

Supporting Information

**Copper-catalyzed Buchner reaction and phenyl cyclopropanation through diyne cyclization**

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## **1. General Information**

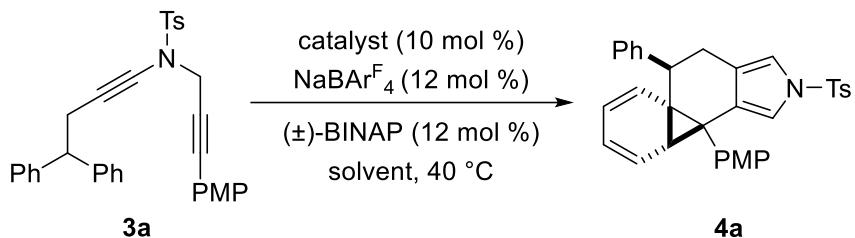
Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1,2-dichloroethane (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available 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-d<sub>3</sub>. 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-d<sub>3</sub>. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

## 2. More Reaction Condition and Scope Studies

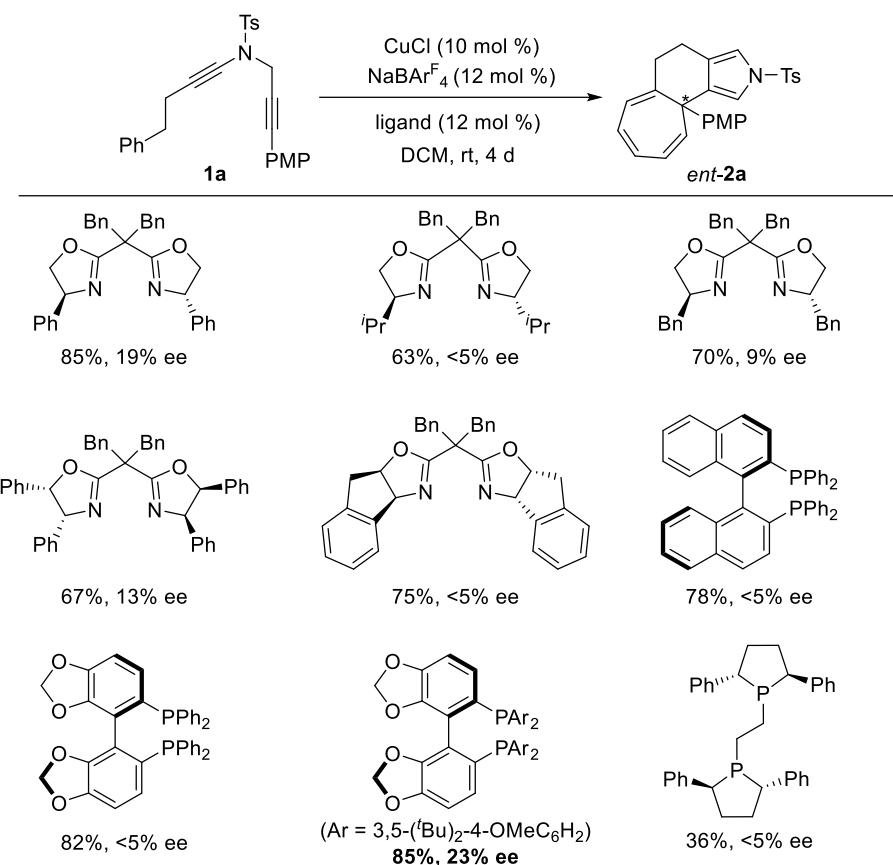
## 2.1 Screening of reaction conditions for the copper-catalyzed phenyl cyclopropanation reaction.<sup>a</sup>



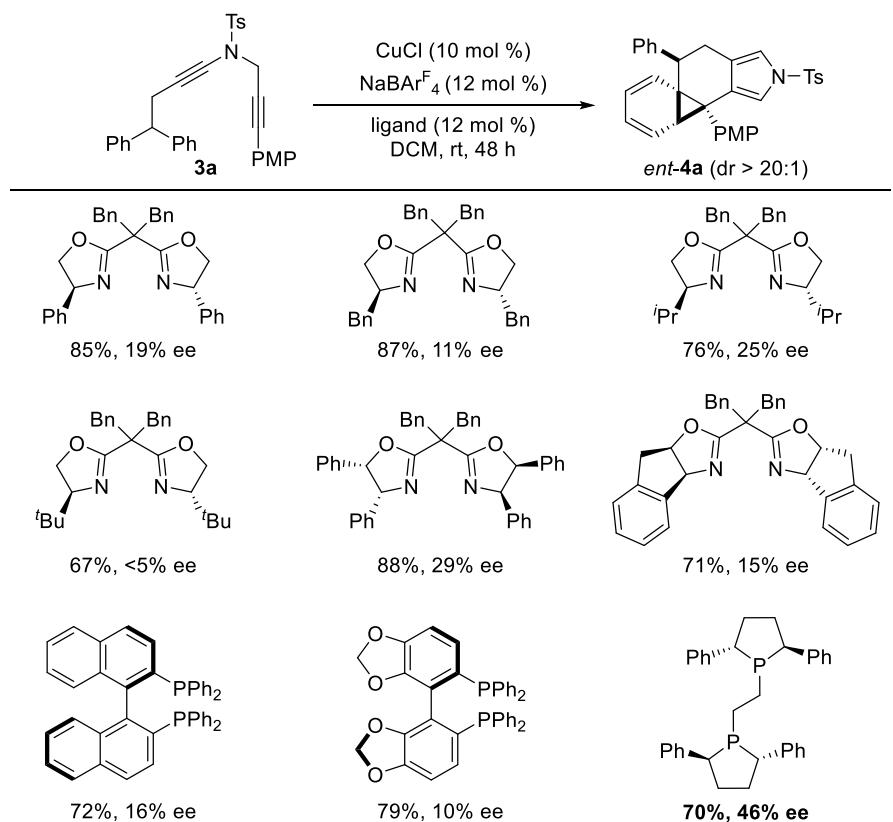
Entry	Catalyst	Reaction conditions	Yield (%) <sup>b</sup>
1	$\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$	toluene, 48 h	50
2	$\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$	DCE, 48 h	45
3	$\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$	DCM, 48 h	73
4	$\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$	THF, 48 h	<5
5	$\text{Cu}(\text{CH}_3\text{CN})_4\text{BF}_4$	DCM, 48 h	78
6	$\text{Cu}(\text{OTf})_2$	DCM, 48 h	<5
7	$\text{Cu}(\text{PPh}_3)_2\text{BH}_4$	DCM, 48 h	<5
8	$\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$	DCM, 48 h	<5
9	CuI	DCM, 72 h	68
10	CuBr	DCM, 72 h	30
<b>11</b>	<b>CuCl</b>	<b>DCM, 53 h</b>	<b>95</b>
12 <sup>c,d</sup>	CuCl	DCM 48 h	15
13 <sup>c</sup>	CuCl	DCM, 48 h	18
14 <sup>d</sup>	CuCl	DCM, 48 h	42

<sup>a</sup> Reaction conditions: **1** (0.05 mmol), [cat.] (0.005 mmol), ( $\pm$ )-BINAP (0.006 mmol), NaBAr<sup>F</sup><sub>4</sub> (0.006 mmol), solvent (1 mL), 40 °C, 48-72 h. <sup>b</sup> Measured by <sup>1</sup>H NMR using diethyl phthalate as internal standard. <sup>c</sup> Without ligand. <sup>d</sup> Without NaBAr<sup>F</sup><sub>4</sub>. PMP = 4-methoxyphenyl, NaBAr<sup>F</sup><sub>4</sub> = sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, DCM = dichloromethane.

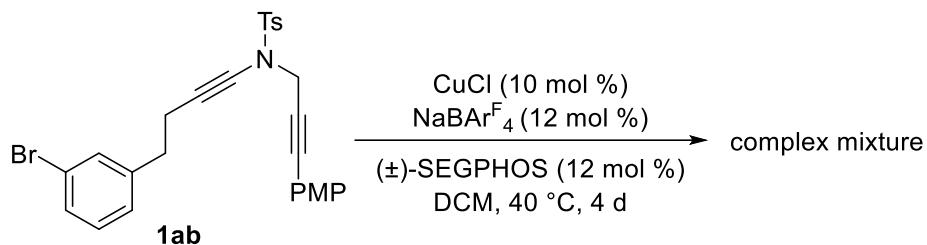
## 2.2 Screening of chiral ligands for the asymmetric Buchner reaction.



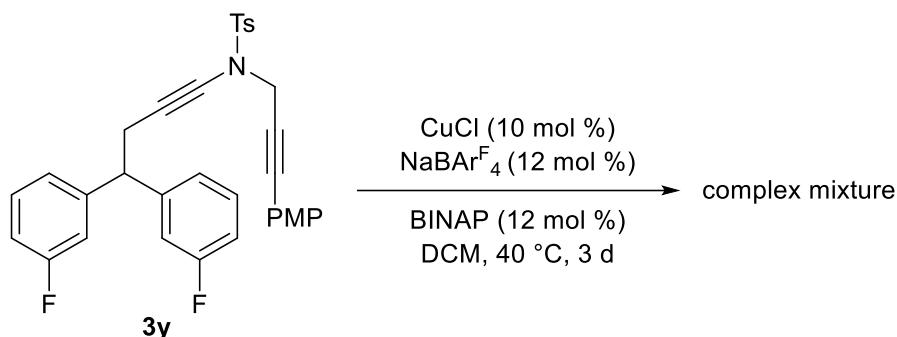
## 2.3 Screening of chiral ligands for the asymmetric phenyl cyclopropanation reaction.



2.4 The reaction of 3-bromophenyl-substituted diyne **1ab** under the standard reaction conditions only gave a complex mixture and no desired product was obtained.

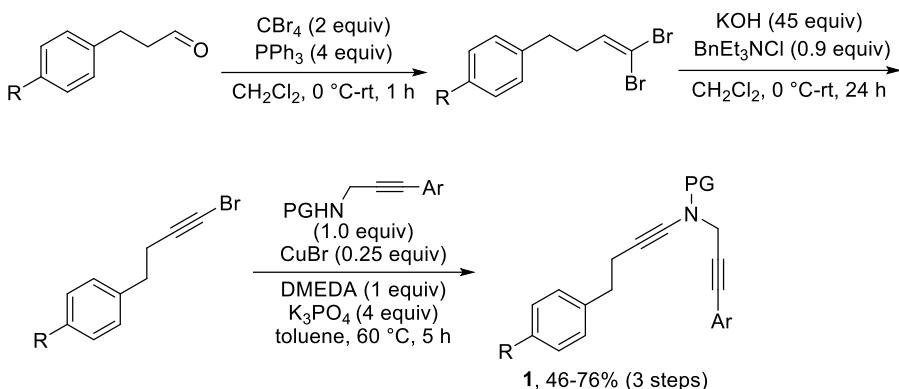


2.5 The reaction of 3-fluorophenyl-substituted diyne **3y** under the standard reaction conditions only gave a complex mixture and no desired product was obtained.



### 3. Preparation of Starting Materials

#### General procedure for the preparation of diynes **1**:

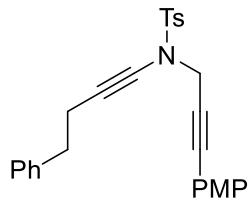


To a solution of  $\text{PPh}_3$  (21.0 g, 80 mmol) in  $\text{CH}_2\text{Cl}_2$  (25 mL) was added  $\text{CBr}_4$  (13.3 g, 40 mmol) at 0 °C. The mixture was stirred at 0 °C for 30 min, followed by adding the corresponding aldehyde (20 mmol). Then the reaction mixture was stirred at room temperature for 1 h. Upon completion, the reaction mixture was diluted with petroleum ether, and filtered through a pad of silica gel. The filtrate was concentrated under reduced pressure, and purified by column chromatography on silica gel (eluent: petroleum ether) to afford the desired product.

To a solution of the above dibromoalkene (10 mmol) and benzyltriethylammonium chloride (2.0 g, 9 mmol) in  $\text{CH}_2\text{Cl}_2$  (25 mL) was added a 10% aqueous solution of KOH (25.8 g solution, 450 mmol KOH) at 0 °C. The mixture was stirred at 0 °C for 30 min, and further stirred at room temperature 24 h. Upon completion, the reaction mixture was extracted with  $\text{CH}_2\text{Cl}_2$ , dried over  $\text{Na}_2\text{SO}_4$ , filtered and concentrated in vacuo. The desired alkynyl bromide product was used in the next step without further purification.

To a solution of the above alkynyl bromide (1.2 mmol) in toluene (6 mL) were added copper bromide (0.25 mmol, 0.036 g), DMEDA (1.0 mmol, 0.107 mL),  $\text{K}_3\text{PO}_4$  (4.0 mmol, 0.849 g) and protected propargylamide derivative (1.2 mmol). The reaction was stirred at 60 °C for 5 h and the progress of the reaction was monitored by TLC. Upon completion, the solution was filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: hexanes/EtOAc) to afford the desired diyne **1** in 46-76% yields.

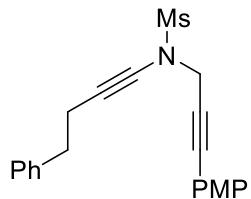
**N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1a)**



**1a**

The compound was isolated in 73% yield according to the general procedure. Yellow solid. M.p = 75 – 76 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J$  = 8.0 Hz, 2H), 7.24 – 7.16 (m, 7H), 7.11 – 7.07 (m, 2H), 6.79 – 6.75 (m, 2H), 4.39 (s, 2H), 3.79 (s, 3H), 2.81 (t,  $J$  = 7.0 Hz, 2H), 2.59 (t,  $J$  = 7.5 Hz, 2H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 144.4, 140.5, 134.5, 133.1, 129.4, 128.5, 128.3, 128.1, 126.2, 114.2, 113.7, 86.0, 80.1, 73.6, 70.0, 55.3, 42.8, 35.2, 21.5, 20.6; IR (neat): 3055, 2987, 2307, 1509, 1428, 1266, 894, 736; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{25}\text{NaO}_3\text{S}^+$  466.1447; Found 466.1444.

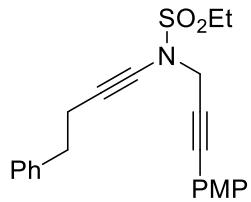
**N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-N-(4-phenylbut-1-yn-1-yl)methanesulfonamide (1b)**



**1b**

The compound was isolated in 69% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 (d,  $J$  = 9.0 Hz, 2H), 7.29 – 7.12 (m, 5H), 6.85 (d,  $J$  = 9.0 Hz, 2H), 4.40 (s, 2H), 3.79 (s, 3H), 3.02 (s, 3H), 2.84 (t,  $J$  = 7.0 Hz, 2H), 2.62 (t,  $J$  = 7.0 Hz, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  160.1, 140.4, 133.3, 128.5, 128.3, 126.2, 114.0, 113.8, 86.4, 80.4, 73.4, 70.3, 55.3, 42.8, 37.9, 35.0, 20.5; IR (neat): 3053, 2986, 2330, 1607, 1509, 1032, 835, 741, 736; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{21}\text{H}_{21}\text{NNaO}_3\text{S}^+$  390.1134; Found 390.1130.

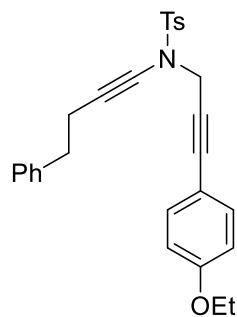
**N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-N-(4-phenylbut-1-yn-1-yl)ethanesulfonamide (1c)**



**1c**

The compound was isolated in 68% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 (d,  $J = 8.5$  Hz, 2H), 7.28 – 7.20 (m, 4H), 7.20 – 7.14 (m, 1H), 6.85 (d,  $J = 8.5$  Hz, 2H), 4.42 (s, 2H), 3.81 (s, 3H), 3.22 (q,  $J = 14.5$  Hz, 2H), 2.84 (t,  $J = 7.0$  Hz, 2H), 2.62 (t,  $J = 7.0$  Hz, 2H), 1.40 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  160.0, 140.5, 133.3, 128.5, 128.3, 126.2, 114.0, 86.2, 80.9, 73.5, 70.0, 55.3, 46.3, 42.5, 35.1, 20.6, 7.7; IR (neat): 3056, 2988, 2306, 1423, 1266, 896, 750, 706; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{22}\text{H}_{23}\text{NNaO}_3\text{S}^+$  404.1291; Found 404.1293.

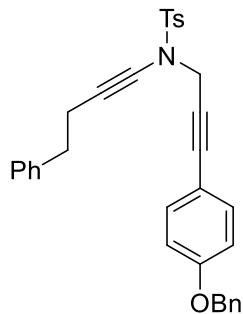
**N-(3-(4-ethoxyphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1d)**



**1d**

The compound was isolated in 70% yield according to the general procedure. Yellow solid. M.p = 77 – 78 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.15 (m, 7H), 7.07 (d,  $J = 8.8$  Hz, 2H), 6.76 (d,  $J = 8.8$  Hz, 2H), 4.39 (s, 2H), 4.00 (q,  $J = 6.8$  Hz, 2H), 2.80 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.35 (s, 3H), 1.40 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 144.3, 140.5, 134.4, 133.1, 129.4, 128.4, 128.3, 128.1, 126.1, 114.2, 114.0, 86.1, 80.0, 73.6, 70.0, 63.5, 42.8, 35.2, 21.5, 20.6, 14.7; IR (neat): 3054, 2986, 2359, 1733, 1170, 741, 736, 705; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_3\text{S}^+$  480.1604; Found 480.1600.

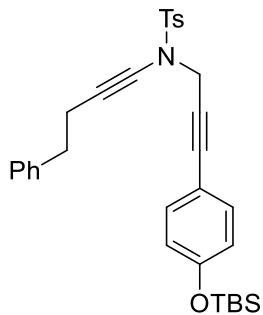
**N-(3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1e)**



**1e**

The compound was isolated in 89% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.4$  Hz, 2H), 7.43 – 7.28 (m, 5H), 7.26 – 7.13 (m, 7H), 7.07 (d,  $J = 8.8$  Hz, 2H), 6.84 (d,  $J = 8.8$  Hz, 2H), 5.04 (s, 2H), 4.38 (s, 2H), 2.79 (t,  $J = 7.2$  Hz, 2H), 2.58 (t,  $J = 7.2$  Hz, 2H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 144.3, 140.5, 136.4, 134.4, 133.1, 129.3, 128.6, 128.4, 128.2, 128.1, 128.0, 127.3, 126.1, 114.6, 114.4, 85.9, 80.1, 73.5, 70.0, 69.9, 42.7, 35.1, 21.5, 20.5; IR (neat): 3056, 2988, 2307, 1509, 1266, 742, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{29}\text{NNaO}_3\text{S}^+$  542.1760; Found 542.1761.

**N-(3-((tert-butyldimethylsilyl)oxy)phenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1f)**

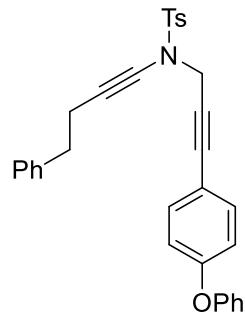


**1f**

The compound was isolated in 45% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.15 (m, 7H), 7.03 (d,  $J = 8.4$  Hz, 2H), 6.71 (d,  $J = 8.8$  Hz, 2H), 4.39 (s, 2H), 2.81 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.36 (s, 3H), 0.97 (s, 9H), 0.19 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.1, 144.3, 140.6, 134.5, 133.1, 129.4, 128.5, 128.3, 128.2, 126.2, 119.9, 114.9, 86.1, 80.2, 73.6, 70.0, 42.8, 35.2, 25.6, 21.6, 20.6, 18.2, -4.4; IR (neat): 3055, 2987, 2306, 1508, 897,

741, 736, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>37</sub>NNaO<sub>3</sub>SSi<sup>+</sup> 566.2156; Found 566.2152.

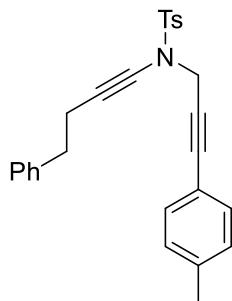
**4-methyl-N-(3-(4-phenoxyphenyl)prop-2-yn-1-yl)-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1g)**



**1g**

The compound was isolated in 74% yield according to the general procedure. Yellow solid. M.p = 96-97 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.79 – 7.75 (d, J = 8.0 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.27 – 7.08 (m, 10H), 7.00 (d, J = 8.0 Hz, 2H), 6.86 (d, J = 8.8 Hz, 2H), 4.40 (s, 2H), 2.81 (t, J = 7.2 Hz, 2H), 2.59 (t, J = 7.2 Hz, 2H), 2.36 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.8, 156.2, 144.4, 140.5, 134.4, 133.2, 129.9, 129.4, 128.4, 128.3, 128.1, 126.2, 123.9, 119.4, 118.0, 116.6, 85.6, 80.8, 73.5, 70.1, 42.7, 35.2, 21.6, 20.6; IR (neat): 3055, 2987, 2306, 1504, 1422, 1169, 896, 737; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>27</sub>NNaO<sub>3</sub>S<sup>+</sup> 528.1604; Found 528.1600.

**N-(3-(4-ethylphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1h)**

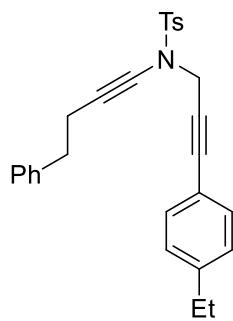


**1h**

The compound was isolated in 61% yield according to the general procedure. Yellow solid. M.p = 73 – 74 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.77 (d, J = 8.0 Hz, 2H), 7.27 – 7.14 (m, 7H), 7.08 – 7.01 (m, 4H), 4.40 (s, 2H), 2.80 (t, J = 7.2 Hz, 2H), 2.59 (t, J = 7.2 Hz, 2H),

2.35 (s, 3H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.4, 140.5, 138.6, 134.4, 131.5, 129.4, 128.8, 128.4, 128.3, 128.1, 126.1, 119.0, 86.2, 80.7, 73.5, 70.0, 42.7, 35.2, 21.5, 21.4, 20.6; IR (neat): 3054, 2986, 2305, 1509, 1265, 896, 741, 736; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{25}\text{NNaO}_2\text{S}^+$  450.1498; Found 450.1495.

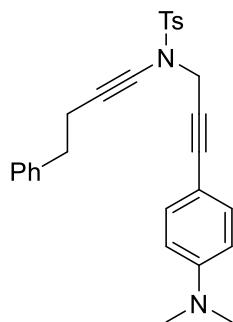
**N-(3-(4-ethylphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1i)**



**1i**

The compound was isolated in 88 % yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.14 (m, 7H), 7.10 – 7.03 (m, 4H), 4.40 (s, 2H), 2.80 (t,  $J = 7.2$  Hz, 2H), 2.67 – 2.55 (m, 4H), 2.34 (s, 3H), 1.21 (t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.9, 144.4, 140.5, 134.4, 131.6, 129.4, 128.4, 128.3, 128.1, 127.6, 126.1, 119.3, 86.2, 80.7, 73.6, 70.0, 42.7, 35.2, 28.7, 21.5, 20.6, 15.3; IR (neat): 3055, 2987, 2306, 1423, 1266, 896, 748, 737; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_2\text{S}^+$  464.1655; Found 464.1657.

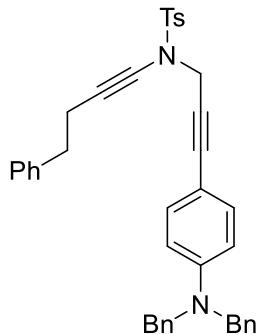
**N-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1j)**



**1j**

The compound was isolated in 87% yield according to the general procedure. Yellow solid. M.p = 111 – 112 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J$  = 8.5 Hz, 2H), 7.25 – 7.18 (m, 7H), 7.04 (d,  $J$  = 9.0 Hz, 2H), 6.55 (d,  $J$  = 9.0 Hz, 2H), 4.40 (s, 2H), 2.96 (s, 6H), 2.80 (t,  $J$  = 7.5 Hz, 2H), 2.58 (t,  $J$  = 7.5 Hz, 2H), 2.37 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  150.6, 144.7, 141.0, 134.9, 133.2, 129.8, 128.9, 128.7, 128.5, 126.5, 111.9, 109.3, 87.6, 79.5, 74.1, 70.4, 43.4, 40.5, 35.6, 21.9(9), 21.9(6), 21.1; IR (neat): 2358, 2250, 1652, 1539, 1361, 1167, 814, 666, 579, 544; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{28}\text{H}_{28}\text{N}_2\text{NaO}_2\text{S}^+$  479.1764; Found 479.1761.

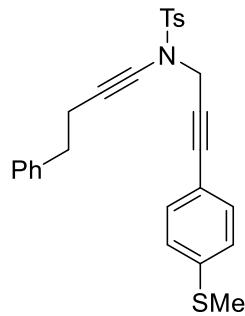
**N-(3-(4-(dibenzylamino)phenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1k)**



**1k**

The compound was isolated in 48% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J$  = 7.6 Hz, 2H), 7.36 – 7.29 (m, 4H), 7.27 – 7.12 (m, 13H), 6.95 (d,  $J$  = 8.0 Hz, 2H), 6.57 (d,  $J$  = 8.0 Hz, 2H), 4.64 (s, 4H), 4.37 (s, 2H), 2.79 (t,  $J$  = 7.2 Hz, 2H), 2.61 (t,  $J$  = 7.2 Hz, 2H), 2.29 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.0, 144.3, 140.6, 137.8, 134.5, 132.9, 129.3, 128.7, 128.5, 128.3, 128.1, 127.1, 126.4, 126.1, 111.8, 109.6, 86.9, 79.2, 73.6, 69.9, 54.1, 43.0, 35.2, 21.5, 20.6; IR (neat): 3604, 3030, 2926, 2253, 2216, 1521, 1363, 815, 736, 698; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{40}\text{H}_{36}\text{N}_2\text{NaO}_2\text{S}^+$  631.2390; Found 631.2392.

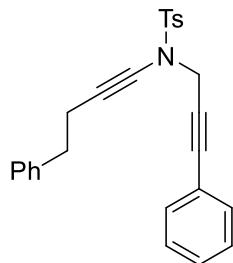
**4-methyl-N-(3-(4-(methylthio)phenyl)prop-2-yn-1-yl)-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1l)**



**1l**

The compound was isolated in 57% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.4$  Hz, 2H), 7.24 – 7.17 (m, 7H), 7.13 – 7.01 (m, 4H), 4.40 (s, 2H), 2.81 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.46 (s, 3H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.4, 140.5, 139.8, 134.4, 131.9, 129.4, 128.4, 128.3, 128.1, 126.2, 125.6, 118.4, 85.8, 81.5, 73.5, 70.1, 42.7, 35.2, 21.6, 20.6, 15.3; IR (neat): 3056, 2988, 2306, 1423, 1366, 1171, 896, 748, 742, 706; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{27}\text{H}_{25}\text{NNaO}_2\text{S}_2^+$  482.1219; Found 482.1216.

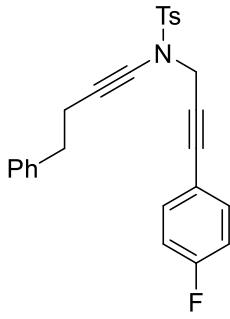
**4-methyl-N-(4-phenylbut-1-yn-1-yl)-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide  
(1m)**



**1m**

The compound was isolated in 76% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.4$  Hz, 2H), 7.32 – 7.10 (m, 12H), 4.41 (s, 2H), 2.81 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.4, 140.5, 134.4, 131.6, 129.4, 128.5, 128.4, 128.3, 128.1(3), 128.0(7), 126.2, 122.1, 86.0, 81.5, 73.5, 70.1, 42.7, 35.2, 21.5, 20.6; IR (neat): 3055, 2987, 2305, 2256, 1365, 1266, 1170, 896, 737, 705; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{26}\text{H}_{23}\text{NNaO}_2\text{S}^+$  436.1342; Found 436.1340.

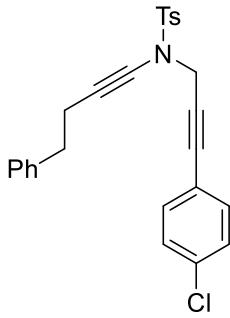
**N-(3-(4-fluorophenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1n)**



**1n**

The compound was isolated in 78% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.0$  Hz, 2H), 7.28 – 7.15 (m, 7H), 7.15 – 7.09 (m, 2H), 6.98 – 6.90 (m, 2H), 4.39 (s, 2H), 2.81 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.5 (d,  $J = 250.1$  Hz), 144.4, 140.5, 134.4, 133.5 (d,  $J = 8.4$  Hz), 129.4, 128.4, 128.3, 128.1, 126.2, 118.2 (d,  $J = 3.5$  Hz), 115.4 (d,  $J = 22.1$  Hz), 85.0, 81.3, 73.5, 70.1, 42.6, 35.2, 21.5, 20.6;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -110.2; IR (neat): 3056, 2989, 2687, 1603, 1423, 1367, 896, 839, 748, 737; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{26}\text{H}_{22}\text{FNNaO}_2\text{S}^+$  454.1247; Found 454.1245.

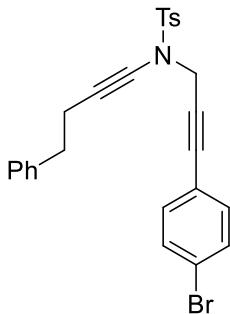
***N*-(3-(4-chlorophenyl)prop-2-yn-1-yl)-4-methyl-*N*-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1o)**



**1o**

The compound was isolated in 71% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.4$  Hz, 2H), 7.26 – 7.15 (m, 9H), 7.05 (d,  $J = 8.4$  Hz, 2H), 4.38 (s, 2H), 2.80 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.4, 140.4, 134.5, 134.3, 132.8, 129.4, 128.4, 128.2, 128.1, 126.1, 120.5, 84.9, 82.5, 73.5, 70.1, 42.6, 35.1, 21.5, 20.5; IR (neat): 3054, 2987, 2307, 1422, 1366, 1265, 1170, 1090, 896, 736, 706; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{26}\text{H}_{22}\text{ClNNaO}_2\text{S}^+$  470.0952; Found 470.0945.

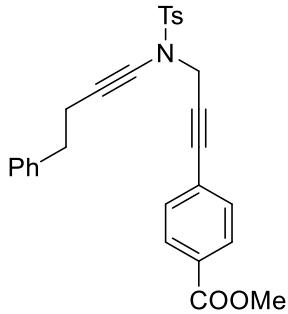
**N-(3-(4-bromophenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1p)**



**1p**

The compound was isolated in 78% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.0$  Hz, 2H), 7.38 (d,  $J = 8.4$  Hz, 2H), 7.27 – 7.15 (m, 7H), 6.98 (d,  $J = 8.4$  Hz, 2H), 4.38 (s, 2H), 2.81 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 7.2$  Hz, 2H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 140.5, 134.4, 133.0, 131.4, 129.4, 128.4, 128.3, 128.1, 126.2, 122.8, 121.0, 85.0, 82.8, 73.5, 70.1, 42.6, 35.1, 21.6, 20.5; IR (neat): 3056, 2989, 2307, 1423, 1266, 897, 742, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{26}\text{H}_{22}\text{BrNNaO}_2\text{S}^+$  514.0447; Found 514.0044.

**methyl 4-((4-methyl-N-(4-phenylbut-1-yn-1-yl)phenyl)sulfonamido)prop-1-yn-1-yl)benzoate (1q)**

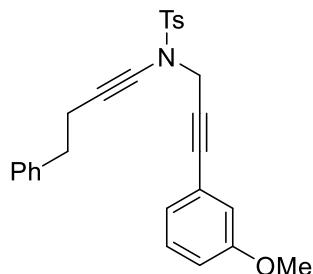


**1q**

The compound was isolated in 60% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 8.4$  Hz, 2H), 7.76 (d,  $J = 8.0$  Hz, 2H), 7.28 – 7.12 (m, 9H), 4.42 (s, 2H), 3.91 (s, 3H), 2.81 (t,  $J = 7.2$  Hz, 2H), 2.60 (t,  $J = 7.2$  Hz, 2H), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.3, 144.5, 140.4, 134.3, 131.5, 129.4, 129.2, 128.4, 128.3, 128.1, 126.7, 126.2, 85.2, 84.5, 73.4, 70.2, 52.2, 42.6, 35.1, 21.5, 20.5;

IR (neat): 3056, 2987, 2307, 1438, 1266, 897, 742, 732, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>25</sub>NNaO<sub>4</sub>S<sup>+</sup> 494.1397; Found 494.1395.

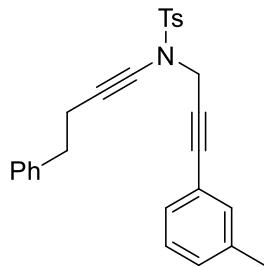
**N-(3-(3-methoxyphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1r)**



**1r**

The compound was isolated in 69% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.24 – 7.13 (m, 8H), 6.87 – 6.82 (m, 1H), 6.76 – 6.66 (m, 2H), 4.40 (s, 2H), 3.76 (s, 3H), 2.81 (t, *J* = 7.2 Hz, 2H), 2.59 (t, *J* = 7.2 Hz, 2H), 2.36 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.1, 144.5, 140.5, 134.4, 129.4, 129.2, 128.4, 128.3, 128.1, 126.2, 124.1, 123.1, 117.0, 114.6, 86.0, 81.3, 73.5, 70.1, 55.2, 42.7, 35.2, 21.5, 20.6; IR (neat): 3056, 2988, 2306, 1423, 1266, 896, 742, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>25</sub>NNaO<sub>3</sub>S<sup>+</sup> 466.1447; Found 466.1445.

**4-methyl-N-(4-phenylbut-1-yn-1-yl)-N-(3-(m-tolyl)prop-2-yn-1-yl)benzenesulfonamide (1s)**

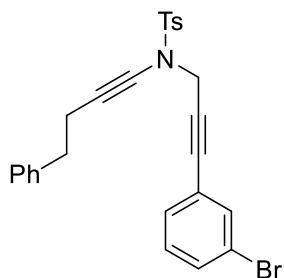


**1s**

The compound was isolated in 80% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.24 – 7.07 (m, 9H), 6.97 – 6.93 (d, *J* = 8.4 Hz, 2H), 4.40 (s, 2H), 2.81 (t, *J* = 7.2 Hz, 2H), 2.59 (t, *J* = 7.2 Hz, 2H), 2.35 (s, 3H), 2.29 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.4, 140.5, 137.7, 134.4, 132.1, 129.4(0), 129.3(6), 128.7, 128.4, 128.3, 128.1, 128.0, 126.1, 121.9, 86.2, 81.1, 73.5,

70.1, 42.7, 35.2, 21.5, 21.2, 20.6; IR (neat): 3056, 2988, 2306, 1423, 1266, 1051, 896, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>25</sub>NNaO<sub>2</sub>S<sup>+</sup> 450.1498; Found 450.1495.

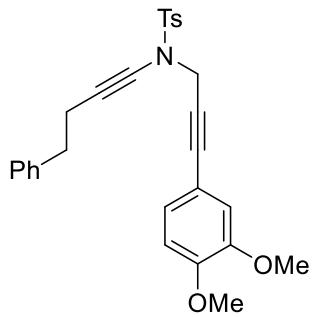
**N-(3-(3-bromophenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1t)**



**1t**

The compound was isolated in 58% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.44 – 7.40 (m, 1H), 7.26 – 7.16 (m, 8H), 7.15 – 7.06 (m, 2H), 4.40 (s, 2H), 2.82 (t, *J* = 7.2 Hz, 2H), 2.61 (t, *J* = 7.2 Hz, 2H), 2.39 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.6, 140.4, 134.4, 131.7, 130.1, 129.6, 129.4, 128.4, 128.3, 128.2, 126.2, 124.0, 121.8, 84.4, 82.9, 73.4, 70.1, 42.6, 35.1, 21.6, 20.5; IR (neat): 3064, 2924, 2256, 1496, 1169, 1090, 1050, 785; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>22</sub>BrNNaO<sub>2</sub>S<sup>+</sup> 514.0447; Found 514.0446.

**N-(3-(3,4-dimethoxyphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1u)**

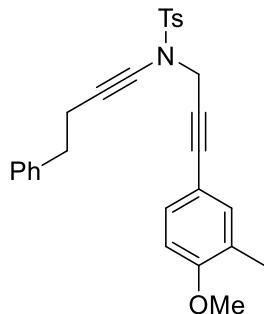


**1u**

The compound was isolated in 52% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.15 (m, 7H), 6.81 – 6.72 (m, 3H), 4.40 (s, 2H), 3.87 (s, 3H), 3.82 (s, 3H), 2.81 (t, *J* = 7.2 Hz, 2H), 2.59 (t, *J* = 7.2 Hz, 2H), 2.36 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 149.7, 148.4, 144.3, 140.5,

134.4, 129.3, 128.4, 128.3, 128.1, 126.2, 125.1, 114.4, 114.3, 110.8, 86.1, 80.0, 73.6, 70.1, 55.9, 42.8, 35.2, 21.6, 20.6; IR (neat): 3056, 2987, 2360, 1365, 1266, 896, 747, 742, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>27</sub>NNaO<sub>4</sub>S<sup>+</sup> 496.1553; Found 496.1550.

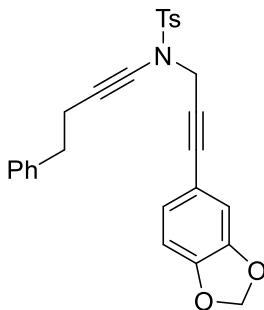
**N-(3-(4-methoxy-3-methylphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1v)**



**1v**

The compound was isolated in 77% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.14 (m, 7H), 7.03 – 6.98 (m, 1H), 6.92 (s, 1H), 6.68 (d, *J* = 8.8 Hz, 1H), 4.39 (s, 2H), 3.81 (s, 3H), 2.80 (t, *J* = 7.2 Hz, 2H), 2.58 (t, *J* = 7.2 Hz, 2H), 2.36 (s, 3H), 2.15 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.0, 144.3, 140.5, 134.5, 133.8, 130.7, 129.4, 128.4, 128.3, 128.1, 126.5, 126.1, 113.6, 109.5, 86.3, 79.6, 73.6, 70.0, 55.3, 42.8, 35.2, 21.6, 20.6, 16.0; IR (neat): 3057, 2927, 2231, 1503, 1266, 814, 742, 737, 704; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>27</sub>NNaO<sub>3</sub>S<sup>+</sup> 480.1604; Found 480.1611.

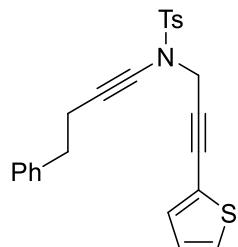
**N-(3-(benzo[d][1,3]dioxol-5-yl)prop-2-yn-1-yl)-4-methyl-N-(4-phenylbut-1-yn-1-yl)benzenesulfonamide (1w)**



**1w**

The compound was isolated in 75% yield according to the general procedure. Yellow solid. M.p = 72 – 73 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J$  = 8.4 Hz, 2H), 7.27 – 7.14 (m, 7H), 6.67 (d,  $J$  = 0.8 Hz, 2H), 6.51 (s, 1H), 5.93 (s, 2H), 4.37 (s, 2H), 2.80 (t,  $J$  = 7.2 Hz, 2H), 2.59 (t,  $J$  = 7.2 Hz, 2H), 2.37 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.0, 147.1, 144.4, 140.5, 134.4, 129.4, 128.4, 128.2, 128.1, 126.2, 126.1, 115.2, 111.6, 108.1, 101.3, 85.9, 79.8, 73.5, 70.0, 42.7, 35.1, 21.5, 20.5; IR (neat): 3057, 2988, 2386, 1599, 1491, 1266, 896, 742, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{23}\text{NNaO}_4\text{S}^+$  480.1240; Found 480.1241.

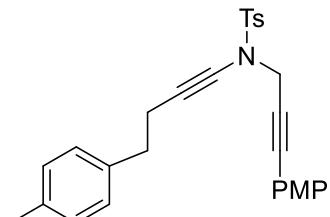
**4-methyl-N-(4-phenylbut-1-yn-1-yl)-N-(3-(thiophen-2-yl)prop-2-yn-1-yl)benzenesulfonamide (1x)**



**1x**

The compound was isolated in 58% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J$  = 8.4 Hz, 2H), 7.28 – 7.14 (m, 8H), 7.00 (d,  $J$  = 2.8 Hz, 1H), 6.94 – 6.89 (m, 1H), 4.42 (s, 2H), 2.81 (t,  $J$  = 7.2 Hz, 2H), 2.59 (t,  $J$  = 7.2 Hz, 2H), 2.38 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 140.5, 134.2, 132.5, 129.5, 128.5, 128.3, 128.1, 127.4, 126.8, 126.2, 122.0, 85.4, 79.4, 73.5, 70.2, 42.8, 35.2, 21.6, 20.6; IR (neat): 3096, 2932, 2307, 1606, 1369, 1249, 834, 728, 700, 672; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{24}\text{H}_{21}\text{NNaO}_2\text{S}_2^+$  442.0906; Found 442.0904.

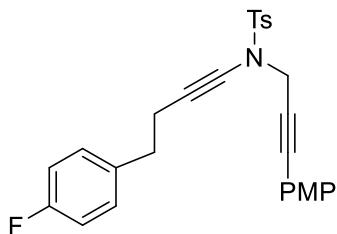
**N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methyl-N-(4-(p-tolyl)but-1-yn-1-yl)benzenesulfonamide (1y)**



**1y**

The compound was isolated in 46% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (d,  $J = 8.4$  Hz, 2H), 7.22 (d,  $J = 8.4$  Hz, 2H), 7.12 – 7.01 (m, 6H), 6.77 (d,  $J = 8.8$  Hz, 2H), 4.40 (s, 2H), 3.79 (s, 3H), 2.80 – 2.74 (t,  $J = 7.2$  Hz, 2H), 2.56 (t,  $J = 7.2$  Hz, 2H), 2.36 (s, 3H), 2.29 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 144.3, 137.5, 135.6, 134.5, 133.1, 129.4, 129.0, 128.3, 128.2, 114.3, 113.7, 86.0, 80.1, 73.5, 70.2, 55.3, 42.8, 34.8, 21.6, 21.0, 20.7; IR (neat): 3056, 2988, 2307, 1511, 1266, 897, 747, 742, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_3\text{S}^+$  480.1604; Found 480.1602.

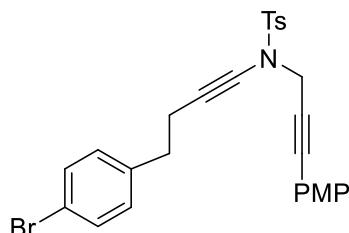
***N*-(4-(4-fluorophenyl)but-1-yn-1-yl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (**1z**)**



**1z**

The compound was isolated in 44% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.4$  Hz, 2H), 7.22 (d,  $J = 8.0$  Hz, 2H), 7.17 – 7.05 (m, 4H), 6.90 – 6.83 (m, 2H), 6.78 (d,  $J = 8.8$  Hz, 2H), 4.39 (s, 2H), 3.80 (s, 3H), 2.76 (t,  $J = 7.2$  Hz, 2H), 2.57 (t,  $J = 7.2$  Hz, 2H), 2.37 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.4 (d,  $J = 242.0$  Hz), 159.8, 144.4, 136.1 (d,  $J = 3.1$  Hz), 134.5, 133.1, 129.9 (d,  $J = 8.0$  Hz), 129.4, 128.1, 115.0 (d,  $J = 21.1$  Hz), 114.1, 113.8, 86.0, 80.0, 73.8, 69.7, 55.3, 42.8, 34.2, 21.5, 20.8;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -117.1; IR (neat): 3053, 2986, 2305, 1421, 1265, 1033, 896, 834, 737; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{27}\text{H}_{24}\text{FNNaO}_3\text{S}^+$  484.1353; Found 484.1345.

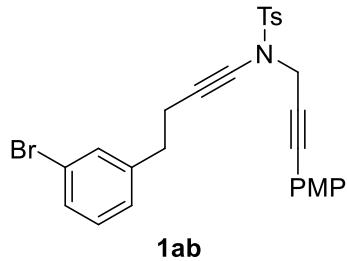
***N*-(4-(4-bromophenyl)but-1-yn-1-yl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (**1aa**)**



### **1aa**

The compound was isolated in 46% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 8.4$  Hz, 2H), 7.29 (d,  $J = 8.0$  Hz, 2H), 7.22 (d,  $J = 8.4$  Hz, 2H), 7.11 – 7.02 (m, 4H), 6.79 (d,  $J = 8.8$  Hz, 2H), 4.39 (s, 2H), 3.80 (s, 3H), 2.74 (t,  $J = 7.2$  Hz, 2H), 2.58 (t,  $J = 7.2$  Hz, 2H), 2.38 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.8, 144.5, 139.4, 134.5, 133.1, 131.3, 130.3, 129.4, 128.1, 120.0, 114.1, 113.8, 86.0, 80.0, 73.9, 69.5, 55.3, 42.8, 34.4, 21.6, 20.4; IR (neat): 3056, 2986, 2256, 1490, 1266, 897, 834, 737, 706; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{27}\text{H}_{24}\text{BrNNaO}_3\text{S}^+$  544.0552; Found 544.0550.

