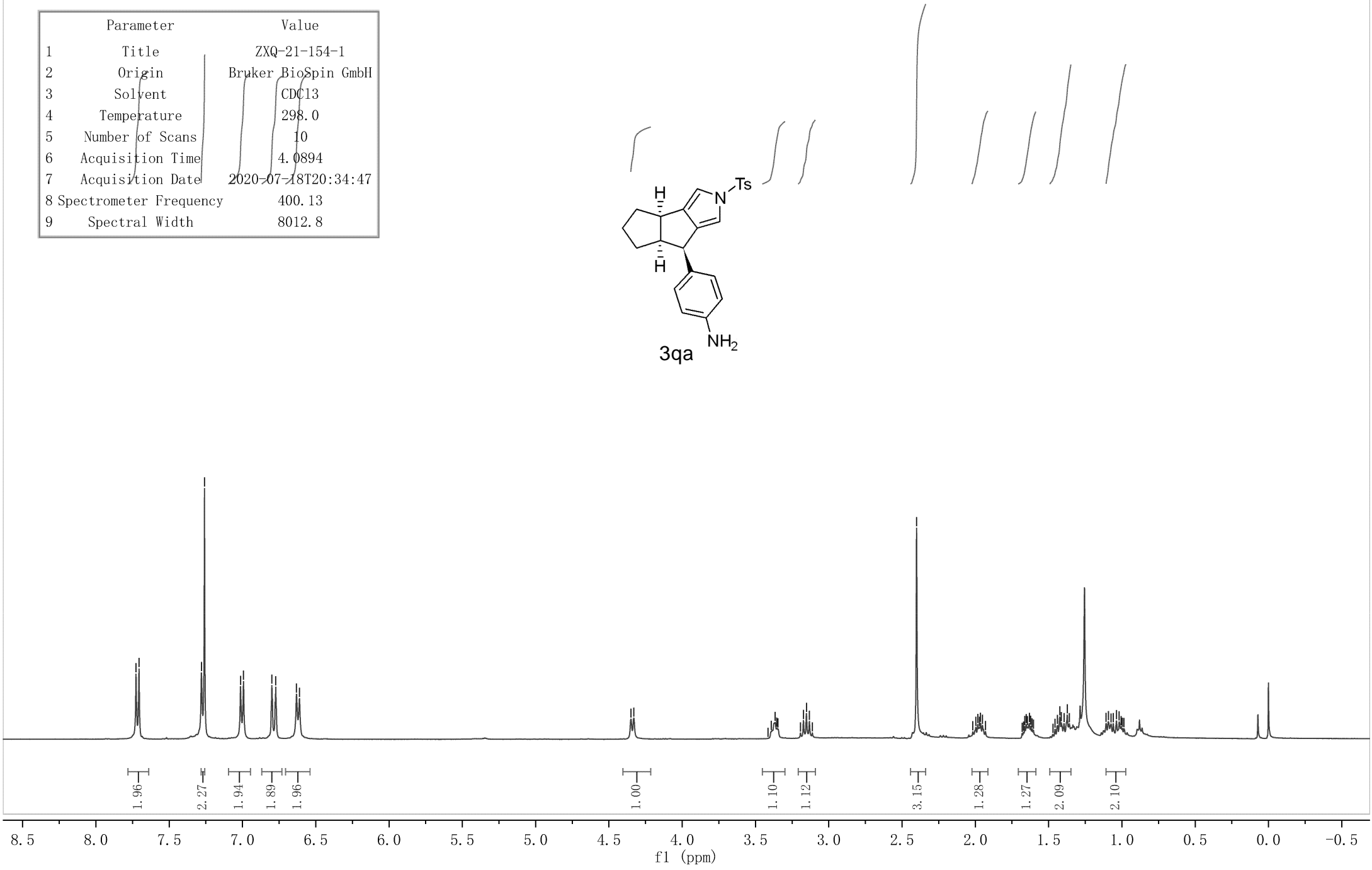
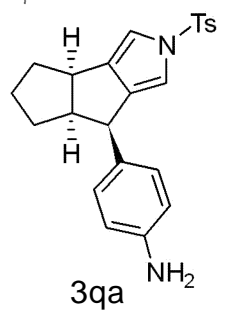
4.349  
4.330

3.414  
3.393  
3.366  
3.355  
3.347  
3.193  
3.173  
3.152  
3.132  
3.112

2.401

1.997  
1.983  
1.972  
1.964  
1.951  
1.632  
1.424  
1.414  
1.395  
1.373  
1.359  
1.108  
1.092  
1.075  
1.059  
1.037  
1.019  
1.005  
0.997  
0.986

Parameter	Value
1 Title	ZXQ-21-154-1
2 Origin	Braker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2020-07-18T20:34:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



Parameter	Value
1 Title	ZXQ-21-154-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	121
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-18T17:44:37
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

144.40  
141.47  
137.49  
136.62

130.97  
129.76  
128.99  
126.68

114.99  
113.54  
112.31

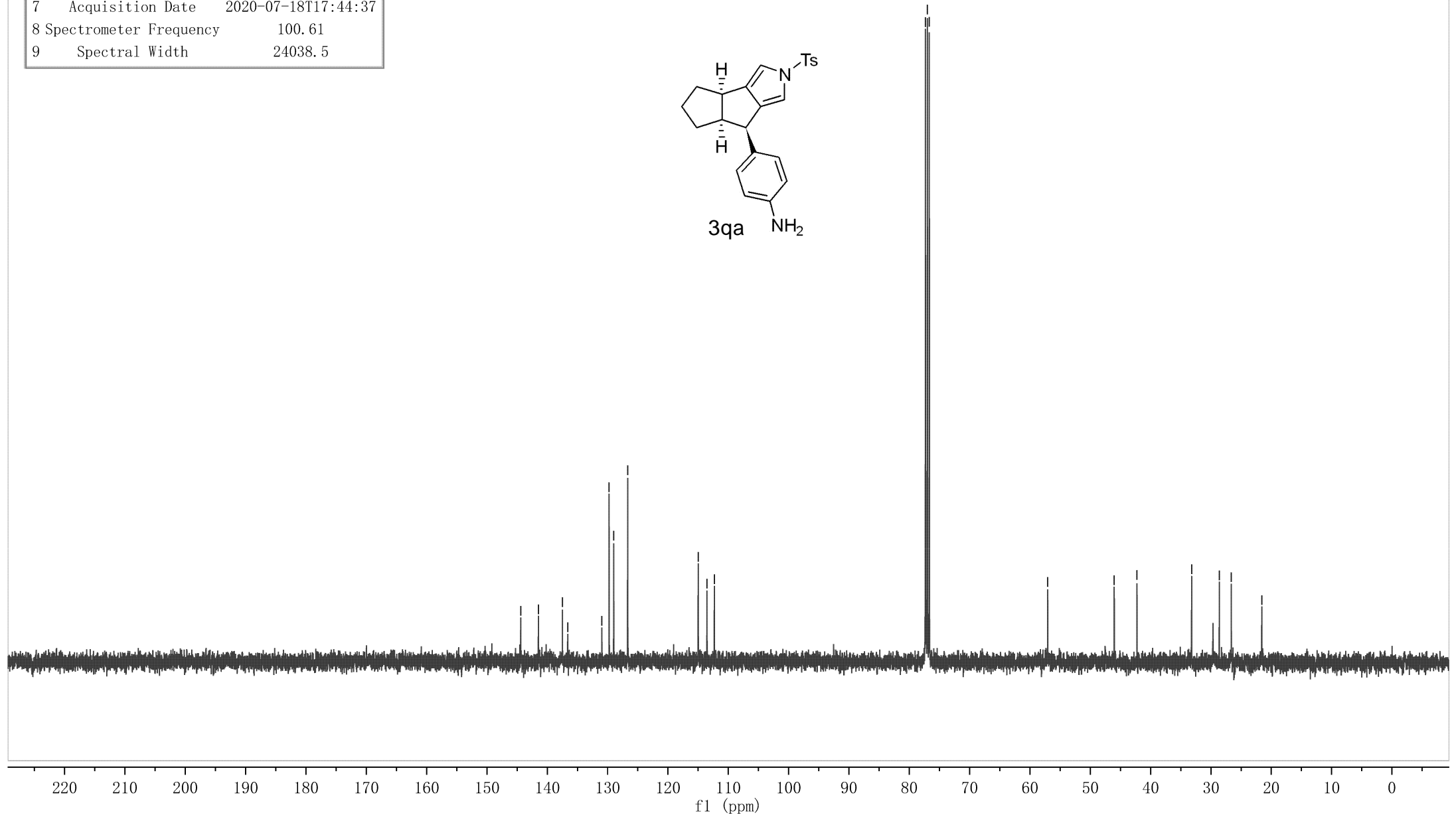
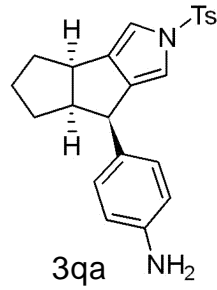
77.32  
77.00  
76.68

57.05

46.03  
42.26

33.20  
28.62  
26.63

21.57



Parameter	Value
1 Title	ZXQ-21-154-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2020-07-18T17:52:35
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

129.79  
129.03  
126.71

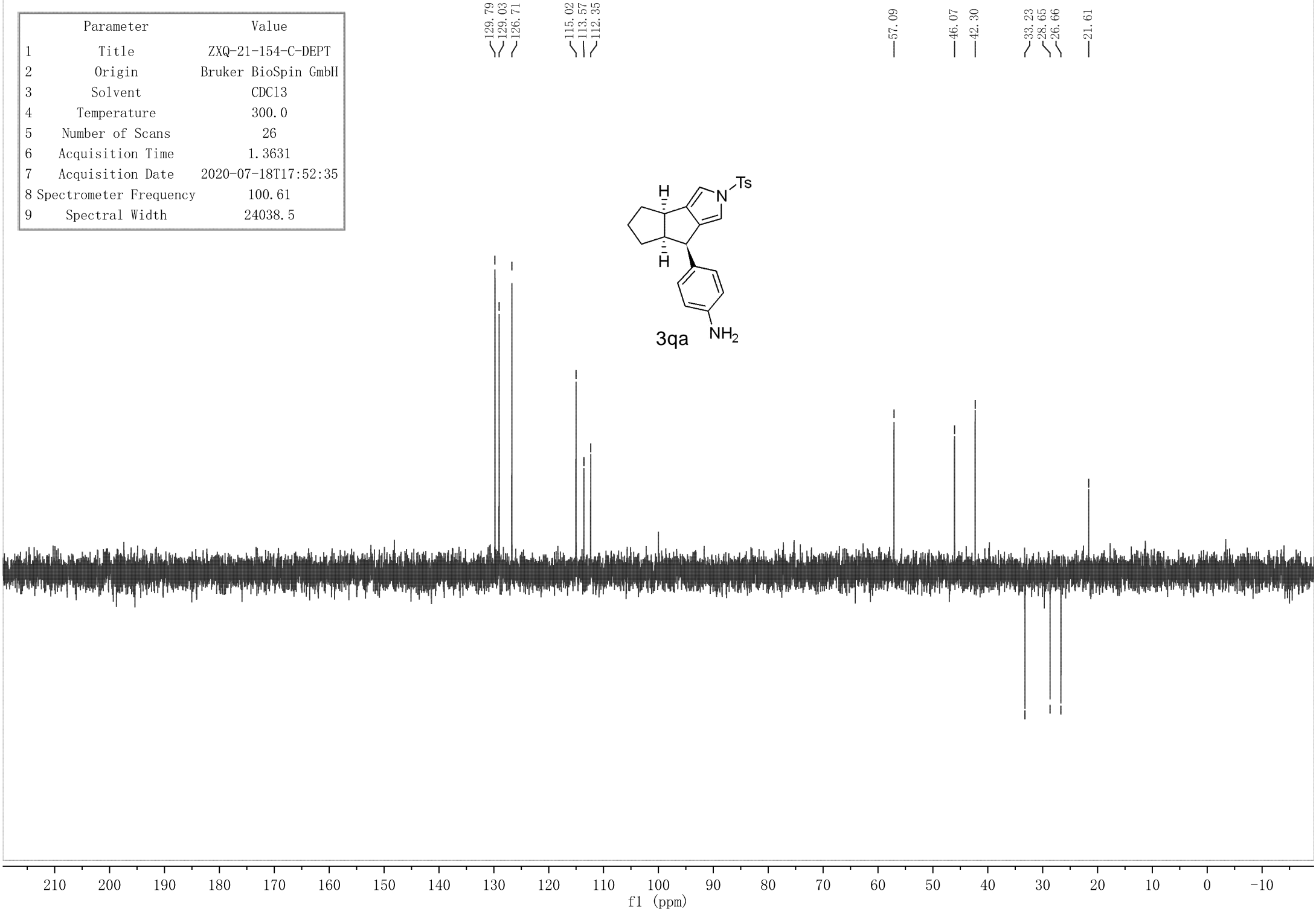
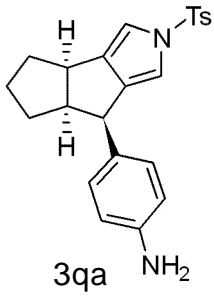
115.02  
113.57  
112.35