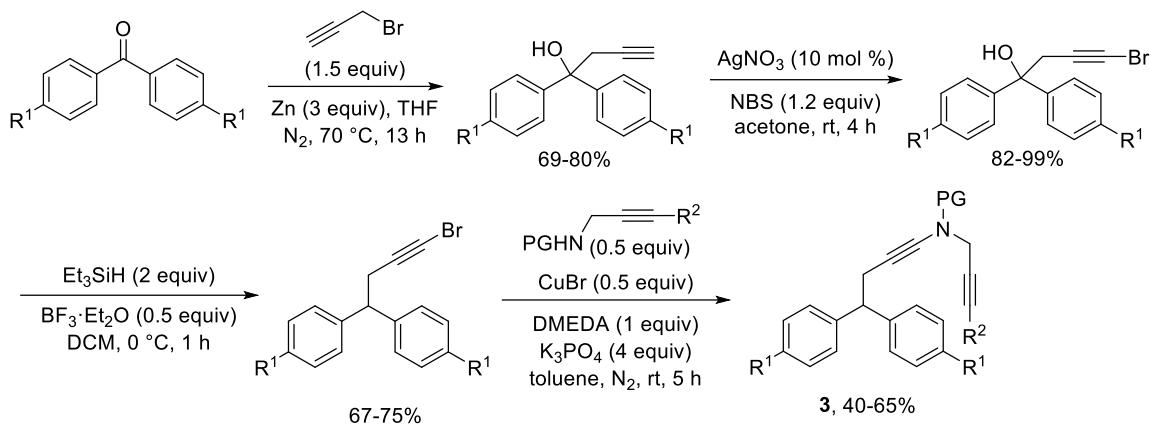
### ***N*-(4-(3-bromophenyl)but-1-yn-1-yl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1ab)**



**1ab**

The compound was isolated in 35% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.4$  Hz, 2H), 7.35 – 7.29 (m, 2H), 7.23 (d,  $J = 8.0$  Hz, 2H), 7.16 – 7.04 (m, 4H), 6.78 (d,  $J = 8.8$  Hz, 2H), 4.39 (s, 2H), 3.80 (s, 3H), 2.77 (t,  $J = 7.2$  Hz, 2H), 2.59 (t,  $J = 6.8$  Hz, 2H), 2.37 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 144.4, 142.8, 134.4, 133.1, 131.5, 129.9, 129.4, 129.3, 128.1, 127.2, 122.3, 114.2, 113.7, 86.1, 80.0, 74.0, 69.5, 55.3, 42.8, 34.7, 21.6, 20.4; IR (neat): 2928, 2836, 2250, 1605, 1566, 1425, 1168, 832, 799, 778, 689, 582, 545; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{27}\text{H}_{24}\text{BrNNaO}_3\text{S}^+$  544.0552; Found 544.0551.

### **General procedure for the preparation of diynes 3:**



Under  $\text{N}_2$  atmosphere, zinc (3.9 g, 60 mmol) was suspended in dry THF (10 mL), and propargyl bromide (2.58 mL, 30 mmol) was added into the mixture dropwise at 0 °C. The reaction mixture was stirred for additional 1 h. Then, a solution of benzophenone derivative (20 mmol) in dry THF (10 mL) was added. The mixture was stirred at 70 °C for 13 h. Upon completion, the reaction was quenched with saturated aqueous  $\text{NH}_4\text{Cl}$  (20 mL). The mixture was then extracted with EtOAc (10 mL) for three times. The combined organic phase was washed with brine, dried over  $\text{MgSO}_4$ , filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography on silica gel (eluent: hexanes/EtOAc) to give the desired propargyl alcohol in 69-80 % yields.

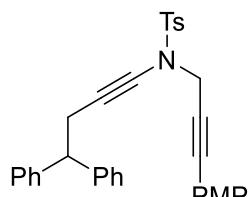
To a solution of propargyl alcohol (10 mmol) in acetone (20 mL) were added NBS (12 mmol, 2.1 g) and  $\text{AgNO}_3$  (1 mmol, 0.17 g) at room temperature. Then, the reaction mixture was stirred at room temperature for 4 h. Upon completion, the mixture was filtered through a pad of celite and concentrated under reduced pressure. The crude alkynyl bromide was used in the next step without further purification (82-99% yields).

To a solution of above alkynyl bromide (3.0 g, 10 mmol) in  $\text{CH}_2\text{Cl}_2$  (10 mL) was added triethylsilane (3.2 mL, 20 mmol) at room temperature. The reaction mixture was cooled to 0 °C before the addition of boron trifluoride diethyl etherate (0.62 mL, 5 mmol). After stirring for 1 h at 0 °C, the reaction was quenched with saturated aqueous  $\text{NaHCO}_3$  (2 mL), extracted with  $\text{CH}_2\text{Cl}_2$ , washed with water, dried over  $\text{Na}_2\text{SO}_4$ , filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography (eluent: hexanes/EtOAc) to afford the desired product in 67-75% yields.

To a solution of the above product (1 mmol) in toluene (6 mL) were added copper bromide (0.5 mmol, 72 mg), DMEDA (1.0 mmol, 0.107 mL),  $\text{K}_3\text{PO}_4$  (4.0 mmol, 0.849 g) and protected propargylamide derivative (0.5 mmol). The reaction was stirred at room temperature for 5 h and the progress of the reaction was monitored by TLC. Upon

completion, the solution was filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: hexanes/EtOAc) to afford the desired diyne **3** in 40-65% yields.

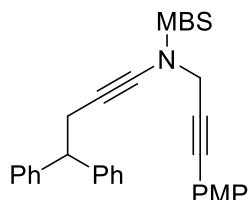
**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3a)**



**3a**

Compound **3a** was prepared in 65% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.4$  Hz, 2H), 7.30 – 7.18 (m, 10H), 7.14 (d,  $J = 8.4$  Hz, 2H), 7.10 – 7.05 (m, 2H), 6.85 – 6.77 (m, 2H). 4.28 (s, 2H), 4.18 (t,  $J = 7.4$  Hz, 1H), 3.77 (s, 3H), 3.00 (d,  $J = 7.6$  Hz, 2H), 2.31 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 144.1, 143.4, 134.4, 133.1, 129.3, 128.3, 127.9(5), 127.9(1), 126.3, 114.1, 113.6, 85.9, 80.0, 74.5, 68.9, 55.2, 50.1, 42.7, 25.3, 21.5; IR (neat): 3027, 2925, 2252, 1508, 1369, 1249, 1169, 1032, 833, 582, 546; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{29}\text{NaO}_3\text{S}^+$  542.1760; Found 542.1754.

**N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4,4-diphenyl-N-((thioxoboraneyl)methyl)but-1-yn-1-amine (3b)**

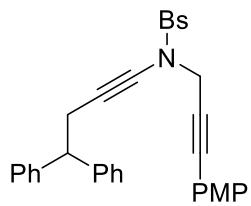


**3b**

Compound **3b** was prepared in 50% yield according to the general procedure. Pale yellow solid. M.p = 108.3 – 108.9 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.56 (m, 2H), 7.27 – 7.13 (m, 10H), 7.08 – 7.03 (m, 2H), 6.80 – 6.71 (m, 4H), 4.29 (s, 2H), 4.19 (t,  $J = 7.5$  Hz, 1H), 3.78 (s, 3H), 3.74 (s, 3H), 3.01 (d,  $J = 7.5$  Hz, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  163.4, 159.7, 143.5, 133.1, 130.2, 129.0, 128.3, 127.9, 126.4, 114.3, 113.9, 113.7, 85.9, 80.1, 74.7, 68.9, 55.4, 55.3, 50.2, 42.6, 25.4; IR (neat): 3027, 2931, 2841, 2254, 1597,

1509, 1363, 1261, 1164, 1031, 832, 701, 583; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NaO<sub>4</sub>S<sup>+</sup> 558.1710; Found 558.1709.

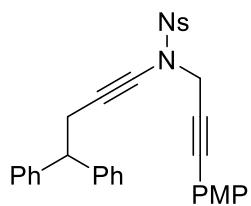
**4-bromo-N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (3c)**



**3c**

Compound **3c** was prepared in 45% yield according to the general procedure. Pale yellow solid. M.p = 90.4 – 91.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.51 – 7.37 (m, 4H), 7.30 – 7.17 (m, 10H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.84 – 6.77 (m, 2H), 4.33 (s, 2H), 4.20 (t, *J* = 7.6 Hz, 1H), 3.82 (s, 3H), 3.02 (d, *J* = 7.6 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.9, 143.4, 136.3, 133.1, 132.0, 129.5, 128.5, 128.4, 127.9, 126.5, 113.9, 86.4, 79.6, 74.0, 69.4, 55.3, 50.2, 43.0, 25.3; IR (neat): 2927, 2219, 2307, 1607, 1510, 1371, 1250, 1173, 1033, 745, 701, 607, 572; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>26</sub>BrNNaO<sub>3</sub>S<sup>+</sup> 606.0709; Found 606.0706.

**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-nitrobenzenesulfonamide (3d)**

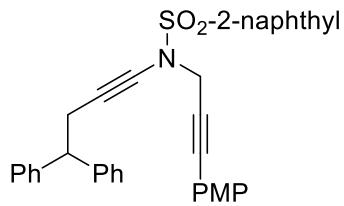


**3d**

Compound **3d** was prepared in 48% yield according to the general procedure. Pale yellow solid. M.p = 114.1 – 115.7 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.01 – 7.98 (m, 2H), 7.74 – 7.71 (m, 2H), 7.30 – 7.17 (m, 10H), 6.98 – 6.95 (m, 2H), 6.77 – 6.73 (m, 2H), 4.37 (s, 2H), 4.21 (t, *J* = 7.5 Hz, 1H), 3.78 (s, 3H), 3.04 (d, *J* = 7.5 Hz, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 160.0, 150.0, 143.2, 142.5, 132.8, 129.1, 128.4, 127.8, 126.5, 123.7, 113.9, 113.3, 86.7, 79.3, 73.4, 69.7, 55.2, 50.1, 43.2, 25.1; IR (neat): 3028, 2932, 2256, 1605,

1510, 1349, 1176, 1032, 834, 701, 572; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>26</sub>N<sub>2</sub>NaO<sub>5</sub>S<sup>+</sup> 573.1455; Found 573.1452.

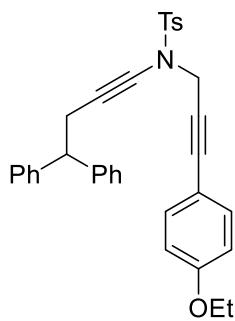
**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)naphthalene-2-sulfonamide (3e)**



**3e**

Compound **3e** was prepared in 42% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.38 (s, 1H), 7.87 – 7.79 (m, 2H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.69 – 7.62 (m, 2H), 7.57 – 7.51 (m, 1H), 7.23 – 7.13 (m, 10H), 6.75 – 6.71 (m, 2H), 6.61 – 6.57 (m, 2H), 4.37 (s, 2H), 4.18 (t, *J* = 7.5 Hz, 1H), 3.75 (s, 3H), 3.01 (d, *J* = 7.0 Hz, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 159.6, 143.4, 135.2, 134.5, 133.0, 131.9, 129.6, 129.5, 128.9, 128.3, 128.0, 127.8, 127.3, 126.4, 123.0, 113.9, 113.5, 86.0, 79.9, 74.5, 69.1, 55.2, 50.1, 42.9, 25.4; IR (neat): 2925, 2230, 1606, 1509, 1249, 1169, 1033, 832, 702, 666, 576, 545; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>36</sub>H<sub>29</sub>NNaO<sub>3</sub>S<sup>+</sup> 578.6812; Found 578.6810.

**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(4-ethoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3f)**

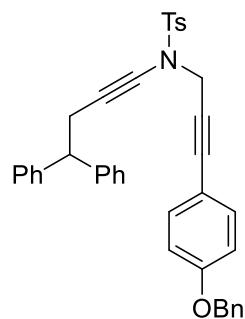


**3f**

Compound **3f** was prepared in 50% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.60 – 7.55 (m, 2H), 7.29 – 7.15 (m, 10H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.08 – 7.00 (m, 2H), 6.79 – 6.73 (m, 2H), 4.29 (s, 2H), 4.19 (t, *J* = 8.0 Hz, 1H), 4.01 (q, *J* = 7.2 Hz 2H), 3.01 (d, *J* = 8.0 Hz, 2H), 2.33 (s, 3H), 1.41 (t, *J* = 7.2 Hz,

3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 144.1, 143.5, 134.4, 133.1, 129.3, 128.3, 128.0(1), 127.9(6), 126.4, 114.2, 114.0, 86.0, 79.9, 74.5, 69.0, 63.5, 50.2, 42.7, 25.4, 21.5, 14.7; IR (neat): 2979, 2923, 2252, 1603, 1508, 1364, 1248, 1044, 812, 738, 701, 546; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{34}\text{H}_{31}\text{NNaO}_3\text{S}^+$  556.1917; Found 556.1716.

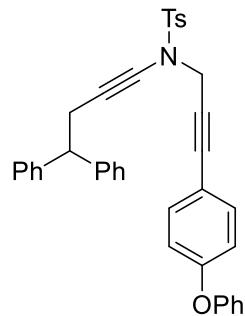
***N*-(3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)-*N*-(4,4-diphenylbut-1-yn-1-yl)-4-methylbenzenesulfonamide (3g)**



**3g**

Compound **3g** was prepared in 59% yield according to the general procedure. Pale yellow solid. M.p = 65 – 65.9 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 – 7.54 (m, 2H), 7.45 – 7.29 (m, 5H), 7.27 – 7.14 (m, 10H), 7.10 (d,  $J$  = 8.0 Hz, 2H), 7.05 – 7.00 (m, 2H), 6.88 – 6.83 (m, 2H), 5.06 (s, 2H), 4.29 (s, 2H), 4.19 (t,  $J$  = 7.2 Hz, 1H), 3.01 (d,  $J$  = 7.6 Hz, 2H), 2.31 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 144.2, 143.5, 136.5, 134.4, 133.1, 129.3, 128.6, 128.3, 128.1, 128.0(3), 127.9(8), 127.4, 126.4, 114.6, 114.5, 85.9, 80.1, 74.5, 70.0, 69.0, 50.2, 42.7, 25.4, 21.5; IR (neat): 3028, 2923, 2258, 1509, 1368, 1244, 1170, 838, 741, 701, 545; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{39}\text{H}_{33}\text{NNaO}_3\text{S}^+$  618.2073; Found 618.2070.

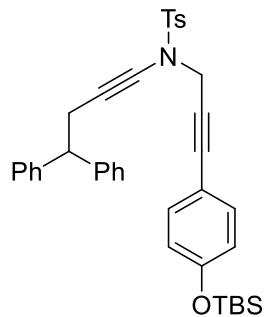
***N*-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-*N*-(3-(4-phenoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (3h)**



### **3h**

Compound **3h** was prepared in 46% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 8.0$  Hz, 2H), 7.36 – 7.31 (m, 2H), 7.25 – 7.07 (m, 13H), 7.06 – 6.97 (m, 4H), 6.87 – 6.84 (m, 2H), 4.29 (s, 2H), 4.19 (t,  $J = 7.5$  Hz, 1H), 3.00 (d,  $J = 7.0$  Hz, 2H), 2.31 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 156.2, 144.2, 143.4, 134.4, 133.2, 129.8, 129.3, 128.3, 128.0, 127.9, 126.4, 123.9, 119.3, 118.0, 116.6, 85.5, 80.8, 74.4, 69.0, 50.1, 42.6, 25.3, 21.5; IR (neat): 3028, 2925, 2257, 1591, 1503, 1369, 1091, 869, 701, 584, 546; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{38}\text{H}_{31}\text{NNaO}_3\text{S}^+$  604.1917; Found 604.1916.

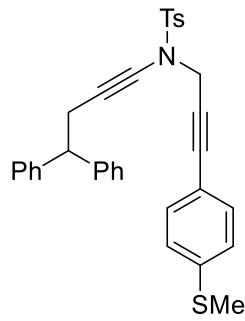
**N-(3-((tert-butyldimethylsilyl)oxy)phenyl)prop-2-yn-1-yl)-N-(4,4-diphenylbut-1-yn-1-yl)-4-methylbenzenesulfonamide (3i)**



**3i**

Compound **3i** was prepared in 41% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 – 7.55 (m, 2H), 7.28 – 7.14 (m, 10H), 7.11 (d,  $J = 8.0$  Hz, 2H), 7.01 – 6.96 (m, 2H), 6.74 – 6.70 (m, 2H), 4.29 (s, 2H), 4.19 (t,  $J = 7.2$  Hz, 1H), 3.01 (d,  $J = 7.2$  Hz, 2H), 2.33 (s, 3H), 0.99 (s, 9H), 0.21 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.1, 144.1, 143.5, 134.4, 133.1, 129.3, 128.3, 128.0, 127.9(7), 126.4, 119.9, 114.9, 86.0, 80.1, 74.5, 69.0, 50.2, 42.7, 25.6, 25.4, 21.5, 18.2, -4.4; IR (neat): 3029, 2859, 2255, 1667, 1603, 1508, 1166, 1091, 783, 581, 545; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{38}\text{H}_{41}\text{NNaO}_3\text{SSi}^+$  642.2469; Found 642.2465.

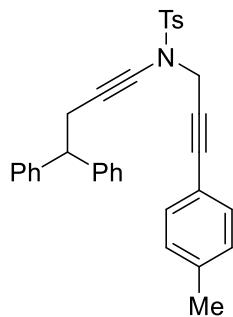
**N-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-N-(3-(4-(methylthio)phenyl)prop-2-yn-1-yl)benzenesulfonamide (3j)**



**3j**

Compound **3j** was prepared in 49% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 – 7.54 (m, 2H), 7.28 – 7.14 (m, 10H), 7.13 – 7.08 (m, 4H), 7.01 – 6.97 (m, 2H), 4.30 (s, 2H), 4.19 (t,  $J = 7.6$  Hz, 1H), 3.01 (d,  $J = 7.2$  Hz, 2H), 2.48 (s, 3H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.2, 143.5, 139.7, 134.4, 131.9, 129.4, 128.4, 128.0, 127.9(8), 126.4, 125.6, 118.4, 85.7, 81.5, 74.5, 69.1, 50.2, 42.7, 25.4, 21.5, 15.3; IR (neat): 3061, 3028, 2923, 2255, 1597, 1493, 1368, 1170, 816, 701, 544; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{33}\text{H}_{29}\text{NNaO}_2\text{S}_2^+$  558.1532; Found 558.1532.

***N*-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-*N*-(3-(p-tolyl)prop-2-yn-1-yl)benzenesulfonamide (**3k**)**

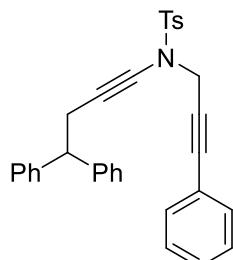


**3k**

Compound **3k** was prepared in 48% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 – 7.54 (m, 2H), 7.26 – 7.15 (m, 10H), 7.10 (d,  $J = 8.4$  Hz, 2H), 7.06 (d,  $J = 8.0$  Hz, 2H), 7.00 – 6.97 (m, 2H), 4.30 (s, 2H), 4.19 (t,  $J = 7.6$  Hz, 1H), 3.01 (d,  $J = 7.6$  Hz, 2H), 2.33 (s, 3H), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.2, 143.5, 138.6, 134.4, 131.5, 129.4, 128.8, 128.3, 128.0, 127.9(7), 126.4, 119.1, 86.1, 80.7, 74.5, 69.0, 50.2, 42.7, 25.4, 21.5, 21.4; IR (neat): 3062, 3028, 2230, 1598,

1495, 1369, 1170, 1091, 759, 701, 594, 546; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NNaO<sub>2</sub>S<sup>+</sup> 526.1811; Found 526.1810.

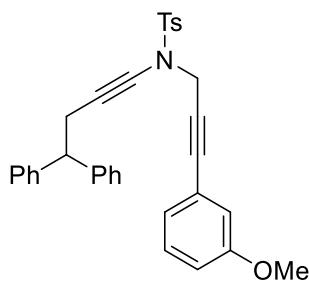
**N-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (3l)**



**3l**

Compound **3l** was prepared in 58% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.58 – 7.52 (m, 2H), 7.27 – 7.11 (m, 13H), 7.09 – 7.02 (m, 4H), 4.30 (s, 2H), 4.19 (t, J = 7.6 Hz, 1H), 3.01 (d, J = 7.6 Hz, 2H), 2.30 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.2, 143.4, 134.3, 131.6, 129.3, 128.4, 128.3, 128.0(2), 127.9(9), 127.9, 126.4, 122.1, 85.9, 81.4, 74.4, 69.0, 50.2, 42.6, 25.3, 21.5; IR (neat): 3059, 3027, 2320, 1597, 1491, 1367, 1169, 1090, 757, 657, 546. HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>27</sub>NNaO<sub>2</sub>S<sup>+</sup> 512.1655; Found 512.1653.

**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(3-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3m)**

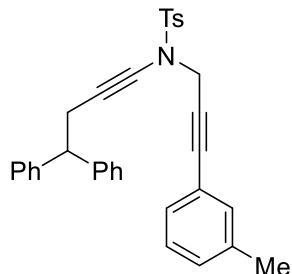


**3m**

Compound **3m** was prepared in 62% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.59 – 7.54 (m, 2H), 7.27 – 7.09 (m, 13H), 6.85 (dd, J = 8.4, 1.6 Hz, 1H), 6.71 – 6.63 (m, 2H), 4.30 (s, 2H), 4.19 (t, J = 7.6 Hz, 1H), 3.76 (s, 3H), 3.01 (d, J = 7.2 Hz, 2H), 2.33 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.1, 144.3, 143.4, 134.3, 129.4, 129.1, 128.3, 128.0, 127.9, 126.4, 124.1, 123.1, 117.1, 114.5, 85.8, 81.2, 74.4, 69.1, 55.2, 50.2, 42.6, 25.4, 21.5; IR (neat): 3063, 3029, 2925, 2256, 1574, 1483,

1320, 1091, 832, 739, 690, 546; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NNaO<sub>3</sub>S<sup>+</sup> 542.1760; Found 542.1758.

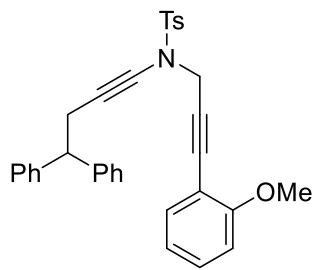
**N-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-N-(3-(m-tolyl)prop-2-yn-1-yl)benzenesulfonamide (3n)**



**3n**

Compound **3n** was prepared in 60% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.08 (m, 14H), 6.93 – 6.88 (m, 2H), 4.31 (s, 2H), 4.20 (t, *J* = 7.2 Hz, 1H), 3.02 (d, *J* = 7.2 Hz, 2H), 2.33 (s, 3H), 2.31 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.2, 143.5, 137.7, 134.4, 132.2, 129.3(9), 129.3(6), 128.8, 128.4, 128.1, 128.0, 126.4, 122.0, 86.1, 81.0, 74.5, 69.0, 50.2, 42.6, 25.4, 21.5, 21.2; IR (neat): 3060, 3028, 2320, 1598, 1451, 1368, 1169, 1050, 813, 738, 546; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NNaO<sub>2</sub>S<sup>+</sup> 526.1811; Found 526.1810.

**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(2-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3o)**

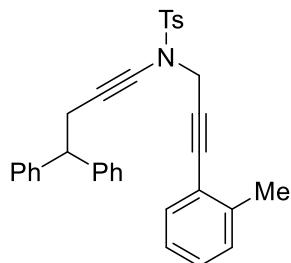


**3o**

Compound **3o** was prepared in 53% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.29 – 7.14 (m, 11H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.91 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.85 – 6.80 (m, 2H), 4.37 (s, 2H), 4.19 (t, *J* = 7.2 Hz, 1H), 3.80 (s, 3H), 3.00 (d, *J* = 7.6 Hz, 2H), 2.31 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.0, 144.1, 143.8, 134.3, 133.9, 129.9, 129.3, 128.3, 128.0, 127.9, 126.4,

120.1, 111.3, 110.5, 85.3, 82.5, 74.4, 69.0, 55.6, 50.2, 42.9, 25.4, 21.5; IR (neat): 3028, 2252, 1597, 1494, 1454, 1263, 1165, 1025, 701, 549; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NNaO<sub>3</sub>S<sup>+</sup> 542.1760; Found 542.1758.

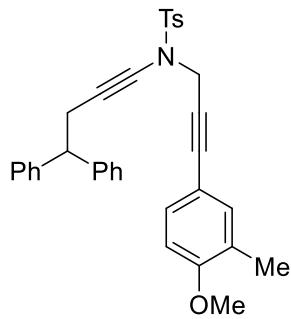
**N-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-N-(3-(*o*-tolyl)prop-2-yn-1-yl)benzenesulfonamide (3p)**



**3p**

Compound **3p** was prepared in 60% yield according to the general procedure. Pale yellow solid. M.p = 59.5 – 60.3 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.54 – 7.51 (m, 2H), 7.27 – 7.16 (m, 11H), 7.14 – 7.11 (m, 1H), 7.08 – 7.04 (m, 4H), 4.35 (s, 2H), 4.19 (t, *J* = 7.6 Hz, 1H), 3.01 (d, *J* = 7.6 Hz, 2H), 2.27 (s, 3H), 2.16 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.3, 143.5, 140.2, 134.3, 132.0, 129.3, 129.2, 128.5, 128.4, 128.0, 127.9, 126.4, 125.3, 122.0, 85.2, 85.0, 74.4, 69.2, 50.3, 42.7, 25.4, 21.5, 20.4; IR (neat): 3063, 2924, 2250, 1596, 1368, 1170, 1049, 813, 701, 594, 546; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NNaO<sub>2</sub>S<sup>+</sup> 526.1811; Found 526.1810.

**N-(4,4-diphenylbut-1-yn-1-yl)-N-(3-(4-methoxy-3-methylphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3q)**

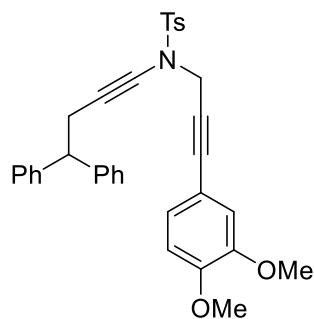


**3q**

Compound **3q** was prepared in 42% yield according to the general procedure. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.26 – 7.14 (m, 10H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.99 – 6.94 (m, 1H), 6.87 (s, 1H), 6.68 (d, *J* = 8.8 Hz, 1H), 4.29 (s, 2H),

4.19 (t, 1H), 3.81 (s, 3H), 3.00 (d,  $J = 7.6$  Hz, 2H), 2.33 (s, 3H), 2.16 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 144.1, 143.5, 134.5, 133.8, 130.7, 129.3, 128.3, 128.0, 127.9, 126.5, 126.3, 113.7, 109.5, 86.2, 79.6, 74.5, 68.9, 55.3, 50.2, 42.7, 25.4, 21.5, 16.0; IR (neat): 3030, 2925, 2253, 1606, 1503, 1368, 1243, 1170, 814, 703, 574, 547; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{34}\text{H}_{31}\text{NNaO}_3\text{S}^+$  556.1917; Found 556.1916.

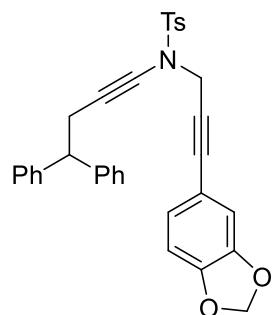
***N*-(3-(3,4-dimethoxyphenyl)prop-2-yn-1-yl)-*N*-(4,4-diphenylbut-1-yn-1-yl)-4-methylbenzenesulfonamide (3r)**



**3r**

Compound **3r** was prepared in 43% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 – 7.56 (m, 2H), 7.29 – 7.11 (m, 12H), 6.76 – 6.68 (m, 3H), 4.31 (s, 2H), 4.19 (t, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.01 (d,  $J = 7.2$  Hz, 2H), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 148.5, 144.1, 143.5, 134.4, 129.3, 128.3, 128.0(3), 127.9(7), 126.4, 125.2, 114.5, 114.4, 110.8, 86.0, 80.0, 74.5, 69.1, 55.9(1), 55.8(9), 50.2, 42.7, 25.4, 21.6; IR (neat): 3061, 3024, 2330, 1598, 1514, 1364, 1244, 1026, 701, 584, 543; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{34}\text{H}_{31}\text{NNaO}_4\text{S}^+$  575.1866; Found 572.1863.

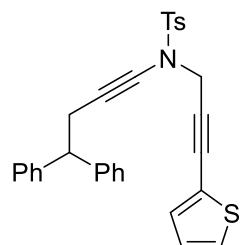
***N*-(3-(benzo[d][1,3]dioxol-5-yl)prop-2-yn-1-yl)-*N*-(4,4-diphenylbut-1-yn-1-yl)-4-methylbenzenesulfonamide (3s)**



**3s**

Compound **3s** was prepared in 40% yield according to the general procedure. White oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 (d,  $J = 8.4$  Hz, 2H), 7.30 – 7.09 (m, 12H), 6.69 – 6.60 (m, 2H), 6.45 (s, 1H), 5.95 (s, 2H), 4.28 (s, 2H), 4.19 (t,  $J = 7.2$  Hz, 1H), 3.01 (d,  $J = 7.6$  Hz, 2H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.0, 147.2, 144.2, 143.4, 134.4, 129.4, 128.3, 128.0(3), 127.9(6), 126.4, 126.2, 115.3, 111.7, 108.2, 101.3, 85.8, 79.7, 74.4, 69.0, 50.2, 42.6, 25.4, 21.5; IR (neat): 3063, 3029, 2922, 2256, 1598, 1444, 1214, 1091, 814, 702, 581, 546; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{27}\text{NNaO}_4\text{S}^+$  556.1553; Found 556.1552.

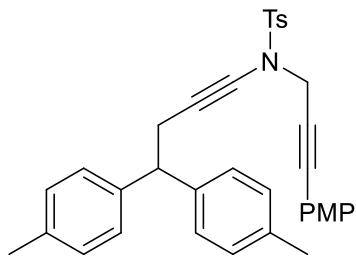
**N-(4,4-diphenylbut-1-yn-1-yl)-4-methyl-N-(3-(thiophen-2-yl)prop-2-yn-1-yl)benzenesulfonamide (3t)**



**3t**

Compound **3t** was prepared in 57% yield according to the general procedure. yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 – 7.53 (m, 2H), 7.28 – 7.11 (m, 13H), 6.98 – 6.90 (m, 2H), 4.32 (s, 2H), 4.20 (t,  $J = 7.6$  Hz, 1H), 3.01 (d,  $J = 7.2$  Hz, 2H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.3, 143.4, 134.2, 132.5, 129.5, 128.3, 128.0, 127.4, 126.8, 126.4, 123.9, 122.0, 85.4, 79.2, 74.4, 69.2, 50.2, 42.7, 25.4, 21.6; IR (neat): 3062, 2924, 2256, 1597, 1495, 1363, 1170, 1039, 813, 701, 546; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{30}\text{H}_{25}\text{NNaO}_2\text{S}_2^+$  518.1219; Found 518.1216.

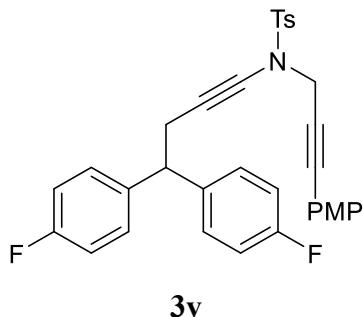
**N-5-(3-chlorophenyl)-11-oxobicyclo[4.4.1]undeca-3,7,9-trien-3-yl)-2,2,2-trifluoroacetamide (3u)**



**3u**

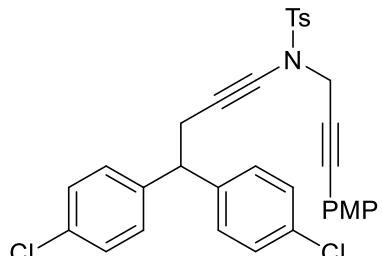
Compound **3u** was prepared in 46% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.56 (m, 2H), 7.14 – 7.09 (m, 6H), 7.08 – 7.02 (m, 6H), 6.81 – 6.75 (m, 2H), 4.30 (s, 2H), 4.13 (t,  $J = 7.2$  Hz, 1H), 3.80 (s, 3H), 2.97 (d,  $J = 7.6$  Hz, 2H), 2.33 (s, 3H), 2.28 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 144.1, 140.8, 135.7, 134.5, 133.1, 129.3, 129.0, 128.1, 127.8, 114.3, 113.7, 85.9, 80.0, 74.3, 69.2, 55.3, 49.4, 42.7, 25.5, 21.5, 21.0; IR (neat): 3050, 2924, 2255, 1606, 1569, 1292, 1092, 833, 737, 585, 545; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{35}\text{H}_{33}\text{NNaO}_3\text{S}^+$  570.2073; Found 570.2072.

**N-(4,4-bis(4-fluorophenyl)but-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3v)**



Compound **3v** was prepared in 51% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 – 7.58 (m, 2H), 7.19 – 7.10 (m, 6H), 7.07 – 7.00 (m, 2H), 6.95 – 6.86 (m, 4H), 6.83 – 6.76 (m, 2H), 4.33 (s, 2H), 4.16 (t,  $J = 7.2$  Hz, 1H), 3.81 (s, 3H), 2.96 (d,  $J = 7.2$  Hz, 2H), 2.37 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.5 (d,  $J = 243.0$  Hz), 159.8, 144.4, 138.9 (d,  $J = 3.0$  Hz), 134.5, 133.1, 129.4 (d,  $J = 8.0$  Hz), 129.3(8), 128.0, 115.1 (d,  $J = 21.0$  Hz), 114.1, 113.8, 86.0, 79.9, 74.9, 68.4, 55.3, 48.5, 42.7, 25.7, 21.5;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -116.2; IR (neat): 2961, 2925, 2256, 1604, 1514, 1364, 1170, 1034, 833, 671, 547. HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{27}\text{F}_2\text{NNaO}_3\text{S}^+$  578.1572; Found 578.1570.

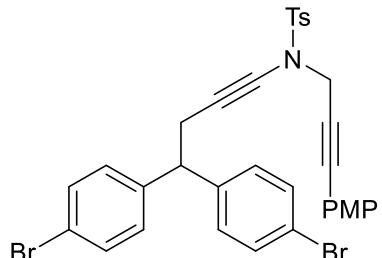
**N-(4,4-bis(4-chlorophenyl)but-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3w)**



**3w**

Compound **3w** was prepared in 54% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 – 7.58 (m, 2H), 7.21 – 7.08 (m, 10H), 7.03 – 6.98 (m, 2H), 6.82 – 6.77 (m, 2H), 4.33 (s, 2H), 4.14 (t,  $J = 7.2$  Hz, 1H), 3.81 (s, 3H), 2.96 (d,  $J = 7.2$  Hz, 2H), 2.38 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.8, 144.5, 141.4, 134.5, 133.1, 132.4, 129.4, 129.3, 128.6, 128.0, 114.0, 113.8, 86.0, 79.9, 75.0, 68.2, 55.3, 48.7, 42.7, 25.3, 21.6; IR (neat): 2926, 2842, 2256, 1604, 1508, 1363, 1170, 1014, 814, 671, 545; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{27}\text{Cl}_2\text{NNaO}_3\text{S}^+$  610.0981; Found 610.0980.

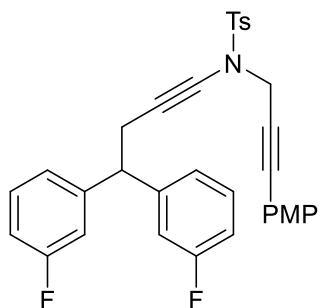
**N-(4,4-bis(4-bromophenyl)but-1-yn-1-yl)-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3x)**



**3x**

Compound **3x** was prepared in 57% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 – 7.57 (m, 2H), 7.36 – 7.30 (m, 4H), 7.16 (d,  $J = 8.0$  Hz, 2H), 7.09 – 6.98 (m, 6H), 6.84 – 6.77 (m, 2H), 4.33 (s, 2H), 4.11 (t,  $J = 7.2$  Hz, 1H), 3.81 (s, 3H), 2.96 (d,  $J = 7.2$  Hz, 2H), 2.39 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.8, 144.5, 141.8, 134.5, 133.1, 131.5, 129.7, 129.5, 127.9, 120.5, 114.0, 113.8, 86.0, 79.9, 75.1, 68.1, 55.3, 48.8, 42.7, 25.1, 21.6; IR (neat): 3052, 2931, 2840, 2256, 1605, 1490, 1405, 1250, 1170, 833, 585, 545; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{27}\text{Br}_2\text{NNaO}_3\text{S}^+$  697.9971; Found 697.9970.

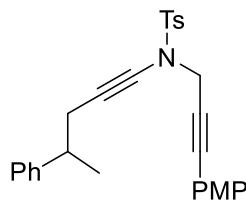
***N*-(4,4-bis(3-fluorophenyl)but-1-yn-1-yl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (3y)**



**3y**

Compound **3y** was prepared in 57% yield. according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.52 (d,  $J = 8.0$  Hz, 2H), 7.31 – 7.20 (m, 2H), 7.17 – 7.09 (m, 6H), 7.02 (d,  $J = 8.8$  Hz, 2H), 6.97 – 6.89 (m, 2H), 6.79 (d,  $J = 8.4$  Hz, 2H), 4.34 (s, 2H), 3.81 (s, 3H), 3.22 (s, 2H), 3.16 – 3.11 (m, 1H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.7 (d,  $J = 244.0$  Hz), 160.0, 147.7 (d,  $J = 7.0$  Hz), 144.8, 134.0, 133.2, 129.8 (d,  $J = 8.0$  Hz), 129.6, 127.9, 121.6 (d,  $J = 3.0$  Hz), 114.3 (d,  $J = 21.0$  Hz), 113.8, 113.7, 113.4 (d,  $J = 22.0$  Hz), 86.4, 79.4, 77.6, 66.2, 55.3, 42.6, 34.1, 33.3, 21.6;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.3, -112.1; IR (neat): 2926, 2854, 2338, 1609, 1510, 1368, 1250, 1170, 1033, 780, 671, 587; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{27}\text{F}_2\text{NNaO}_3\text{S}^+$  578.1572; Found 578.1570.

***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methyl-*N*-(4-phenylpent-1-yn-1-yl)benzenesulfonamide (3z)**



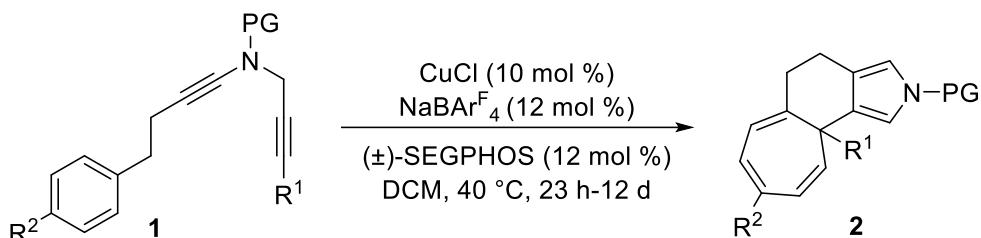
**3z**

The compound was isolated in 46% yield according to the general procedure. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 8.0$  Hz, 2H), 7.26 – 7.15 (m, 7H), 7.08 (d,  $J = 8.8$  Hz, 2H), 6.77 (d,  $J = 8.8$  Hz, 2H), 4.39 (s, 2H), 3.79 (s, 3H), 2.97 – 2.90 (m, 1H), 2.64 – 2.45 (m, 2H), 2.36 (s, 3H), 1.31 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 145.7, 144.4, 134.5, 133.1, 129.4, 128.3, 128.1, 126.9, 126.2, 114.2, 113.7, 86.0, 80.1, 74.1, 69.3, 55.3, 42.8, 39.2, 27.6, 21.6, 20.6. IR (neat): 3028, 2962, 2925, 2252, 1606,

1568, 1495, 1292, 833, 762, 670, 583; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>27</sub>NNaO<sub>3</sub>S<sup>+</sup> 480.1604; Found 480.1602.

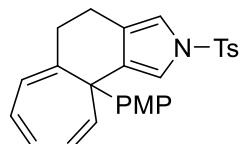
#### 4. General Procedures

##### 4.1 Synthesis of cycloheptatriene fused pyrroles 2



The powdered CuCl (0.02 mmol, 2.0 mg), ( $\pm$ )-SEGPHOS (0.024 mmol, 14.6 mg) and NaBAr<sup>F</sup><sub>4</sub> (0.024 mmol, 21.3 mg) were introduced into an oven-dried Schlenk tube under nitrogen atmosphere. After DCM (1 mL) was injected into the Schlenk tube, the solution was stirred at 40 °C for 0.5 h. Then *N*-propargyl ynamide **1** (0.2 mmol) in DCM (1 mL) was introduced into the system dropwise. The resulting mixture was stirred at 40 °C for 23 h-12 d, and the progress of the reaction was monitored by TLC. Upon completion, the reaction was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (eluent: hexanes/ethyl acetate) to give the cycloheptatriene fused pyrrole **2**.

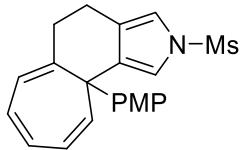
##### **10a-(3-methoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2a)**



**2a**

Compound **2a** was prepared in 95% yield (84.2 mg) according to the general procedure. 23 h. Yellow solid. M.p = 121 – 122 °C. 18 h. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H),, 7.02 – 6.97 (m, 2H), 6.81 (s, 1H), 6.64 – 6.59 (m, 2H), 6.53 (d, *J* = 2.0 Hz, 1H), 6.28 – 6.22 (m, 2H), 6.16 – 6.08 (m, 2H), 4.69 (d, *J* = 8.5 Hz, 1H), 3.73 (s, 3H), 2.75 – 2.57 (m, 3H), 2.45 – 2.33 (m, 4H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.4, 144.5, 136.4, 135.8, 134.7, 129.8, 129.0, 128.0, 127.4, 126.6 125.1, 124.9, 124.2, 117.8, 115.1, 112.2, 106.9, 55.0, 41.3, 33.4, 21.6, 21.5; IR (neat): 3056, 2988, 1734, 1509, 1423, 1174, 896, 742, 737; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>25</sub>NNaO<sub>3</sub>S<sup>+</sup> 466.1447; Found 466.1444.

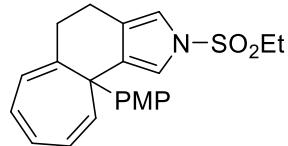
**10a-(3-methoxyphenyl)-2-(methylsulfonyl)-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2b)**



**2b**

Compound **2b** was prepared in 94% yield (69.7 mg) according to the general procedure. 3 d. Yellow solid. M.p = 151 – 153 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.04 (d,  $J$  = 8.5 Hz, 2H), 6.82 (s, 1H), 6.62 (d,  $J$  = 8.5 Hz, 2H), 6.48 (d,  $J$  = 2.0 Hz, 1H), 6.34 – 6.25 (m, 2H), 6.19 – 6.10 (m, 2H), 4.77 (d,  $J$  = 8.5 Hz, 1H), 3.72 (s, 3H), 3.03 (s, 3H), 2.83 – 2.64 (m, 3H), 2.55 – 2.40 (m, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.5, 135.8, 134.6, 129.1, 128.1, 127.4, 125.1, 124.7, 124.2, 117.3, 114.9, 114.8, 112.3, 106.6, 55.0, 42.5, 41.3, 33.5, 21.5; IR (neat): 3054, 2937, 1609, 1443, 1266, 1067, 985, 736, 732; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{21}\text{H}_{21}\text{NNaO}_3\text{S}^+$  390.1134; Found 390.1131.

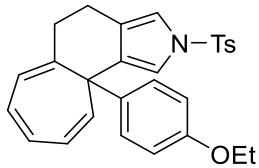
**2-(ethylsulfonyl)-10a-(4-methoxyphenyl)-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2c)**



**2c**

Compound **2c** was prepared in 73% yield (55.3 mg) according to the general procedure. 4 d. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.03 (d,  $J$  = 8.8 Hz, 2H), 6.80 (s, 1H), 6.61 (d,  $J$  = 8.4 Hz, 2H), 6.48 – 6.44 (d,  $J$  = 1.6 Hz, 1H), 6.32 – 6.26 (m, 2H), 6.20 – 6.10 (m, 2H), 4.81 (d,  $J$  = 8.8 Hz, 1H), 3.71 (s, 3H), 3.12 (q,  $J$  = 7.2 Hz, 2H), 2.85 – 2.64 (m, 3H), 2.51 – 2.42 (m, 1H), 1.16 (t,  $J$  = 7.2 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.4, 135.4, 134.8, 128.9, 128.1, 127.5, 125.2, 124.3, 124.1, 117.8, 116.7, 115.3, 112.2, 108.2, 55.0, 49.9, 41.7, 33.6, 21.6, 8.0; IR (neat): 3053, 2986, 1507, 1421, 1162, 896, 740, 736, 705; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{22}\text{H}_{23}\text{NNaO}_3\text{S}^+$  404.1291; Found 404.1290.

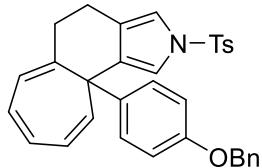
**10a-(4-ethoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2d)**



**2d**

Compound **2d** was prepared in 77% yield (73.0 mg) according to the general procedure. 3 d. Yellow solid. M.p = 118 – 119 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 – 7.58 (d,  $J$  = 8.0 Hz, 2H), 7.22 (d,  $J$  = 8.4 Hz, 2H), 6.98 (d,  $J$  = 8.4 Hz, 2H), 6.80 (s, 1H), 6.59 (d,  $J$  = 8.4 Hz, 2H), 6.53 (d,  $J$  = 2.0 Hz, 1H), 6.27 – 6.21 (m, 2H), 6.16 – 6.00 (m, 2H), 4.68 (d,  $J$  = 8.8 Hz, 1H), 3.94 (q,  $J$  = 7.2 Hz, 2H), 2.75 – 2.57 (m, 3H), 2.44 – 2.36 (m, 4H), 1.36 (t,  $J$  = 7.2 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.9, 144.5, 136.5, 135.9, 134.6, 129.9, 129.1, 128.1, 127.5, 126.7, 125.2, 125.0, 124.3, 117.9, 115.2, 115.1, 112.8, 106.8, 63.2, 41.4, 33.5, 21.7, 21.6, 15.0; IR (neat): 3055, 2988, 1423, 1266, 1064, 896, 748, 743, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_3\text{S}^+$  480.1604; Found 480.1602.

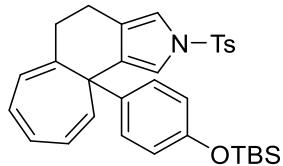
**10a-(4-(benzyloxy)phenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2e)**



**2e**

Compound **2e** was prepared in 89% yield (95.0 mg) according to the general procedure. 27 h. yield Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J$  = 8.4 Hz, 2H), 7.44 – 7.31 (m, 5H), 7.21 (d,  $J$  = 8.0 Hz, 2H), 7.00 (d,  $J$  = 8.8 Hz, 2H), 6.81 (s, 1H), 6.69 (d,  $J$  = 8.4 Hz, 2H), 6.54 (d,  $J$  = 2.0 Hz, 1H), 6.28 – 6.22 (m, 2H), 6.18 – 6.07 (m, 2H), 4.95 (s, 2H), 4.70 (d,  $J$  = 8.8 Hz, 1H), 2.74 – 2.59 (m, 3H), 2.39 – 2.35 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.8, 144.4, 137.2, 136.3, 135.7, 135.0, 129.8, 129.0, 128.5, 128.0, 127.8, 127.6, 127.4, 126.6, 125.1, 124.9, 124.1, 117.7, 115.5, 115.0, 113.1, 107.2, 69.9, 41.4, 33.4, 21.6, 21.5; IR (neat): 3054, 2926, 2306, 1459, 1265, 896, 742, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{29}\text{NNaO}_3\text{S}^+$  542.1760; Found 542.1764.

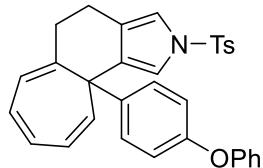
**10a-(4-((tert-butyldimethylsilyl)oxy)phenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2f)**



**2f**

Compound **2f** was prepared in 74% yield (82.0 mg) according to the general procedure. 65 h. yield Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 (d,  $J = 8.4$  Hz, 2H),  $\delta$  7.07 (d,  $J = 8.4$  Hz, 2H), 6.77 (d,  $J = 8.8$  Hz, 2H), 6.66 (s, 1H), 6.41 – 6.36 (m, 3H), 6.12 – 6.06 (m, 2H), 6.00 – 5.90 (m, 2H), 4.57 (d,  $J = 8.4$  Hz, 1H), 2.60 – 2.45 (m, 3H), 2.30 – 2.18 (m, 4H), 0.80 (s, 9H), 0.00 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.3, 144.4, 136.3, 135.8, 135.4, 129.8, 129.0, 128.1, 127.4, 126.6, 125.1, 124.9, 124.1, 118.2, 117.7, 116.4, 115.0, 108.1, 41.7, 33.5, 25.6, 21.6, 21.5, 18.1, -4.4, -4.5; IR (neat): 3056, 2988, 1508, 1266, 1064, 896, 740, 705; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{32}\text{H}_{37}\text{NNaO}_3\text{SSi}^+$  566.2156; Found 566.2147.

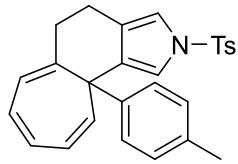
#### **10a-(4-phenoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2g)**



**2g**

Compound **2g** was prepared in 90% yield (94.0 mg) according to the general procedure. 4 d. Yellow solid. M.p = 55 – 57 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 8.0$  Hz, 2H), 7.33 – 7.23 (m, 5H), 7.21 – 7.17 (m, 2H), 7.15 – 7.10 (m, 1H), 7.08 – 7.03 (m, 2H), 6.96 (d,  $J = 7.6$  Hz, 2H), 6.90 (s, 1H), 6.86 – 6.77 (m, 4H), 5.10 (s, 1H), 2.92 – 2.76 (m, 2H), 2.62 – 2.47 (m, 2H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.2, 155.3, 144.7, 141.9, 141.0, 138.7, 136.1, 130.4, 129.9, 129.8, 129.6, 128.6, 127.5, 126.9, 126.8, 126.4, 126.3, 123.1, 119.1, 118.8, 118.7, 118.3, 48.0, 31.1, 25.0, 21.5; IR (neat): 3055, 2988, 1590, 1490, 1371, 1266, 896, 748, 736, 706; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{32}\text{H}_{27}\text{NNaO}_3\text{S}^+$  528.1604; Found 528.1603.

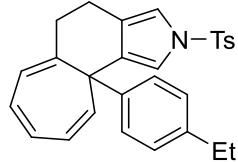
#### **10a-(*p*-tolyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2h)**



**2h**

Compound **2h** was prepared in 68% yield (60.0 mg) according to the general procedure. 5 d. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.4$  Hz, 2H), 7.23 (d,  $J = 8.0$  Hz, 2H), 6.97 (d,  $J = 8.0$  Hz, 2H), 6.86 (d,  $J = 7.6$  Hz, 2H), 6.80 (s, 1H), 6.56 (d,  $J = 2.0$  Hz, 1H), 6.30 – 6.23 (m, 2H), 6.19 – 6.09 (m, 2H), 4.80 (d,  $J = 8.8$  Hz, 1H), 2.77 – 2.60 (m, 3H), 2.41 – 2.37 (m, 4H), 2.23 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 139.8, 136.4, 135.7, 135.1, 129.8, 128.2, 127.8, 127.6, 127.5, 126.6, 125.2, 125.0, 124.0, 117.8, 115.0, 109.9, 42.6, 33.7, 21.6(4), 21.5(9), 21.0; IR (neat): 3055, 2988, 2307, 1422, 1266, 1063, 896, 749, 736, 705; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{25}\text{NNaO}_2\text{S}^+$  450.1498; Found 450.1499.

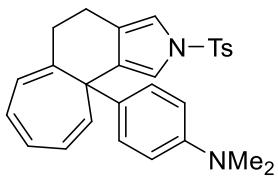
**10a-(4-ethylphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2i)**



**2i**

Compound **2i** was prepared in 75% yield (69.0 mg) according to the general procedure. 7 d. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.4$  Hz, 2H), 7.23 (d,  $J = 8.0$  Hz, 2H), 6.99 (d,  $J = 8.0$  Hz, 2H), 6.89 (d,  $J = 8.0$  Hz, 2H), 6.80 (s, 1H), 6.58 (d,  $J = 2.0$  Hz, 1H), 6.32 – 6.25 (m, 2H), 6.22 – 6.11 (m, 2H), 4.84 (d,  $J = 8.8$  Hz, 1H), 2.80 – 2.62 (m, 3H), 2.55 (q,  $J = 7.6$  Hz, 2H), 2.48 – 2.37 (m, 4H), 1.18 (t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 141.3, 140.2, 136.3, 135.8, 129.8, 128.3, 127.7, 127.6, 126.6, 126.3, 125.2, 125.1, 123.9, 117.9, 115.0, 111.0, 42.9, 33.7, 28.3, 21.7, 21.6, 15.2; IR (neat): 3055, 2988, 1590, 1490, 1371, 1266, 896, 748, 736, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_2\text{S}^+$  464.1655; Found 464.1662.

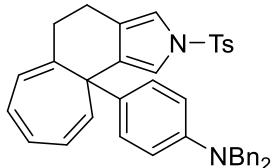
**N,N-dimethyl-4-(2-tosyl-4,5-dihydrocyclohepta[e]isoindol-10a(2H)-yl)aniline (2j)**



**2j**

Compound **2j** was prepared in 65% yield (59.0 mg) according to the general procedure. 4 d. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 (d,  $J = 8.4$  Hz, 2H), 7.23 (d,  $J = 8.4$  Hz, 2H), 6.93 (d,  $J = 8.8$  Hz, 2H), 6.79 (s, 1H), 6.57 (d,  $J = 2.4$  Hz, 1H), 6.46 (d,  $J = 8.8$  Hz, 2H), 6.27 – 6.21 (m, 2H), 6.18 – 6.08 (m, 2H), 4.66 (d,  $J = 8.4$  Hz, 1H), 2.87 (s, 6H), 2.75 – 2.54 (m, 3H), 2.41 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.4, 144.4, 136.4, 136.2, 129.8, 128.7, 127.9, 127.2, 126.6, 125.0, 124.1, 117.7, 115.0, 114.5, 111.2, 106.4, 41.0, 40.6, 33.5, 21.6, 21.5; IR (neat): 3056, 2987, 2307, 1422, 1265, 896, 747, 741, 736; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{28}\text{H}_{28}\text{N}_2\text{NaO}_2\text{S}^+$  479.1764; Found 479.1762.

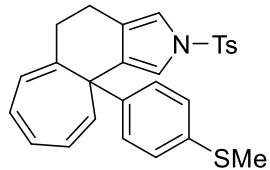
#### N,N-dibenzyl-3-(2-tosyl-4,5-dihydrocyclohepta[e]isoindol-10a(2H)-yl)aniline (**2k**)



**2k**

Compound **2k** was prepared in 71% yield (88.0 mg) according to the general procedure. 48 h. Yellow solid. M.p = 66 – 68 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 8.4$  Hz, 2H), 7.34 – 7.15 (m, 12H), 6.84 (d,  $J = 8.4$  Hz, 2H), 6.78 (s, 1H), 6.59 (d,  $J = 2.0$  Hz, 1H), 6.46 (d,  $J = 8.8$  Hz, 2H), 6.24 – 6.08 (m, 4H), 4.68 (d,  $J = 8.8$  Hz, 1H), 4.54 (s, 4H), 2.71 – 2.55 (m, 3H), 2.39 – 2.35 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.4, 144.3, 139.0, 136.4, 131.1, 129.7, 128.6, 128.5, 128.1, 127.4, 126.9, 126.7, 126.6, 125.2, 125.0, 123.9, 117.9, 117.2, 114.9, 111.3, 108.8, 54.2, 41.7, 33.7, 21.6; IR (neat): 3055, 2987, 1438, 1265, 896, 747, 742, 706; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{40}\text{H}_{36}\text{N}_2\text{NaO}_2\text{S}^+$  631.2390; Found 631.2391.

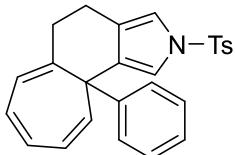
#### 10a-(4-(methylthio)phenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (**2l**)



**2l**

Compound **2l** was prepared in 80% yield (53.0 mg) according to the general procedure. 12 d. Yellow solid. M.p = 121 – 122 °C..  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J$  = 8.0 Hz, 2H), 7.24 (d,  $J$  = 8.0 Hz, 2H), 7.04 – 6.92 (m, 4H), 6.81 (s, 1H), 6.56 (d,  $J$  = 1.2 Hz, 1H), 6.31 – 6.23 (m, 2H), 6.18 – 6.08 (m, 2H), 4.80 (d,  $J$  = 8.8 Hz, 1H), 2.76 – 2.67 (m, 3H), 2.44 – 2.40 (m, 4H), 2.39 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 140.1, 136.3, 135.3, 135.1, 129.8, 128.4, 128.3, 127.6, 126.7, 125.2, 124.9, 124.0, 117.8, 117.8, 115.1, 109.5, 42.4, 33.5, 21.6, 15.8; IR (neat): 3055, 2987, 1422, 1266, 896, 747, 736, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{25}\text{NNaO}_2\text{S}_2^+$  482.1219; Found 482.1216.

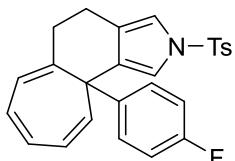
#### **10a-phenyl-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2m)**



**2m**

Compound **2m** was prepared in 78% yield (67.0 mg) according to the general procedure. 4 d. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J$  = 8.4 Hz, 2H), 7.23 (d,  $J$  = 8.4 Hz, 2H), 7.12 – 7.05 (m, 5H), 6.81 (s, 1H), 6.55 (d,  $J$  = 2.4 Hz, 1H), 6.32 – 6.26 (m, 2H), 6.19 – 6.08 (m, 2H), 4.84 (d,  $J$  = 8.8 Hz, 1H), 2.79 – 2.62 (m, 3H), 2.43 – 2.38 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.5, 143.0, 136.3, 135.5, 129.8, 128.3, 127.9, 127.6, 126.8, 126.6, 125.8, 125.2, 125.0, 124.0, 118.7, 117.9, 115.1, 110.4, 43.1, 33.7, 21.6(4), 21.5(8); IR (neat): 3054, 2987, 1422, 1266, 896, 741, 736, 705; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{26}\text{H}_{23}\text{NNaO}_2\text{S}^+$  436.1342; Found 436.1335.

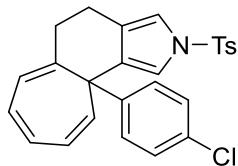
#### **10a-(4-fluorophenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2n)**



## 2n

Compound **2n** was prepared in 77% yield (69.0 mg) according to the general procedure. 54 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.8$  Hz, 2H), 7.22 (d,  $J = 8.0$  Hz, 2H), 7.05 (dd,  $J = 6.0, 5.6$  Hz, 2H), 6.82 (s, 1H), 6.78 – 6.70 (m, 2H), 6.52 (d,  $J = 1.6$  Hz 1H), 6.30 – 6.22 (m, 2H), 6.11 (m, 2H), 4.74 (d,  $J = 8.4$  Hz, 1H), 2.78 – 2.57 (m, 3H), 2.41 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.8 (d,  $J = 243.9$  Hz), 144.6, 138.4 (d,  $J = 3.1$  Hz), 136.2, 135.2, 129.8, 129.4 (d,  $J = 8.0$  Hz), 128.2, 127.5, 126.6, 125.2, 124.7, 124.2, 117.6, 116.0, 115.2, 113.6 (d,  $J = 21.2$  Hz) 107.7, 41.7, 33.3, 21.6, 21.5;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -117.2; IR (neat): 3055, 2988, 1422, 1266, 1064, 896, 739, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{26}\text{H}_{22}\text{FNNaO}_2\text{S}^+$  454.1247; Found 454.1244.

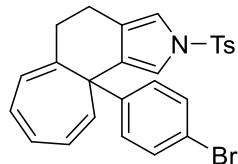
### 10a-(4-chlorophenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (**2o**)



## 2o

Compound **2o** was prepared in 83% yield (76.0 mg) according to the general procedure 29 h. Yellow solid. M.p = 89 – 91 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.4$  Hz, 2H), 7.23 (d,  $J = 8.0$  Hz, 2H), 7.06 – 7.00 (m, 4H), 6.83 (s, 1H), 6.54 (d,  $J = 2.0$  Hz, 1H), 6.31 – 6.24 (m, 2H), 6.18 – 6.10 (m, 2H), 4.82 (d,  $J = 8.8$  Hz, 1H), 2.78 – 2.59 (m, 3H), 2.46 – 2.38 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.6, 141.6, 136.2, 134.9, 131.2, 129.8, 129.2, 128.4, 127.7, 127.0, 126.6, 125.3, 124.8, 124.1, 118.4, 117.7, 115.2, 110.0, 42.5, 33.4, 21.6, 21.5; IR (neat): 3134, 2852, 1599, 1489, 1289, 1064, 814, 704, 673; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{26}\text{H}_{22}\text{ClNNaO}_2\text{S}^+$  470.0952; Found 470.0950.

### 10a-(4-bromophenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (**2p**)

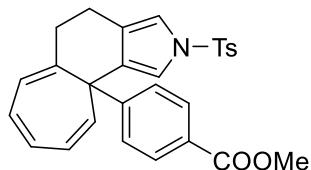


## 2p

Compound **2p** was prepared in 83% yield (94.1 mg) according to the general procedure. 81 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.8$  Hz, 2H), 7.24 (d,  $J =$

8.4 Hz, 2H), 7.17 (d,  $J$  = 8.4 Hz, 2H), 6.97 (d,  $J$  = 8.4 Hz, 2H), 6.82 (s, 1H), 6.55 (d,  $J$  = 2.0 Hz, 1H), 6.32 – 6.24 (m, 2H), 6.19 – 6.09 (m, 2H), 4.83 (d,  $J$  = 8.8 Hz, 1H), 2.78 – 2.61 (m, 3H), 2.41 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.6, 142.2, 136.2, 134.8, 129.9, 129.8, 129.6, 128.5, 127.8, 126.6, 125.3, 124.8, 124.1, 119.4, 118.7, 117.7, 115.2, 110.3, 42.7, 33.5, 21.6, 21.5; IR (neat): 3054, 2987, 1422, 1265, 896, 740, 736, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{26}\text{H}_{22}\text{BrNNaO}_2\text{S}^+$  514.0447; Found 514.0444.

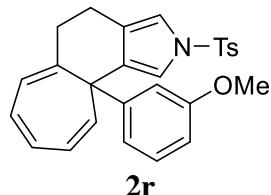
**methyl 4-(2-tosyl-4,5-dihydrocyclohepta[e]isoindol-10a(2H)-yl)benzoate (2q)**



**2q**

Compound **2q** was prepared in 80% yield (77.6 mg) according to the general procedure. 6 d. Yellow solid. M.p = 75 – 77 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J$  = 8.0 Hz, 2H), 7.59 (d,  $J$  = 8.0 Hz, 2H), 7.24 – 7.14 (m, 4H), 6.83 (s, 1H), 6.54 (s, 1H), 6.35 – 6.27 (m, 2H), 6.19 – 6.07 (m, 2H), 4.95 (d,  $J$  = 8.8 Hz, 1H), 3.86 (s, 3H), 2.80 – 2.64 (m, 3H), 2.41 – 2.38 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.0, 148.9, 144.6, 136.1, 134.5, 129.8, 128.6, 128.2, 127.9, 127.7, 126.6, 125.4, 124.8, 124.0, 121.3, 117.7, 115.2, 112.8, 51.9, 43.9, 33.6, 21.7, 21.6; IR (neat): 3055, 2987, 2305, 1720, 1437, 1266, 896, 747, 741, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{28}\text{H}_{25}\text{NNaO}_4\text{S}^+$  494.1397; Found 494.1398.

**10a-(3-methoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2r)**

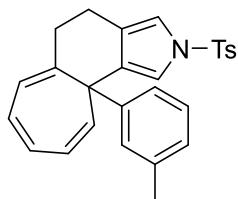


**2r**

Compound **2r** was prepared in 74% yield (68.0 mg) according to the general procedure. 46 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J$  = 8.0 Hz, 2H), 7.22 (d,  $J$  = 8.0 Hz, 2H), 7.00 – 6.97 (m, 1H), 6.81 (s, 1H), 6.73 – 6.56 (m, 4H), 6.29 – 6.27 (m, 2H), 6.20 – 6.17 (m, 2H), 4.92 (d,  $J$  = 8.8 Hz, 1H), 3.71 (s, 3H), 2.79 – 2.61 (m, 3H), 2.41 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 145.0, 144.5, 136.3, 135.4, 129.8,

128.5, 127.8, 127.6, 126.6, 125.3, 125.1, 123.9, 122.3, 120.5, 117.9, 115.0, 114.5, 113.8, 110.3, 55.0, 44.1, 33.9, 21.8, 21.6; IR (neat): 3056, 2988, 1423, 1266, 896, 742, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>25</sub>NNaO<sub>3</sub>S<sup>+</sup> 466.1447; Found 466.1449.

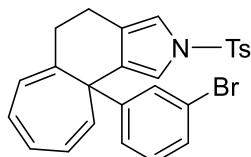
**10a-(m-tolyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2s)**



**2s**

Compound **2s** was prepared in 94% yield (83.0 mg) according to the general procedure. 48 h. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.60 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 6.97 – 6.83 (m, 4H), 6.80 (s, 1H), 6.56 (d, J = 2.0 Hz, 1H), 6.31 – 6.23 (m, 2H), 6.16 – 6.12 (m, 2H), 4.83 (d, J = 8.8 Hz, 1H), 2.78 – 2.60 (m, 3H), 2.41 – 2.37 (m, 4H), 2.21 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.4, 143.0, 136.3, 136.1, 135.7, 129.7, 128.6, 128.2, 127.6, 126.6(1), 126.5(7), 126.5, 125.2, 125.1, 124.9, 124.0, 119.5, 117.9, 115.0, 111.2, 43.2, 33.8, 21.7, 21.6, 21.5; IR (neat): 3055, 2988, 2307, 1422, 1266, 1094, 1064, 896, 749, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>25</sub>NNaO<sub>2</sub>S<sup>+</sup> 450.1498; Found 450.1500.

**10a-(3-bromophenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2t)**

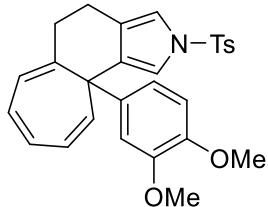


**2t**

Compound **2t** was prepared in 88% yield (89.0 mg) according to the general procedure. 48 h. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.8 Hz, 2H), 7.17 (d, J = 7.6 Hz, 2H), 7.05 (d, J = 8.0 Hz, 1H), 6.95 – 6.91 (m, 1H), 6.82 (s, 1H), 6.56 (d, J = 2.0 Hz, 1H), 6.34 – 6.27 (m, 2H), 6.23 – 6.12 (m, 2H), 4.89 (d, J = 8.8 Hz, 1H), 2.71 (m, 3H), 2.41 – 2.37 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 145.7, 144.6, 136.2, 134.9, 130.8, 129.8, 128.9, 128.7, 128.4, 128.0, 126.7, 126.4, 125.5, 125.0, 124.1, 121.1, 121.0, 117.8, 115.3, 112.5, 43.6, 33.7, 21.7, 21.6; IR (neat): 3054, 2987, 1422, 1265,

1174, 1064, 896, 737, 705; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>22</sub>BrNNaO<sub>2</sub>S<sup>+</sup> 514.0447; Found 514.0444.

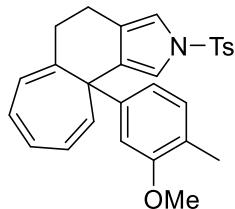
**10a-(3,4-dimethoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2u)**



**2u**

Compound **2u** was prepared in 85% yield (82.4 mg) according to the general procedure. 48 h. Yellow solid. M.p = 145 – 147 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 6.82 (s, 1H), 6.66 – 6.55 (m, 4H), 6.30 – 6.23 (m, 2H), 6.20 – 6.10 (m, 2H), 4.76 (d, *J* = 8.4 Hz, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 2.76 – 2.58 (m, 3H), 2.41 – 2.37 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 147.4, 146.9, 144.5, 136.3, 135.7, 135.4, 129.8, 128.2, 127.5, 126.7, 125.2, 124.9, 124.1, 120.4, 117.7, 116.7, 115.1, 112.0, 109.5, 108.4, 55.8, 55.6, 42.2, 33.5, 21.6(0), 21.5(8); IR (neat): 3056, 2988, 2307, 1514, 1423, 1266, 896, 738, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>27</sub>NNaO<sub>4</sub>S<sup>+</sup> 496.1553; Found 496.1555.

**10a-(3-methoxy-4-methylphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2v)**

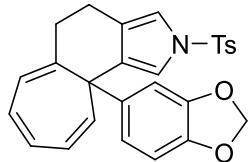


**2v**

Compound **2v** was prepared in 88% yield (83.0 mg) according to the general procedure. 35 h. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 6.87 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.80 (s, 2H), 6.56 – 6.49 (m, 2H), 6.28 – 6.22 (m, 2H), 6.19 – 6.09 (m, 2H), 4.73 (d, *J* = 8.8 Hz, 1H), 3.75 (s, 3H), 2.77 – 2.57 (m, 3H), 2.41 – 2.35 (m, 4H), 2.08 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.6, 144.4, 136.4, 136.1, 134.3, 130.4, 129.7, 128.1, 127.4, 126.6, 126.0, 125.1(1), 125.0(7), 124.6, 124.1, 117.8, 117.1, 115.0, 108.7, 108.1, 55.1, 41.9, 33.7, 21.6(1), 21.5(9), 16.4; IR (neat): 3055,

2987, 1422, 1266, 1064, 896, 747, 742; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>27</sub>NNaO<sub>3</sub>S<sup>+</sup> 480.1604; Found 480.1607.

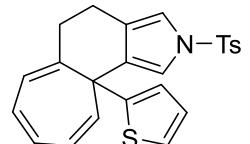
**10a-(benzo[d][1,3]dioxol-5-yl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2w)**



**2w**

Compound **2w** was prepared in 86% yield (84.0 mg) according to the general procedure. 4 d. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.82 (s, 1H), 6.60 – 6.49 (m, 4H), 6.30 – 6.11 (m, 4H), 5.85 (d, *J* = 2.8 Hz, 2H), 4.73 (d, *J* = 8.4 Hz, 1H), 2.76 – 2.58 (m, 3H), 2.41 – 2.37 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 146.2, 145.3, 144.5, 136.8, 136.3, 135.5, 129.8, 128.2, 127.6, 126.7, 125.2, 124.9, 124.2, 121.1, 117.7, 117.0, 115.1, 108.9, 108.7, 106.7, 100.6, 42.3, 33.5, 21.6, 21.5; IR (neat): 3055, 2927, 1437, 1267, 1064, 896, 741, 737, 706; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>23</sub>NNaO<sub>4</sub>S<sup>+</sup> 480.1240; Found 480.1243.

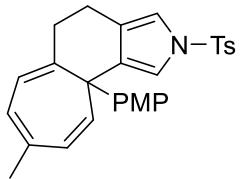
**10a-(thiophen-3-yl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2x)**



**2x**

Compound **2x** was prepared in 76% yield (64.0 mg) according to the general procedure. 4 d. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 6.82 (s, 1H), 6.69 – 6.65 (m, 1H), 6.63 (d, *J* = 2.4 Hz, 1H), 6.36 – 6.24 (m, 4H), 5.16 (d, *J* = 8.8 Hz, 1H), 2.78 – 2.70 (m, 2H), 2.65 – 2.56 (m, 1H), 2.52 – 2.43 (m, 1H), 2.39 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 148.6, 144.6, 136.3, 135.4, 129.8, 129.1, 128.4, 126.6, 125.8, 125.2, 125.1, 124.8, 124.1, 122.1, 119.1, 117.9, 115.0, 41.8, 33.7, 21.9, 21.6; IR (neat): 3055, 2987, 1422, 1265, 1064, 896, 740, 705; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>24</sub>H<sub>21</sub>NNaO<sub>2</sub>S<sub>2</sub><sup>+</sup> 442.0906; Found 442.0905.

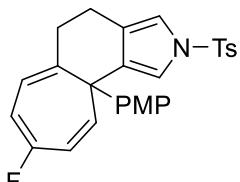
**10a-(4-methoxyphenyl)-8-methyl-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2y)**



**2y**

Compound **2y** was prepared in 49% yield (46.0 mg) according to the general procedure. 3 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 8.0$  Hz, 2H), 7.22 (d,  $J = 8.0$  Hz, 2H), 6.98 (d,  $J = 8.4$  Hz, 2H), 6.80 (s, 1H), 6.61 (d,  $J = 8.4$  Hz, 2H), 6.47 (s, 1H), 6.11 – 6.05 (d,  $J = 7.2$  Hz, 1H), 5.99 (d,  $J = 8.4$  Hz, 1H), 5.81 (d,  $J = 7.2$  Hz, 1H), 4.39 (d,  $J = 8.4$  Hz, 1H), 3.73 (s, 3H), 2.75 – 2.47 (m, 3H), 2.41 – 2.37 (m, 4H), 1.71 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.3, 144.4, 136.4, 135.6, 134.7, 129.7, 129.3, 126.9, 126.6, 125.4, 124.7, 117.7, 115.1, 112.2, 105.2, 98.3, 55.0, 39.0, 32.5, 22.4, 21.5, 21.1; IR (neat): 3054, 2932, 2854, 1609, 1266, 1064, 896, 736, 705, 672; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_3\text{S}^+$  480.1604; Found 480.1600.

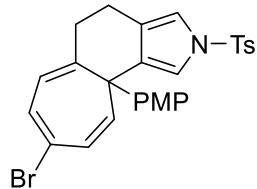
**8-fluoro-10a-(4-methoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2z)**



**2z**

Compound **2z** was prepared in 61% yield (58.0 mg) according to the general procedure. 64 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.0$  Hz, 2H), 7.23 (d,  $J = 8.0$  Hz, 2H), 7.01 (d,  $J = 8.8$  Hz, 2H), 6.81 (s, 1H), 6.62 – 5.58 (m, 3H), 6.25 – 6.21 (m, 2H), 5.93 – 5.89 (m, 1H), 5.16 – 5.12 (m, 1H), 3.73 (s, 3H), 2.80 – 2.61 (m, 3H), 2.41 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.7 (d,  $J = 244.4$  Hz), 157.7, 144.6, 136.2, 135.5 (d,  $J = 24.9$  Hz), 129.8, 128.1, 126.6, 125.1, 121.6 (d,  $J = 10.7$  Hz), 120.3 (d,  $J = 12.5$  Hz), 117.8, 117.0, 116.7, 115.1, 112.5, 111.7 (d,  $J = 26.5$  Hz), 55.0, 44.7, 34.2, 22.1, 21.6;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -107.2; IR (neat): 3054, 2987, 2685, 1422, 1265, 1064, 896, 741, 736, 705; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{24}\text{FNNaO}_3\text{S}^+$  484.1353; Found 484.1350.

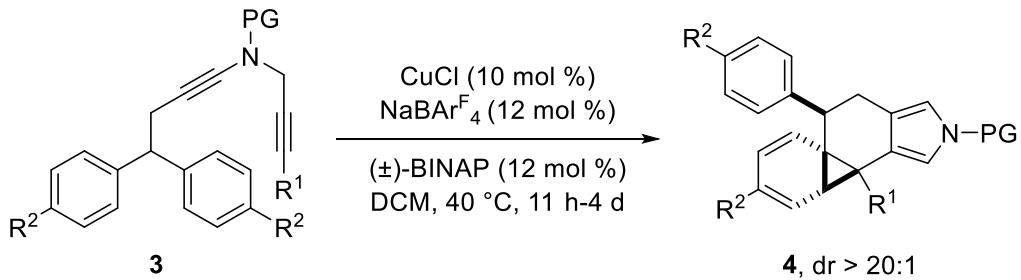
**8-bromo-10a-(4-methoxyphenyl)-2-tosyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole (2aa)**



**2aa**

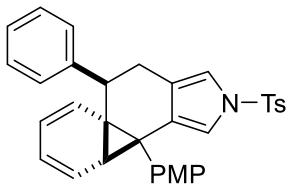
Compound **2aa** was prepared in 63% yield (67.0 mg) according to the general procedure. 48 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.0$  Hz, 2H), 7.23 (d,  $J = 8.0$  Hz, 2H), 6.97 (d,  $J = 8.4$  Hz, 2H), 6.82 (s, 1H), 6.64 (d,  $J = 8.8$  Hz, 2H), 6.51 (d,  $J = 2.0$  Hz, 1H), 6.37 (d,  $J = 8.8$  Hz, 2H), 6.11 (d,  $J = 7.6$  Hz, 1H), 4.73 (d,  $J = 9.6$  Hz, 1H), 3.74 (s, 3H), 2.77 – 2.56 (m, 3H), 2.41 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 144.6, 136.2, 135.0, 134.3, 130.9, 129.8, 128.4, 127.7, 126.7, 124.6, 124.0, 121.4, 121.1, 117.9, 115.2, 112.6, 112.5, 55.1, 42.9, 33.4, 21.6, 21.5; IR (neat): 3054, 2987, 2685, 1422, 1266, 1064, 896, 747, 742, 731, 706; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{27}\text{H}_{24}\text{BrNNaO}_3\text{S}^+$  544.0552; Found 544.0555.

#### 4.2 Synthesis of norcaradiene derived pyrroles 4



The powdered  $\text{CuCl}$  (0.02 mmol, 2.0 mg),  $(\pm)$ -BINAP (0.024 mmol, 14.9 mg) and  $\text{NaBAr}^{\text{F}}_4$  (0.024 mmol, 21.3 mg) were introduced into an oven-dried Schlenk tube. After  $\text{DCM}$  (1 mL) was injected into the Schlenk tube, the solution was stirred at 40 °C for 0.5 h. Then compound **3** (0.2 mmol) in  $\text{DCM}$  (1 mL) was introduced into the system dropwise. The resulting mixture was stirred at 40 °C for 11 h-4 d, and the progress of the reaction was monitored by TLC. Upon completion, the reaction was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (eluent: hexanes/ethyl acetate) to give the norcaradiene derived pyrrole **4**.

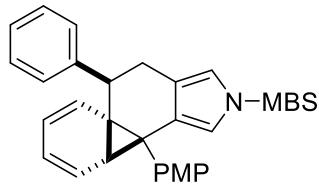
**3b-(4-methoxyphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4a)**



**4a**

Compound **4a** was prepared in 99% yield (103.8 mg) according to the general procedure. 53 h. White solid. M.p = 93.4 – 94.2 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J$  = 8.5 Hz, 2H), 7.28 – 7.10 (m, 7H), 7.05 – 7.00 (m, 2H), 6.84 – 6.82 (m, 1H), 6.72 – 6.67 (m, 2H), 6.37 (d,  $J$  = 2.5 Hz, 1H), 6.23 – 6.18 (m, 1H), 5.83 – 5.79 (m, 1H), 5.68 – 5.63 (m, 2H), 3.76 (s, 3H), 3.65 (dd,  $J$  = 12.0, 4.5 Hz, 1H), 3.50 (d,  $J$  = 8.0 Hz, 1H), 2.77 (dd,  $J$  = 16.0, 5.0 Hz, 1H), 2.43 – 2.33 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.6, 144.8, 144.5, 136.3, 133.6, 131.8, 130.8, 129.8, 128.4, 128.0, 127.8(9), 126.8, 126.5, 125.1, 124.8, 123.9, 122.8, 117.7, 115.5, 112.5, 67.7, 59.1, 55.0, 46.0, 29.5, 27.7, 21.6; IR (neat): 3034, 2933, 1532, 1370, 1246, 1172, 1062, 796, 703, 674, 585, 538; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{29}\text{NNaO}_3\text{S}^+$  558.2073; Found 558.2072.

**3b-(4-methoxyphenyl)-2-((4-methoxyphenyl)sulfonyl)-8-phenyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4b)**

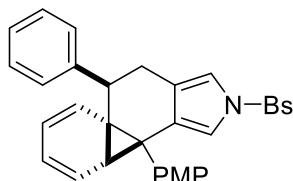


**4b**

Compound **4b** was prepared in 70% yield (77.2 mg) according to the general procedure. 42 h. Pale yellow solid. M.p = 77.7 – 78.4 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 – 7.65 (m, 2H), 7.28 – 7.21 (m, 2H), 7.20 – 7.14 (m, 1H), 7.12 (d,  $J$  = 7.0 Hz, 2H), 7.02 – 6.99 (m, 2H), 6.92 – 6.88 (m, 2H), 6.80 (s, 1H), 6.70 – 6.66 (m, 2H), 6.35 (d,  $J$  = 2.0 Hz, 1H), 6.25 – 6.19 (m, 1H), 5.82 – 5.78 (m, 1H), 5.67 – 5.61 (m, 2H), 3.83 (s, 3H), 3.76 (s, 3H), 3.65 (dd,  $J$  = 12.5, 5.0 Hz, 1H), 3.49 (d,  $J$  = 7.0 Hz, 1H), 2.77 (dd,  $J$  = 15.5, 5.0 Hz, 1H), 2.42 – 2.33 (m, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  163.5, 157.5, 144.9, 133.5, 131.8, 130.8, 130.7, 129.0, 128.4, 127.9(4), 127.8(9), 126.5, 125.1, 124.8, 123.9, 122.7, 117.6,

115.4, 114.3, 112.5, 67.7, 59.1, 55.6, 55.0, 46.0, 29.5, 27.7; IR (neat): 2924, 1574, 1509, 1374, 1176, 1062, 745, 701, 631, 582; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>29</sub>NNaO<sub>4</sub>S<sup>+</sup> 574.2023; Found 574.2022.

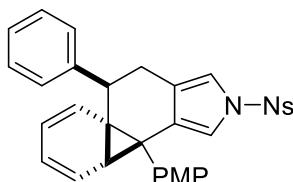
**2-((4-bromophenyl)sulfonyl)-3b-(4-methoxyphenyl)-8-phenyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4c)**



**4c**

Compound **4c** was prepared in 87% yield (104.2 mg) according to the general procedure. 56 h. Pale yellow solid. M.p = 79.3 – 79.6 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.63 – 7.56 (m, 4H), 7.28 – 7.08 (m, 5H), 7.02 – 6.98 (m, 2H), 6.81 (s, 1H), 6.71 – 6.65 (m, 2H), 6.34 (d, *J* = 2.4 Hz, 1H), 6.25 – 6.20 (m, 1H), 5.82 – 5.76 (m, 1H), 5.67 – 5.61 (m, 2H), 3.77 (s, 3H), 3.65 (dd, *J* = 12.0, 4.8 Hz, 1H), 3.48 (d, *J* = 6.8 Hz, 1H), 2.78 (dd, *J* = 15.6, 4.8 Hz, 1H), 2.43 – 2.31 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.6, 144.7, 138.1, 134.4, 132.5, 131.9, 130.6, 128.7, 128.5, 128.2, 127.9(4), 127.9(0), 126.5, 125.2, 124.9, 123.9, 123.4, 117.7, 115.6, 112.6, 66.8, 58.3, 55.0, 45.8, 29.4, 27.5; IR (neat): 3034, 2925, 2853, 2183, 1656, 1510, 1375, 1176, 745, 583; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>26</sub>BrNNaO<sub>3</sub>S<sup>+</sup> 622.1022; Found 622.1020.

**3b-(4-methoxyphenyl)-2-((4-nitrophenyl)sulfonyl)-8-phenyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4d)**

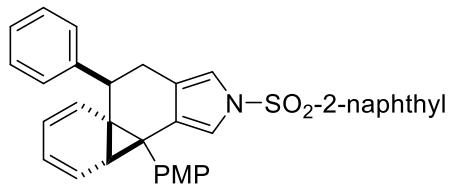


**4d**

Compound **4d** was prepared in 72% yield (83.8 mg) according to the general procedure. 56 h. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 – 8.36 (m, 2H), 8.02 – 7.96 (m, 2H), 7.37 – 7.26 (m, 3H), 7.23 – 7.18 (m, 2H), 7.12 – 7.06 (m, 2H), 6.92 (s, 1H), 6.81 – 6.75 (m, 2H), 6.44 (d, *J* = 2.4 Hz, 1H), 6.35 – 6.28 (m, 1H), 5.94 – 5.87 (m, 1H), 5.79 – 5.69 (m, 2H), 3.86 (s, 3H), 3.72 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.54 (d, *J* = 6.8 Hz, 1H), 2.87

(dd,  $J = 15.6, 4.8$  Hz, 1H), 2.52 – 2.42 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 150.5, 144.5, 135.4, 131.9, 130.4, 128.5, 128.0, 127.9, 126.6, 125.3, 125.0, 124.5, 124.3, 123.8, 117.8, 115.8, 112.6, 57.6, 55.1, 45.7, 29.3, 27.3, 15.9; IR (neat): 2956, 2925, 2854, 1609, 1533, 1350, 1250, 1181, 1060, 741, 701; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{32}\text{H}_{26}\text{NNaO}_5\text{S}^+$  605.2081; Found 605.2080.

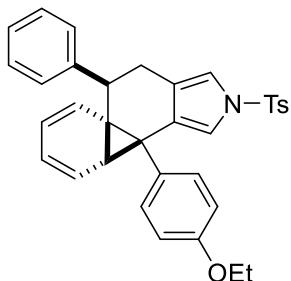
**3b-(4-methoxyphenyl)-2-(naphthalen-2-yl)-8-phenyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4e)**



**4e**

Compound **4e** was prepared in 82% yield (93.7 mg) according to the general procedure. 54 h. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.36 (s, 1H), 7.95 – 7.85 (m, 3H), 7.70 – 7.58 (m, 3H), 7.28 – 7.22 (m, 2H), 7.20 – 7.16 (m, 1H), 7.12 (d,  $J = 7.0$  Hz, 2H), 7.04 – 7.01 (m, 2H), 6.91 (s, 1H), 6.73 – 6.69 (m, 2H), 6.46 (d,  $J = 2.5$  Hz, 1H), 6.25 – 6.19 (m, 1H), 5.84 – 5.79 (m, 1H), 5.68 – 5.62 (m, 2H), 3.76 (s, 3H), 3.63 (dd,  $J = 12.5, 5.0$  Hz, 1H), 3.48 (d,  $J = 6.5$  Hz, 1H), 2.76 (dd,  $J = 16.0, 5.0$  Hz, 1H), 2.43 – 2.33 (m, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.6, 144.8, 136.0, 135.1, 133.9, 132.0, 131.9, 130.7, 129.6, 129.4, 129.3, 128.4, 128.3, 127.9(2), 127.8(9), 127.7, 126.5, 125.1, 124.8, 123.9, 123.0, 121.7, 117.9, 115.7, 112.5, 66.9, 58.3, 55.0, 45.9, 29.4, 27.5; IR (neat): 2925, 1510, 1365, 1245, 1174, 1061, 737, 641, 578; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{36}\text{H}_{29}\text{NNaO}_3\text{S}^+$  594.2073; Found 594.2071.

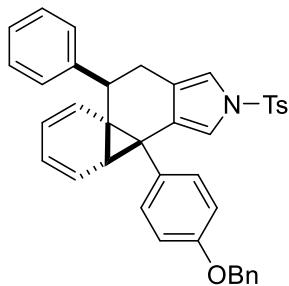
**3b-(4-ethoxyphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4f)**



**4f**

Compound **4f** was prepared in 79% yield (86.8 mg) according to the general procedure. **4d**. White solid. M.p = 156.7 – 157.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.66 – 7.62 (m, 2H), 7.28 – 7.10 (m, 7H), 7.03 – 6.99 (m, 2H), 6.84 – 6.81 (m, 1H), 6.71 – 6.66 (m, 2H), 6.37 (d, *J* = 2.0 Hz, 1H), 6.25 – 6.19 (m, 1H), 5.84 – 5.78 (m, 1H), 5.69 – 5.60 (m, 2H), 3.98 (q, *J* = 7.2 Hz, 2H), 3.65 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.50 (d, *J* = 6.8 Hz, 1H), 2.77 (dd, *J* = 15.6, 4.8 Hz, 1H), 2.43 – 2.34 (m, 4H), 1.39 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.0, 144.9, 144.5, 136.3, 133.7, 131.8, 130.6, 129.8, 128.4, 128.0, 127.9, 126.8, 126.5, 125.1, 124.9, 123.9, 122.8, 117.8, 115.5, 113.0, 67.9, 63.1, 59.3, 46.0, 29.5, 27.8, 21.6, 14.9; IR (neat): 3033, 2979, 2927, 1609, 1509, 1369, 1243, 1171, 1061, 702, 674, 586; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>35</sub>H<sub>35</sub>NNaO<sub>3</sub>S<sup>+</sup> 572.2230; Found 572.2229.

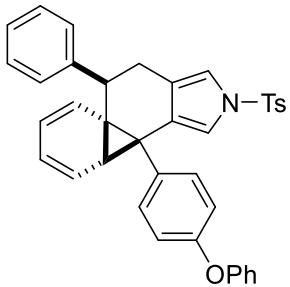
### **3b-(4-(benzyloxy)phenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4g)**



**4g**

Compound **4g** was prepared in 87% yield (106.3 mg) according to the general procedure. 96 h. Yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.67 – 7.62 (m, 2H), 7.46 – 7.18 (m, 10H), 7.16 – 7.12 (m, 2H), 7.06 – 7.01 (m, 2H), 6.85 – 6.76 (m, 3H), 6.39 (d, *J* = 2.4 Hz, 1H), 6.25 – 6.19 (m, 1H), 5.88 – 5.81 (m, 1H), 5.72 – 5.63 (m, 2H), 5.00 (s, 2H), 3.66 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.52 (d, *J* = 6.8 Hz, 1H), 2.78 (dd, *J* = 15.6, 4.8 Hz, 1H), 2.44 – 2.34 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 157.0, 144.8, 144.5, 137.2, 136.3, 133.6, 131.8, 131.2, 129.9, 129.8, 128.5, 128.4, 128.0, 127.9, 127.8, 127.7, 126.8, 126.5, 125.2, 124.9, 123.9, 122.8, 117.8, 115.5, 113.4, 70.0, 59.9, 46.0, 29.5, 28.0, 21.6; IR (neat): 2925, 2855, 1603, 1508, 1351, 1164, 1093, 832, 737, 701. HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>40</sub>H<sub>37</sub>NNaO<sub>3</sub>S<sup>+</sup> 634.2386; Found 634.2385.

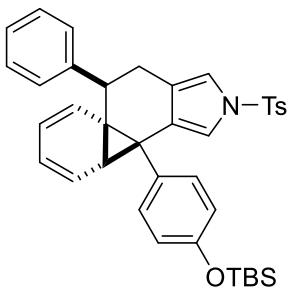
### **3b-(4-phenoxyphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4h)**



**4h**

Compound **4h** was prepared in 83% yield (99.1 mg) according to the general procedure. 56 h. Pale yellow solid. M.p = 123.8 – 125.3 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 – 7.64 (m, 2H), 7.35 – 7.31 (m, 2H), 7.29 – 7.24 (m, 4H), 7.22 – 7.18 (m, 1H), 7.15 – 7.12 (m, 2H), 7.10 – 7.05 (m, 3H), 7.02 – 6.98 (m, 2H), 6.85 – 6.83 (m, 1H), 6.81 – 6.77 (m, 2H), 6.42 (d,  $J$  = 2.0 Hz, 1H), 6.26 – 6.20 (m, 1H), 5.89 – 5.80 (m, 1H), 5.73 – 5.63 (m, 2H), 3.67 (dd,  $J$  = 12.5, 5.0 Hz, 1H), 3.57 (d,  $J$  = 7.0 Hz, 1H), 2.79 (dd,  $J$  = 15.5, 5.0 Hz, 1H), 2.44 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.2, 155.2, 144.7, 144.6, 136.3, 133.6, 133.3, 132.0, 129.8, 129.6, 128.5, 128.0, 127.8, 126.8, 126.5, 125.3, 125.1, 123.9, 123.1, 122.8, 118.9, 117.7, 117.3, 115.6, 70.0, 61.2, 46.1, 29.5, 28.5, 21.6; IR (neat): 3035, 2923, 1590, 1504, 1489, 1237, 1172, 1061, 673, 584; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{39}\text{H}_{35}\text{NNaO}_3\text{S}^+$  620.2230; Found 620.2228.