57.09

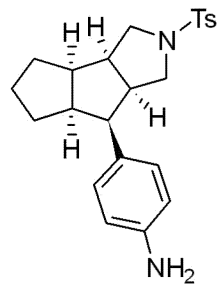
46.07  
42.30

33.23  
28.65  
26.66

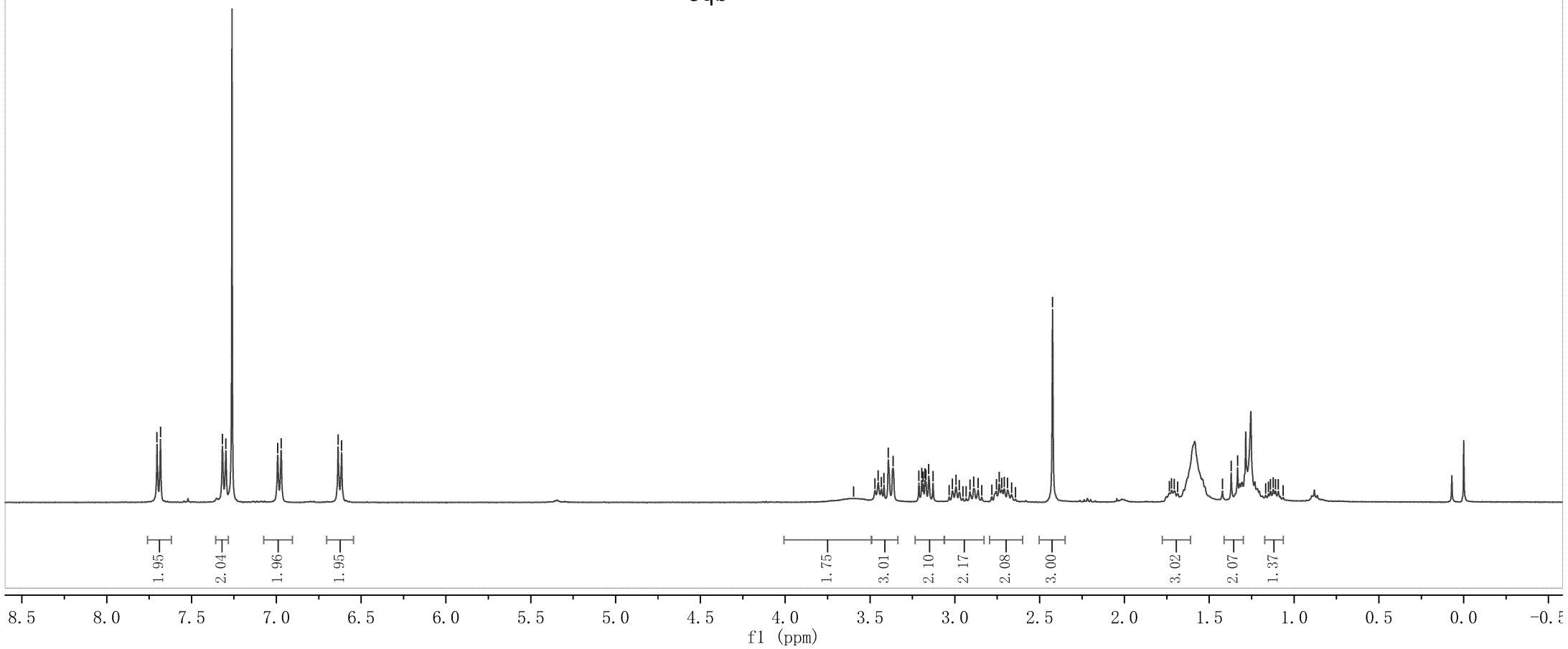
21.61



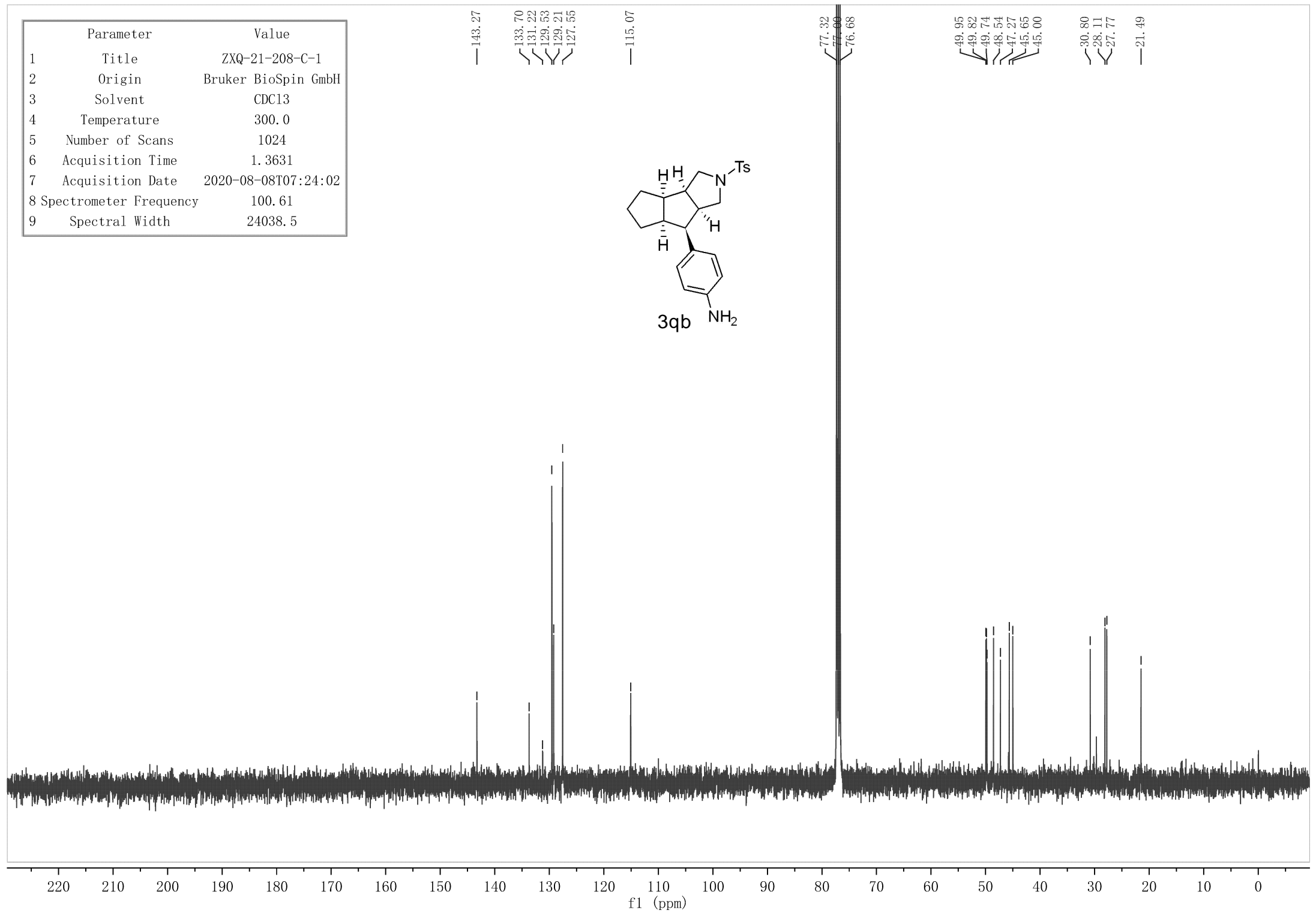
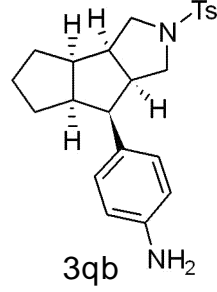
Parameter	Value
1 Title	ZXQ-21-208
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2020-08-07T11:20:41
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



3qb



Parameter	Value
1 Title	ZXQ-21-208-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	1024
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-08T07:24:02
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5





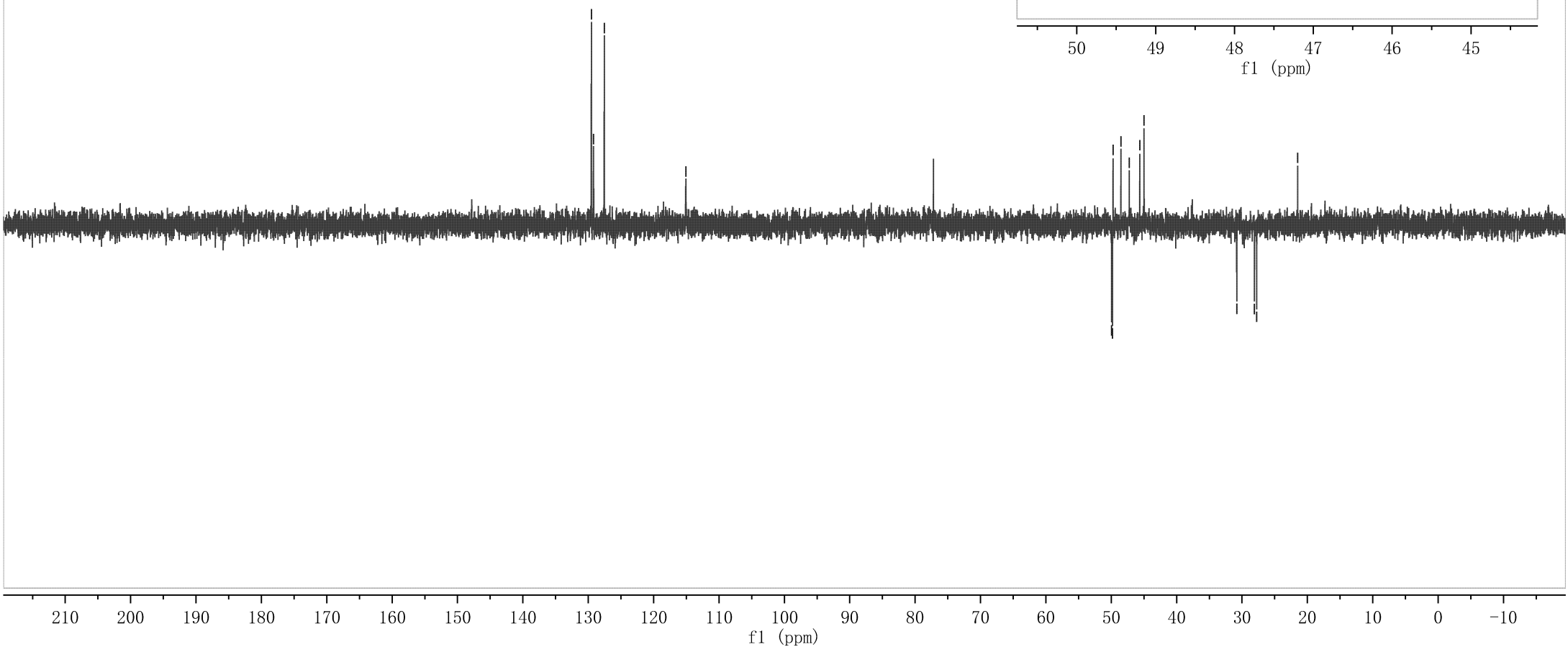
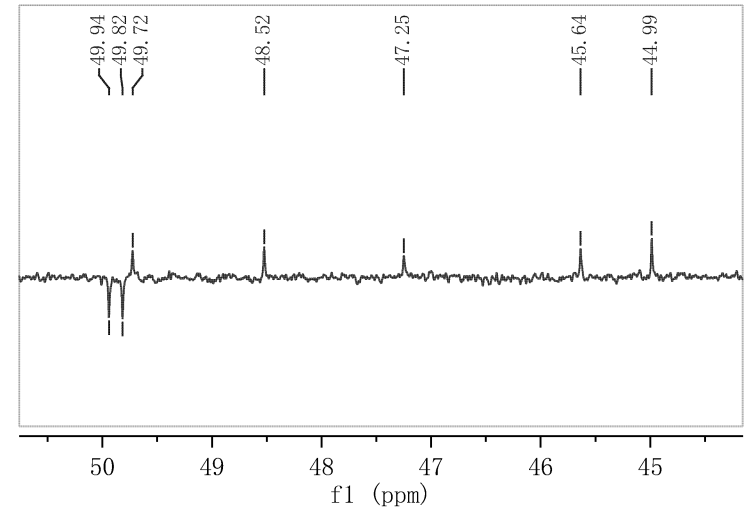
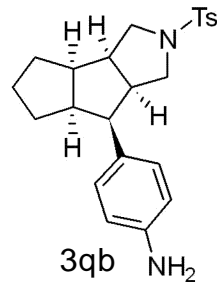
Parameter	Value
1 Title	ZXQ-21-208-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.6
5 Number of Scans	198
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-12T17:38:53
8 Spectrometer Frequency	100.59
9 Spectral Width	24038.5