**3b-((tert-butyldimethylsilyl)oxy)phenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4i)**

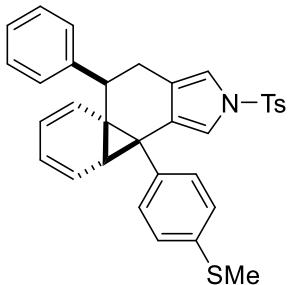


**4i**

Compound **4i** was prepared in 80% yield (101.6 mg) according to the general procedure. 11 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 – 7.61 (m, 2H), 7.29 – 7.11 (m, 7H), 6.98 – 6.92 (m, 2H), 6.84 – 6.81 (m, 1H), 6.64 – 6.60 (m, 2H), 6.37 (d,  $J$  = 2.4 Hz, 1H), 6.25 – 6.19 (m, 1H), 5.83 – 5.77 (m, 1H), 5.67 – 5.60 (m, 2H), 3.65 (dd,  $J$  = 12.4, 5.2 Hz, 1H), 3.54 (d,  $J$  = 6.8 Hz, 1H), 2.77 (dd,  $J$  = 15.6, 4.8 Hz, 1H), 2.45 – 2.33 (m, 4H), 0.97 (s, 9H), 0.18 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.6, 144.9, 144.5, 136.3,

133.7, 131.7, 131.6, 129.8, 128.4, 128.0, 127.8, 126.8, 126.5, 125.2, 125.0, 123.9, 122.8, 118.6, 117.8, 115.5, 69.6, 60.9, 46.1, 29.5, 28.4, 25.7, 21.6, 18.2, -4.3(7), -4.3(9); IR (neat): 2931, 2858, 1604, 1508, 1255, 1173, 1062, 840, 781, 702, 585, 538; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>39</sub>H<sub>45</sub>NNaO<sub>3</sub>SSi<sup>+</sup> 658.2782; Found 658.2781.

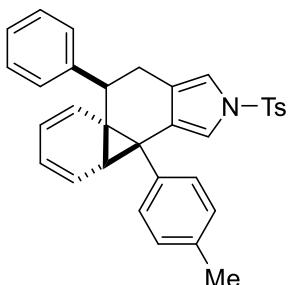
**3b-(4-(methylthio)phenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4j)**



**4j**

Compound **4j** was prepared in 78% yield (86.0 mg) according to the general procedure 48 h. Pale yellow solid. M.p = 88.8 – 90.2 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.72 – 7.67 (m, 2H), 7.35 – 7.15 (m, 7H), 7.11 – 7.02 (m, 4H), 6.83 (s, 1H), 6.38 (d, *J* = 2.4 Hz, 1H), 6.25 – 6.20 (m, 1H), 5.90 – 5.85 (m, 1H), 5.76 – 5.68 (m, 2H), 3.67 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.59 (d, *J* = 7.2 Hz, 1H), 2.78 (dd, *J* = 15.6, 4.8 Hz, 1H), 2.52 – 2.39 (m, 7H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.7, 144.5, 136.3, 135.8, 135.6, 133.2, 131.1, 129.8, 128.5, 128.0, 127.7, 126.8, 126.5, 125.4, 125.3, 125.2, 123.9, 122.8, 117.7, 115.6, 71.1, 62.3, 46.2, 29.5, 29.0, 21.6, 15.7; IR (neat): 3029, 2923, 2855, 1597, 1494, 1369, 1171, 1062, 812, 674, 585, 538; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>34</sub>H<sub>33</sub>NNaO<sub>2</sub>S<sub>2</sub><sup>+</sup> 574.1845; Found 574.1842.

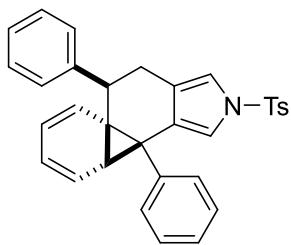
**8-phenyl-3b-(*p*-tolyl)-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4k)**



**4k**

Compound **4k** was prepared in 65% yield (67.5 mg) according to the general procedure. 3 d. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 – 7.61 (m, 2H), 7.31 – 7.12 (m, 7H), 7.01 – 6.93 (m, 4H), 6.84 – 6.80 (m, 1H), 6.37 (d,  $J$  = 2.4 Hz, 1H), 6.25 – 6.20 (t,  $J$  = 7.6 Hz, 1H), 5.86 – 5.79 (m, 1H), 5.71 – 5.63 (m, 2H), 3.68 (dd,  $J$  = 12.4, 5.2 Hz, 1H), 3.58 (d,  $J$  = 6.8 Hz, 1H), 2.78 (dd,  $J$  = 15.6, 5.2 Hz, 1H), 2.45 – 2.36 (m, 4H), 2.28 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.8, 144.5, 136.4, 135.8, 135.4, 133.6, 130.5, 129.8, 128.4, 128.0, 127.8(3), 127.7(9), 126.8, 126.5, 125.2, 125.0, 124.0, 123.0, 117.9, 115.5, 71.0, 62.2, 46.2, 29.6, 29.1, 21.6, 21.2; IR (neat): 2949, 2925, 2856, 1453, 1369, 1172, 1061, 811, 674, 585; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{34}\text{H}_{33}\text{NNaO}_2\text{S}^+$  542.2124; Found 542.2122.

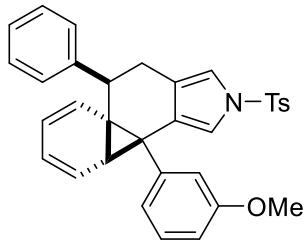
**3b,8-diphenyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4l)**



**4l**

Compound **4l** was prepared in 85% yield (85.9 mg) according to the general procedure. 96 h. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 – 7.60 (m, 2H), 7.31 – 7.09 (m, 12H), 6.85 – 6.81 (m, 1H), 6.36 (d,  $J$  = 2.0 Hz, 1H), 6.26 – 6.20 (m, 1H), 5.85 – 5.80 (m, 1H), 5.67 (d,  $J$  = 4.5 Hz, 2H), 3.69 (dd,  $J$  = 12.0, 5.0 Hz, 1H), 3.64 (d,  $J$  = 7.0 Hz, 1H), 2.80 (dd,  $J$  = 15.5, 4.5 Hz, 1H), 2.46 – 2.38 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  144.7, 144.5, 139.0, 136.3, 133.4, 130.6, 129.8, 128.4, 128.0, 127.8, 127.0, 126.8, 126.5, 126.1, 125.3, 125.1, 124.0, 123.0, 117.8, 115.5, 72.1, 63.2, 46.3, 29.7, 29.6, 21.6; IR (neat): 3029, 2926, 1737, 1597, 1445, 1369, 1171, 1061, 812, 752, 674, 586, 524; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{33}\text{H}_{31}\text{NNaO}_2\text{S}^+$  528.1968; Found 528.1967.

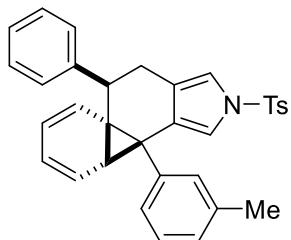
**3b-(3-methoxyphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4m)**



**4m**

Compound **4m** was prepared in 79% yield (84.6 mg) according to the general procedure. 89 h. Pale yellow solid. M.p = 171.5 – 172.2 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 – 7.58 (m, 2H), 7.28 – 7.20 (m, 4H), 7.20 – 7.10 (m, 4H), 7.01 – 6.98 (m, 1H), 6.81 – 6.72 (m, 3H), 6.36 (s, 1H), 6.20 – 6.14 (m, 1H), 5.67 – 5.64 (m, 1H), 5.54 (d,  $J$  = 9.6 Hz, 1H), 5.45 – 5.35 (m, 1H), 3.68 – 3.52 (m, 4H), 2.86 (d,  $J$  = 6.0 Hz, 1H), 2.71 (dd,  $J$  = 16.0, 5.2 Hz, 1H), 2.38 (s, 3H), 2.31 – 2.20 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 145.5, 144.3, 136.5, 133.7, 129.7, 128.4, 128.0, 127.9, 126.7, 126.3, 124.6, 122.6, 119.0, 117.2, 115.6, 111.2, 55.2, 44.0, 36.9, 29.7, 29.1, 21.6, 18.7; IR (neat): 3039, 2931, 1596, 1494, 1369, 1172, 1062, 741, 675, 585; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{34}\text{H}_{33}\text{NNaO}_3\text{S}^+$  558.2073; Found 558.2072.

**8-phenyl-3b-(*m*-tolyl)-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (**4n**)**

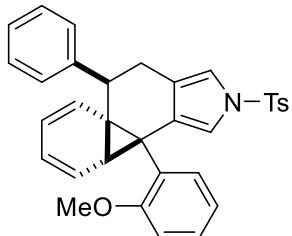


**4n**

Compound **4n** was prepared in 82% yield (85.1 mg) according to the general procedure. 65 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 – 7.59 (m, 2H), 7.27 – 7.09 (m, 9H), 7.04 – 6.99 (m, 1H), 6.94 – 6.86 (m, 3H), 6.82 – 6.79 (m, 1H), 6.37 (d,  $J$  = 2.4 Hz, 1H), 6.25 – 6.19 (m, 1H), 5.84 – 5.79 (m, 1H), 5.69 – 5.63 (m, 2H), 3.69 (dd,  $J$  = 12.4, 4.9 Hz, 1H), 3.63 (d,  $J$  = 7.2 Hz, 1H), 2.79 (dd,  $J$  = 15.6, 5.2 Hz, 1H), 2.44 – 2.33 (m, 4H), 2.26 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.8, 144.5, 138.9, 136.4, 136.3, 133.6, 131.3, 129.8, 128.4, 128.0, 127.7, 127.6, 126.9, 126.8, 126.7, 126.5, 125.3, 125.0, 124.0, 123.0, 117.9, 115.5, 72.5, 63.7, 46.3, 29.8, 29.6, 21.6, 21.4; IR (neat): 3027, 2921, 2852,

1598, 1449, 1352, 1163, 1092, 701, 544; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>34</sub>H<sub>33</sub>NNaO<sub>2</sub>S<sup>+</sup> 542.2124; Found 542.2123.

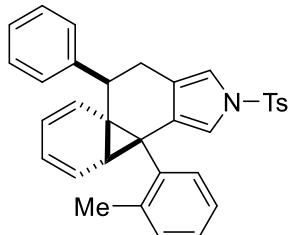
**3b-(2-methoxyphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4o)**



**4o**

Compound **4o** was prepared in 85% yield (91.0 mg) according to the general procedure. 56 h. White solid. M.p = 72.7 – 74.1 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.62 (d, *J* = 7.0 Hz, 2H), 7.28 – 7.22 (m, 4H), 7.19 – 7.12 (m, 4H), 7.02 (s, 1H), 6.83 – 6.71 (m, 3H), 6.37 (s, 1H), 6.22 – 6.14 (m, 1H), 5.67 (s, 1H), 5.55 (d, *J* = 9.5 Hz, 1H), 5.40 (s, 1H), 3.67 – 3.52 (m, 4H), 2.87 (d, *J* = 6.5 Hz, 1H), 2.72 (dd, *J* = 16.0, 5.5 Hz, 1H), 2.39 (s, 3H), 2.27 (t, *J* = 13.0 Hz, 1H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.2, 145.4, 144.3, 136.5, 133.6, 132.0, 129.7, 129.3, 129.0, 128.3, 128.0, 127.9, 126.7, 126.3, 124.5, 123.8, 122.6, 121.5, 119.0, 117.1, 115.6, 111.1, 55.2, 44.5, 44.0, 36.8, 29.0, 21.5, 18.7; IR (neat): 3032, 2929, 1598, 1492, 1428, 1369, 1285, 1172, 1062, 737, 701, 584; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>34</sub>H<sub>33</sub>NNaO<sub>3</sub>S<sup>+</sup> 558.2073; Found 558.2072.

**8-phenyl-3b-(*o*-tolyl)-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4p)**

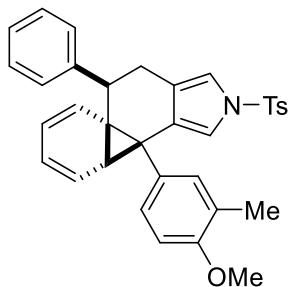


**4p**

Compound **4p** was prepared in 83% yield (83.5 mg) according to the general procedure. 70 h. White solid. M.p = 172.0 – 172.6 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.22 (m, 4H), 7.14 – 6.96 (m, 7H), 6.82 (s, 1H), 6.34 – 6.25 (m, 2H), 5.75 – 5.70 (m, 1H), 5.59 (d, *J* = 9.5 Hz, 1H), 5.47 – 5.42 (m, 1H), 3.47 (dd, *J* = 12.5, 5.0 Hz,

1H), 2.88 (d,  $J$  = 6.0 Hz, 1H), 2.73 (dd,  $J$  = 15.5, 5.0 Hz, 1H), 2.39 (s, 3H), 2.28 (t,  $J$  = 13.0 Hz, 1H), 1.97 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  144.9, 144.4, 138.0, 136.2, 134.4, 133.0, 131.5, 130.6, 129.7, 128.4, 127.7, 127.1, 126.8, 126.6, 126.5, 124.0(3), 123.9(6), 123.5, 122.7, 122.4, 117.6, 115.9, 43.8, 42.7, 34.4, 28.9, 21.6, 20.8, 19.6; IR (neat): 3033, 2923, 1493, 1369, 1173, 1093, 1061, 750, 675, 614, 585; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{33}\text{H}_{29}\text{NNaO}_2\text{S}^+$  526.1811; Found 526.1810.

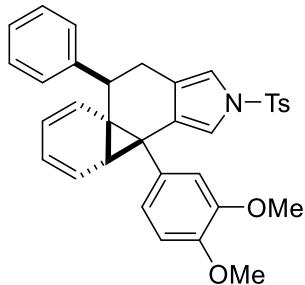
**3b-(4-methoxy-3-methylphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4q)**



**4q**

Compound **4q** was prepared in 72% yield (79.1 mg) according to the general procedure. 56 h. Pale yellow solid. M.p = 97 – 98.3 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J$  = 8.5 Hz, 2H), 7.29 – 7.18 (m, 5H), 7.15 – 7.11 (m, 2H), 6.89 (dd,  $J$  = 8.5, 2.5 Hz, 1H), 6.85 – 6.80 (m, 2H), 6.60 (d,  $J$  = 8.5 Hz, 1H), 6.38 (d,  $J$  = 2.0 Hz, 1H), 6.22 (t,  $J$  = 8.0 Hz, 1H), 5.82 (t,  $J$  = 7.0 Hz, 1H), 5.69 – 5.61 (m, 2H), 3.78 (s, 3H), 3.66 (dd,  $J$  = 12.5, 5.0 Hz, 1H), 3.50 (d,  $J$  = 7.0 Hz, 1H), 2.77 (dd,  $J$  = 15.5, 5.0 Hz, 1H), 2.43 – 2.36 (m, 4H), 2.12 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 144.9, 144.5, 136.3, 133.9, 133.0, 130.3, 129.8, 128.9, 128.4, 128.0, 127.9, 126.7, 126.4, 125.1, 124.9, 124.8, 123.9, 122.9, 117.9, 115.5, 108.4, 68.8, 60.2, 55.0, 46.1, 29.5, 28.1, 21.6, 16.3; IR (neat): 2926, 2855, 1597, 1503, 1369, 1243, 1172, 1061, 810, 674, 585; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{35}\text{H}_{35}\text{NNaO}_3\text{S}^+$  572.2230; Found 572.2229.

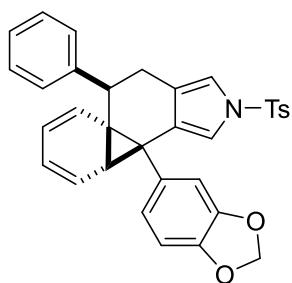
**3b-(3,4-dimethoxyphenyl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4r)**



**4r**

Compound **4r** was prepared in 80% yield (90.4 mg) according to the general procedure. 58 h. Pale yellow solid. M.p = 72.6 – 73.9 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J$  = 8.5 Hz, 2H), 7.26 – 7.23 (m, 4H), 7.21 – 7.17 (m, 1H), 7.15 – 7.12 (m, 2H), 6.85 – 6.81 (m, 1H), 6.68 – 6.58 (m, 3H), 6.41 (d,  $J$  = 2.5 Hz, 1H), 6.26 – 6.19 (m, 1H), 5.85 – 5.81 (m, 1H), 5.70 – 5.61 (m, 2H), 3.83 (s, 3H), 3.77 (s, 3H), 3.67 (dd,  $J$  = 12.5, 5.0 Hz, 1H), 3.53 (d,  $J$  = 7.0 Hz, 1H), 2.78 (dd,  $J$  = 15.5, 5.0 Hz, 1H), 2.43 – 2.36 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  147.5, 147.0, 144.7, 144.5, 136.2, 133.5, 131.2, 129.8, 128.4, 127.9, 127.8, 126.7, 126.4, 125.2, 124.9, 123.8, 123.3, 122.7, 117.6, 115.5, 114.4, 109.8, 68.1, 59.5, 55.8, 55.6, 45.9, 29.4, 28.2, 21.5; IR (neat): 3031, 2932, 2856, 1598, 1369, 1188, 1093, 812, 737, 675, 584; HRMS (ESI/QTOF) m/z: [M + Na] $^+$  Calcd for  $\text{C}_{35}\text{H}_{35}\text{NNaO}_4\text{S}^+$  588.2179; Found 588.2178.

**3b-(benzo[d][1,3]dioxol-5-yl)-8-phenyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4s)**

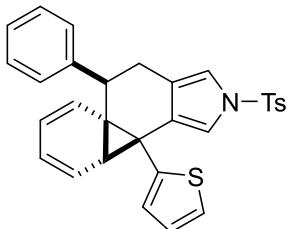


**4s**

Compound **4s** was prepared in 87% yield (95.5 mg) according to the general procedure. 55 h. Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 – 7.64 (m, 2H), 7.28 – 7.10 (m, 7H), 6.84 – 6.82 (m, 1H), 6.64 – 6.55 (m, 3H), 6.44 (d,  $J$  = 2.0 Hz, 1H), 6.25 – 6.20 (m, 1H), 5.94 – 5.84 (m, 3H), 5.74 – 5.62 (m, 2H), 3.65 (dd,  $J$  = 12.4, 4.8 Hz, 1H), 3.56 (d,  $J$  = 6.8 Hz, 1H), 2.78 (dd,  $J$  = 15.6, 4.8 Hz, 1H), 2.46 – 2.34 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.2, 145.5, 144.7, 144.5, 136.3, 133.4, 132.6, 129.8, 128.4, 127.9, 127.7,

126.8, 126.5, 125.4, 125.1, 124.0, 123.8, 122.8, 117.7, 115.5, 111.3, 107.1, 100.7, 70.9, 62.1, 46.1, 29.5, 29.0, 21.6; IR (neat): 2925, 1490, 1369, 1226, 1061, 1040, 812, 702, 674, 585. HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>34</sub>H<sub>31</sub>NNaO<sub>4</sub>S<sup>+</sup> 572.1866; Found 572.1865.

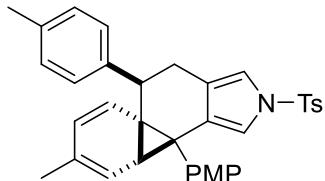
**8-phenyl-3b-(thiophen-2-yl)-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4t)**



**4t**

Compound **4t** was prepared in 87% yield (88.9 mg) according to the general procedure. 50 h. Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.67 – 7.63 (m, 2H), 7.29 – 7.22 (m, 4H), 7.22 – 7.16 (m, 1H), 7.13 – 7.09 (m, 2H), 7.02 (dd, *J* = 4.8, 1.2 Hz, 1H), 6.85 – 6.82 (m, 1H), 6.77 – 6.74 (m, 1H), 6.69 – 6.65 (m, 2H), 6.25 – 6.20 (m, 1H), 6.10 – 6.00 (m, 1H), 5.92 – 5.85 (m, 1H), 5.67 (d, *J* = 8.4 Hz, 1H), 4.05 (d, *J* = 7.2 Hz, 1H), 3.75 (dd, *J* = 12.0, 4.8 Hz, 1H), 2.83 (dd, *J* = 15.2, 4.8 Hz, 1H), 2.53 – 2.38 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 144.6, 144.3, 143.3, 136.3, 133.5, 129.8, 128.4, 128.2, 128.0, 127.5, 126.7, 126.6, 126.5, 126.3, 124.8, 124.1, 123.2, 123.0, 117.9, 115.6, 85.9, 46.5, 29.5, 28.2, 21.6; IR (neat): 3029, 2926, 2855, 1733, 1597, 1453, 1266, 1171, 1018, 814, 674, 586. HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>31</sub>H<sub>29</sub>NNaO<sub>2</sub>S<sup>+</sup> 534.1532; Found 534.1531.

**3b-(4-methoxyphenyl)-5-methyl-8-(*p*-tolyl)-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4u)**

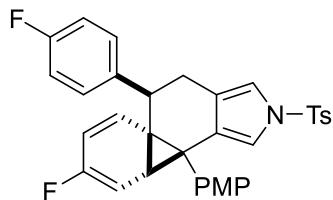


**4u**

Compound **4u** was prepared in 50% yield (54.7 mg) according to the general procedure. 40 h. yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.65 – 7.61 (m, 2H), 7.27 – 7.23 (m, 3H),

7.09 – 6.97 (m, 5H), 6.81 – 6.78 (m, 1H), 6.72 – 6.66 (m, 2H), 6.34 (d,  $J$  = 2.4 Hz, 1H), 5.90 (d,  $J$  = 6.8 Hz, 1H), 5.56 (d,  $J$  = 9.6 Hz, 1H), 5.43 (d,  $J$  = 9.2 Hz, 1H), 3.77 (s, 3H), 3.56 (dd,  $J$  = 12.4, 4.8 Hz, 1H), 3.27 (d,  $J$  = 6.8 Hz, 1H), 2.72 (dd,  $J$  = 15.6, 5.2 Hz, 1H), 2.40 (s, 3H), 2.32 – 2.28 (s, 4H), 1.56 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.5, 144.4, 142.1, 136.4, 135.9, 133.8, 133.0, 132.1, 131.0, 129.8, 129.1, 128.3, 127.8, 127.0, 126.8, 122.9, 120.4, 117.6, 115.4, 112.4, 60.8, 55.1, 53.3, 45.0, 29.6, 26.5, 21.6, 21.4, 21.0; IR (neat): 3023, 2926, 2858, 1597, 1514, 1369, 1172, 1062, 814, 672, 539. HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{35}\text{H}_{33}\text{NNaO}_3\text{S}^+$  570.2073; Found 570.2072.

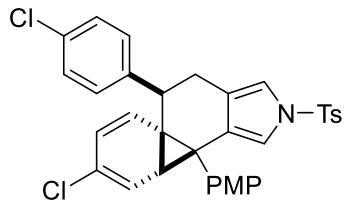
**5-fluoro-8-(4-fluorophenyl)-3b-(4-methoxyphenyl)-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4v)**



**4v**

Compound **4v** was prepared in 98% yield (108.8 mg) according to the general procedure. 40 h. Pale yellow solid. M.p = 92.2 – 93.5 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 – 7.61 (m, 2H), 7.27 – 7.23 (m, 2H), 7.10 – 7.01 (m, 4H), 6.99 – 6.92 (m, 2H), 6.84 (s, 1H), 6.72 – 6.67 (m, 2H), 6.43 (d,  $J$  = 2.4 Hz, 1H), 5.97 – 5.91 (m, 1H), 5.75 – 5.70 (m, 1H), 5.65 – 5.58 (m, 1H), 4.03 – 3.97 (m, 1H), 3.78 – 3.67 (m, 4H), 2.81 (dd,  $J$  = 15.6, 4.8 Hz, 1H), 2.47 – 2.37 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.6 (d,  $J$  = 243.0 Hz), 159.2 (d,  $J$  = 233.0 Hz), 157.9, 144.6, 139.9 (d,  $J$  = 3.0 Hz), 136.2, 133.6, 131.5, 130.5, 129.8, 129.4 (d,  $J$  = 8.0 Hz), 128.4 (d,  $J$  = 10.0 Hz), 126.7, 122.8, 117.9, 115.6 (d,  $J$  = 5.0 Hz), 115.4 (d,  $J$  = 21.0 Hz), 115.3, 112.8, 108.3 (d,  $J$  = 27.0 Hz), 85.5, 55.0, 46.2, 33.4, 29.9, 21.6;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -116.1, -112.6; IR (neat): 2921, 2858, 1369, 1248, 1172, 1062, 825, 672, 540; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for  $\text{C}_{33}\text{H}_{27}\text{F}_2\text{NNaO}_3\text{S}^+$  578.1572; Found 578.1571.

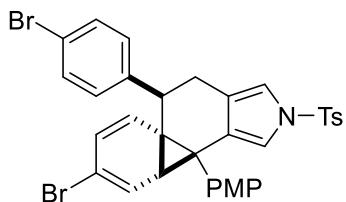
**5-chloro-8-(4-chlorophenyl)-3b-(4-methoxyphenyl)-2-tosyl-3b,3c,8,9-tetrahydro-2*H*-benzo[2,3]cyclopropa[1,2-*e*]isoindole (4w)**



**4w**

Compound **4w** was prepared in 57% yield (74.0 mg) according to the general procedure. 65 h. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J = 8.5$  Hz, 2H), 7.27 – 7.22 (m, 4H), 7.05 (d,  $J = 8.5$  Hz, 2H), 6.99 (d,  $J = 9.0$  Hz, 2H), 6.83 (s, 1H), 6.72 (d,  $J = 9.0$  Hz, 2H), 6.39 (d,  $J = 2.5$  Hz 1H), 6.23 (d,  $J = 7.5$  Hz, 1H), 5.66 – 5.62 (m, 2H), 3.78 (s, 3H), 3.66 – 3.58 (m, 2H), 2.77 (dd,  $J = 15.5$  Hz, 1H), 2.42 – 2.31 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 144.7, 142.7, 136.2, 132.7, 132.5, 131.2, 130.4, 130.1, 129.8, 129.2, 129.1, 128.8, 126.8, 126.6, 122.2, 121.8, 118.1, 115.7, 112.9, 65.2, 55.1, 45.5, 31.5, 30.5, 22.6, 21.6; IR (neat): 3285, 2203, 1704, 1532, 1491, 1322, 1184, 1093, 830, 527; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{34}\text{H}_{31}\text{Cl}_2\text{NNaO}_3\text{S}^+$  627.1924; Found 627.1923.

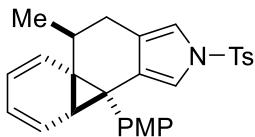
**5-bromo-8-(4-bromophenyl)-3b-(4-methoxyphenyl)-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4x)**



**4x**

Compound **4x** was prepared in 88% yield (110.6 mg) according to the general procedure. 55 h. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 (d,  $J = 8.0$  Hz, 2H), 7.39 (d,  $J = 8.5$  Hz, 2H), 7.26 (d,  $J = 7.5$  Hz, 2H), 7.02 – 6.95 (m, 4H), 6.83 (s, 1H), 6.72 (d,  $J = 8.5$  Hz, 2H), 6.43 – 6.37 (m, 2H), 5.84 (d,  $J = 9.0$  Hz, 1H), 5.57 (d,  $J = 9.0$  Hz, 1H), 3.78 (s, 3H), 3.67 – 3.59 (m, 2H), 2.78 (dd,  $J = 15.5$  Hz, 1H), 2.42 – 2.31 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  157.9, 144.7, 143.1, 136.1, 132.6, 131.7, 131.0, 130.4, 129.8, 129.6, 129.1, 128.9, 126.8, 125.2, 122.2, 120.5, 118.9, 118.0, 115.7, 112.8, 68.1, 55.1, 45.7, 31.0, 29.3, 21.6; IR (neat): 3051, 2932, 2837, 1609, 1489, 1369, 1248, 1171, 1062, 816, 738, 676, 538; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{34}\text{H}_{31}\text{Br}_2\text{NNaO}_3\text{S}^+$  714.0284; Found 714.0284.

**3b-(4-methoxyphenyl)-8-methyl-2-tosyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (4z)**

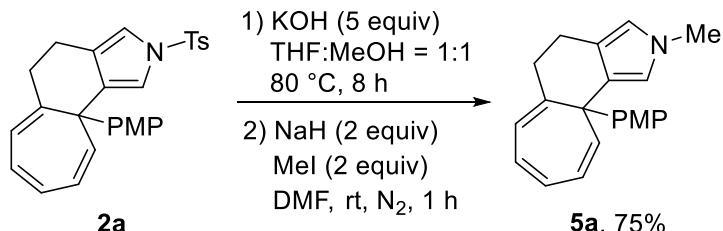


**4z**

Compound **4z** was prepared in 94% yield (86.0 mg) according to the general procedure. 48 h. Pale yellow oil.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 8.5$  Hz, 2H), 7.22 (d,  $J = 8.0$  Hz, 2H), 6.97 (d,  $J = 8.5$  Hz, 2H), 6.80 – 6.76 (m, 1H), 6.64 (d,  $J = 8.5$  Hz, 2H), 6.44 (d,  $J = 2.0$  Hz, 1H), 6.19 – 6.13 (m, 1H), 6.06 (d,  $J = 8.0$  Hz, 1H), 5.96 – 5.88 (m, 2H), 3.77 – 3.72 (m, 4H), 2.67 (dd,  $J = 15.0, 4.5$  Hz, 1H), 2.60 – 2.55 (m, 1H), 2.38 (s, 3H), 2.09 – 2.02 (m, 1H), 1.06 (d,  $J = 6.5$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.4, 144.4, 136.4, 134.5, 132.8, 130.7, 129.7, 126.6, 126.4, 125.6, 125.2, 124.7, 123.2, 117.6, 115.4, 112.3, 55.0, 34.8, 34.4, 33.7, 28.3, 21.6, 21.6, 20.0. IR (neat): 2954, 2925, 2855, 1609, 1509, 1460, 1291, 1172, 1062, 812, 789, 674, 605, 583, 538; HRMS (ESI/QTOF) m/z:  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{28}\text{H}_{27}\text{NNaO}_3\text{S}^+$  480.1604; Found 480.1598.

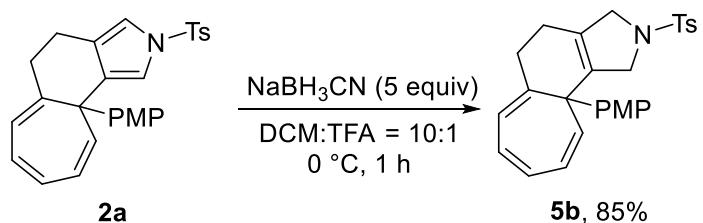
### 4.3 Synthetic transformations

**10a-(4-methoxyphenyl)-2-methyl-2,4,5,10a-tetrahydrocyclohepta[e]isoindole(5a)**



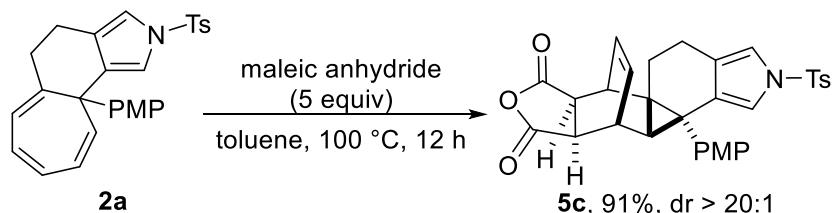
Compound **5a** was prepared in 75% yield according to the known procedure (0.1 mmol scale, 22.5 mg).<sup>1,2</sup> Pale yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.07 (d,  $J = 8.8$  Hz, 2H), 6.60 (d,  $J = 8.4$  Hz, 2H), 6.36 – 6.25 (m, 3H), 6.21 – 6.15 (m, 2H), 6.00 (d,  $J = 2.0$  Hz, 1H), 5.07 (d,  $J = 8.8$  Hz, 1H), 3.70 (s, 3H), 3.48 (s, 3H), 2.85 – 2.69 (m, 3H), 2.59 – 2.44 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  157.0, 137.2, 130.4, 128.5, 128.4, 127.5, 125.6, 124.7, 123.4, 118.9, 118.5, 116.8, 116.3, 111.9, 54.9, 43.8, 36.0, 35.1, 21.8; IR (neat): 2924, 2849, 1702, 1607, 1459, 1394, 1243, 1174, 823, 789, 703; HRESIMS Calcd for  $[\text{C}_{21}\text{H}_{21}\text{NNaO}]^+ [\text{M} + \text{Na}]^+$  326.1515, found 326.1514.

**10a-(3-methoxyphenyl)-2-tosyl-1,2,3,4,5,10a-hexahydrocyclohepta[e]isoindole(5b)**



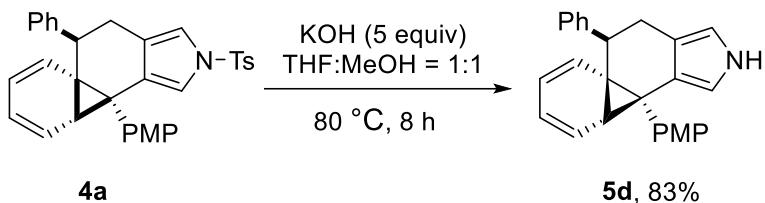
Compound **5b** was prepared in 85% yield according to the known procedure (0.1 mmol scale, 37.8 mg).<sup>1</sup> Pale yellow oil. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.73 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.22 – 7.13 (m, 3H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.91 (d, *J* = 8.5 Hz, 2H), 6.71 (d, *J* = 9.0 Hz, 2H), 4.35 – 4.31 (m, 2H), 4.21 – 4.19 (m, 1H), 4.11 – 4.08 (m, 1H), 4.01 – 3.98 (m, 1H), 3.75 (s, 3H), 2.91 – 2.80 (m, 1H), 2.49 – 2.34 (m, 4H), 2.29 – 2.27 (m, 1H), 2.10 – 2.05 (m, 1H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.9, 143.4, 142.6, 140.0, 133.8, 133.3, 132.6, 130.2, 129.8, 129.3, 129.3, 128.1, 127.5, 127.3, 126.2, 113.6, 59.6, 59.4, 55.2, 48.0, 30.5, 27.1, 21.5; IR (neat): 2923, 1733, 1654, 1595, 1456, 1256, 1180, 1090, 700, 664, 583, 541; HRESIMS Calcd for [C<sub>27</sub>H<sub>27</sub>NNaO<sub>3</sub>S]<sup>+</sup> [M + Na<sup>+</sup>] 468.1604, found 468.1602.

### **3b-(4-methoxyphenyl)-2-tosyl-3b,3c,4,4a,7a,8,9,10-octahydro-7*H*-4,8-ethenoisobenzofuro[5',6':2,3]cyclopropa[1,2-*e*]isoindole-5,7(2*H*)-dione(**5c**)**



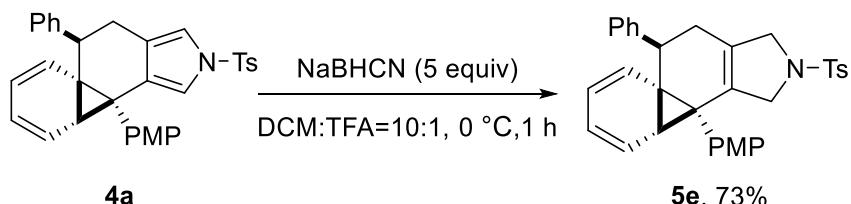
Compound **5c** was prepared in 91% yield (dr > 20:1) according to the known procedure (0.1 mmol scale, 49.3 mg).<sup>3</sup> Pale yellow oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 – 7.53 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 6.91 – 6.65 (m, 5H), 6.02 (s, 1H), 5.42 – 5.22 (m, 2H), 3.81 (s, 3H), 3.62 – 3.60 (m, 2H), 3.40 – 3.38 (m, 1H), 3.21 – 3.18 (m, 1H), 2.65 – 2.63 (m, 1H), 2.39 (s, 3H), 2.30 – 2.17 (m, 1H), 2.09 – 2.06 (m, 2H), 1.65 – 1.63 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 172.3, 171.7, 157.8, 144.6, 136.1, 133.3, 133.1, 131.0, 130.0, 129.8, 126.7, 122.1, 117.9, 115.7, 114.6, 113.6, 55.2, 45.5, 44.6, 38.8, 33.9, 32.5, 31.7, 29.5, 23.7, 21.6, 19.7; IR (neat): 2954, 2343, 1791, 1660, 1507, 1169, 1062, 932, 816, 702, 668; HRESIMS Calcd for [C<sub>31</sub>H<sub>27</sub>NNaO<sub>6</sub>S]<sup>+</sup> [M + Na<sup>+</sup>] 564.1451, found 564.1452.

**3b-(4-methoxyphenyl)-8-phenyl-3b,3c,8,9-tetrahydro-2H-benzo[2,3]cyclopropa[1,2-e]isoindole (5d)**



Compound **5d** was prepared in 83% yield (60.4 mg) according to the known procedure (0.2 mmol scale).<sup>1</sup> Yellow solid. M.p = 160.8 – 162.5 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.81 (s, 1H), 7.33 – 7.29 (m, 2H), 7.29 – 7.24 (m, 3H), 7.20 – 7.11 (m, 2H), 6.70 – 6.67 (m, 2H), 6.50 (s, 1H), 6.35 – 6.29 (m, 1H), 6.11 – 6.05 (m, 1H), 5.95 – 5.85 (m, 1H), 5.82 – 5.70 (m, 2H), 3.83 – 3.75 (m, 2H), 3.74 (s, 3H), 2.89 (dd, *J* = 15.5, 5.0 Hz, 1H), 2.65 – 2.49 (m, 1H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.2, 145.8, 133.0, 131.4, 128.3, 128.2, 127.7, 126.2, 125.1, 125.0, 124.2, 116.9, 115.3, 112.9, 112.2, 77.9, 68.8, 55.0, 47.5, 30.5, 30.1; IR (neat): 3357, 3337, 1612, 1511, 1246, 1060, 1034, 786, 768, 699, 531; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>22</sub>NNaOS<sup>+</sup> 387.1594; Found 387.1593.

**3b-(4-methoxyphenyl)-8-phenyl-2-tosyl-2,3,3b,3c,8,9-hexahydro-1*H*-benzo[2,3]cyclopropano[1,2-*e*]isoindole (5e)**

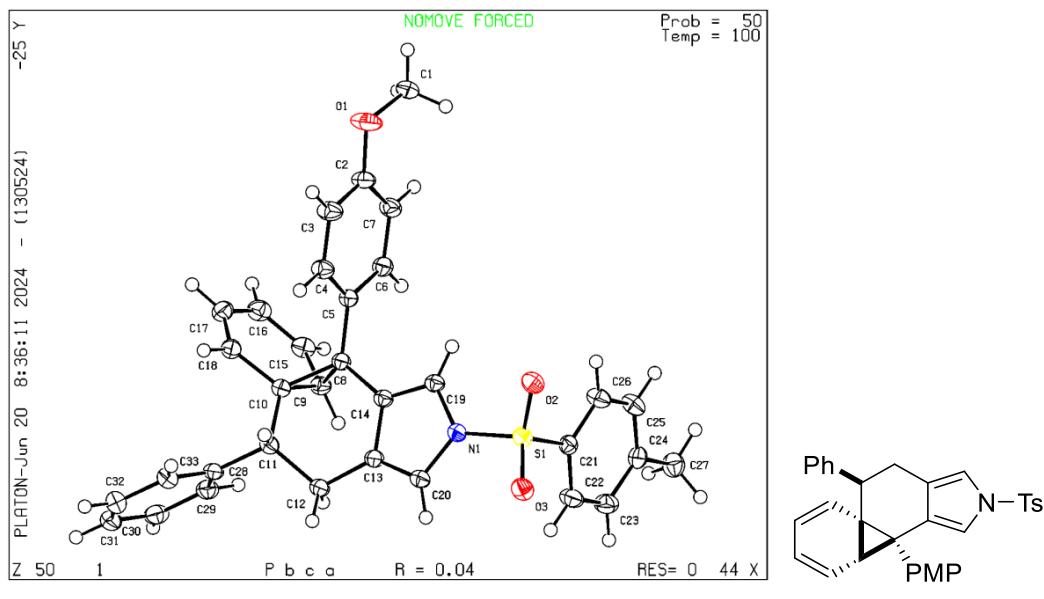


Compound **5e** was prepared in 73% yield (76.1 mg) according to the known procedure (0.2 mmol scale).<sup>2</sup> Yellow solid. M.p = 61.2 – 62.2 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.66 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.18 – 7.14 (m, 3H), 7.10 – 7.06 (m, 2H), 7.01 – 6.96 (m, 3H), 6.87 – 6.83 (m, 1H), 6.74 – 6.70 (m, 2H), 6.67 – 6.63 (m, 2H), 4.93 (s, 1H), 4.56 (dd, *J* = 9.0, 3.0 Hz, 1H), 4.26 – 4.18 (m, 1H), 4.09 (d, *J* = 11 Hz, 2H), 3.82 – 3.73 (m, 4H), 2.87 – 2.75 (m, 1H), 2.59 (d, *J* = 18.0 Hz, 1H), 2.44 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.0, 143.4, 143.1, 142.2, 141.1, 133.7, 131.0, 130.9, 130.2, 130.1, 129.7, 129.6, 129.2, 128.3, 127.8, 127.5, 126.8, 126.4, 126.3, 113.6, 60.1, 59.3, 55.2, 47.9, 46.2, 31.0, 21.5; IR (neat): 2925, 1609, 1509, 1344, 1253, 1163, 1098, 1033, 815, 736, 671; HRMS (ESI/QTOF) m/z: [M + Na]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>31</sub>NNaO<sub>3</sub>S<sup>+</sup> 544.1917; Found 544.1916.

## 5. Crystal Data

Crystal data and structure refinement for **4a**. CCDC Number = 2410274

ORTEP drawing of **4a** (thermal ellipsoids set at 50% probability). Recrystallization from *n*-hexane/DCM afforded single crystals suitable for X-ray diffraction analysis.



Bond precision: C-C = 0.0021 Å Wavelength=0.71073

Cell:  $a=13.4398(8)$   $b=16.1210(9)$   $c=24.2005(11)$   
 $\alpha=90$   $\beta=90$   $\gamma=90$

Temperature: 100 K

	Calculated	Reported
Volume	5243.4(5)	5243.4(5)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C33 H29 N O3 S	C33 H29 N O3 S
Sum formula	C33 H29 N O3 S	C33 H29 N O3 S
Mr	519.63	519.63
Dx, g cm <sup>-3</sup>	1.316	1.317
Z	8	8
μ (mm <sup>-1</sup> )	0.160	0.160
F000	2192.0	2192.0
F000'	2193.89	
h, k, lmax	17, 21, 32	17, 21, 32
Nref	6523	6519
Tmin, Tmax	0.962, 0.972	0.702, 0.746
Tmin'	0.962	

Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta (max) = 28.321

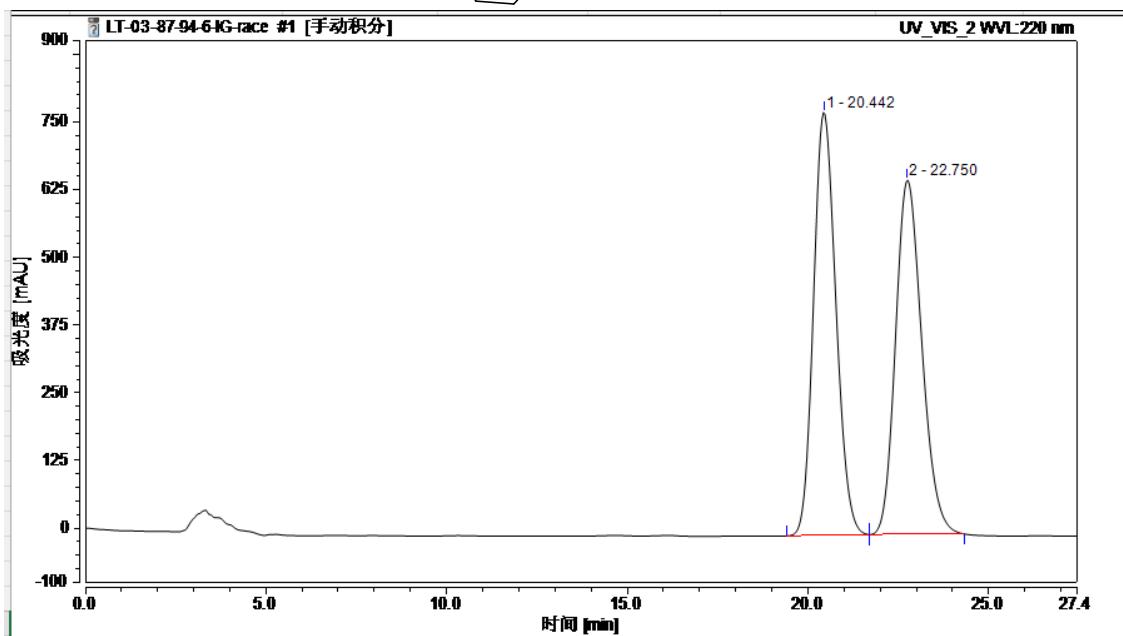
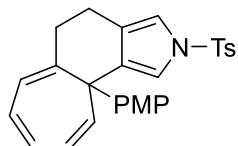
R(reflections)= 0.0442( 5445) wR2 (reflections)=  
S = 1.070 Npar= 345 0.1064( 6519)

## Reference

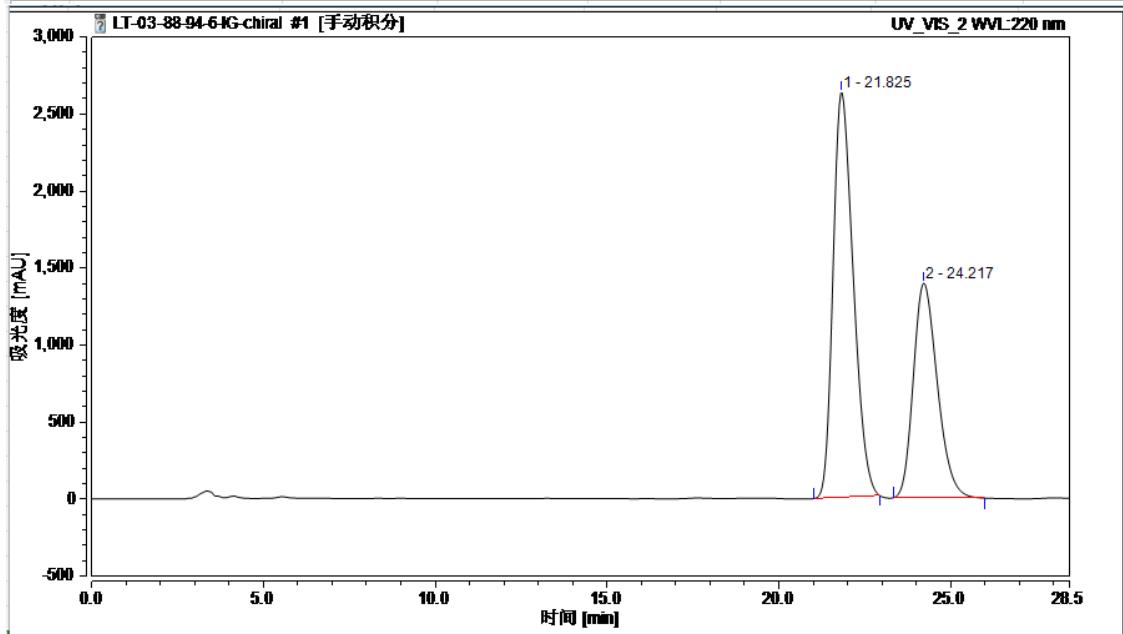
1. Y.-B. Chen, L.-G. Liu, Z.-Q. Wang, R. Chang, X. Lu, B. Zhou and L.-W. Ye, Enantioselective Functionalization of Unactivated C(sp<sup>3</sup>)–H Bonds through Copper-Catalyzed Diyne Cyclization by Kinetic Resolution, *Nat. Commun.*, 2024, **15**, 2232.
2. Y.-B. Chen, L.-G. Liu, C.-M. Chen, Y.-X. Liu, B. Zhou, X. Lu, Z. Xu, and L.-W. Ye, Construction of Axially Chiral Arylpyrroles via Atroposelective Diyne Cyclization, *Angew. Chem. Int. Ed.*, 2023, **62**, e202303670.
3. T. Ito, S. Harada, H. Homma, H. Takenaka, S. Hirose and T. Nemoto, Asymmetric Intramolecular Dearomatization of Nonactivated Arenes with Ynamides for Rapid Assembly of Fused Ring System under Silver Catalysis, *J. Am. Chem. Soc.*, 2021, **143**, 604.

## 6. HPLC Chromatograms

**ent-2a:** IC, *n*-hexane/2-propanol = 94/6, v = 1.0 mL·min<sup>-1</sup>, λ = 220 nm

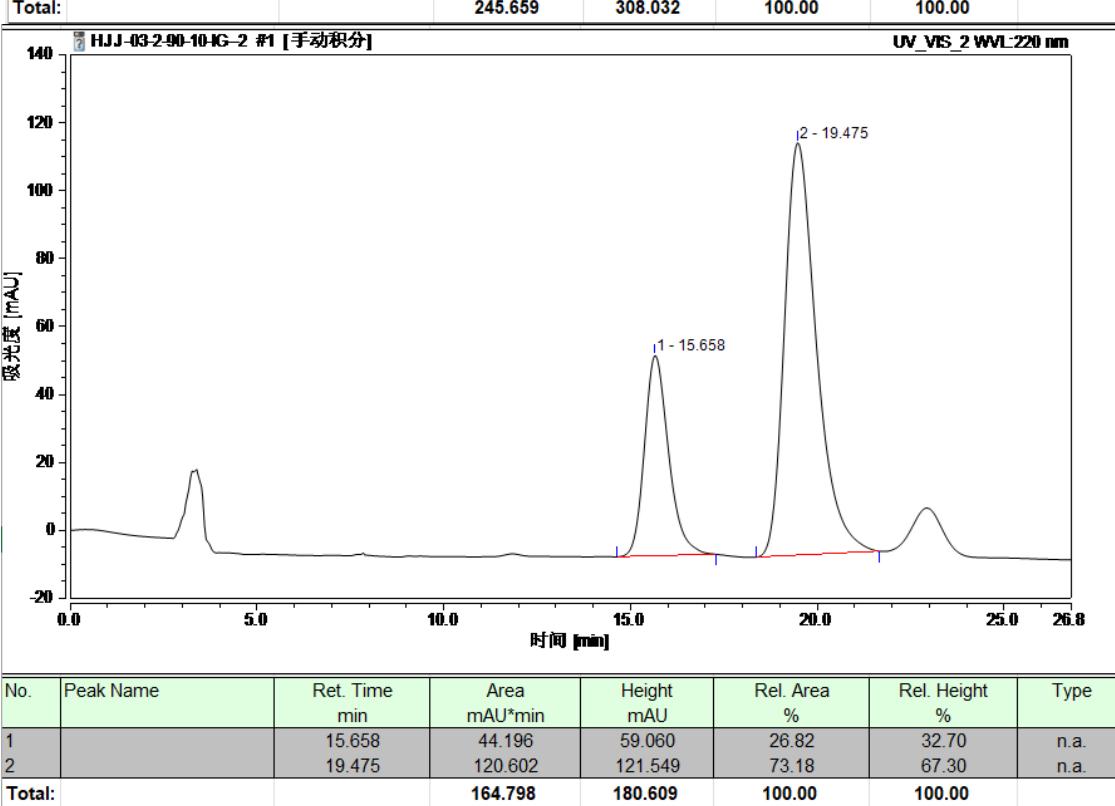
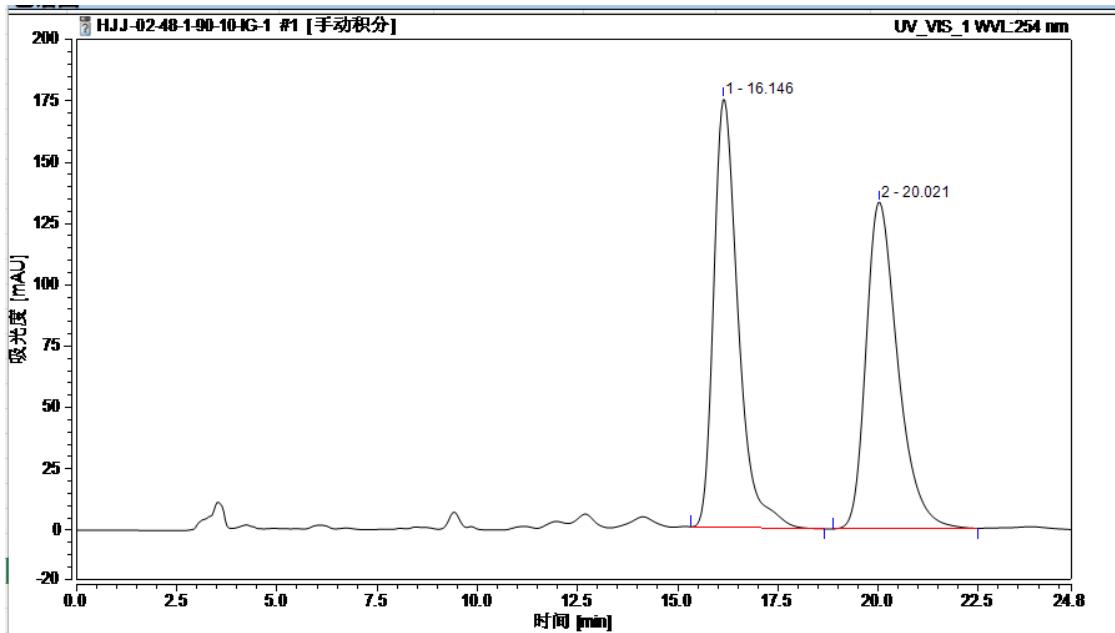
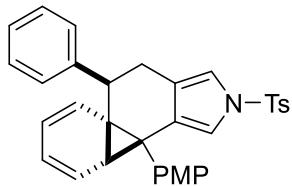


No.	Peak Name	Ret. Time min	Area mAU*min	Height mAU	Rel. Area %	Rel. Height %	Type
1		20.442	559.600	782.126	50.40	54.44	n.a.
2		22.750	550.823	654.632	49.60	45.56	n.a.
<b>Total:</b>			<b>1110.422</b>	<b>1436.758</b>	<b>100.00</b>	<b>100.00</b>	



No.	Peak Name	Ret. Time min	Area mAU*min	Height mAU	Rel. Area %	Rel. Height %	Type
1		21.825	1784.571	2632.975	61.30	65.37	n.a.
2		24.217	1126.467	1394.726	38.70	34.63	n.a.
<b>Total:</b>			<b>2911.038</b>	<b>4027.701</b>	<b>100.00</b>	<b>100.00</b>	

*ent*-4a: IC, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min<sup>-1</sup>, λ = 254 nm



7.777  
7.761  
7.234  
7.224  
7.220  
7.207  
7.200  
7.193  
7.187  
7.177  
7.177  
7.163  
7.098  
7.094  
7.084  
7.080  
6.783  
6.779  
6.769  
6.765

—4.392

—3.793

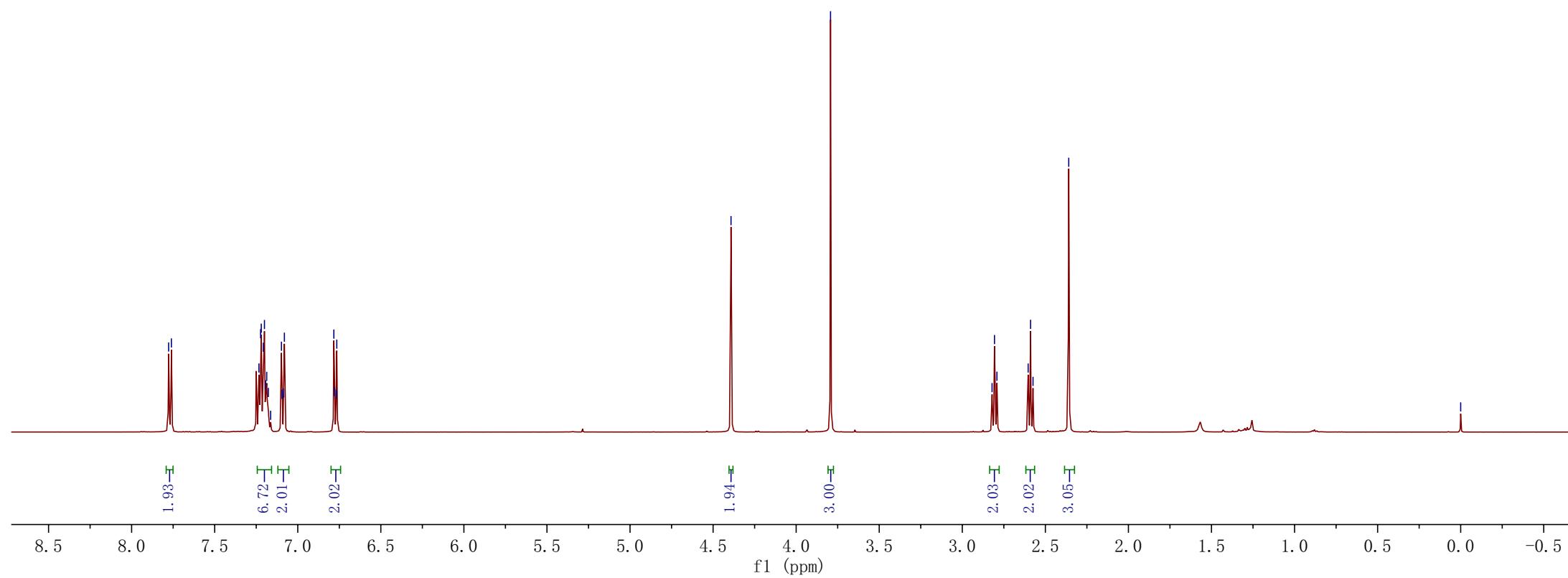
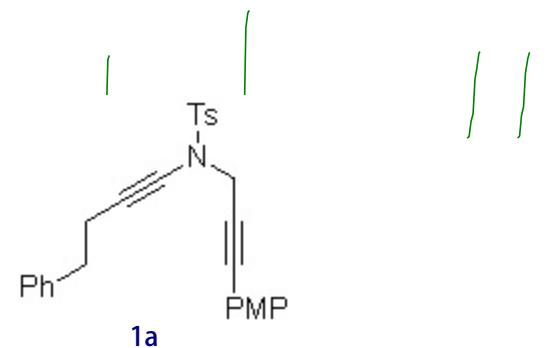
2.821  
2.806  
2.792  
2.604  
2.589  
2.574  
2.359

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

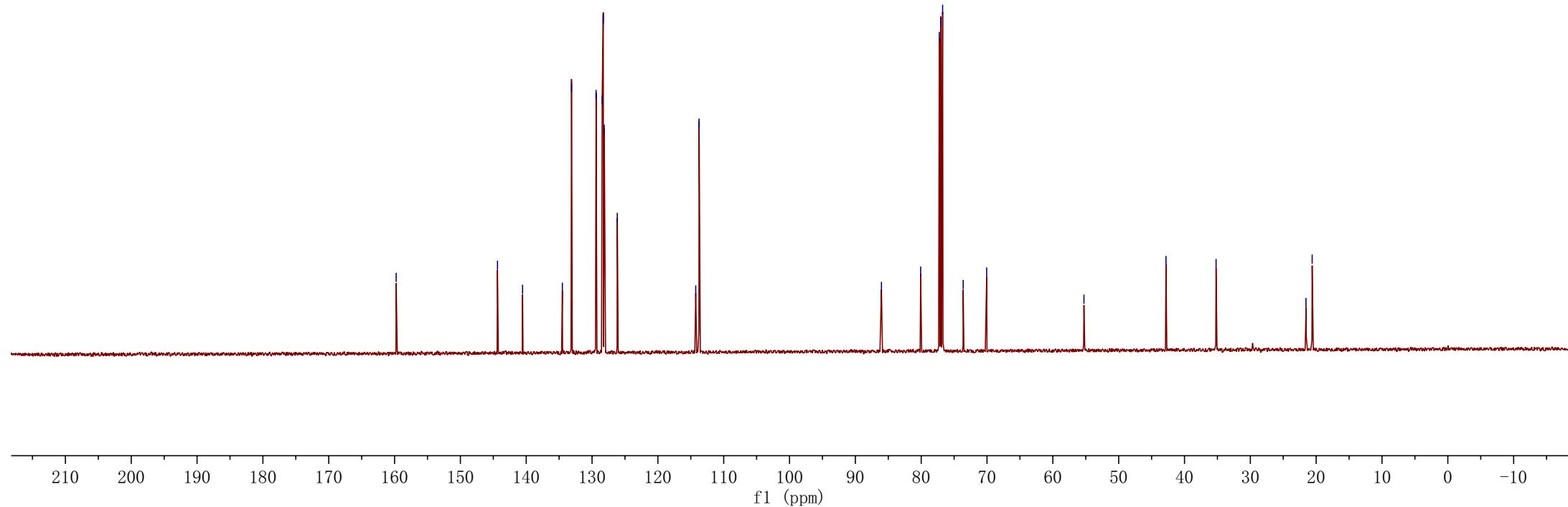
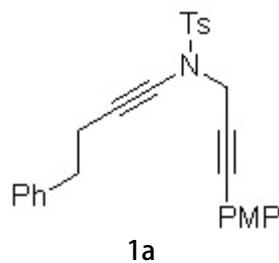
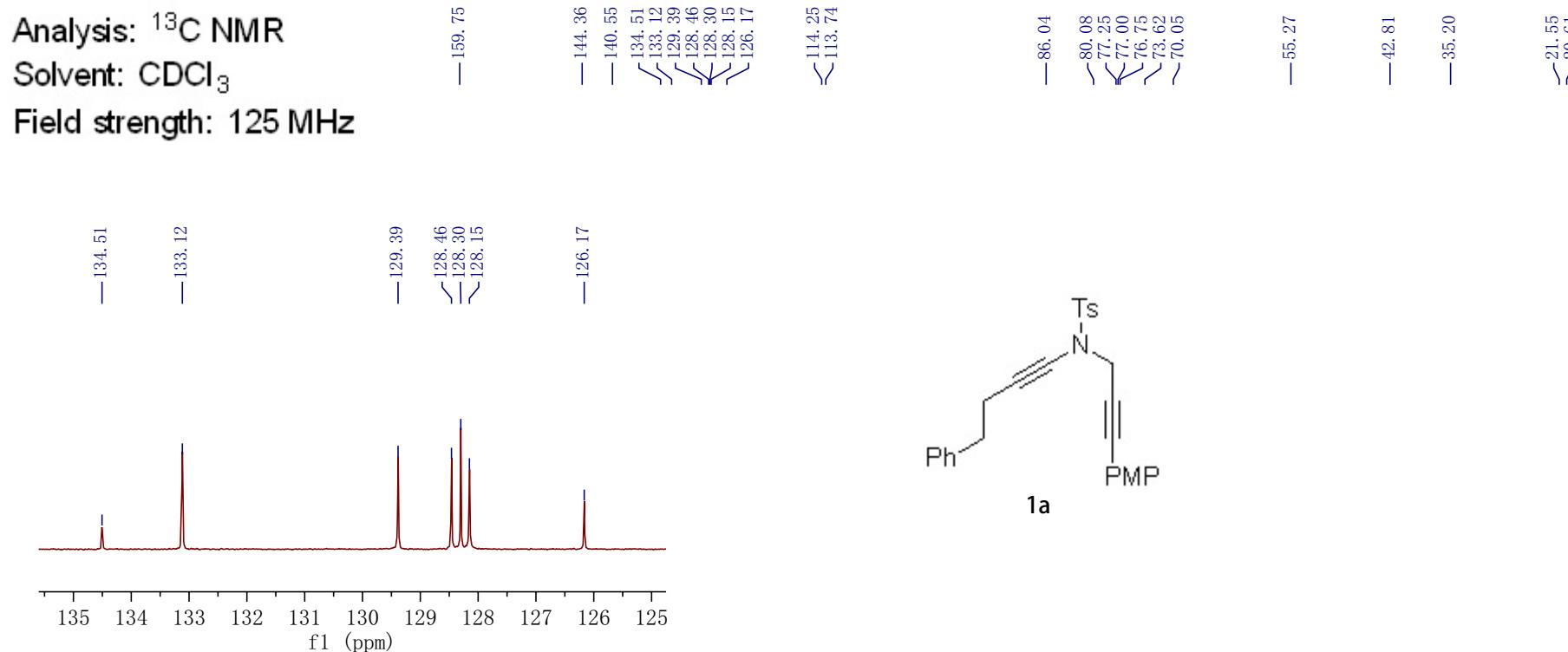
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz

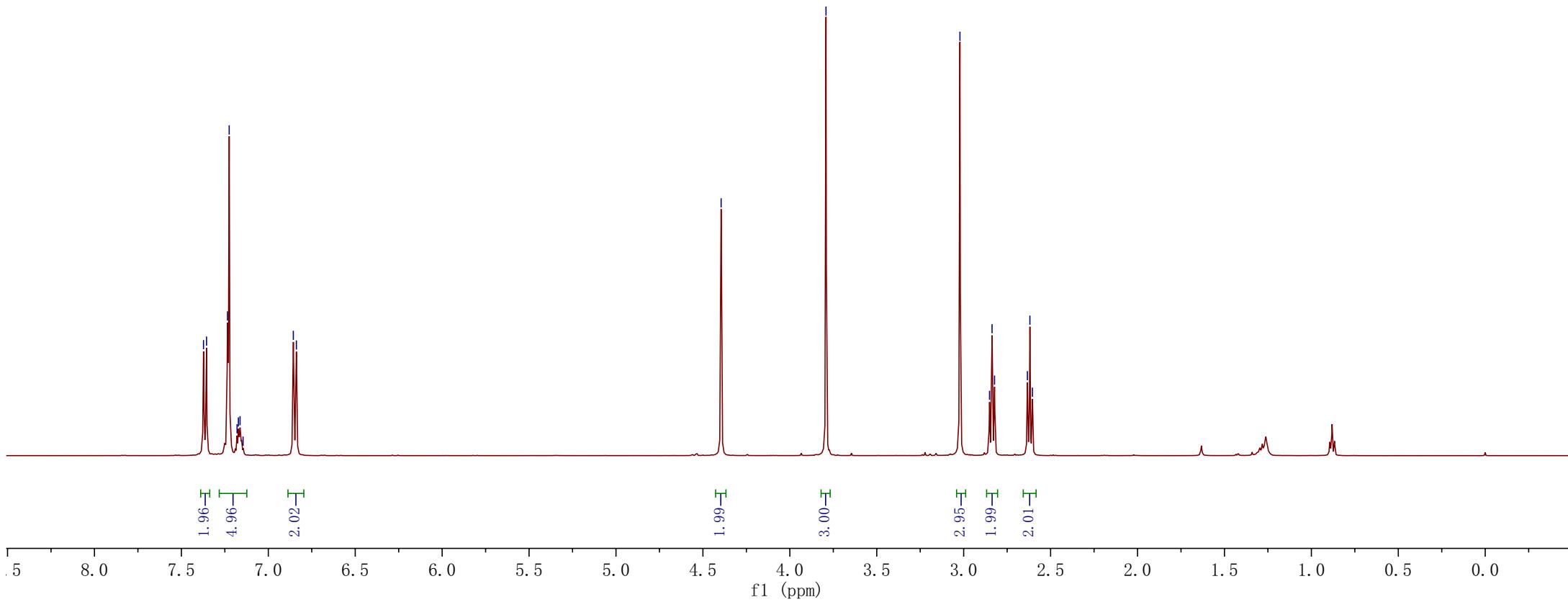
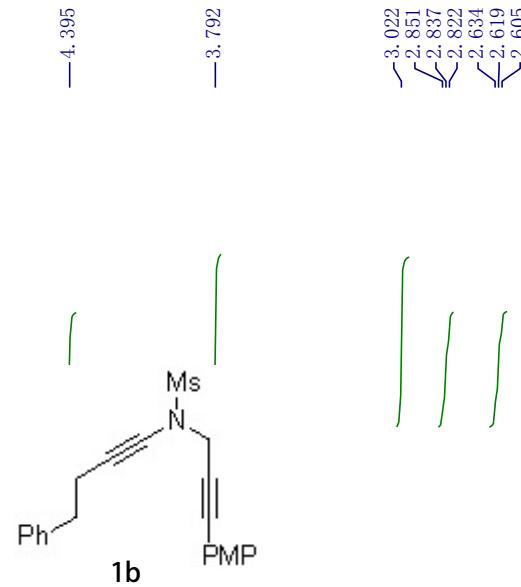


7.373  
7.355  
7.235  
7.225  
7.180  
7.172  
7.163  
7.145  
6.856  
6.838

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

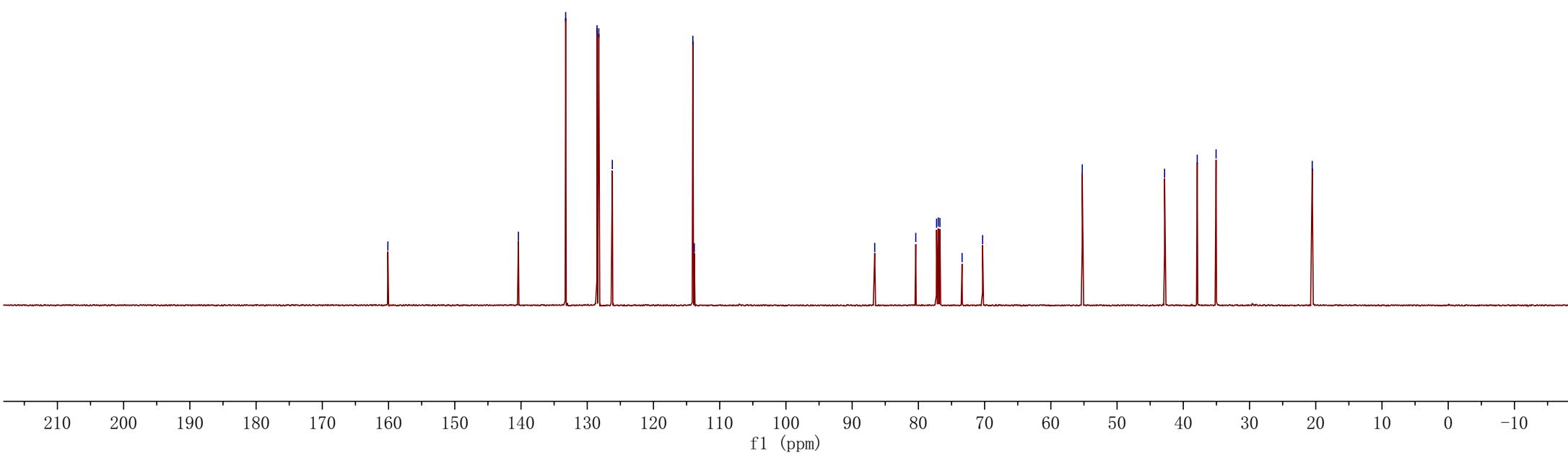
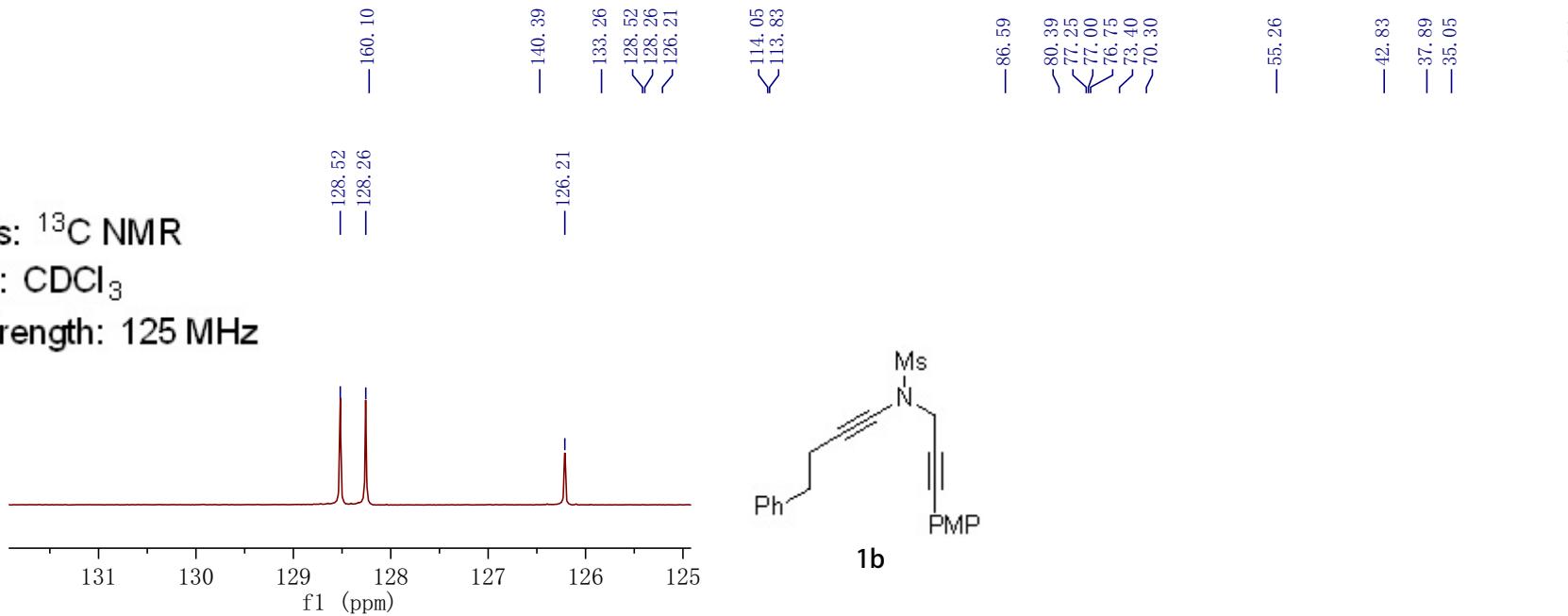
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



7.374  
7.357  
7.247  
7.262  
7.233  
7.220  
7.190  
7.186  
7.179  
7.173  
7.166  
7.160  
6.861  
6.844

—4.417

—3.811

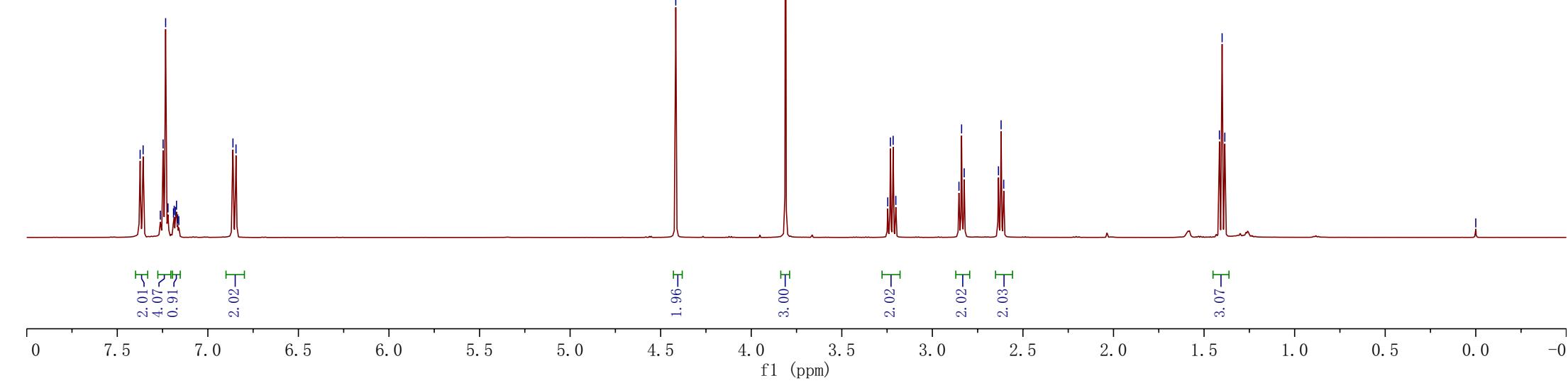
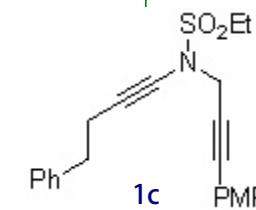
1.415  
1.400  
1.386

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

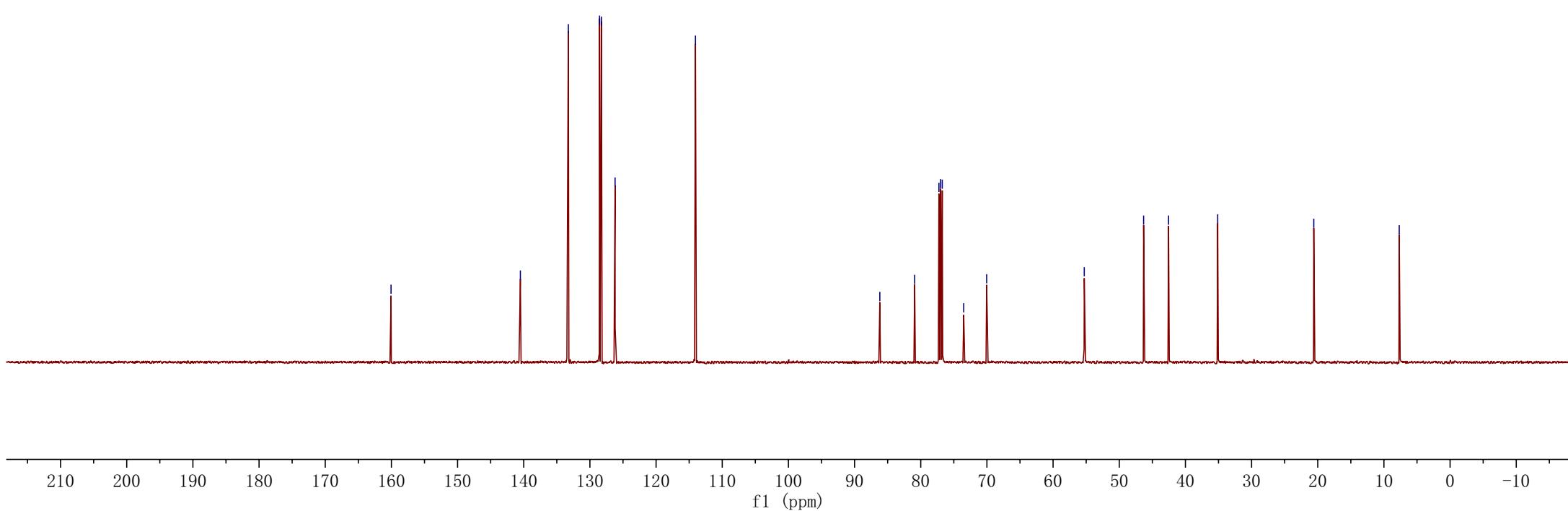
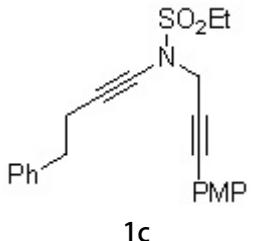
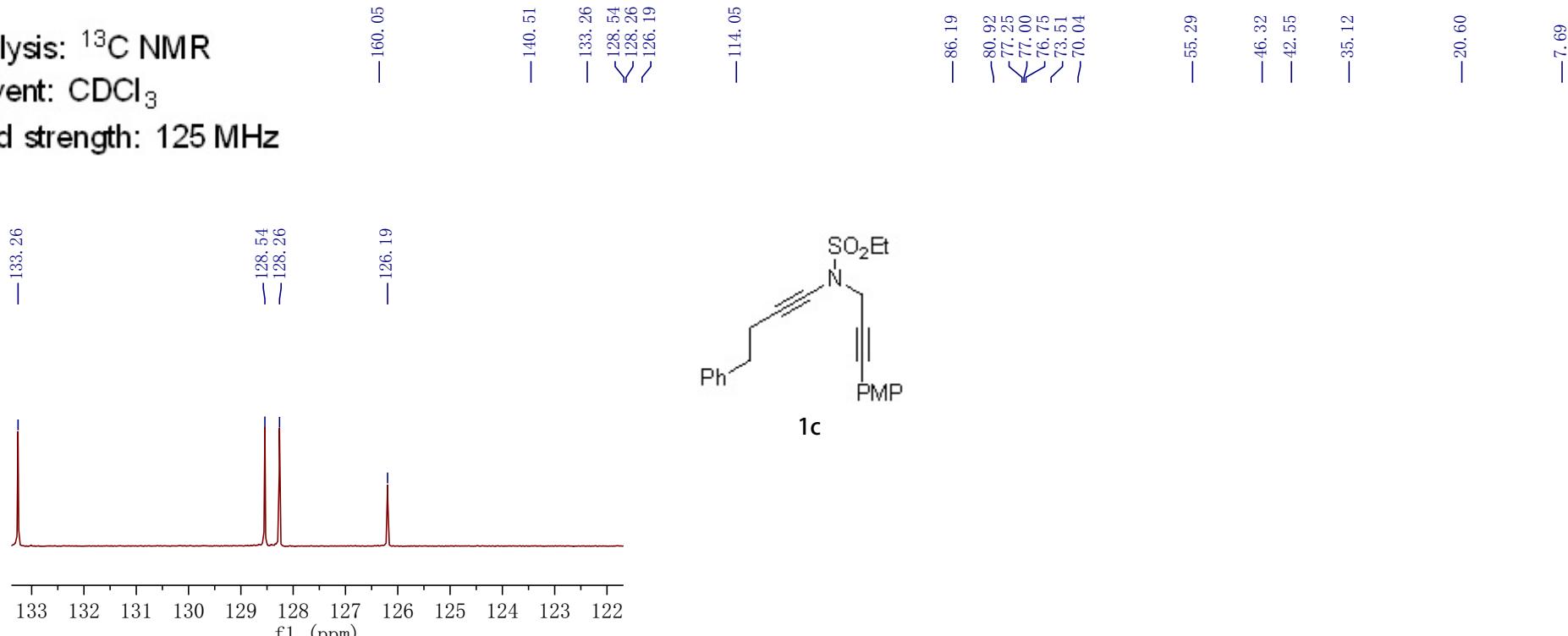
Field strength: 500 MHz

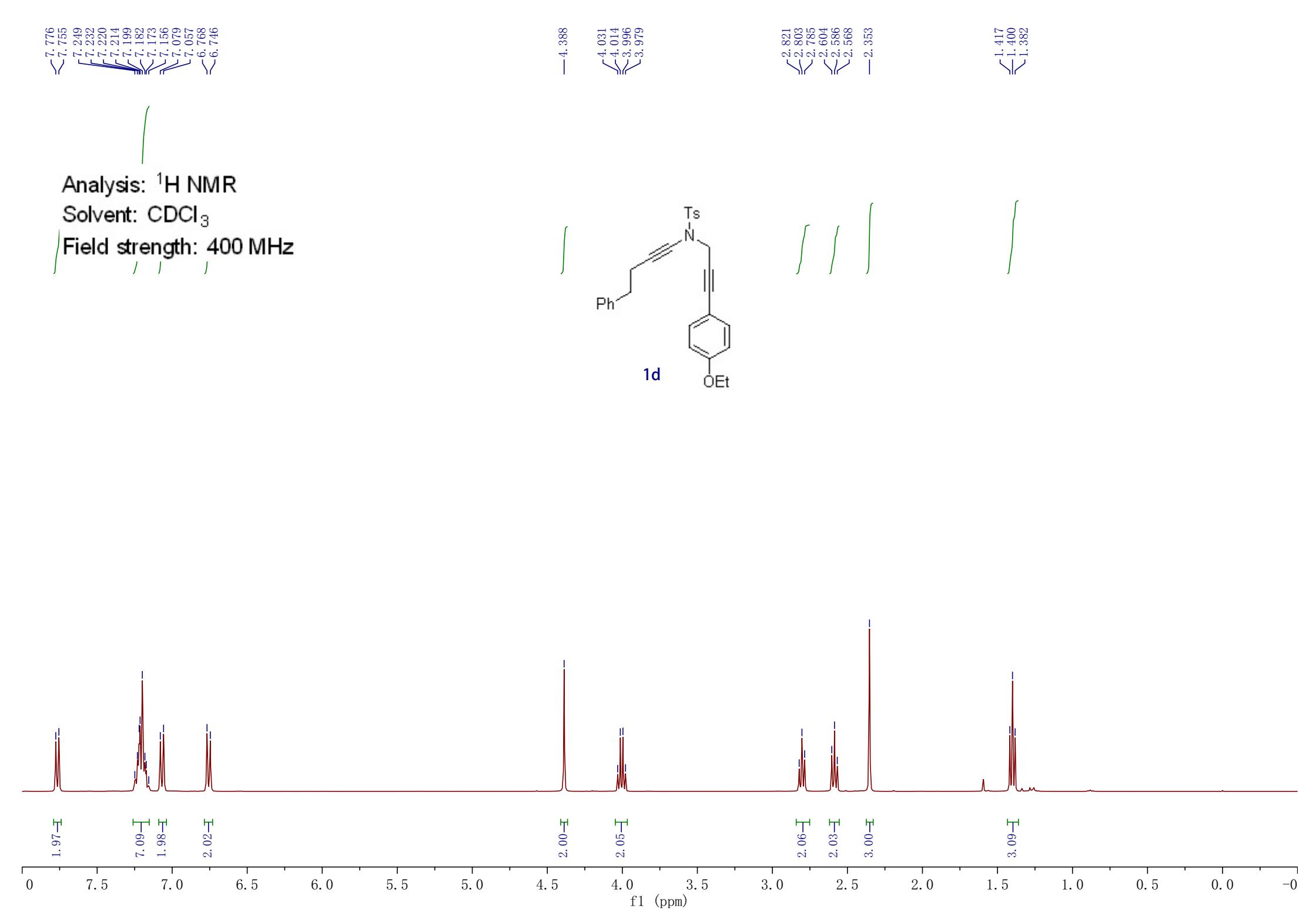


Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz

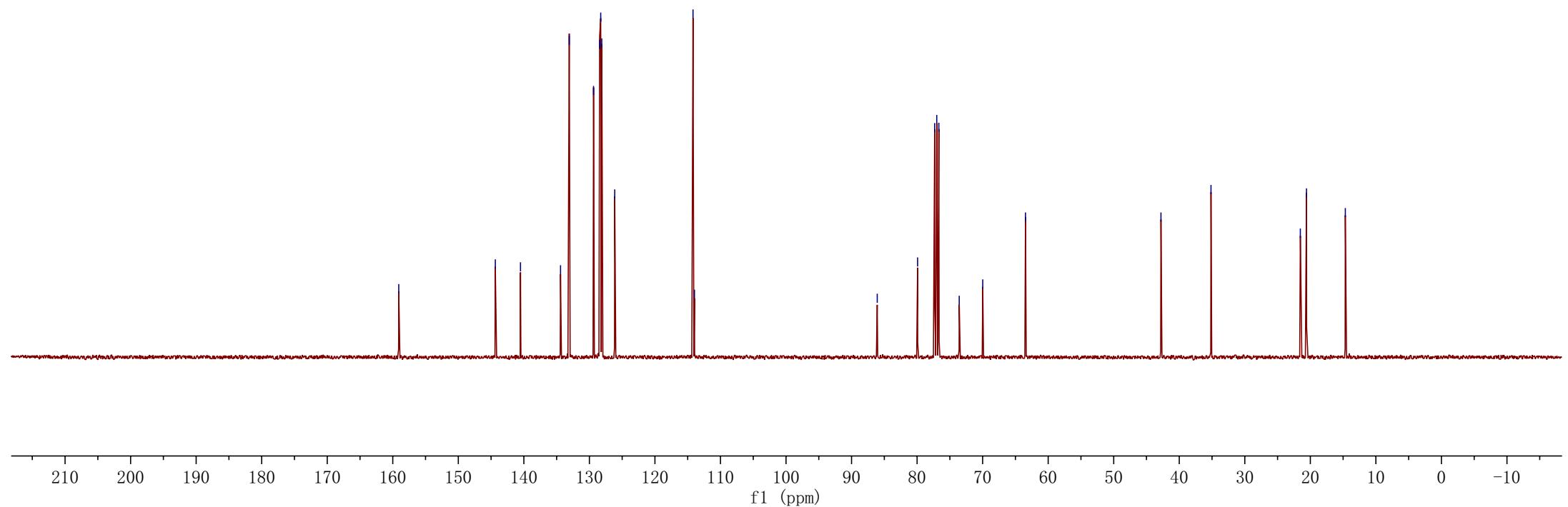
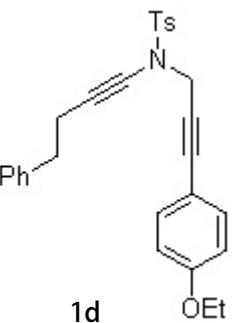
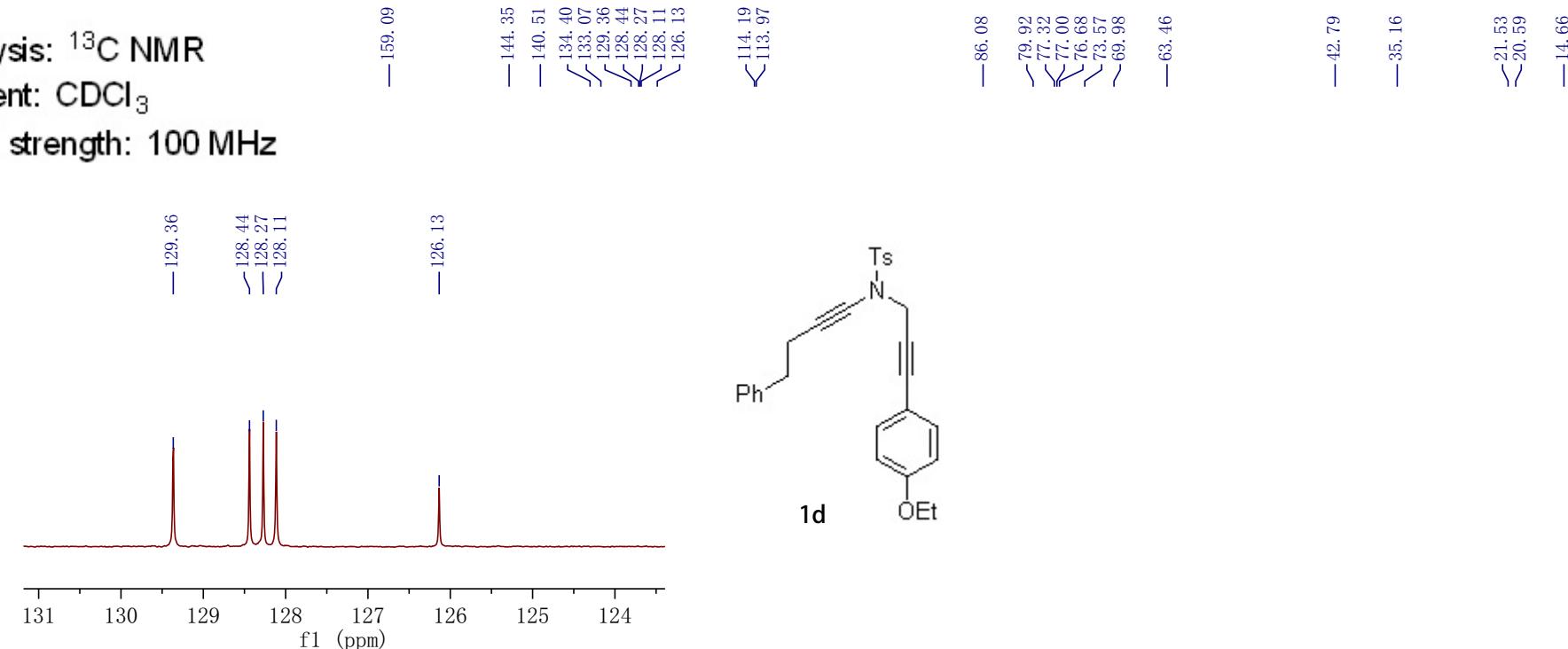




Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.768  
7.747  
7.7408  
7.387  
7.369  
7.350  
7.331  
7.314  
7.297  
7.240  
7.223  
7.204  
7.191  
7.162  
7.081  
7.059  
6.848  
6.826