129.52  
129.20  
127.55

115.07

49.94  
49.82  
49.72  
48.52  
47.25  
45.64  
44.99

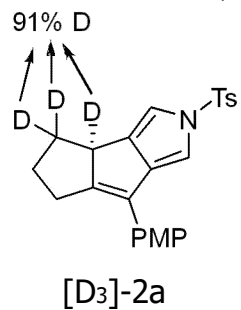
30.80  
28.10  
27.76  
21.49



Parameter	Value
1 Title	ZXQ-22-6
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2020-08-14T16:56:10
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

7.757  
7.736  
7.463  
7.441  
7.274  
7.257  
7.252  
7.237  
7.088  
7.066  
7.053  
7.050  
6.971  
6.971  
6.967  
6.953  
6.949  
6.932

3.831  
3.569  
3.550  
3.535  
2.740  
2.728  
2.718  
2.706  
2.696  
2.683  
2.675  
2.662  
2.662  
2.441  
2.420  
2.402  
2.365  
2.227  
2.212  
2.199  
2.190  
2.178  
2.167  
2.157  
2.134  
2.049  
2.049  
1.034  
1.021  
1.013  
1.001



1.95  
1.84  
2.36  
1.01  
2.80

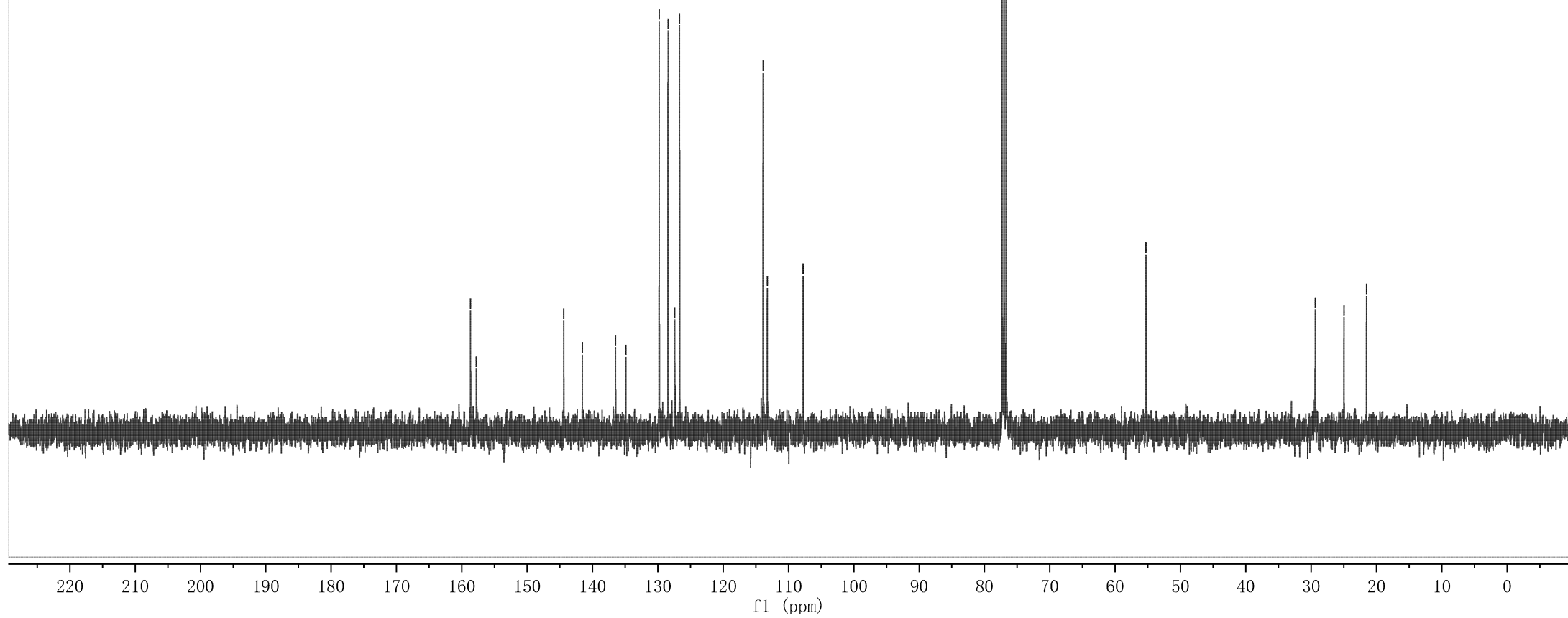
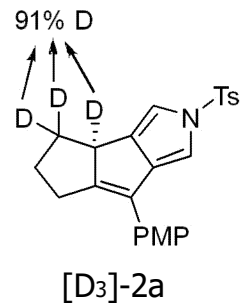
3.00  
0.09  
0.94  
1.06  
2.95  
1.87  
0.09  
0.09

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.

f1 (ppm)

Parameter	Value
1 Title	ZXQ-22-6-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	35
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-14T16:57:13
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

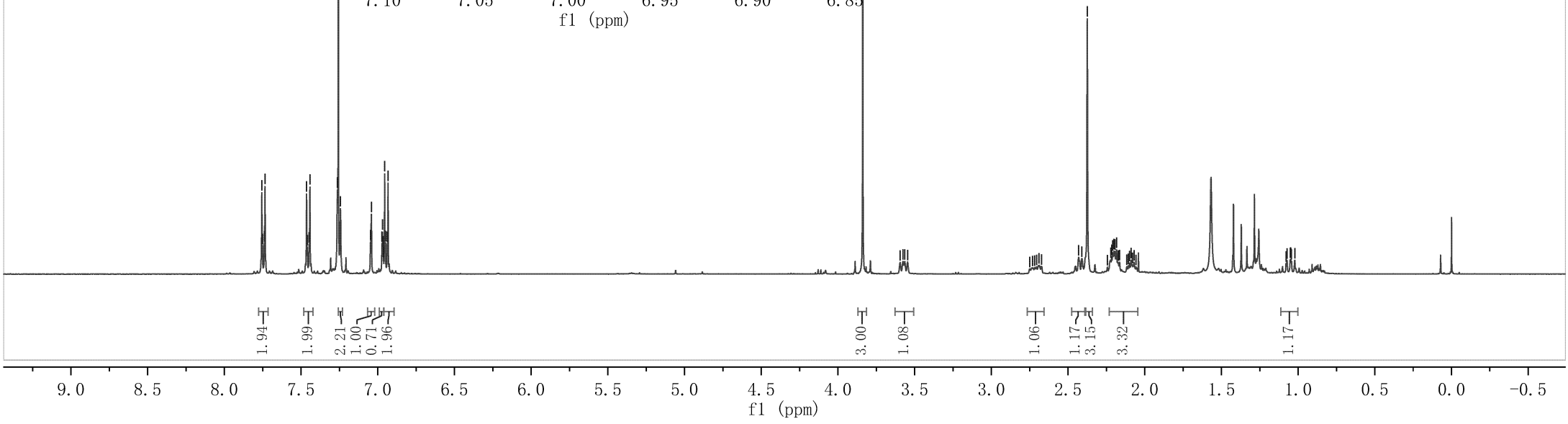
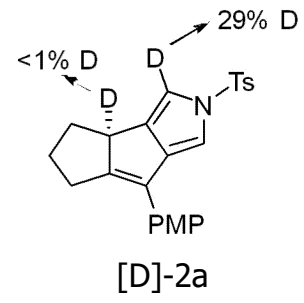
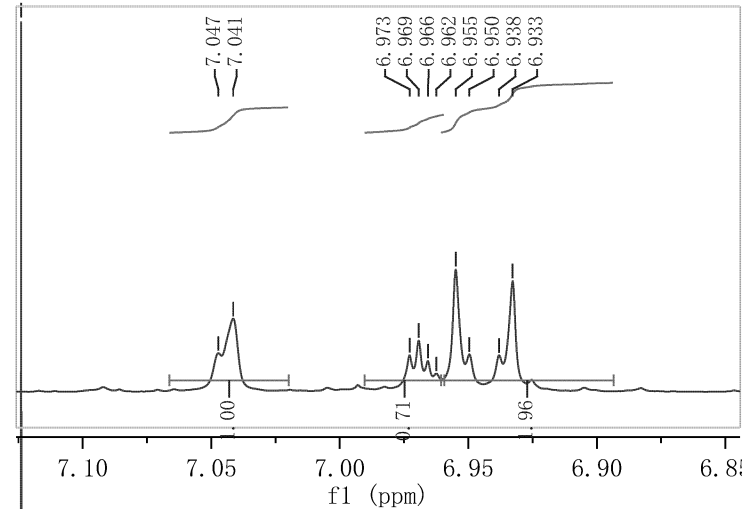
158.66 157.77 144.40 141.55 136.48 134.90 129.79 128.43 127.43 126.67 113.88 113.25 107.76 77.32 77.00 76.68 55.28 29.37 24.97 21.52