—5.035  
—4.376

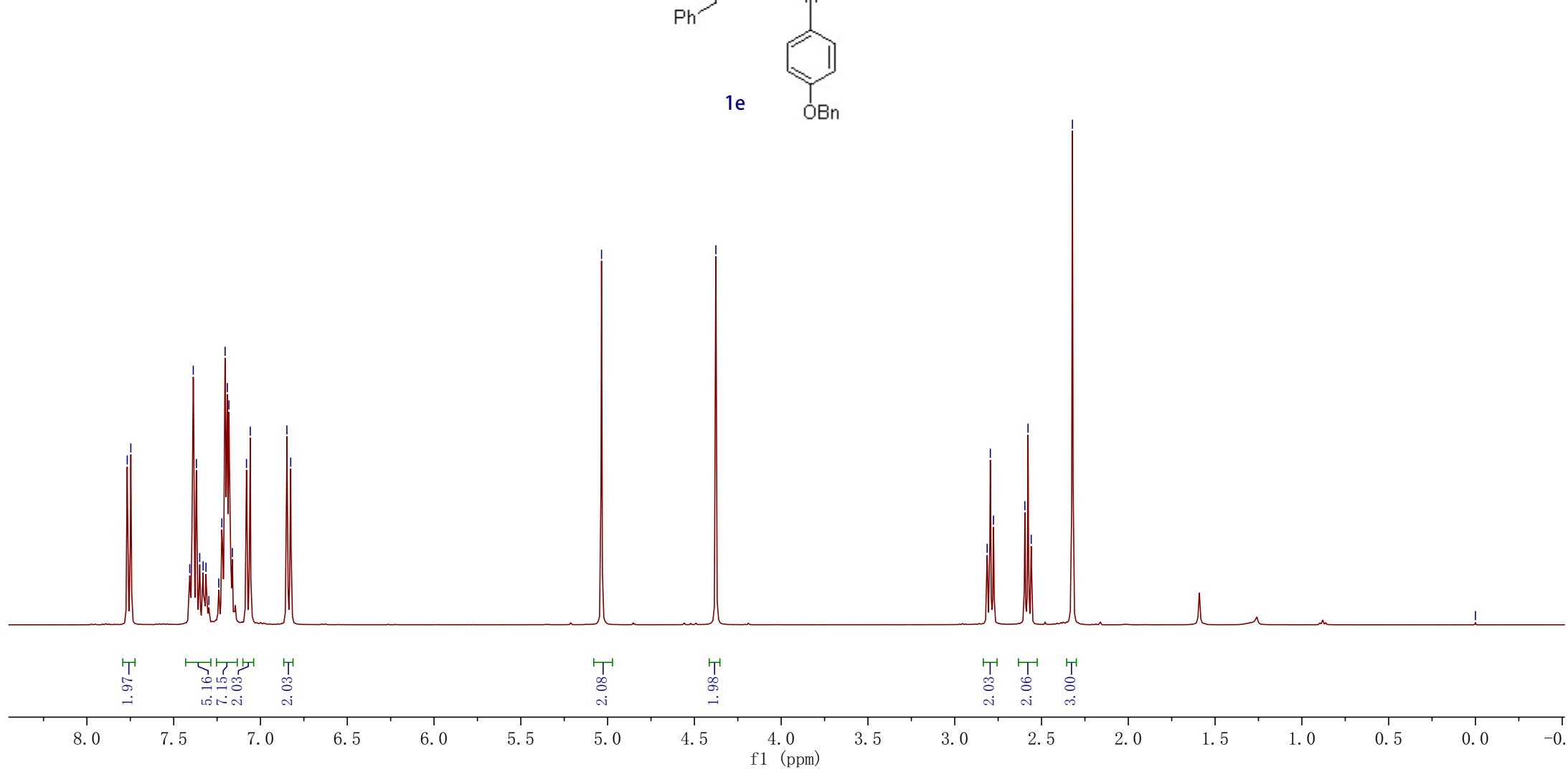
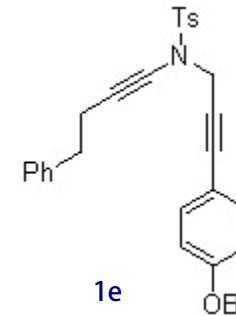
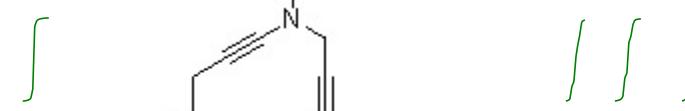
2.813  
2.795  
2.777  
2.596  
2.578  
2.559  
—2.322

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

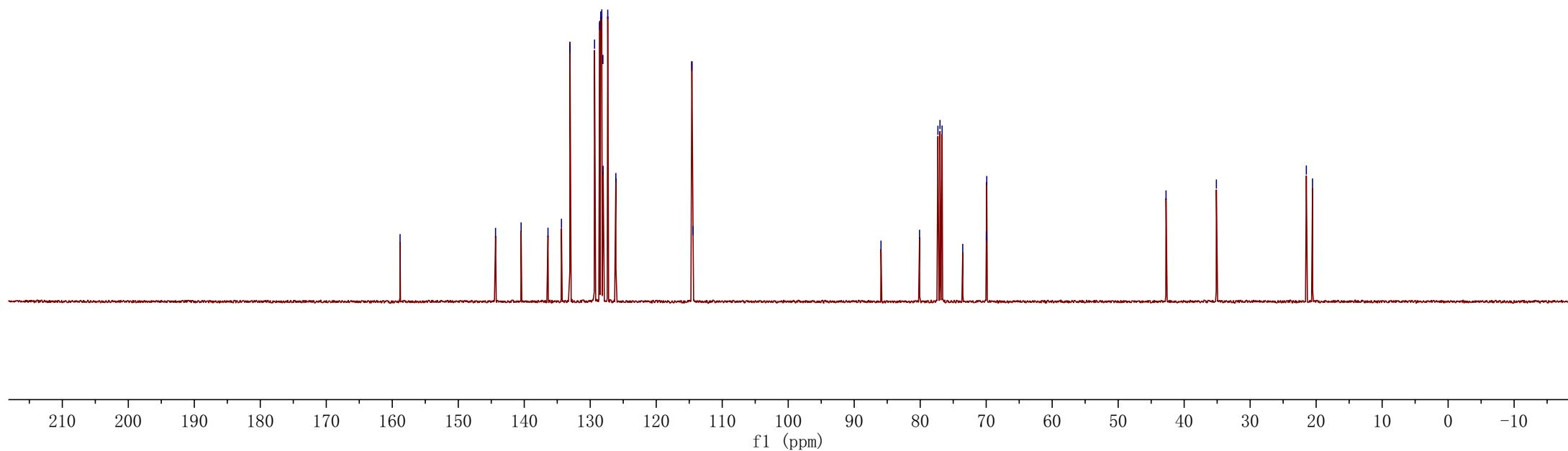
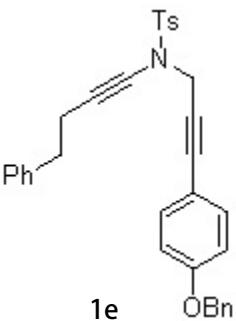
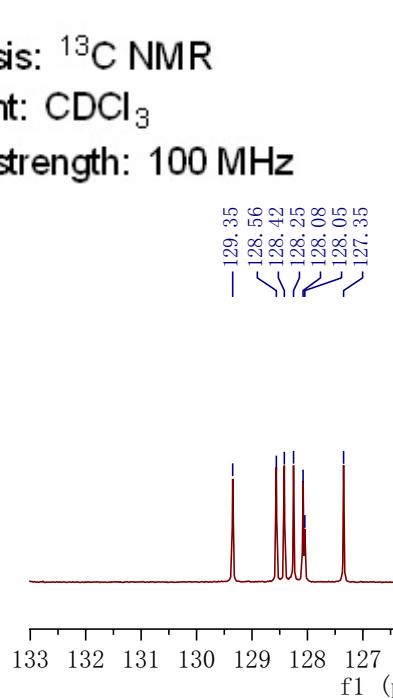
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.778  
<7.757  
7.251  
7.229  
7.221  
7.212  
7.201  
7.192  
7.185  
7.172  
7.039  
7.018  
6.720  
<6.699

—4.390

2.827  
2.809  
2.791  
2.609  
2.591  
2.572  
—2.357

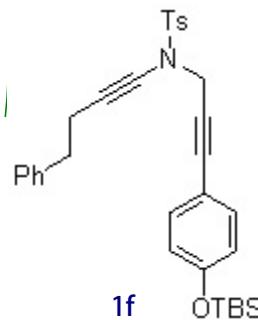
—0.973

—0.191  
—0.000

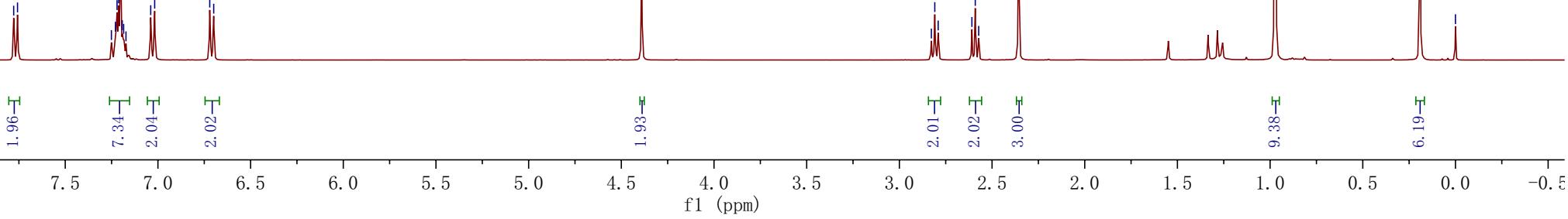
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



**1f**

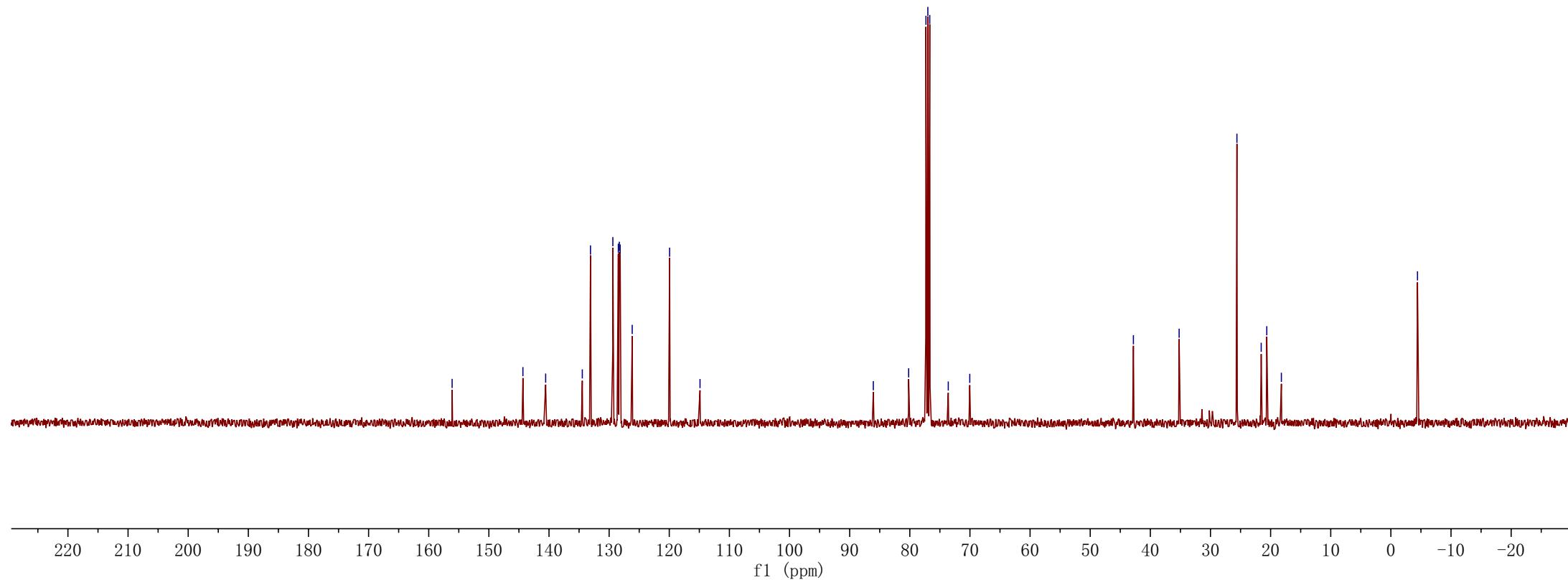
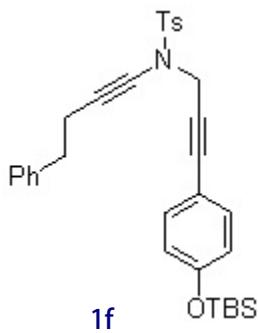


Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

—156.11  
—144.34  
—140.56  
—134.46  
—133.10  
—129.38  
—128.47  
—128.30  
—128.17  
—126.16  
—119.94  
—114.89  
—86.07  
—80.19  
—77.32  
—77.00  
—76.68  
—73.60  
—70.03  
—42.82  
—35.21  
—25.60  
—21.56  
—20.64  
—18.21  
—4.43



<7.780  
<7.760  
7.370  
7.351  
7.331  
7.251  
7.229  
7.215  
7.209  
7.199  
7.182  
7.174  
7.159  
7.140  
7.121  
7.115  
7.093  
7.011  
6.991  
6.871  
6.849

—4.395

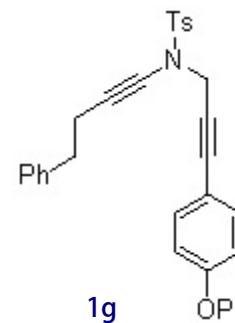
<2.825  
<2.806  
<2.788  
<2.609  
<2.591  
<2.572  
—2.356

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



1.94 [T]  
1.94 [T]  
10.14 [T]  
1.95 [T]  
1.96 [T]

1.98 [T]

1.98 [T]  
1.98 [T]  
3.00 [T]

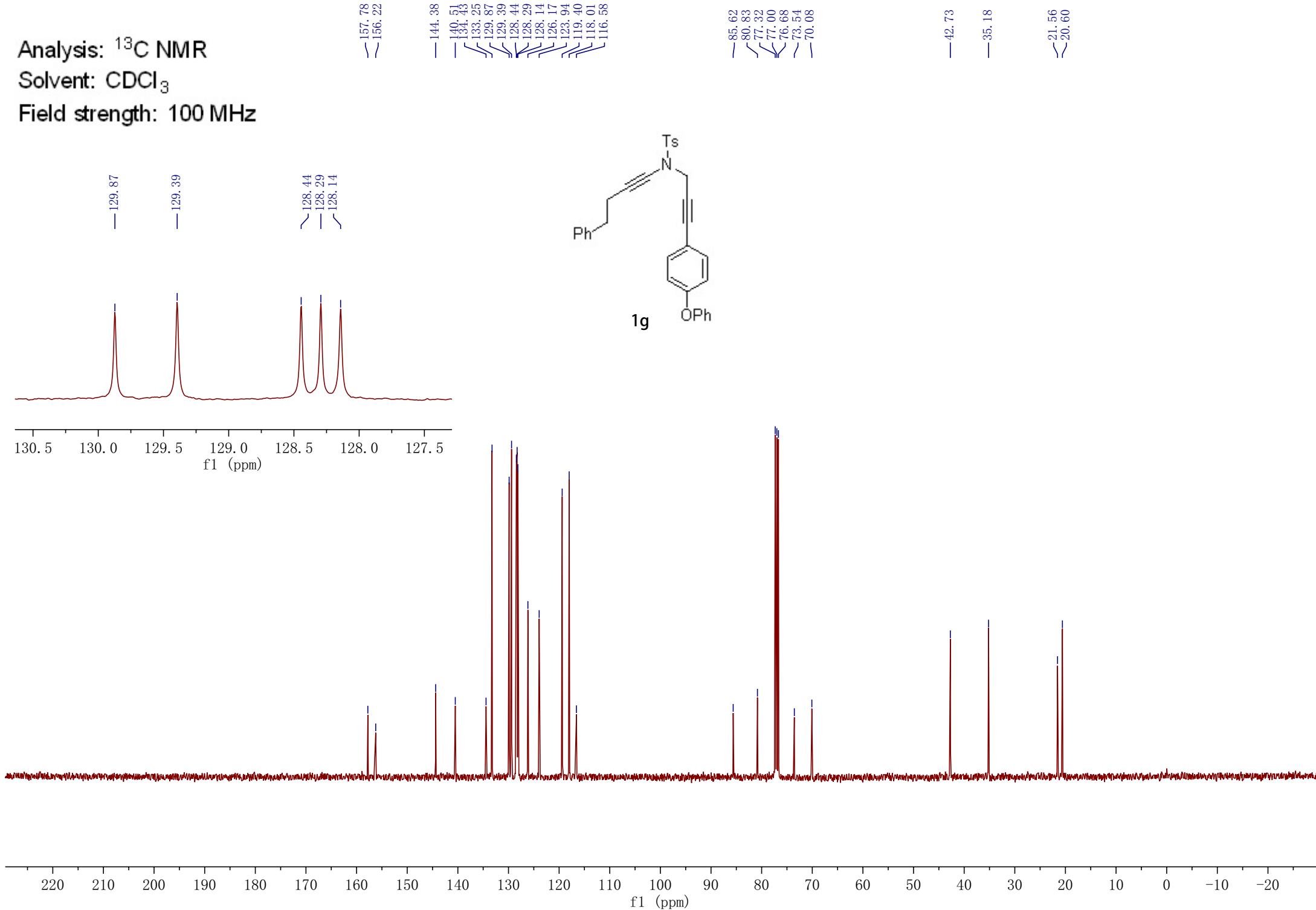
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



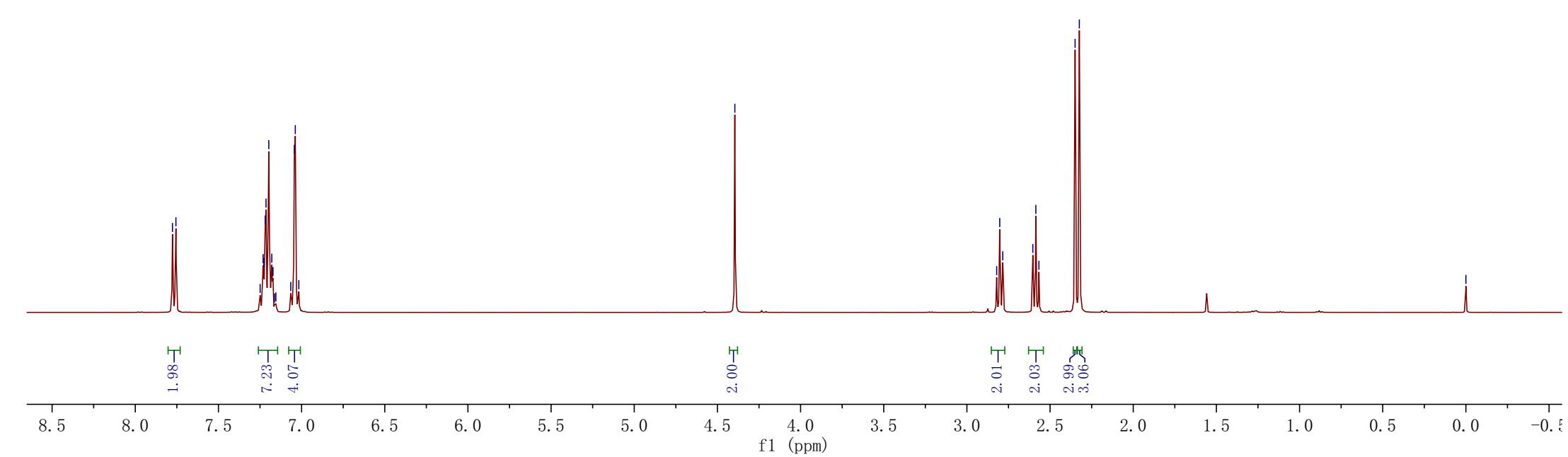
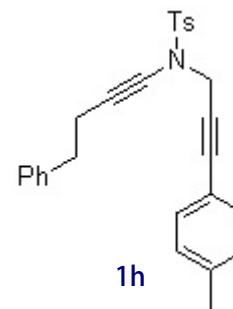
7.776  
7.756  
7.249  
7.231  
7.228  
7.219  
7.214  
7.197  
7.179  
7.172  
7.163  
7.155  
7.065  
7.044  
7.038  
7.017

—4.395  
—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

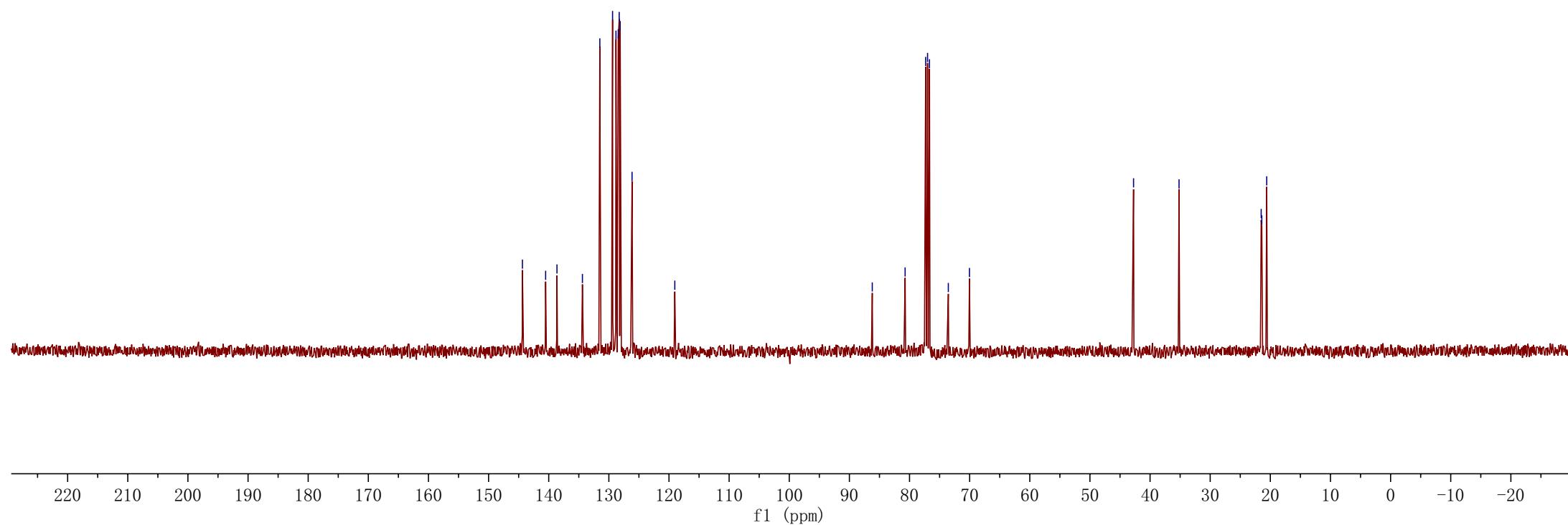
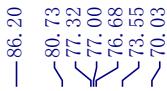
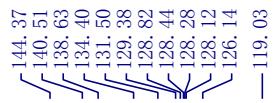
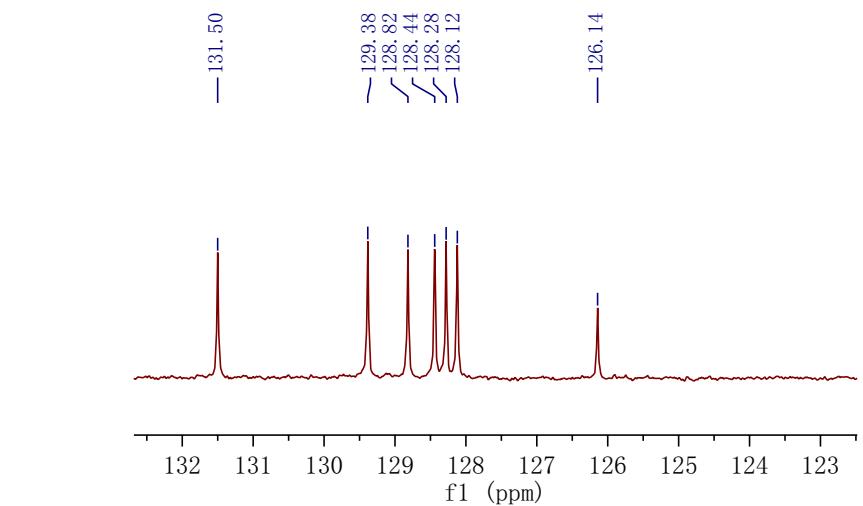
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.778  
<7.757  
7.247  
7.229  
7.226  
7.217  
7.212  
7.197  
7.189  
<7.180  
7.169  
7.152  
7.091  
7.069  
7.044

-4.396

2.822  
2.804  
2.786  
2.647  
2.627  
2.605  
2.586  
2.567  
2.343

<1.228  
<1.209  
1.190

-0.000

Analysis:  $^1\text{H}$  NMR

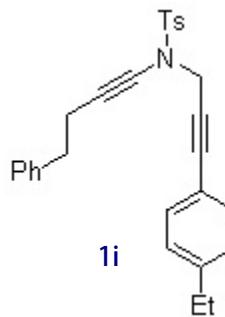
Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

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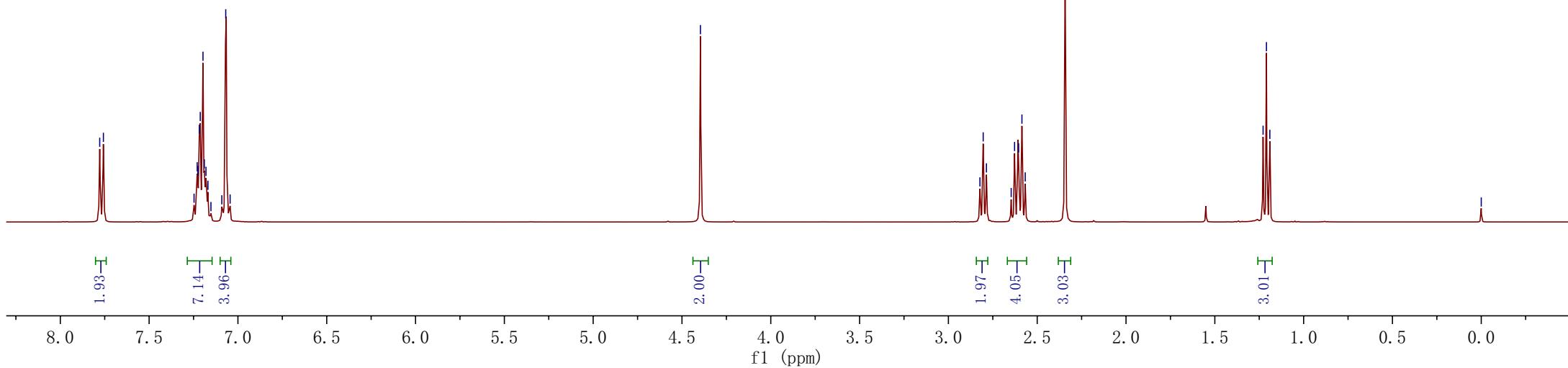
]

]



]

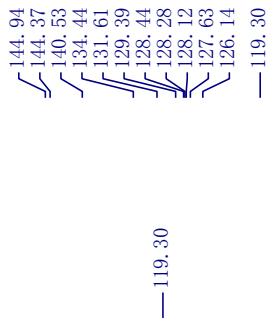
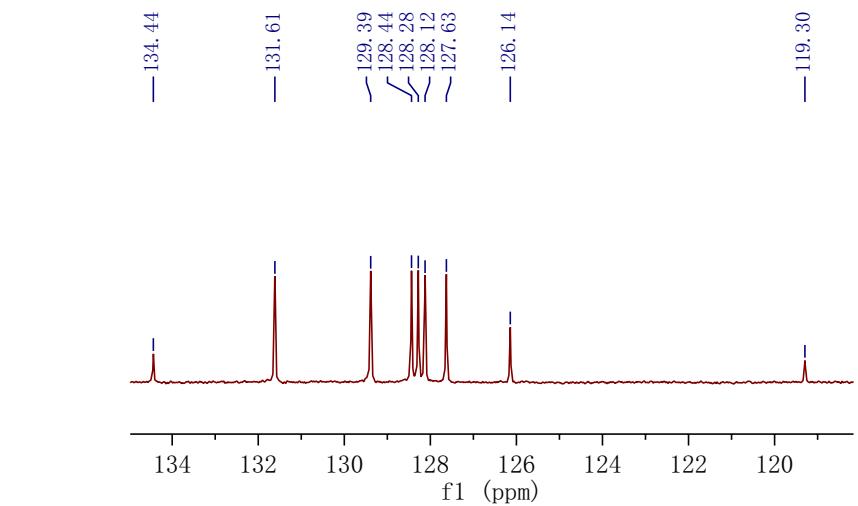
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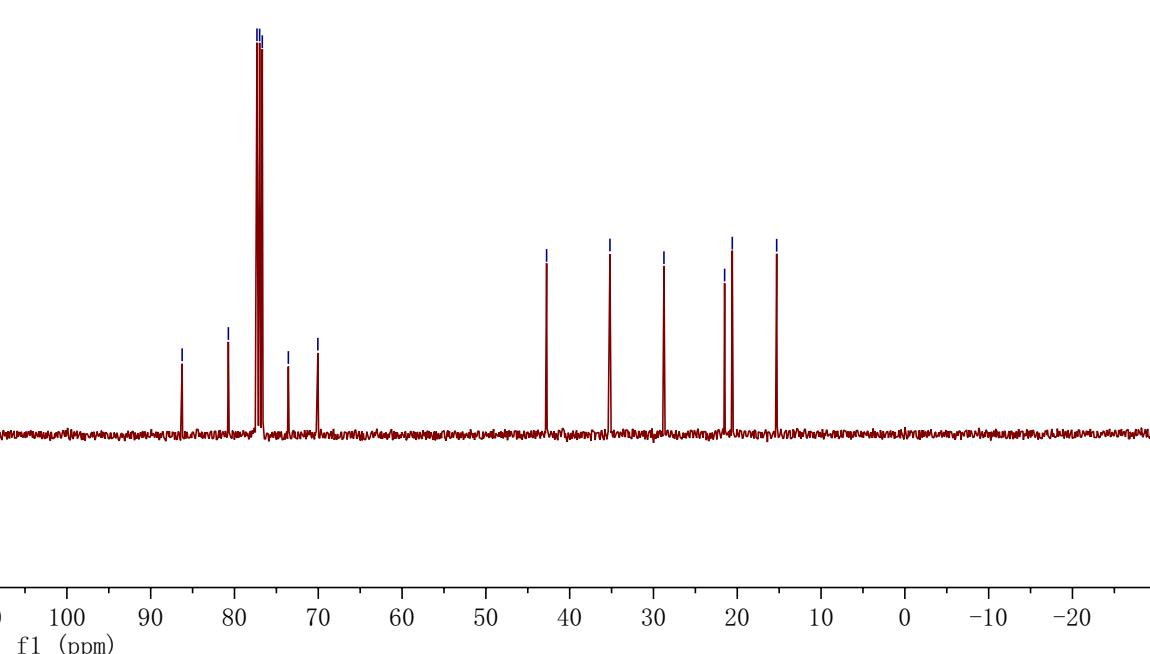
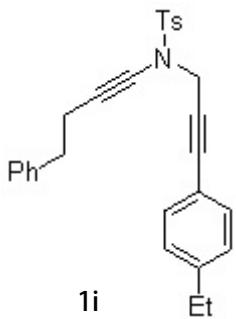
Analysis:  $^{13}\text{C}$  NMR

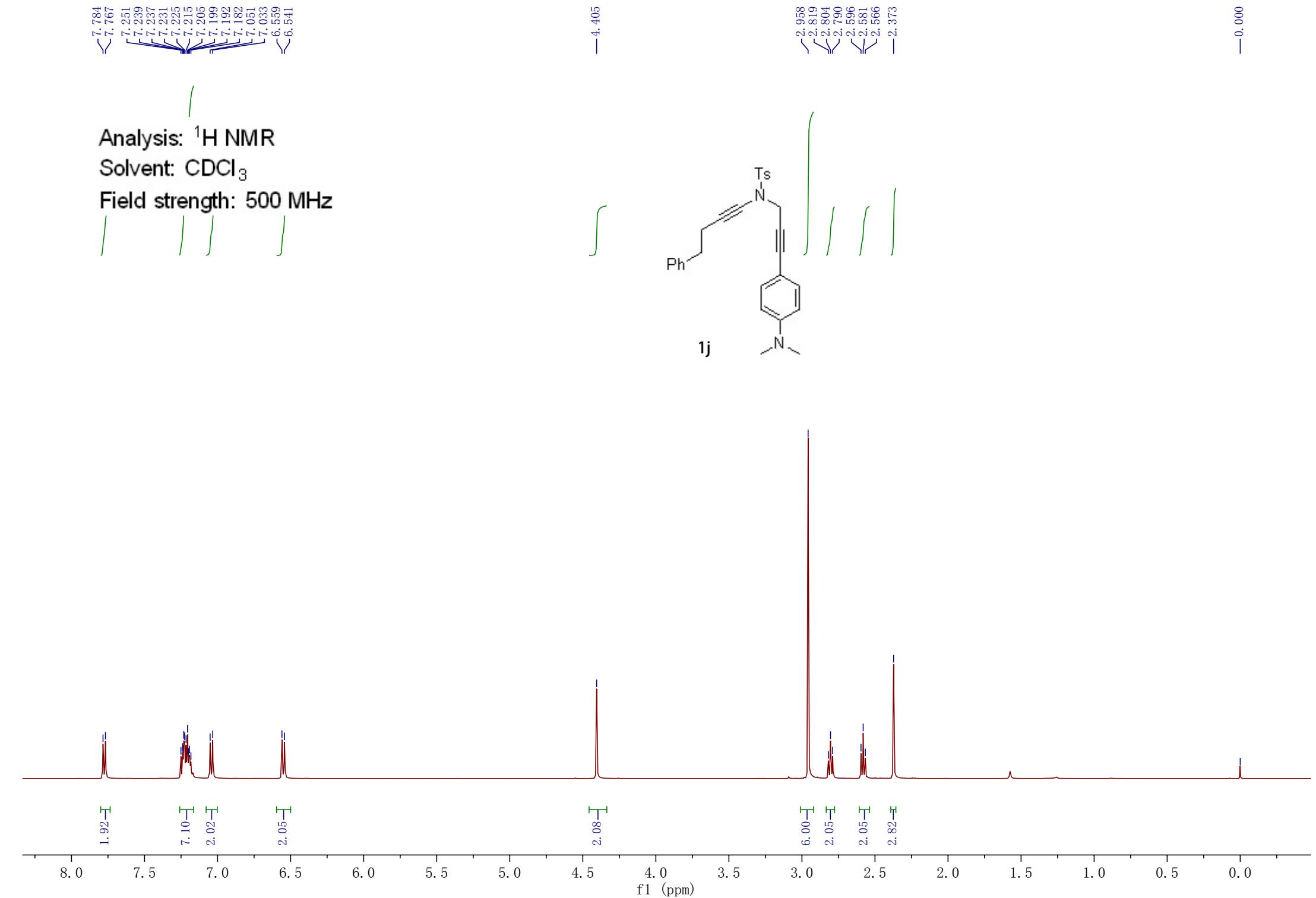
Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



—134.44  
—131.61  
—129.39  
—128.44  
—128.28  
—128.12  
—127.63  
—126.14  
—119.30  
—144.94  
—144.37  
—140.53  
—134.44  
—131.61  
—129.39  
—128.44  
—128.28  
—128.12  
—127.63  
—126.14  
—119.30  
—86.25  
—80.73  
—77.32  
—77.00  
—76.68  
—73.57  
—70.05  
—42.75  
—35.19  
—28.75  
—21.51  
—20.59  
—15.30



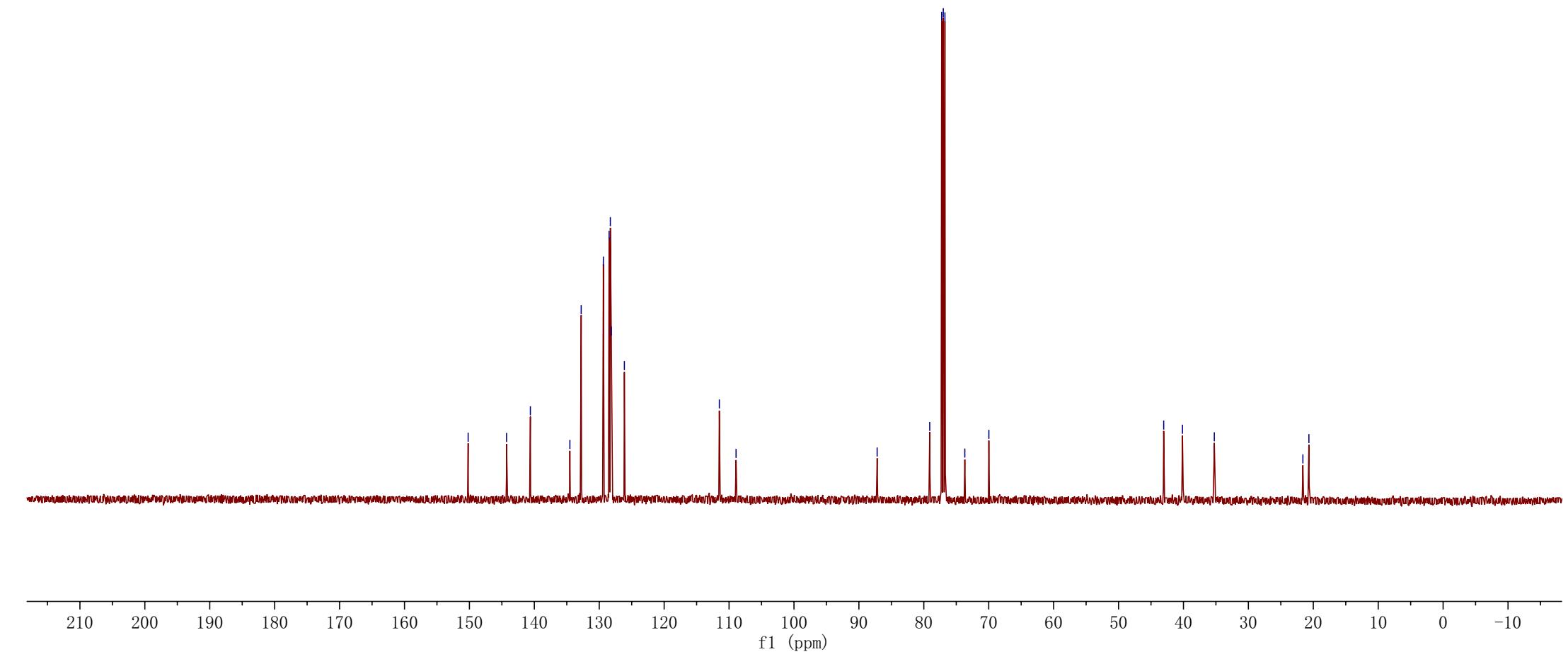
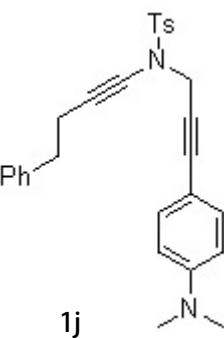


— 150.20  
— 144.28  
— 140.61  
— 134.52  
— 132.78  
— 129.36  
— 128.48  
— 128.29  
— 128.14  
— 126.13  
— 111.50  
— 108.92  
— 87.19  
— 79.09  
— 77.25  
— 77.00  
— 76.75  
— 73.68  
— 69.98  
— 43.04  
— 40.15  
— 35.25  
— 21.60  
— 20.68

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



7.755  
7.736  
7.336  
7.319  
7.301  
7.253  
7.233  
7.207  
7.187  
7.168  
7.152  
6.961  
6.941

6.584  
6.564

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

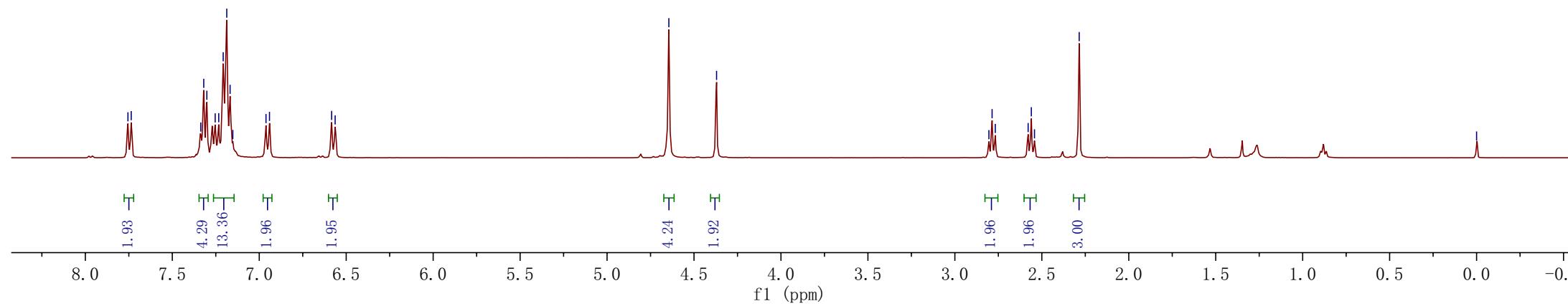
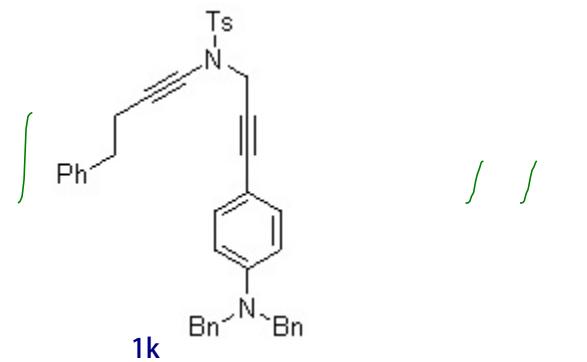
Field strength: 400 MHz



—4.645  
—4.370

2.804  
2.786  
2.768  
2.579  
2.560  
2.542  
—2.285

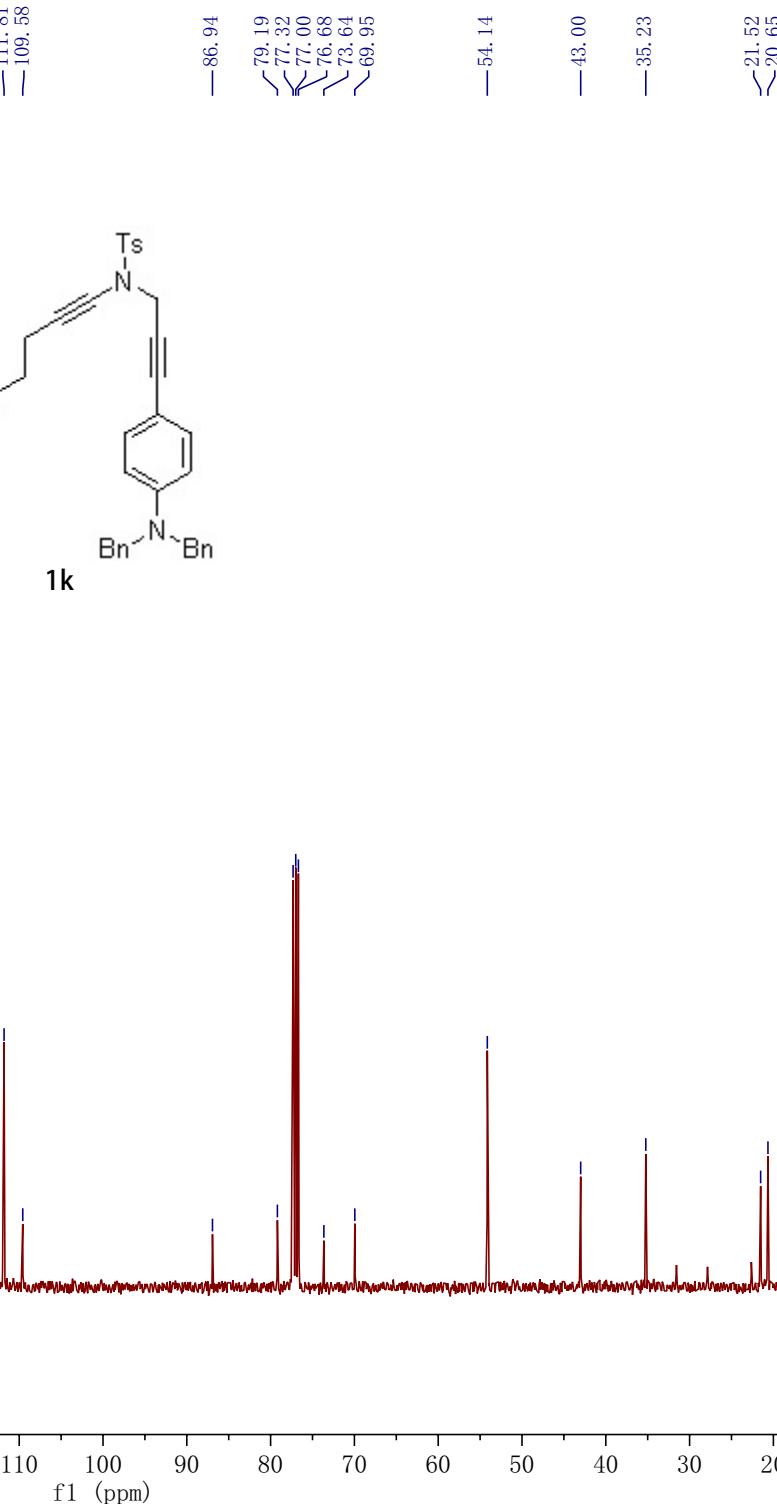
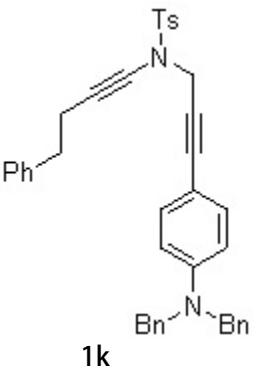
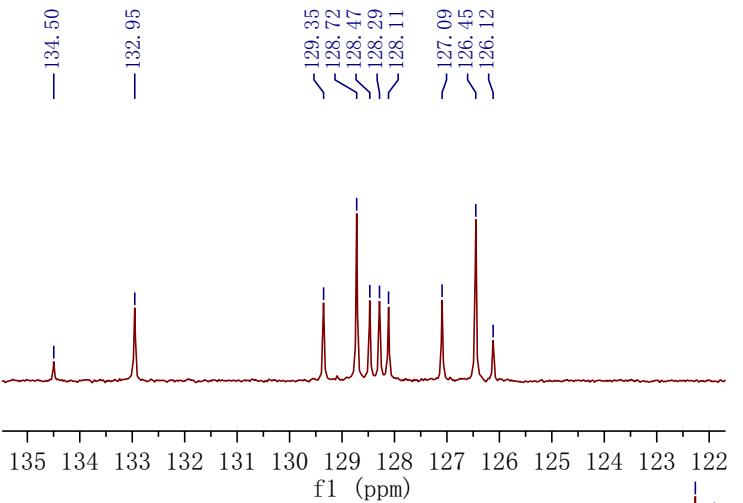
—0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.774  
7.753

7.236  
7.224

7.219  
7.200

7.182  
7.116

7.095  
7.057

7.036

-4.395

2.824  
2.806

2.788  
2.608

2.590  
2.572

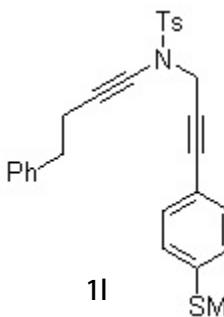
2.464  
2.357

-0.000

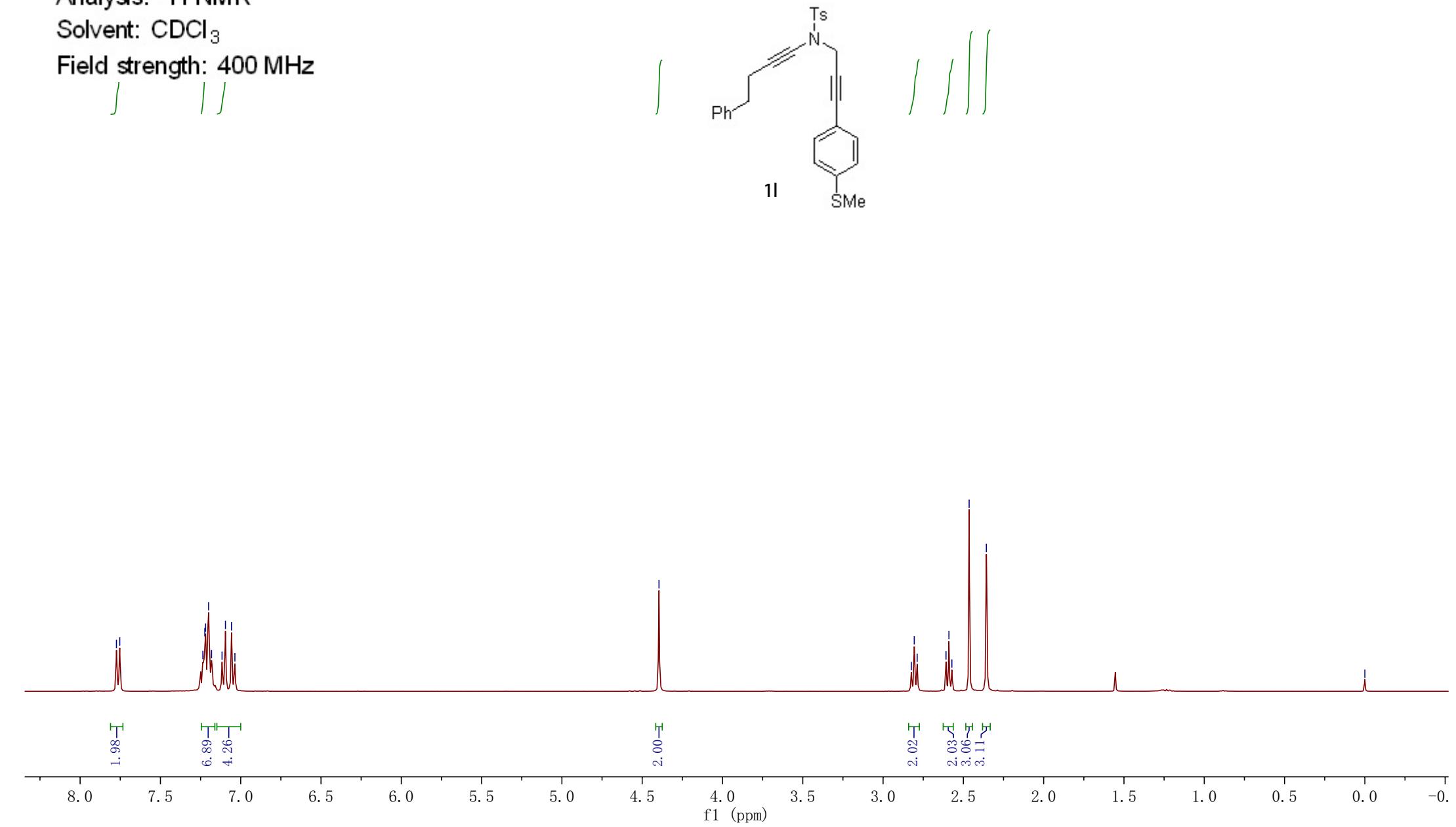
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



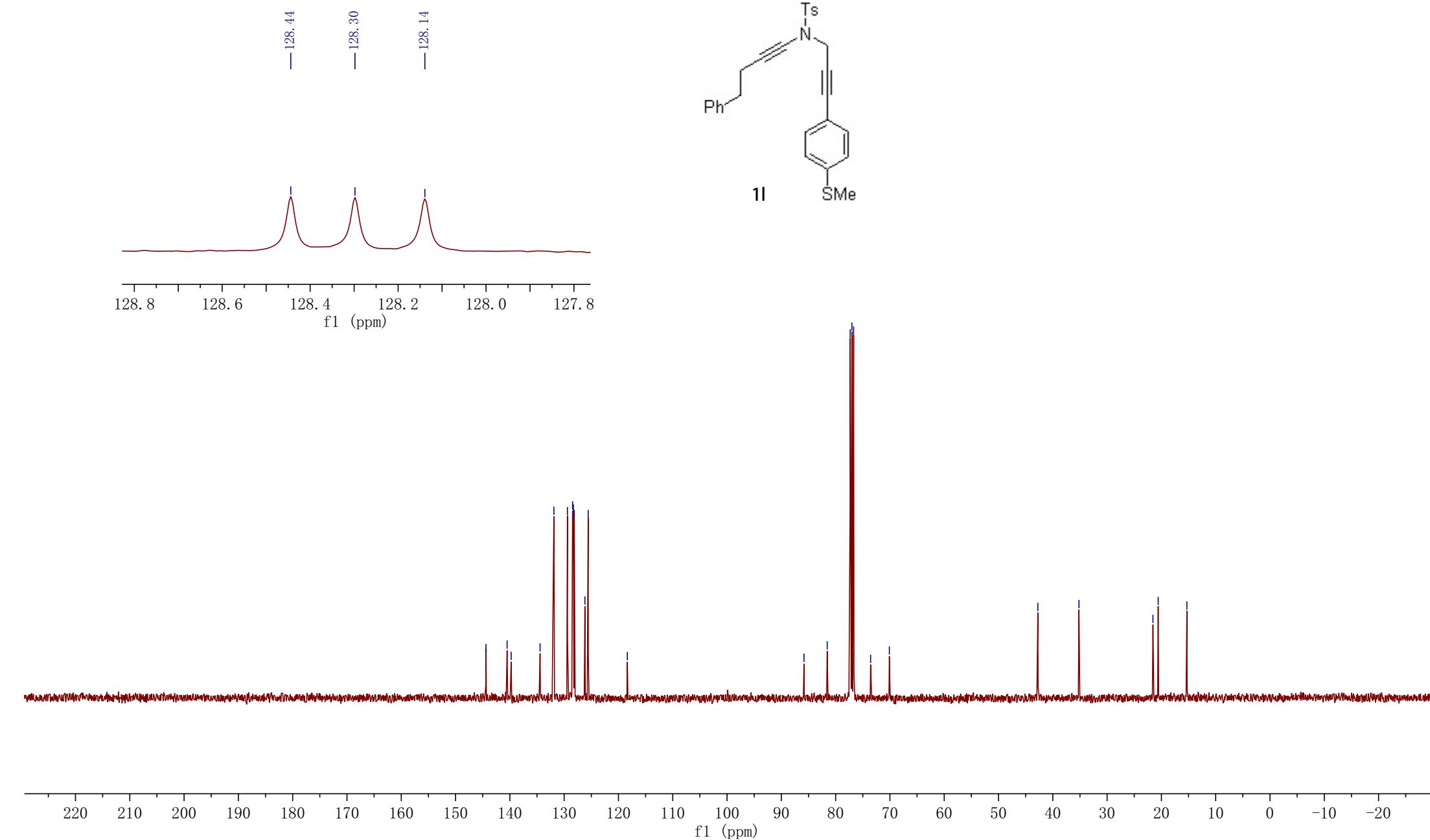
II



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.780  
<7.759  
7.309  
7.273  
7.262  
7.243  
7.230  
7.227  
7.213  
7.199  
7.183  
7.170  
7.142  
7.124

—4.405

2.828  
2.809  
2.791  
2.612  
2.594  
2.575  
—2.339

—0.000

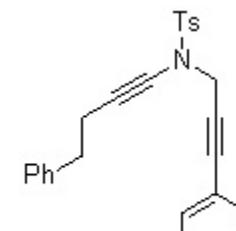
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

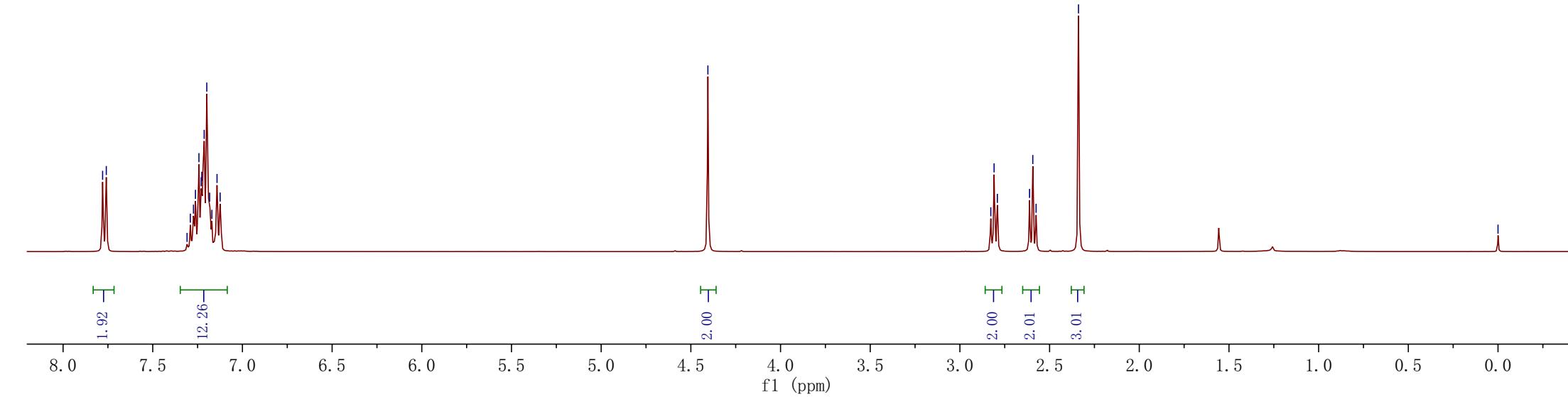
Field strength: 400 MHz

ʃ ʃ

ʃ ʃ ʃ



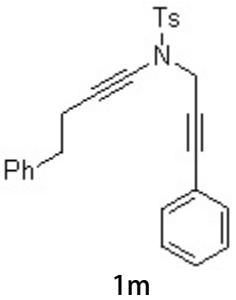
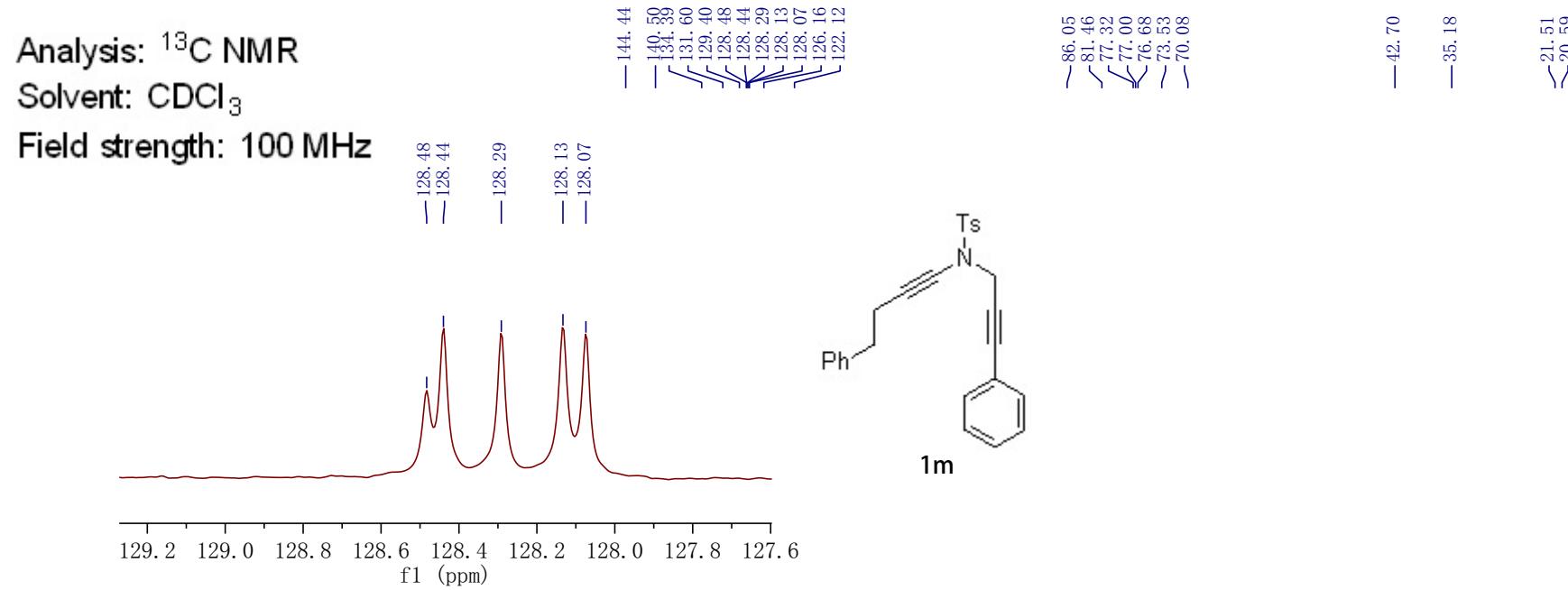
1m



### Analysis: $^{13}\text{C}$ NMR

Solvent: CDCl<sub>3</sub>

Field strength: 100 MHz



7.773  
7.753  
7.252  
7.246  
7.234  
7.224  
7.217  
7.201  
7.182  
7.177  
7.158  
7.135  
7.130  
7.121  
7.113  
7.105  
7.100  
6.963  
6.942  
6.920

-4.385

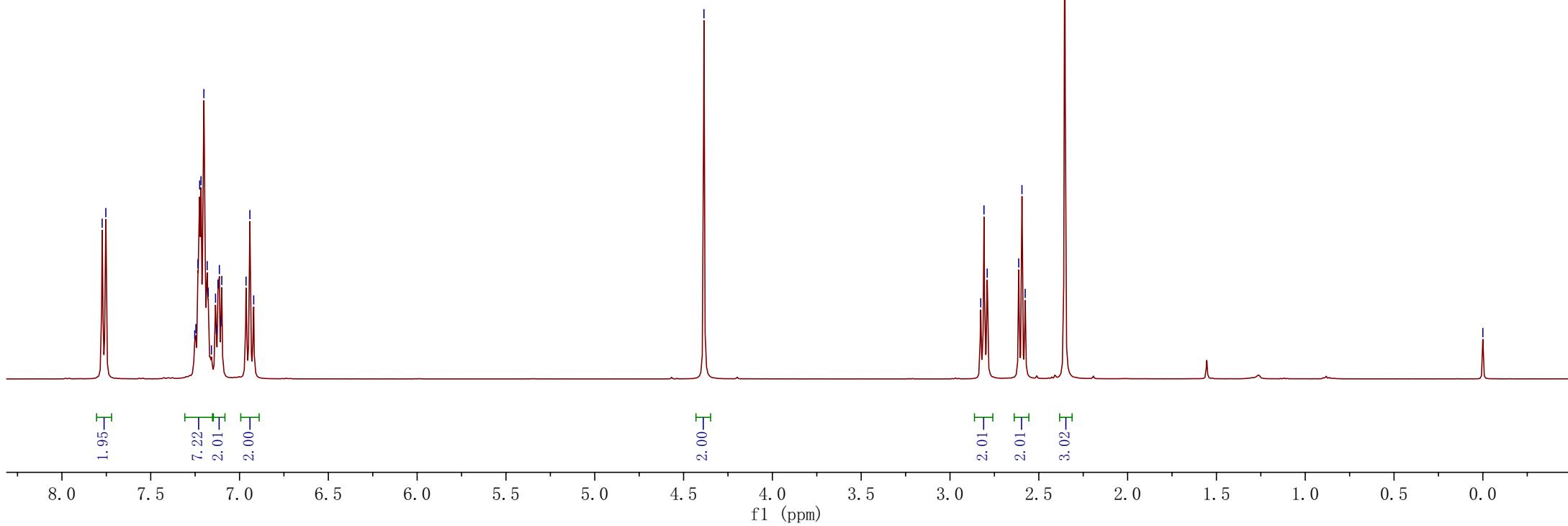
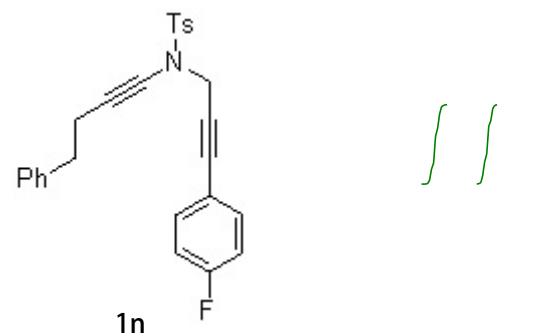
2.827  
2.809  
2.791  
2.613  
2.595  
2.577  
-2.354

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

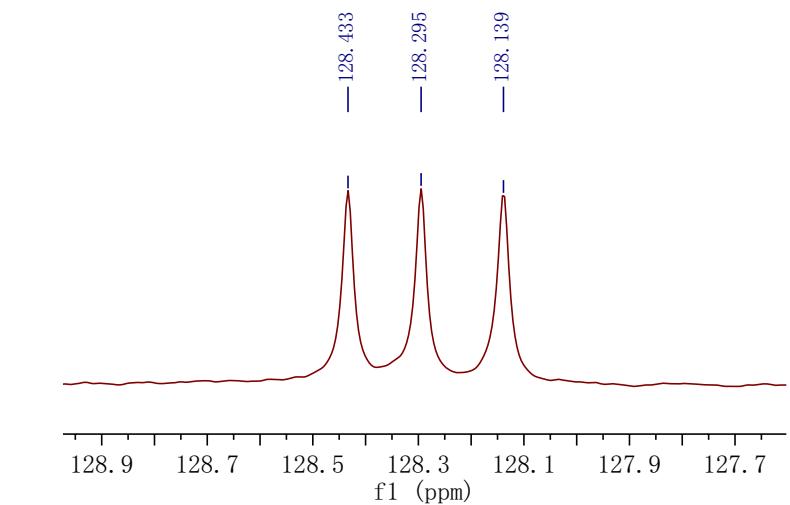
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

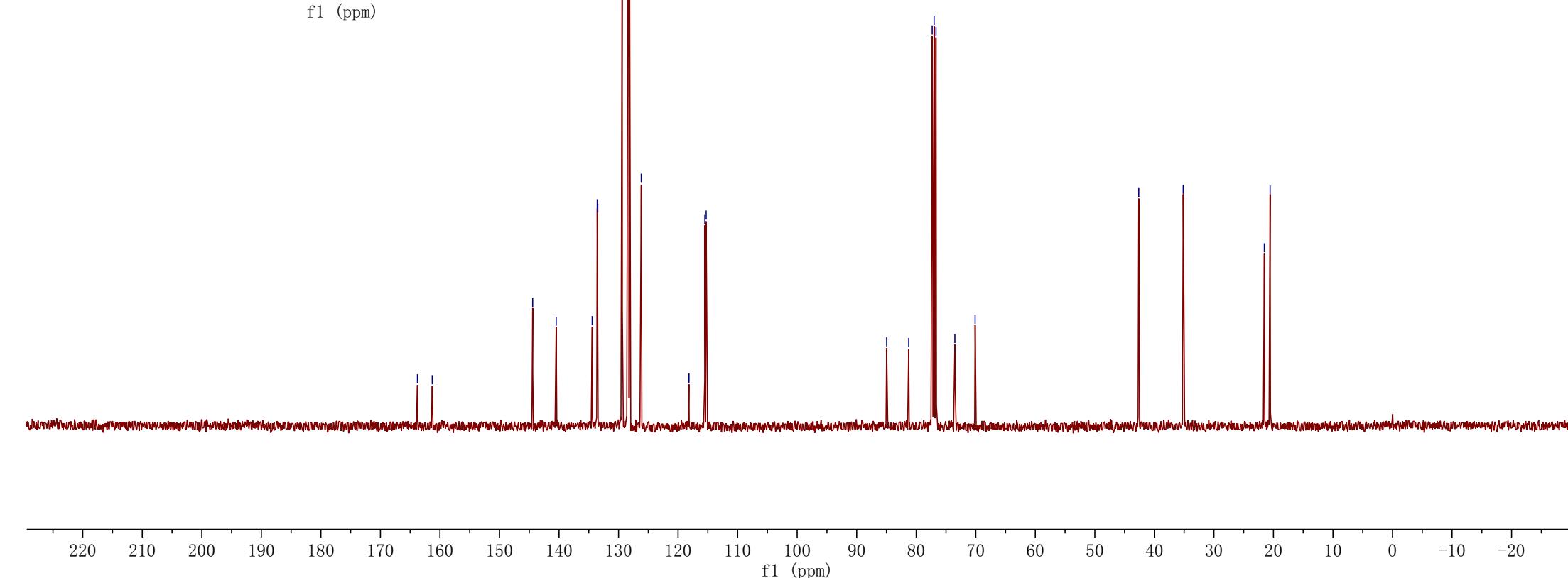
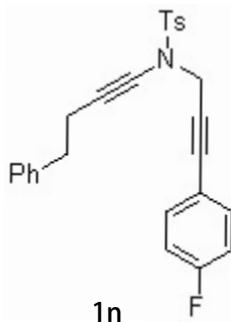


— 144.426  
— 140.478  
— 134.428  
— 133.581  
— 133.498  
— 129.392  
— 128.433  
— 128.295  
— 128.139  
— 126.185  
— 118.213  
— 118.178  
— 115.502  
— 115.283

— 84.966  
— 81.262  
— 77.318  
— 77.000  
— 76.683  
— 73.512  
— 70.110

— 42.622  
— 35.155

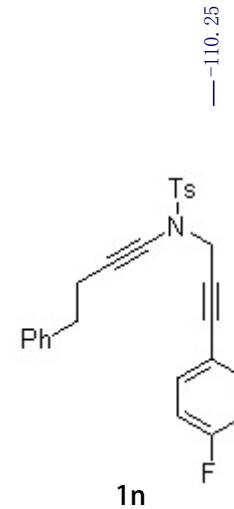
— 21.529  
— 20.560



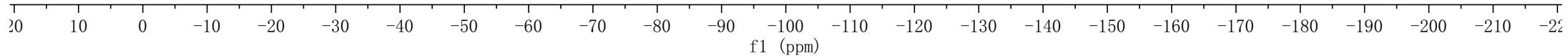
Analysis:  $^{19}\text{F}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz



— -110.25



<7.765  
<7.744  
7.248  
7.227  
7.212  
7.206  
7.194  
7.176  
7.057  
7.036

-4.382

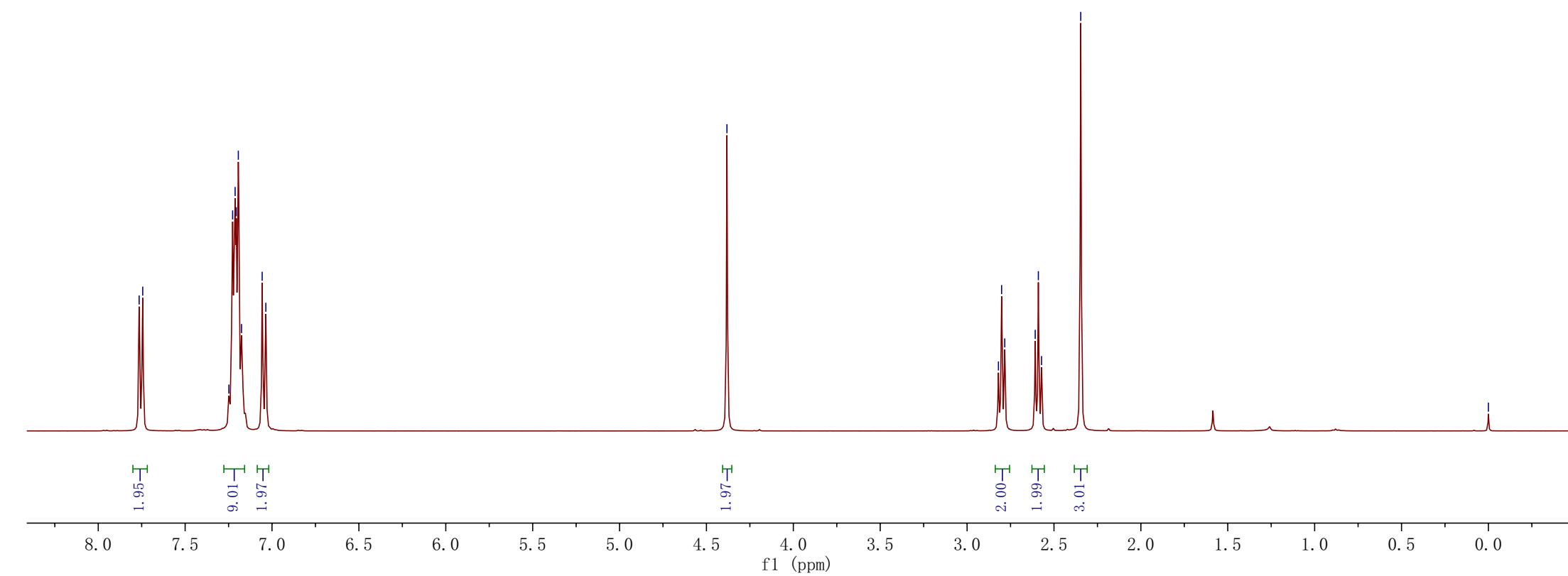
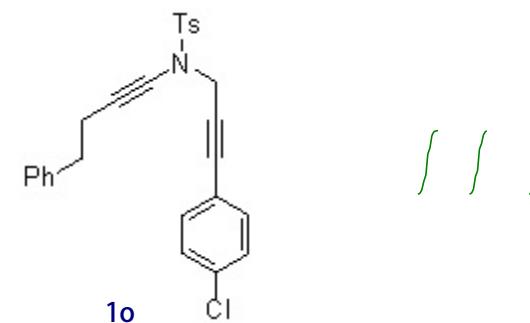
2.820  
2.801  
2.783  
2.608  
2.590  
2.572  
2.346

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

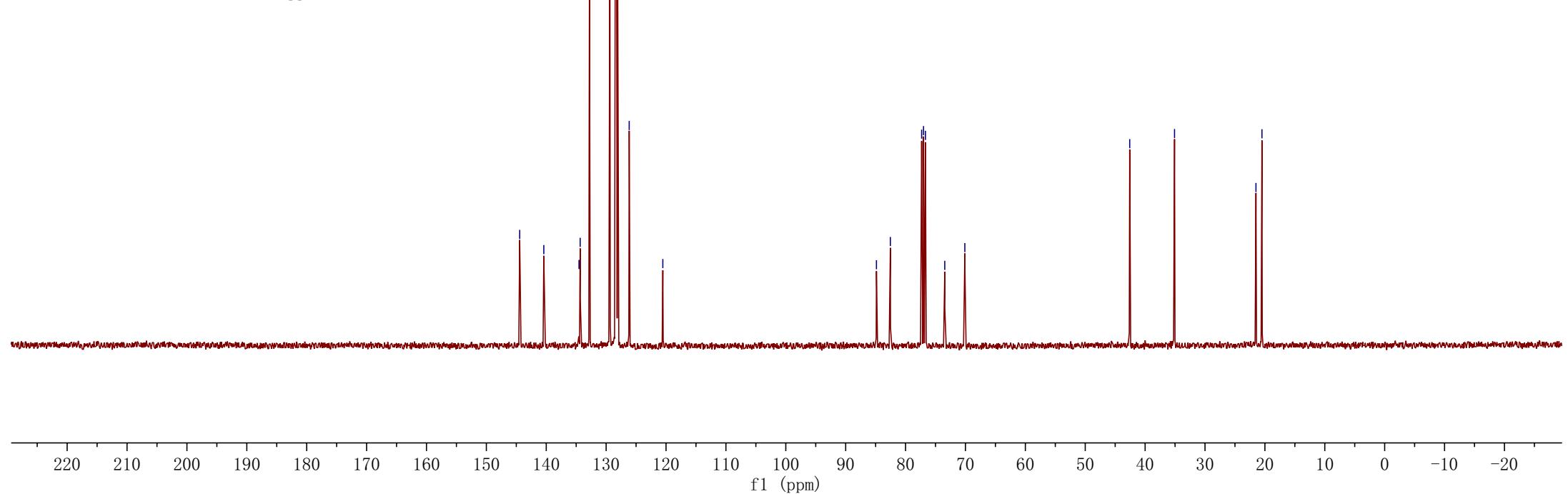
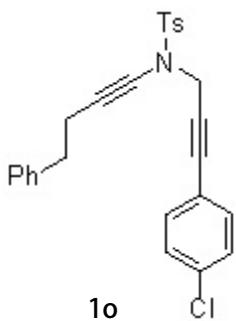
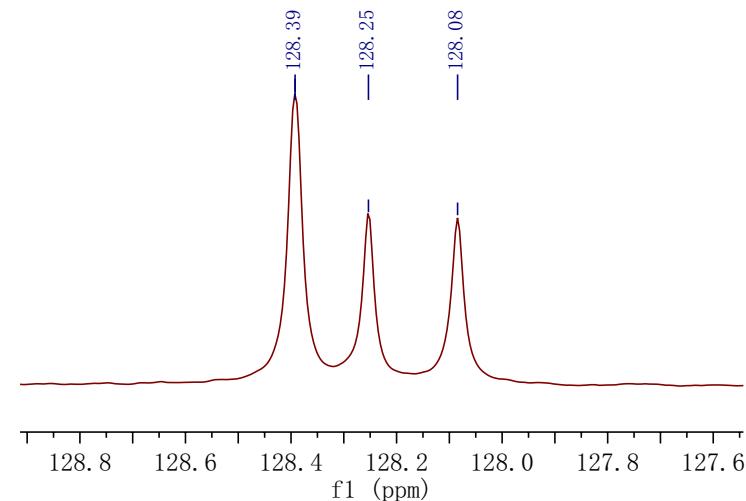
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.766  
7.746  
7.394  
7.373  
7.256  
7.251  
7.236  
7.198  
7.180  
7.162  
6.994  
6.973

—4.382

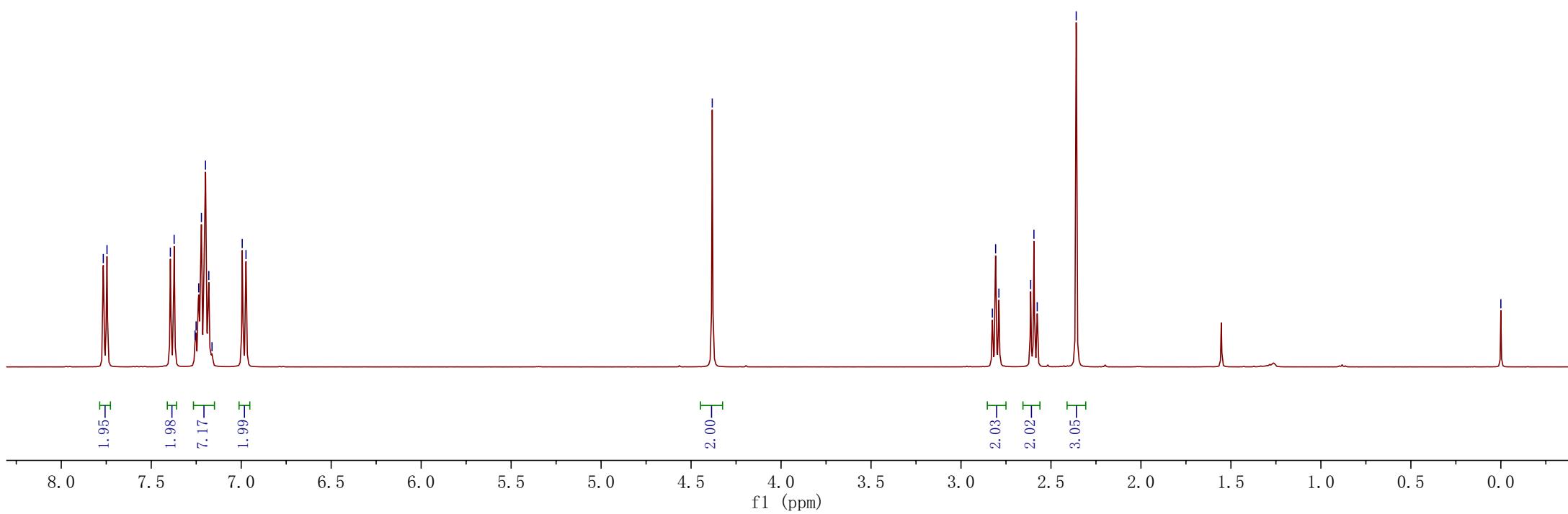
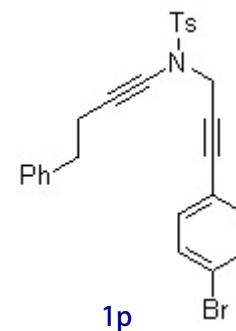
2.826  
2.808  
2.789  
2.613  
2.595  
2.576  
—2.360

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

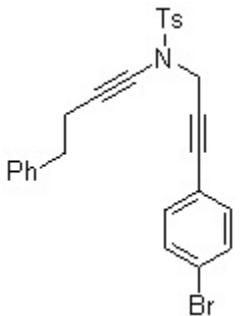
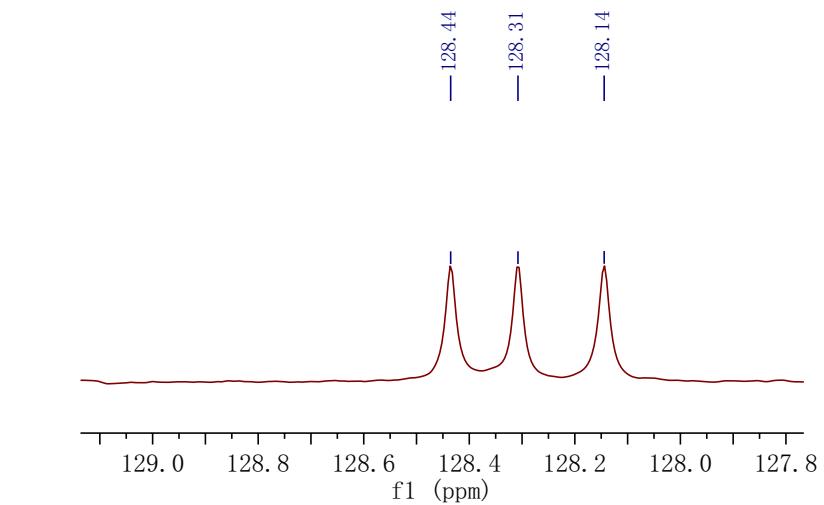
Field strength: 400 MHz



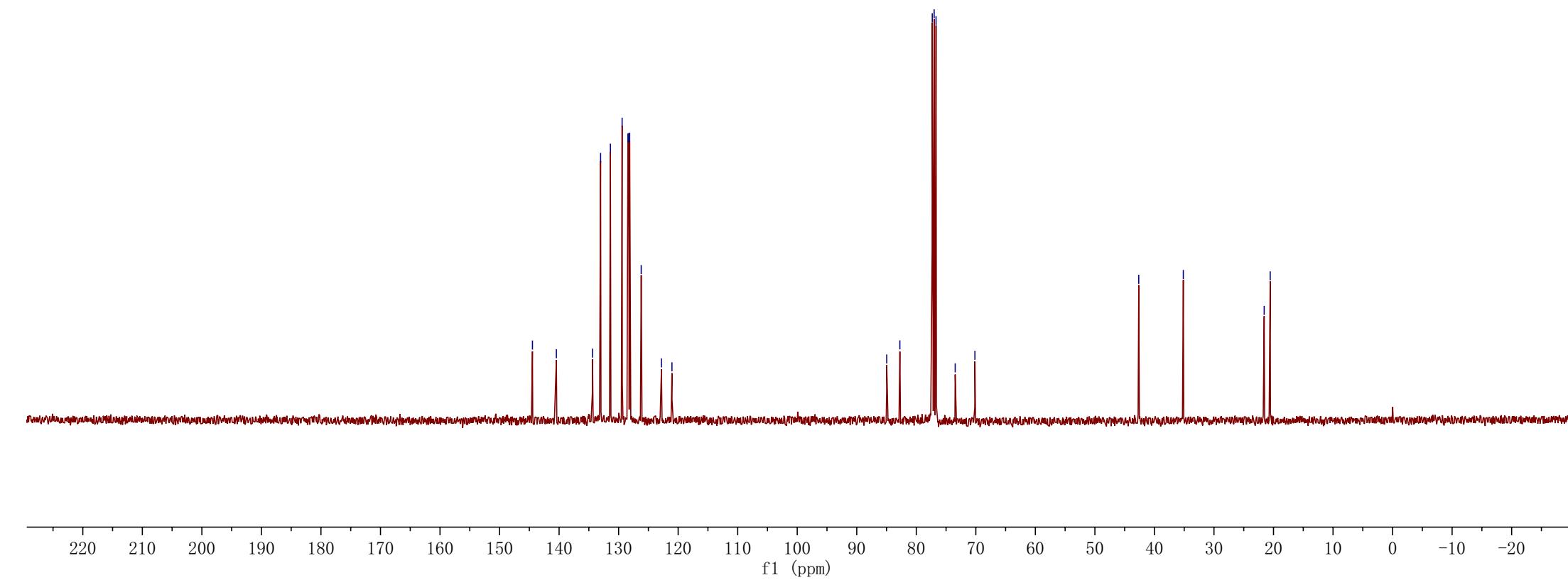
Analysis:  $^{13}\text{C}$  NMR

Solvent: CDCl<sub>3</sub>

Field strength: 100 MHz



1 p



<7.931  
<7.910  
<7.772  
<7.752

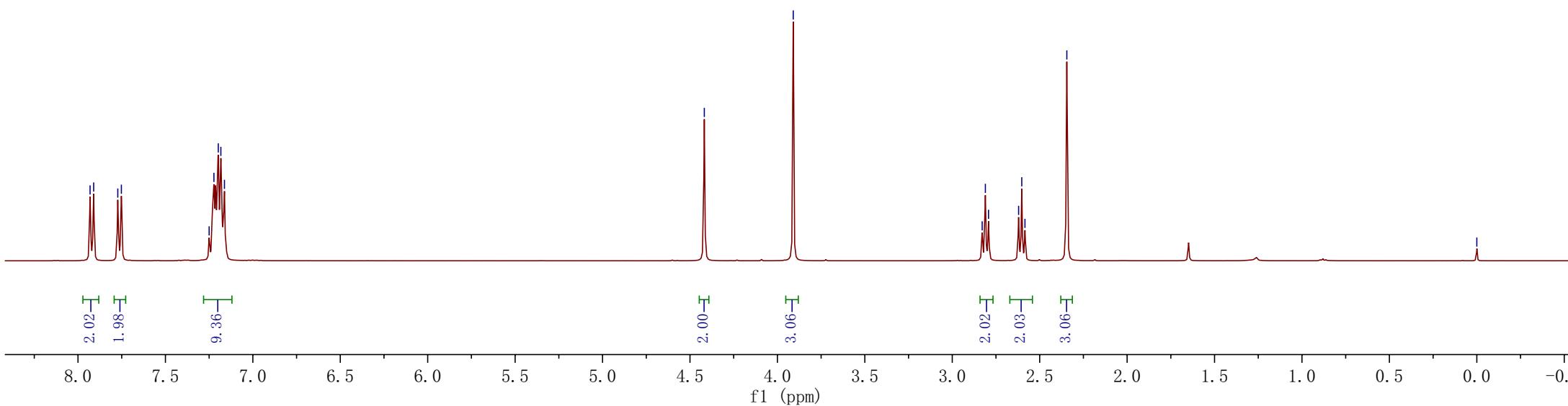
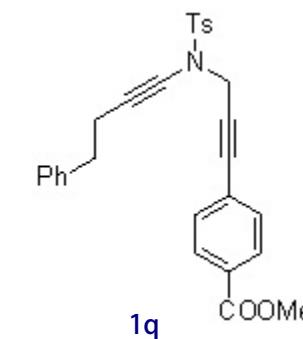
7.250  
7.223  
7.198  
7.183  
7.162

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

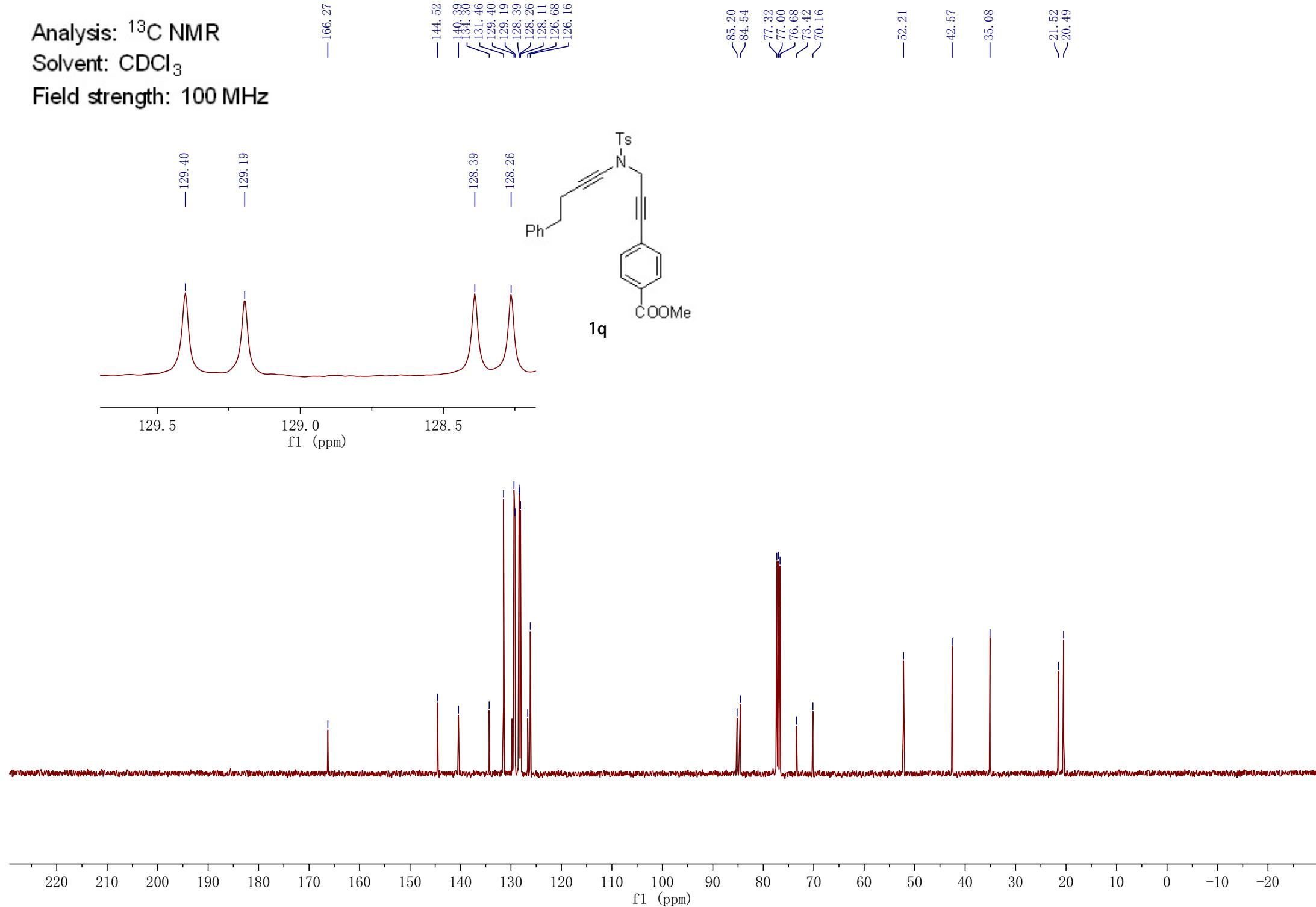
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