Parameter	Value
1 Title	ZXQ-22-14-1-D20-
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	301.6
5 Number of Scans	9
6 Acquisition Time	3.9846
7 Acquisition Date	2020-08-17T21:55:22
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7

7.756  
7.752  
7.739  
7.735  
7.464  
7.459  
7.447  
7.442  
7.263  
7.257  
7.243  
7.047  
7.041  
6.973  
6.969  
6.966  
6.962  
6.955  
6.950  
6.938  
6.933

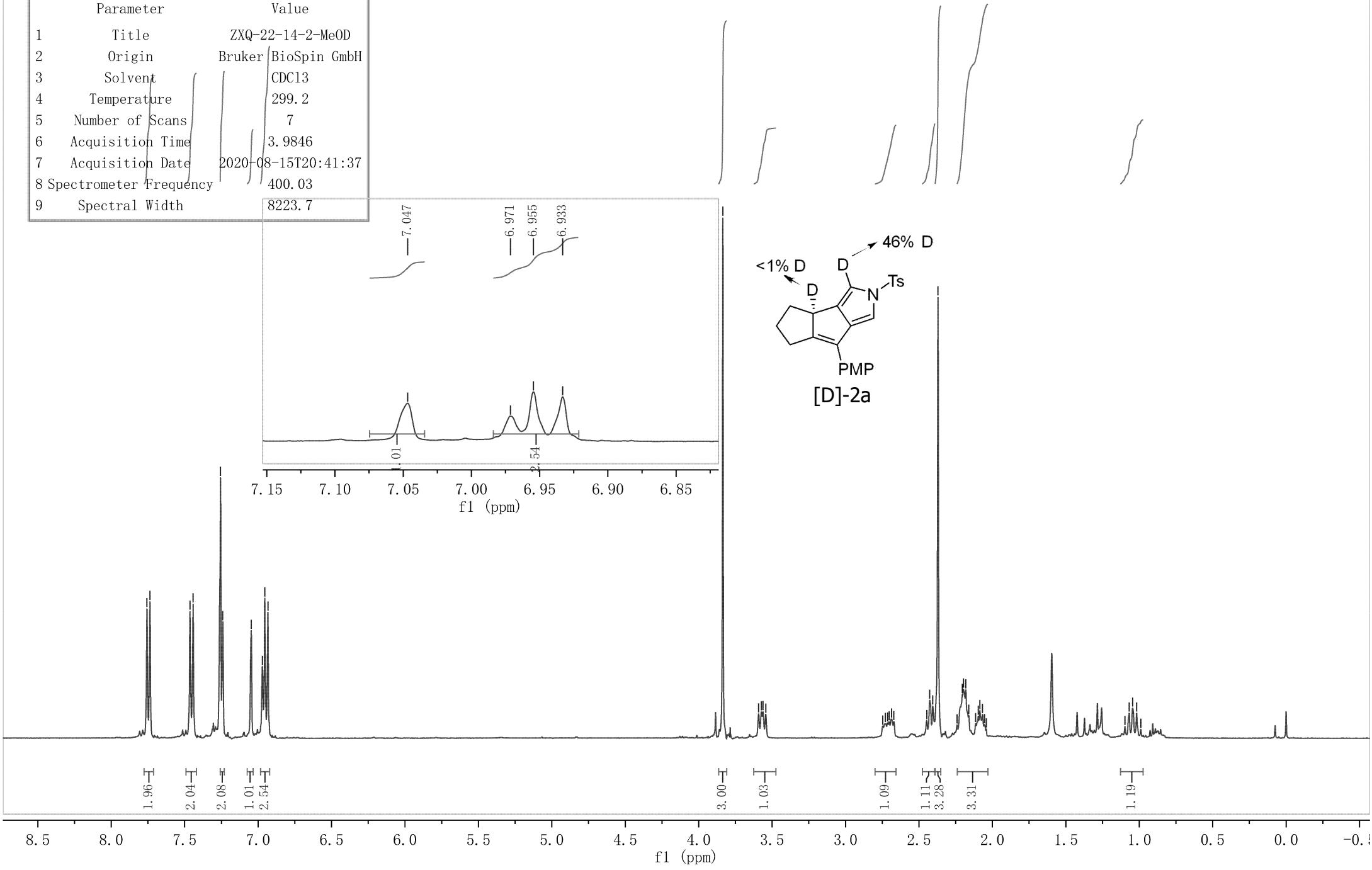
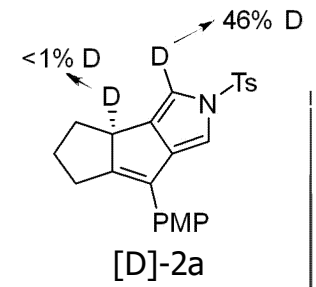
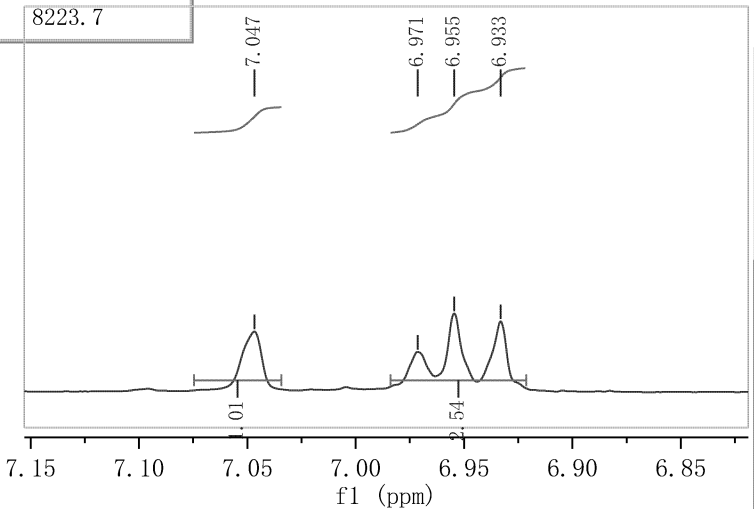
3.838  
3.595  
3.576  
3.564  
3.546  
2.749  
2.731  
2.717  
2.704  
2.689  
2.673  
2.430  
2.409  
2.374  
2.221  
2.215  
2.209  
2.201  
2.194  
2.184  
2.164  
2.088  
1.072  
1.052  
1.048  
1.043  
1.022



7.757  
7.736  
7.464  
7.442  
7.256  
7.241  
7.047  
6.971  
6.955  
6.933

3.835  
3.592  
3.573  
3.562  
3.543  
2.747  
2.729  
2.714  
2.703  
2.686  
2.671  
2.447  
2.426  
2.406  
2.370  
2.205  
2.197  
2.181  
2.114  
2.096  
2.085  
2.068  
2.054  
1.069  
1.045  
1.018  
0.989

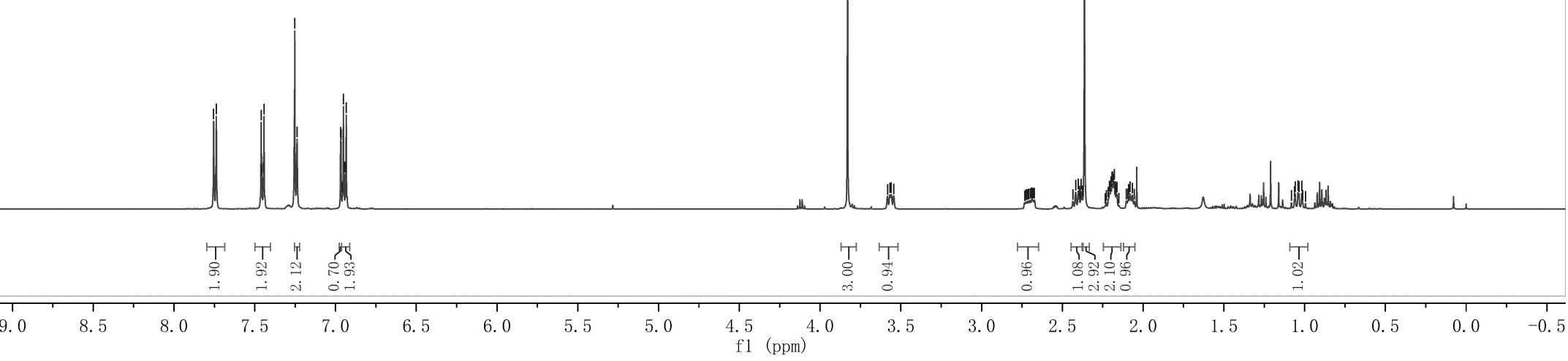
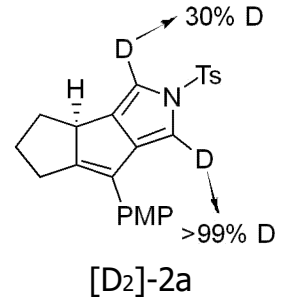
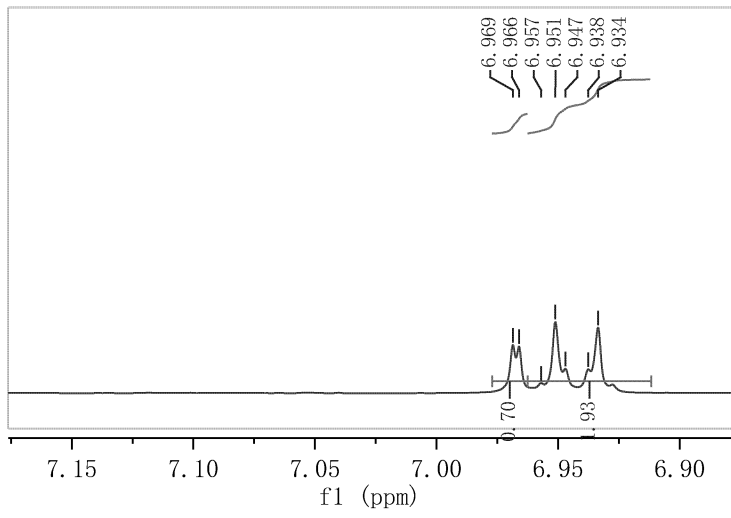
Parameter	Value
1 Title	ZXQ-22-14-2-MeOD
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	299.2
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2020-08-15T20:41:37
8 Spectrometer Frequency	400.03
9 Spectral Width	8223.7



Parameter	Value
1 Title	ZXQ-23-192
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.4
5 Number of Scans	13
6 Acquisition Time	3.1719
7 Acquisition Date	2020-12-25T16:54:12
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6

7.755  
7.738  
7.460  
7.447  
7.443  
7.252  
6.969  
6.966  
6.957  
6.951  
6.947  
6.938  
6.934

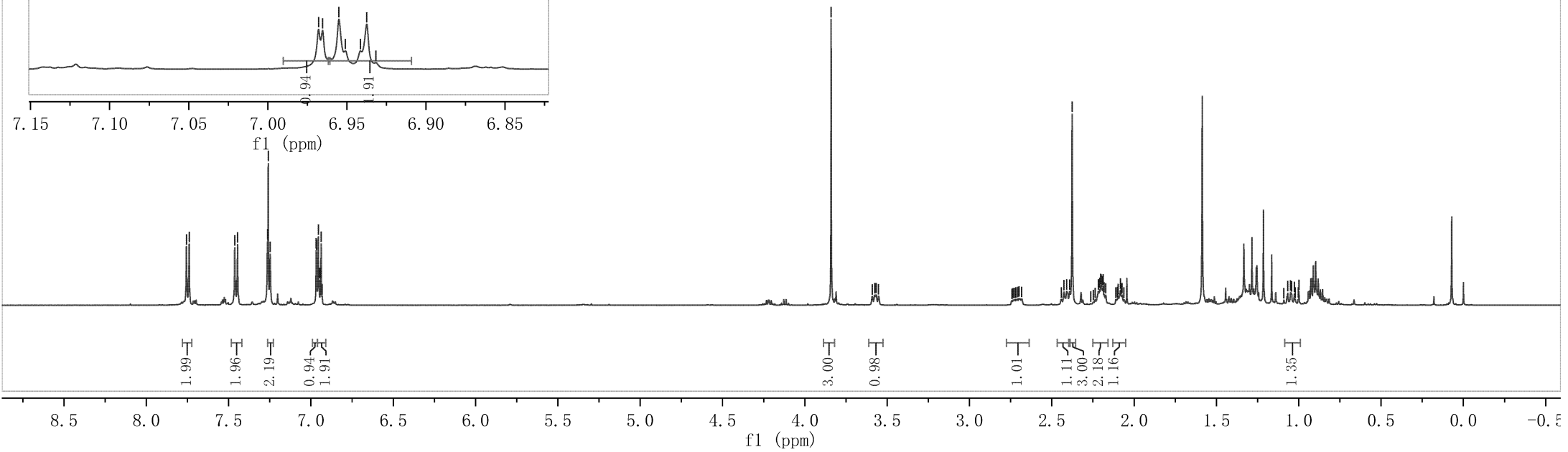
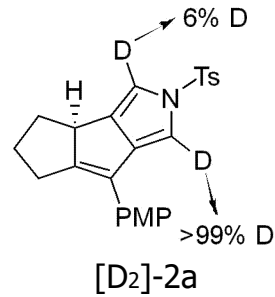
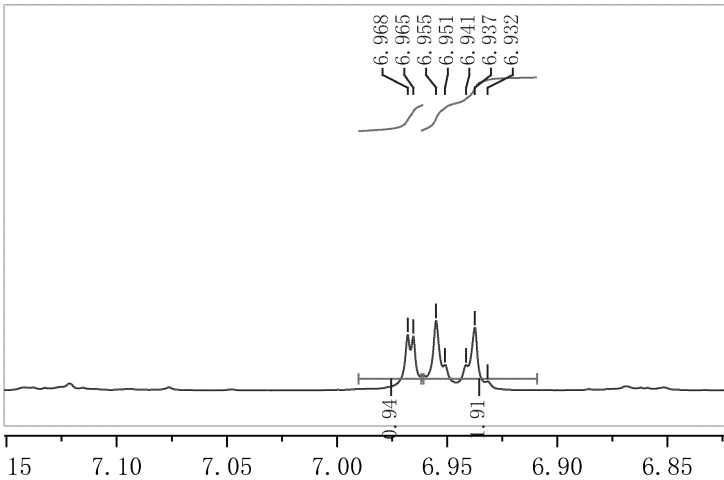
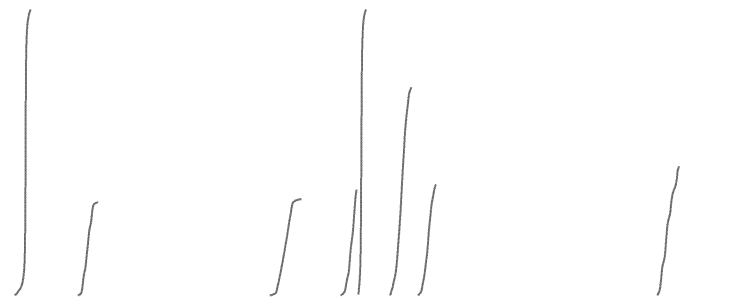
3.830  
3.582  
3.567  
3.560  
3.544  
2.708  
2.698  
2.690  
2.686  
2.682  
2.674  
2.418  
2.401  
2.384  
2.363  
2.208  
2.198  
2.193  
2.189  
2.185  
2.178  
1.082  
1.058  
1.041  
1.035  
1.018  
1.012  
0.995



7.756  
7.739  
7.463  
7.445  
7.263  
7.259  
7.247  
6.968  
6.965  
6.955  
6.951  
6.941  
6.937  
6.932

3.840  
3.590  
3.575  
3.575  
3.568  
3.552  
2.742  
2.734  
2.726  
2.718  
2.708  
2.699  
2.683  
2.426  
2.409  
2.392  
2.376  
2.218  
2.208  
2.203  
2.200  
2.196  
2.188  
2.182  
2.084  
2.080  
1.067  
1.050  
1.044  
1.026  
1.021  
1.003  
0.999

Parameter	Value
1 Title	ZXQ-23-182
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	3.1719
7 Acquisition Date	2020-12-23T17:15:44
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6

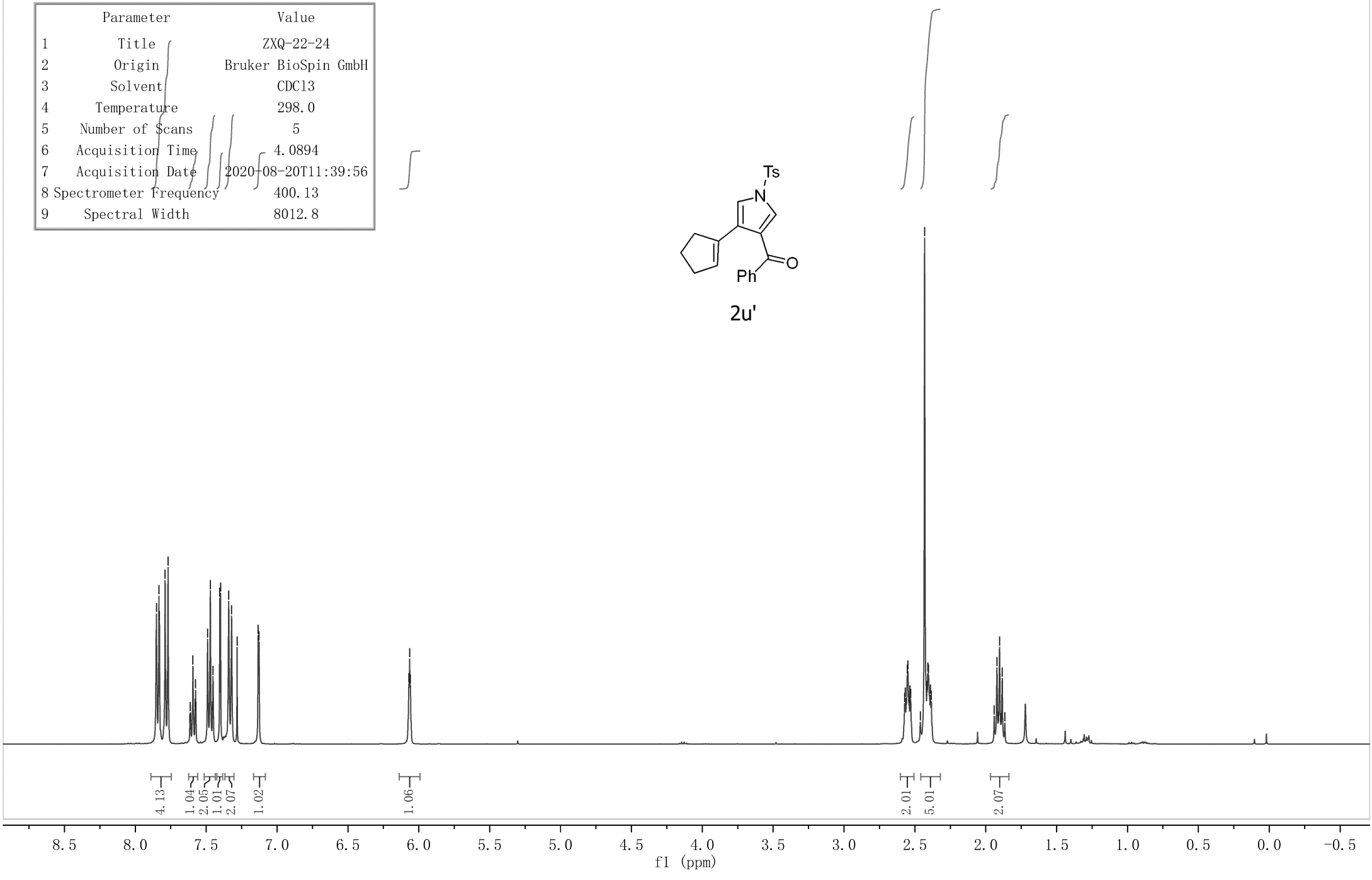
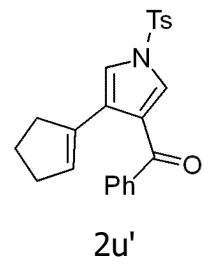


7.851  
7.833  
7.830  
7.790  
7.769  
7.615  
7.612  
7.609  
7.594  
7.578  
7.575  
7.572  
7.490  
7.471  
7.456  
7.452  
7.405  
7.399  
7.341  
7.321  
7.282  
7.133  
7.127

6.070  
6.065  
6.060

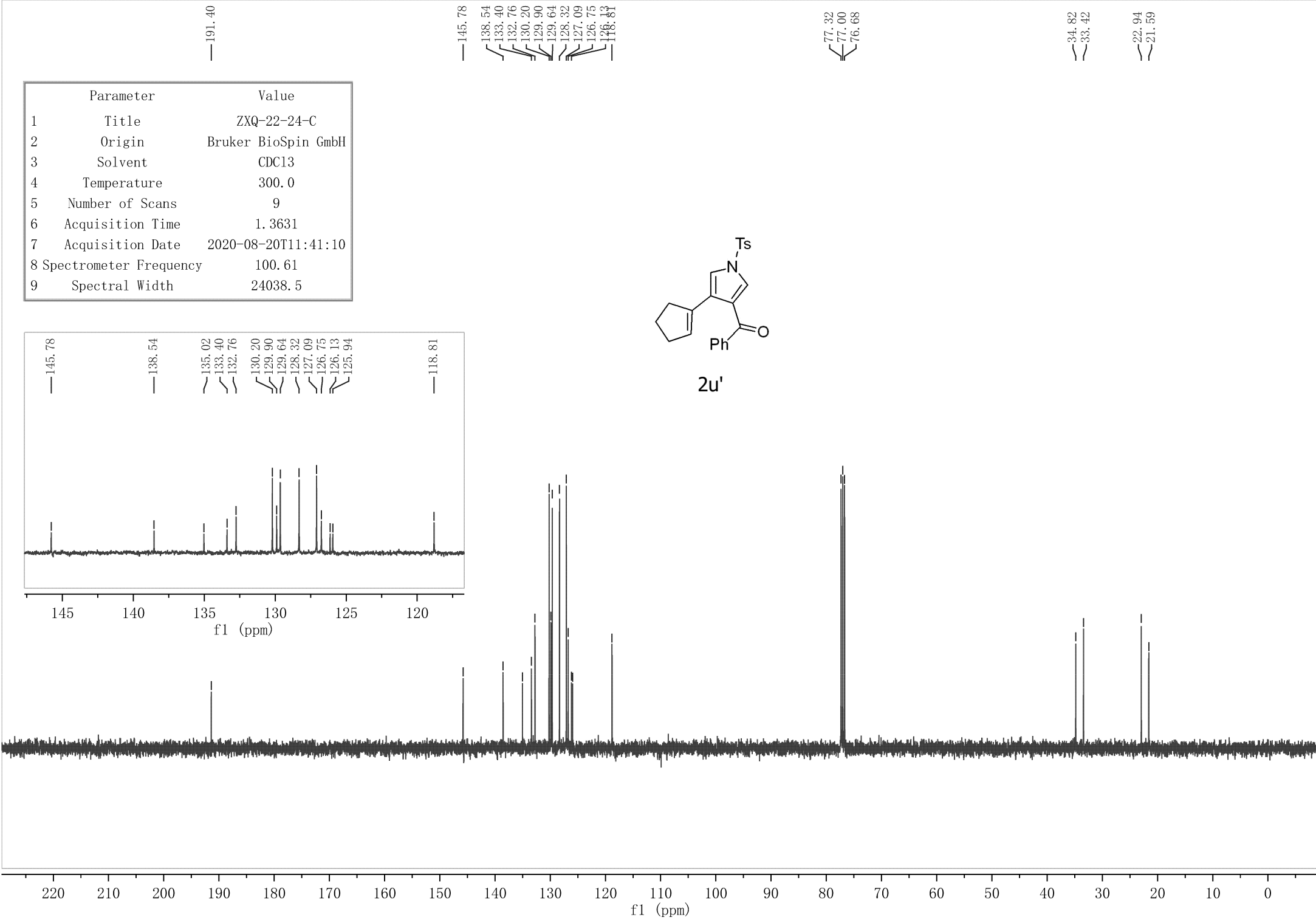
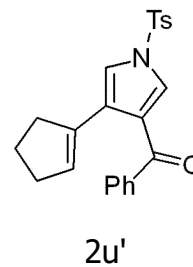
2.572  
2.567  
2.554  
2.549  
2.540  
2.535  
2.530  
2.462  
2.432  
2.415  
2.409  
2.404  
2.390  
2.385  
1.940  
1.921  
1.913  
1.903  
1.893  
1.884  
1.865

Parameter	Value
1 Title	ZXQ-22-24
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2020-08-20T11:39:56
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8





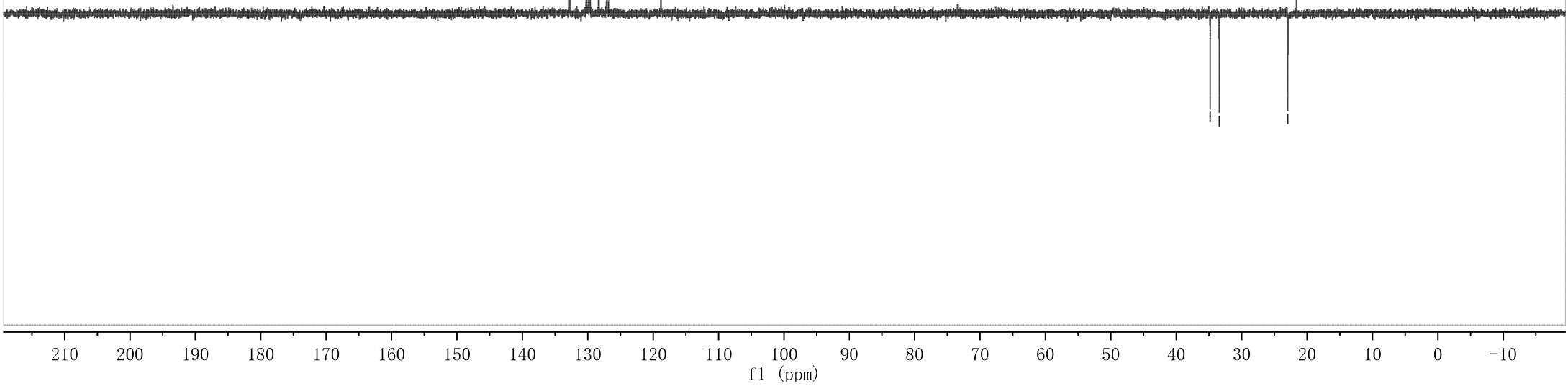
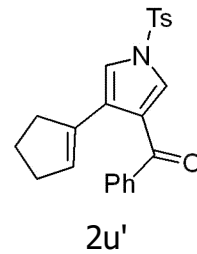
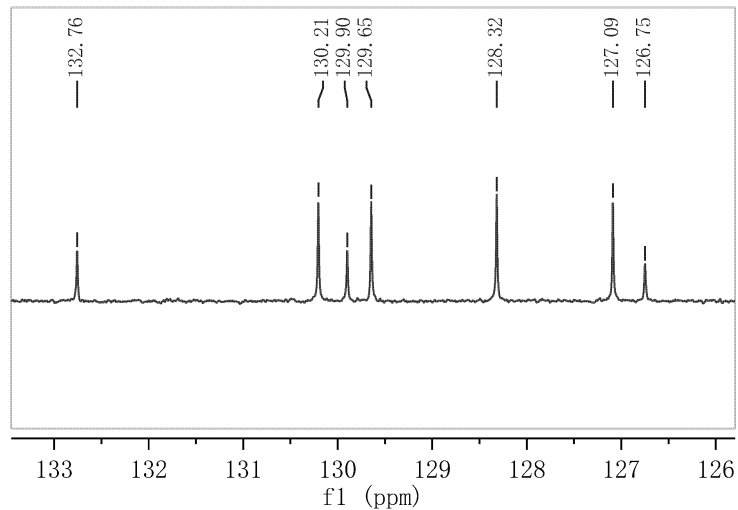
Parameter	Value
1 Title	ZXQ-22-24-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	9
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-20T11:41:10
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZXQ-22-24-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	7
6 Acquisition Time	1.3631
7 Acquisition Date	2020-08-20T11:42:14
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

132.76  
130.21  
129.90  
129.65  
128.32  
127.09  
126.75  
118.81

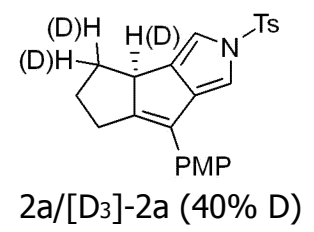
34.82  
33.42  
22.95  
21.59



7.756  
7.740  
7.463  
7.450  
7.446  
7.200  
7.248  
7.047  
6.974  
6.971  
6.961  
6.955  
6.951  
6.942  
6.937  
6.932

3.841  
3.590  
3.575  
3.565  
3.553  
3.553  
2.731  
2.722  
2.712  
2.705  
2.705  
2.695  
2.687  
2.442  
2.425  
2.408  
2.403  
2.389  
2.377  
2.218  
2.203  
2.196  
2.189  
2.178  
2.169  
1.091  
1.072  
1.067  
1.050  
1.044  
1.027  
1.004

Parameter	Value
1 Title	ZXQ-22-130-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	297.8
5 Number of Scans	7
6 Acquisition Time	3.1719
7 Acquisition Date	2020-09-18T20:52:45
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6



1.93  
1.99  
2.00  
3.92

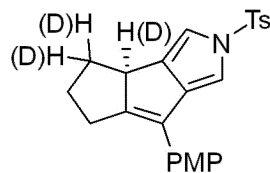
3.00  
0.60  
1.03  
1.03  
3.20  
2.23  
0.60

0.60

40% D  
40% D  
40% D

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5  
f1 (ppm)

Parameter	Value
1 Title	ZXQ-24-75
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	298.5
5 Number of Scans	9
6 Acquisition Time	3.1719
7 Acquisition Date	2021-03-10T16:52:27
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6



2a/[D<sub>3</sub>]-2a (41% D)

7.758  
7.741  
7.465  
7.448  
7.262  
7.250  
7.050  
7.048  
6.975  
6.972  
6.963  
6.957  
6.953  
6.943  
6.939  
6.933

3.843  
3.592  
3.577  
3.568  
3.555  
2.742  
2.732  
2.723  
2.714  
2.707  
2.697  
2.689  
2.427  
2.410  
2.405  
2.391  
2.379  
2.220  
2.205  
2.198  
2.190  
2.180  
2.174  
1.893  
1.074  
1.069  
1.053  
1.046  
1.029  
1.006

1.95  
2.01  
2.10  
4.00

2.97  
0.59  
0.99  
0.97  
3.01  
2.24  
0.59

0.59

41% D

41% D

41% D

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5  
f1 (ppm)