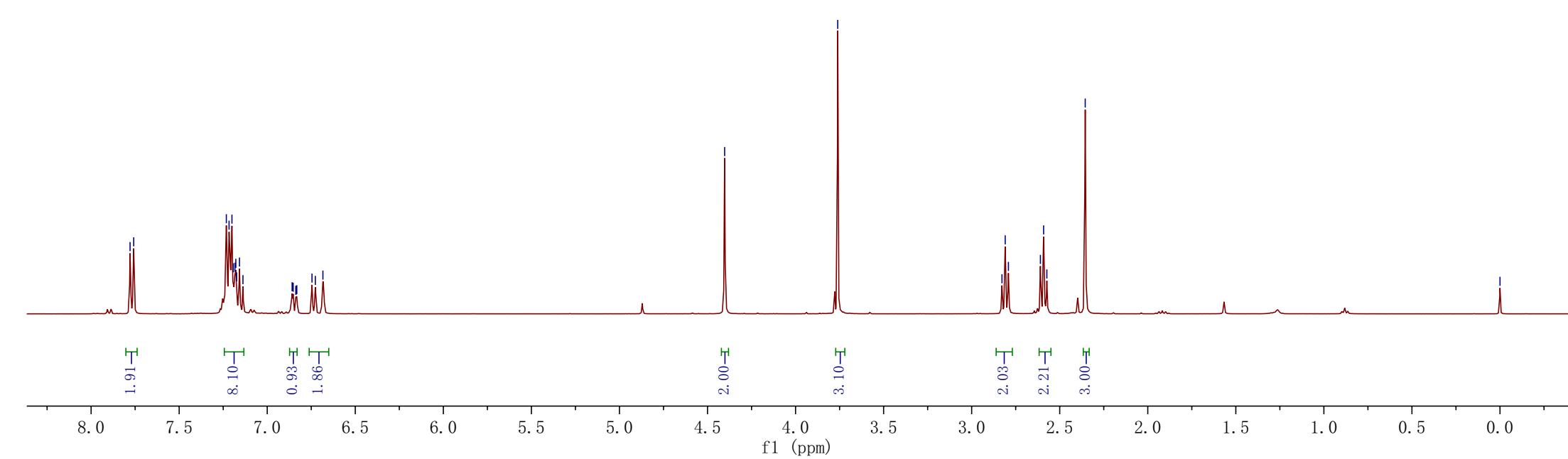
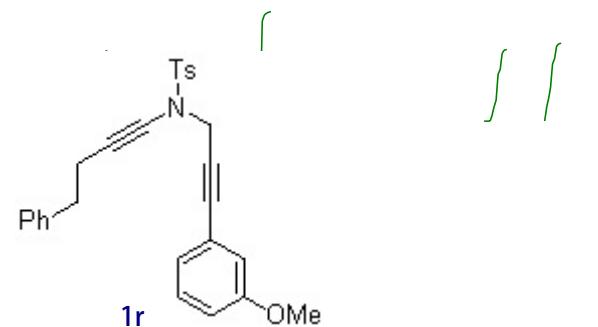
7.779  
7.758  
7.232  
7.217  
7.200  
7.193  
7.183  
7.178  
7.174  
7.158  
7.138  
6.859  
6.853  
6.838  
6.832  
6.746  
6.727  
6.684

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

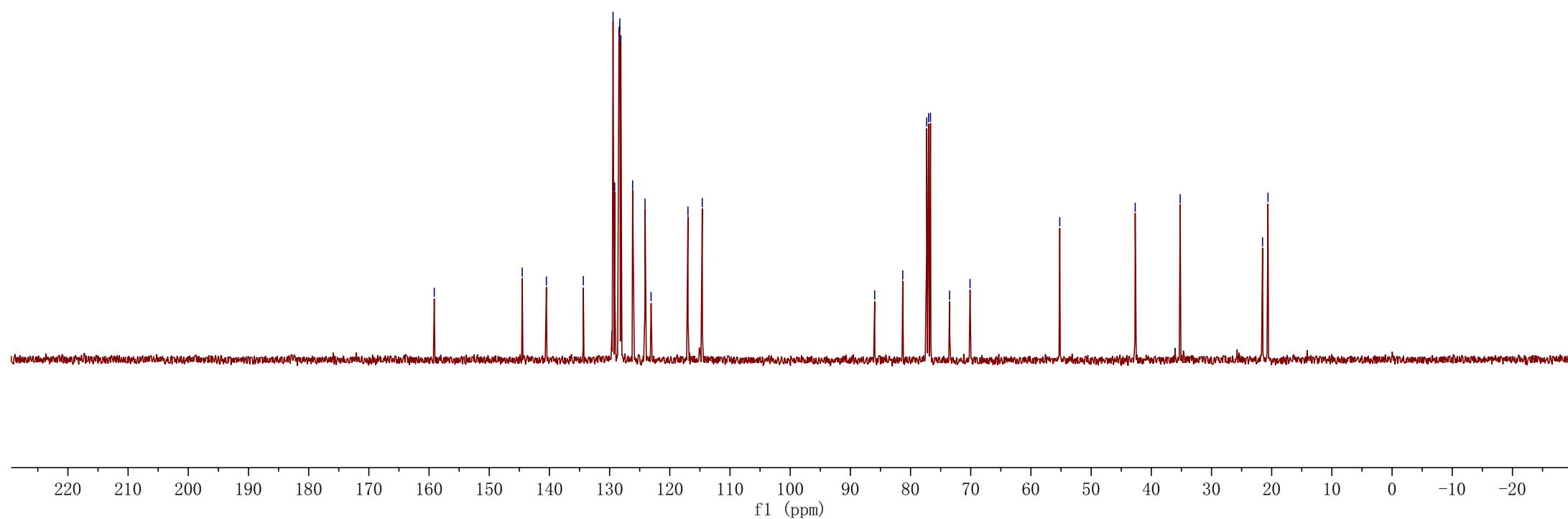
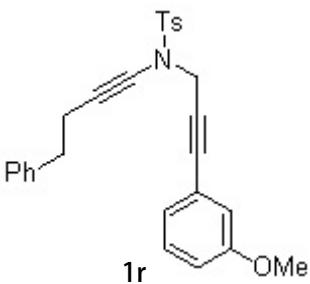
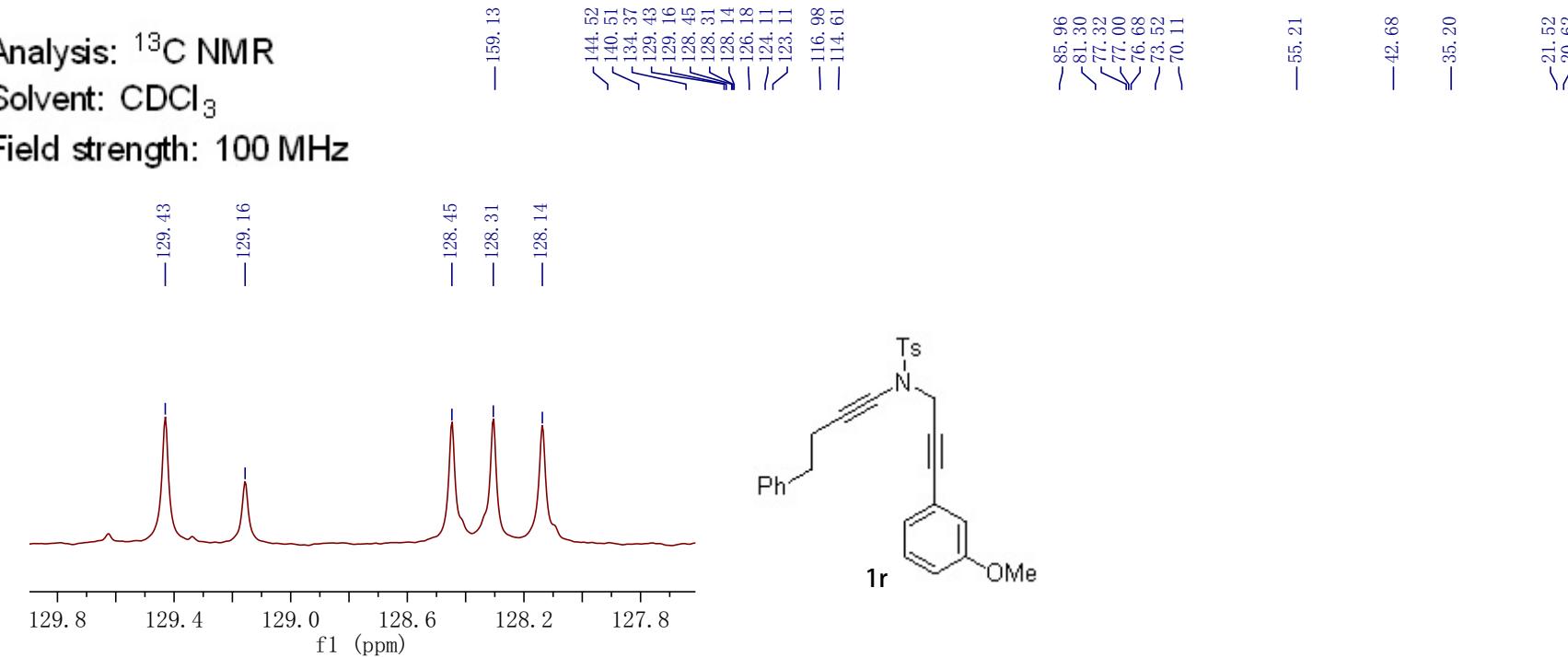
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.782  
<7.761  
7.241  
7.229  
7.213  
7.208  
7.200  
7.191  
7.183  
7.171  
7.155  
7.136  
7.118  
7.107  
7.088  
6.959  
6.936

-4.402

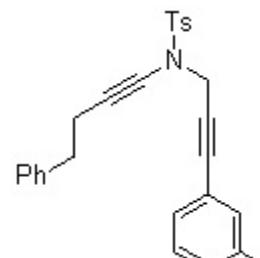
<2.828  
<2.809  
<2.791  
<2.609  
<2.591  
<2.572  
-2.354  
-2.292

-0.000

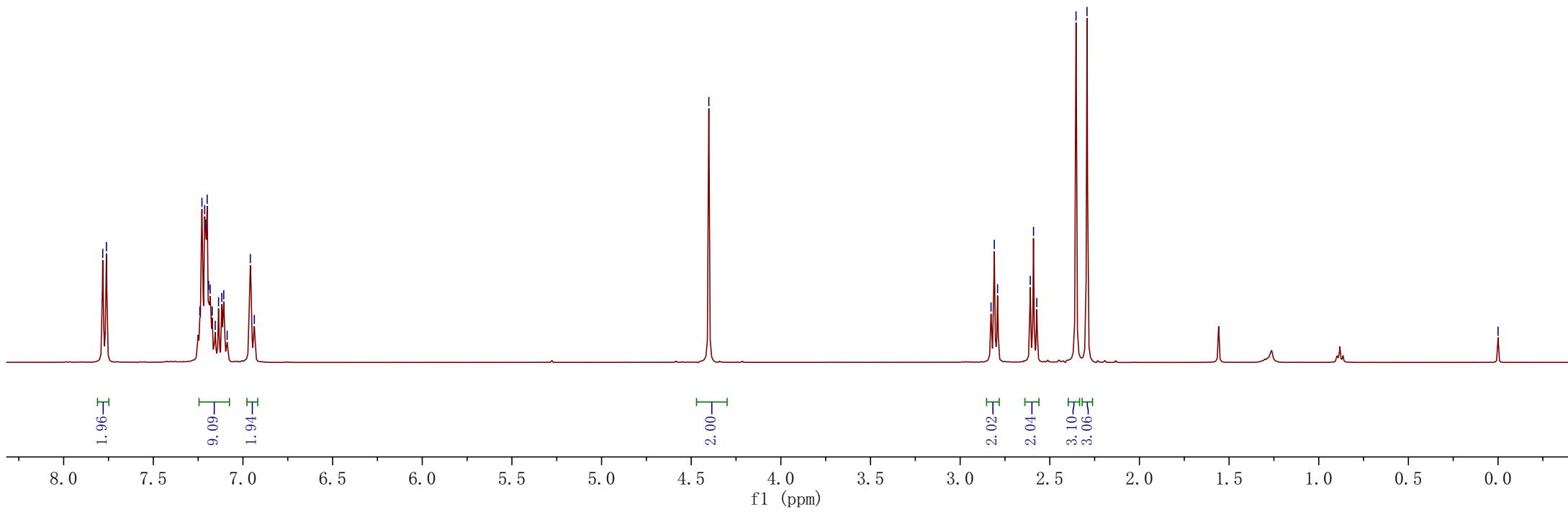
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



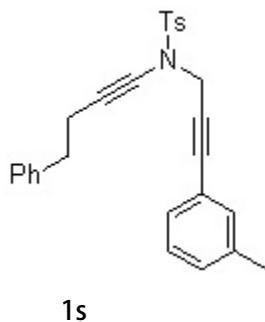
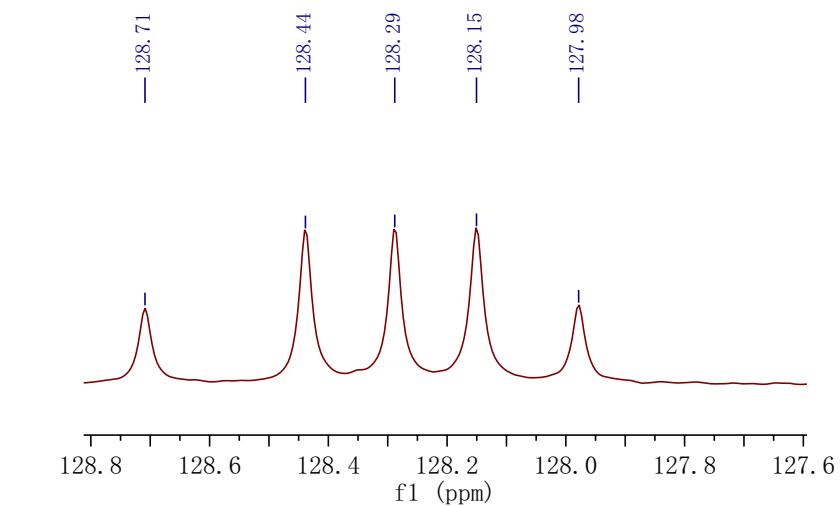
1s



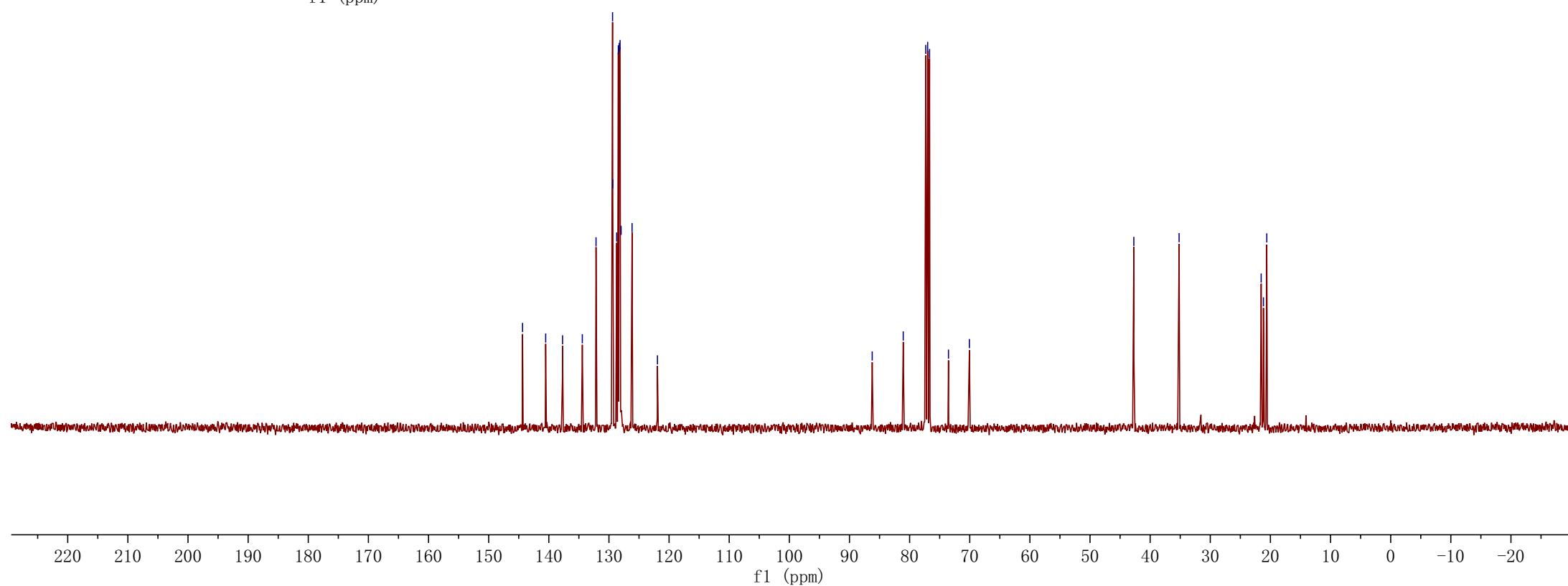
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**1s**



< 7.772  
< 7.751  
< 7.438  
< 7.434  
< 7.430  
< 7.419  
< 7.415  
< 7.411  
< 7.248  
< 7.225  
< 7.204  
< 7.185  
< 7.164  
< 7.141  
< 7.122  
< 7.103  
< 7.089  
< 7.073  
< 7.070

-4.400

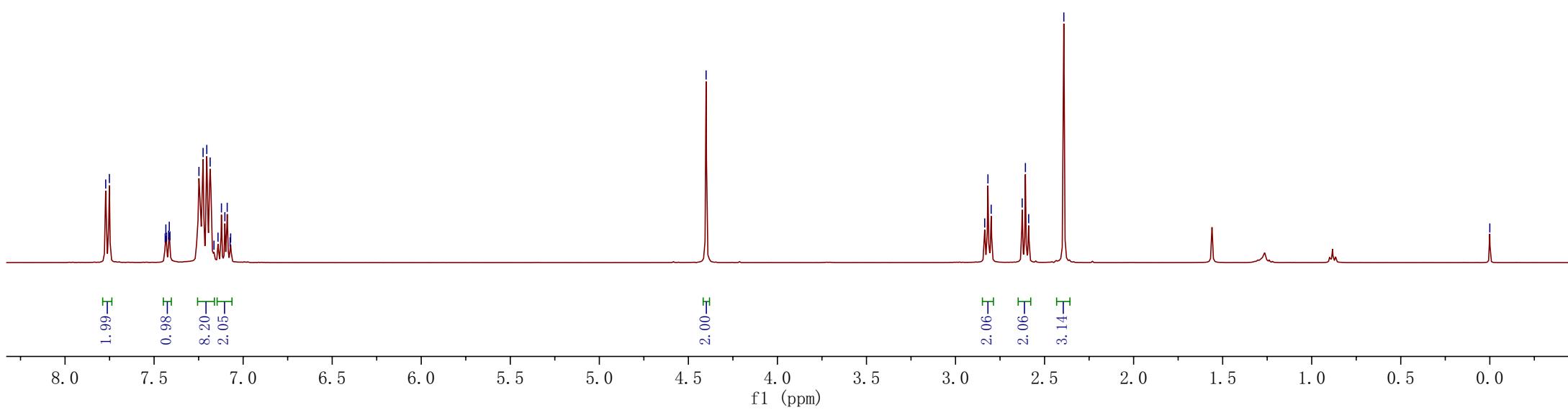
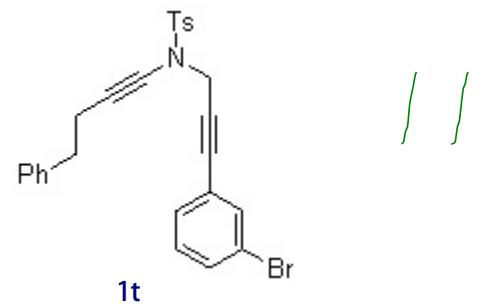
< 2.836  
< 2.818  
< 2.800  
< 2.626  
< 2.608  
< 2.589  
< 2.392

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

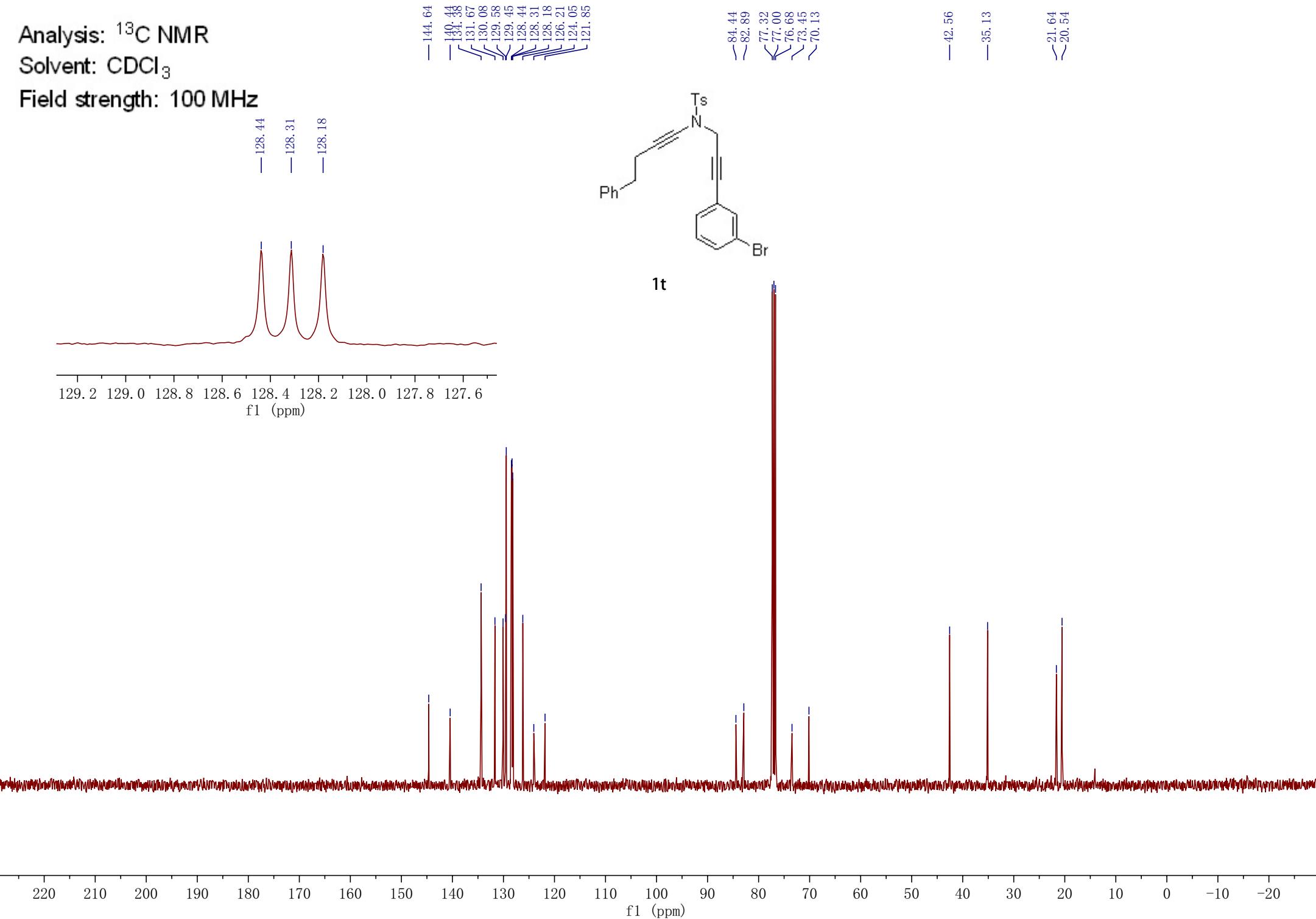
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



< 7.785  
7.764  
7.254  
7.236  
7.217  
7.201  
7.194  
7.184  
7.174  
7.157  
6.800  
6.796  
6.779  
6.775  
6.750  
6.736  
6.732

-4.401

> 3.871  
> 3.821

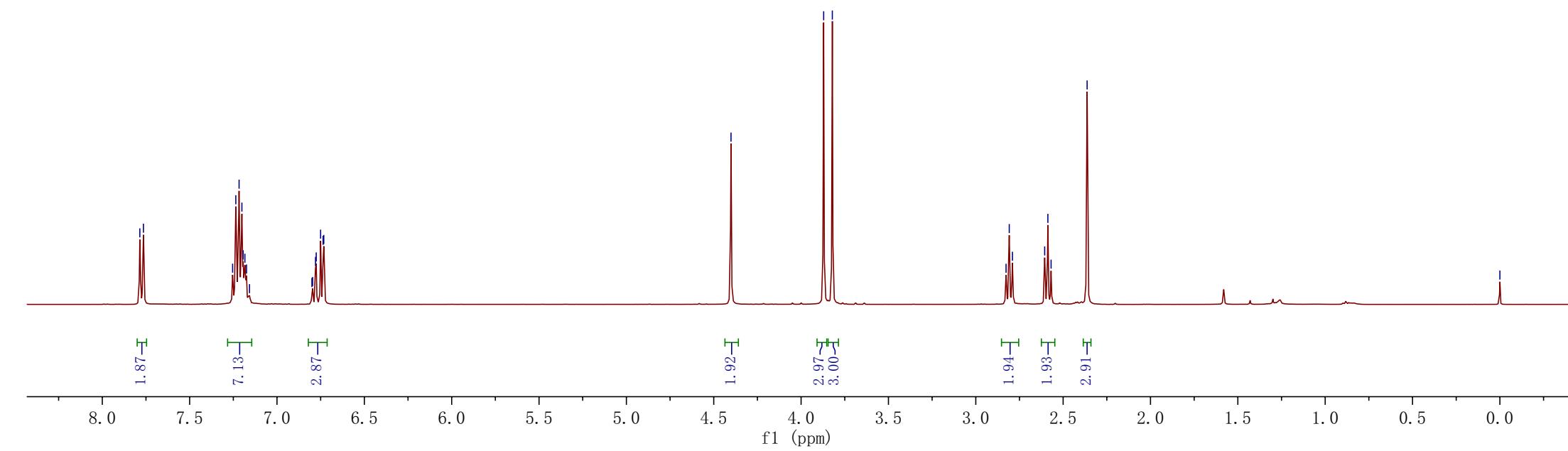
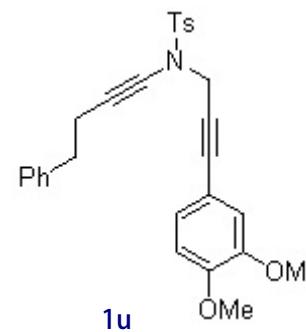
< 2.827  
< 2.808  
< 2.790  
< 2.606  
< 2.587  
< 2.569  
< 2.363

--0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

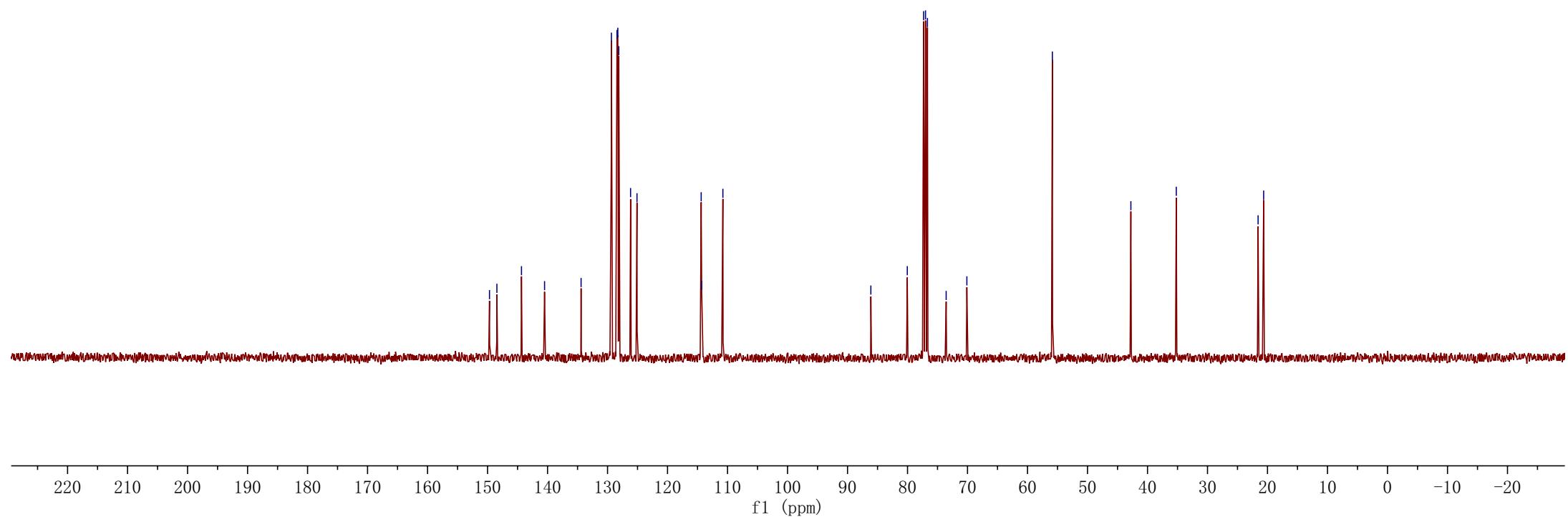
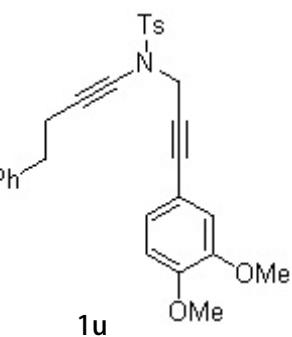
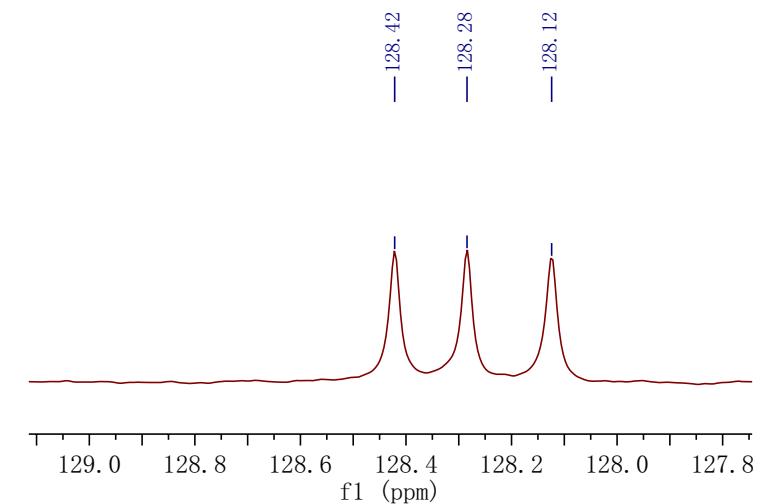
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.782  
7.762  
7.250  
7.231  
7.213  
7.198  
7.181  
7.173  
7.155  
7.017  
7.014  
6.996  
6.993  
6.918  
6.690  
6.668

—4.390

—3.806

2.823  
2.805  
2.786  
2.603  
2.584  
2.566  
—2.364

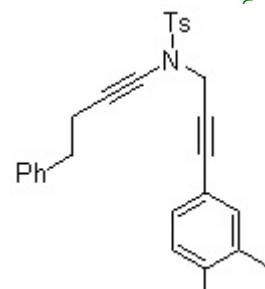
—2.149

—0.000

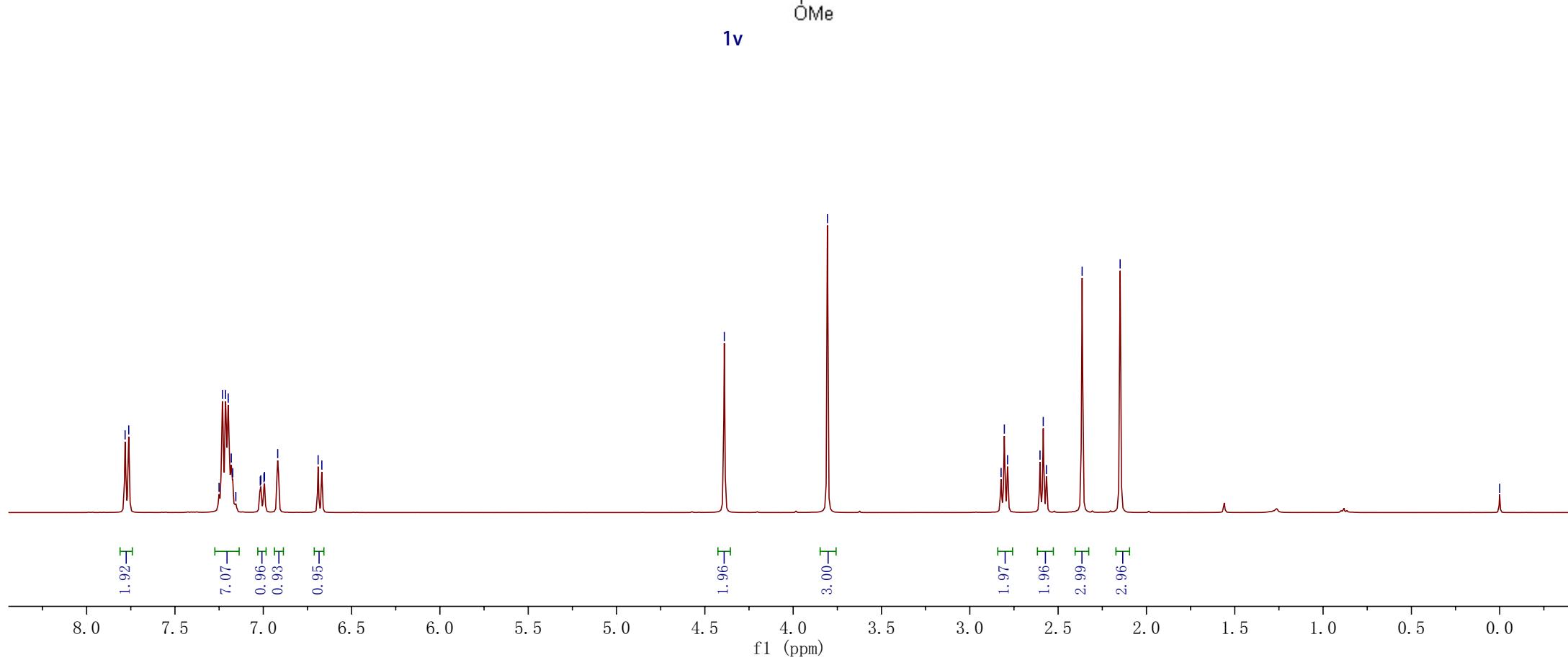
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



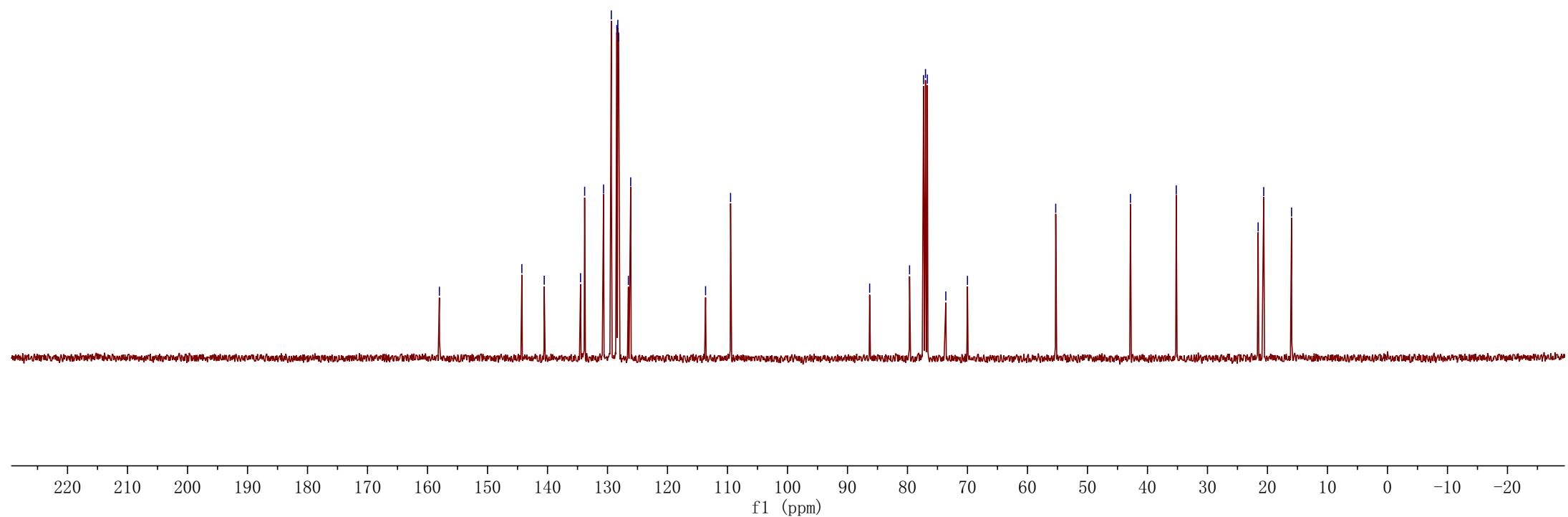
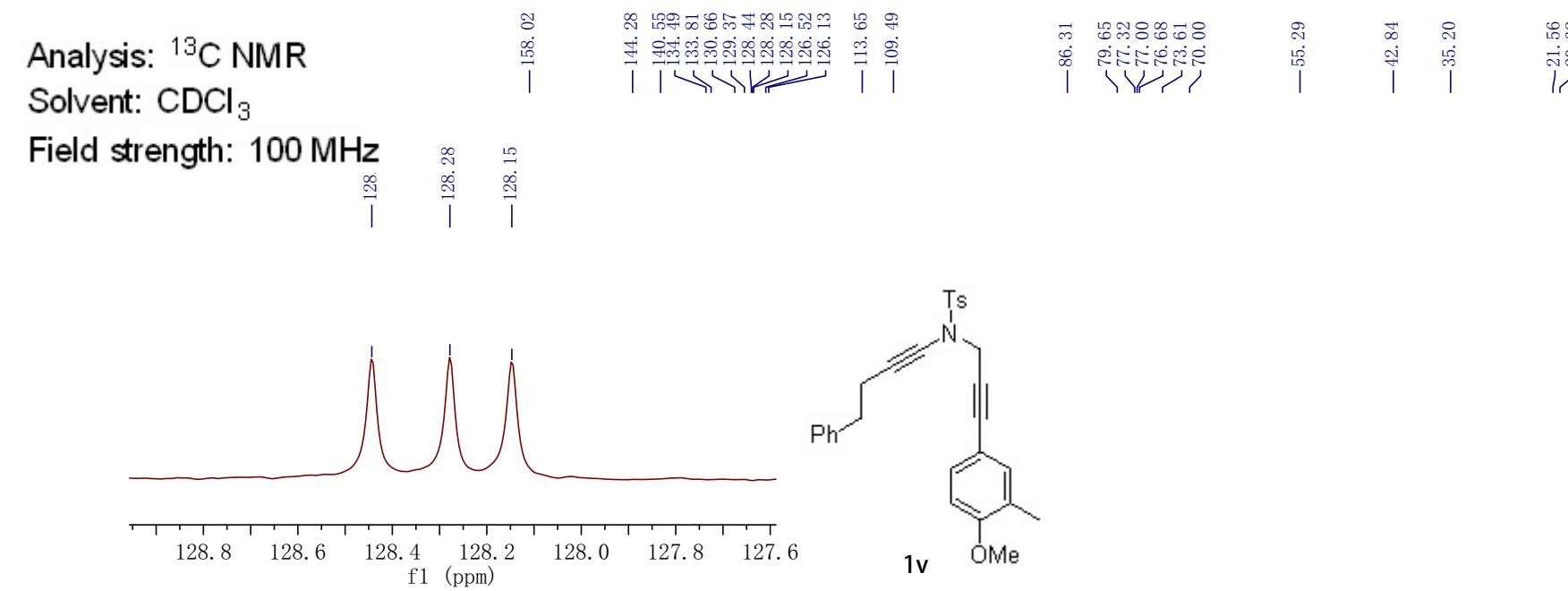
**1v**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.768  
7.747  
7.253  
7.235  
7.218  
7.197  
7.179  
7.175  
7.167  
7.163  
7.158

6.674  
6.672  
6.511

5.934

4.370

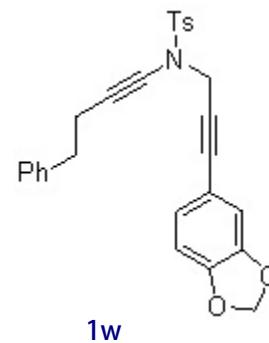
2.820  
2.801  
2.783  
2.605  
2.387  
2.569  
2.373

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

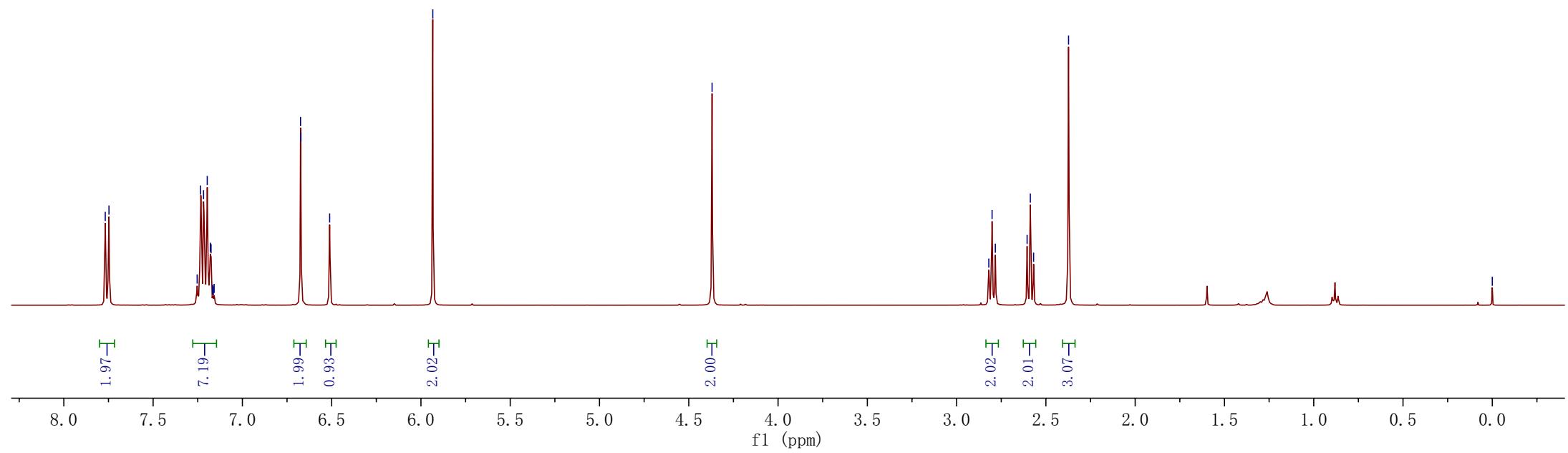
Field strength: 400 MHz



**1w**

{ { } }

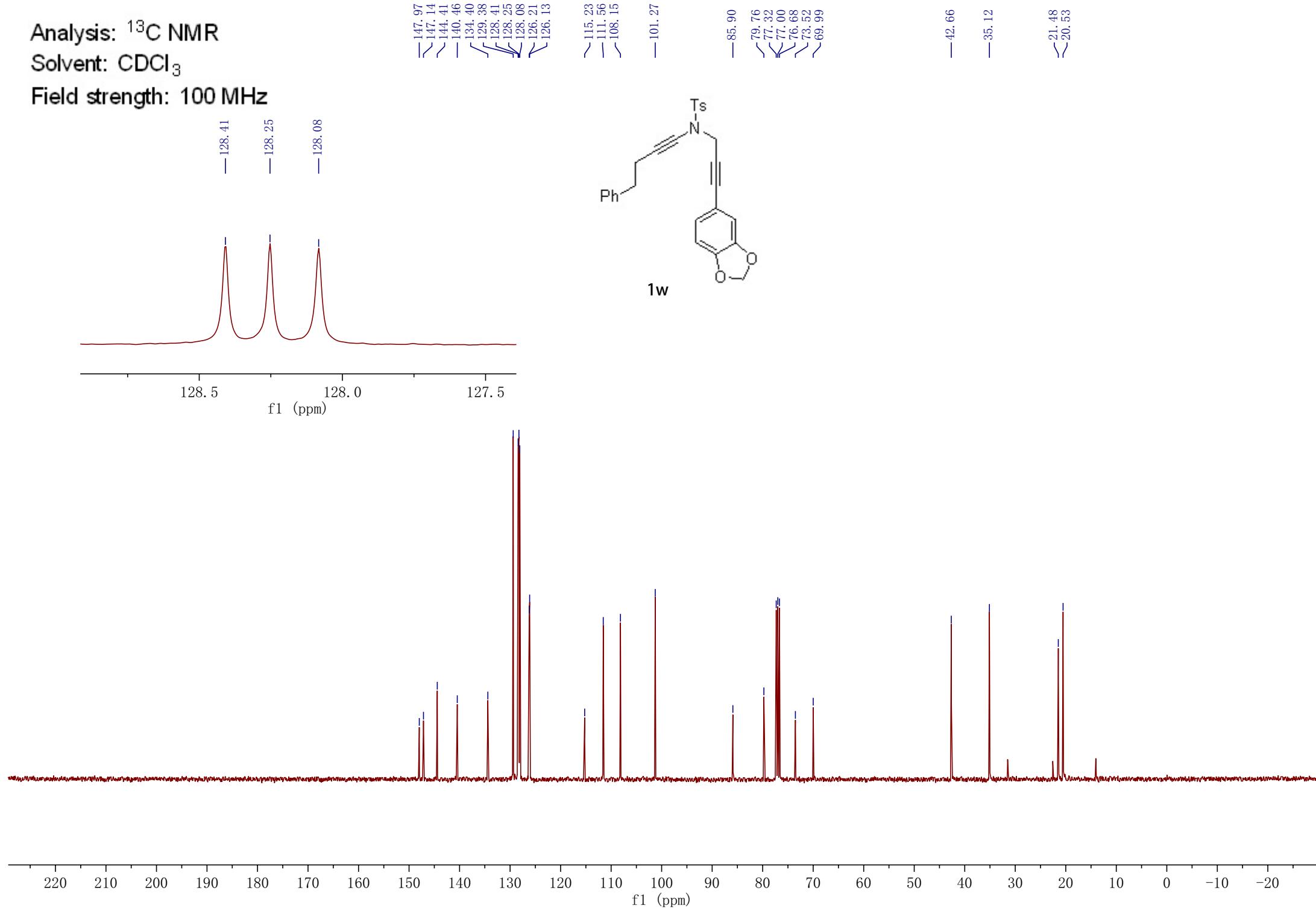
{ { } }



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.771  
7.750  
7.250  
7.237  
7.230  
7.229  
7.219  
7.219  
7.199  
7.182  
7.178  
7.178  
7.169  
7.165  
7.160  
7.002  
6.995  
6.932  
6.922  
6.919  
6.910

-4.420

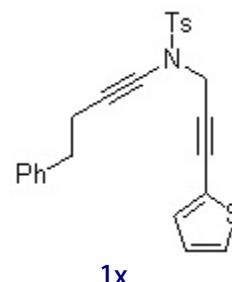
<2.827  
<2.808  
<2.790  
<2.605  
<2.587  
<2.568  
<2.376

--0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

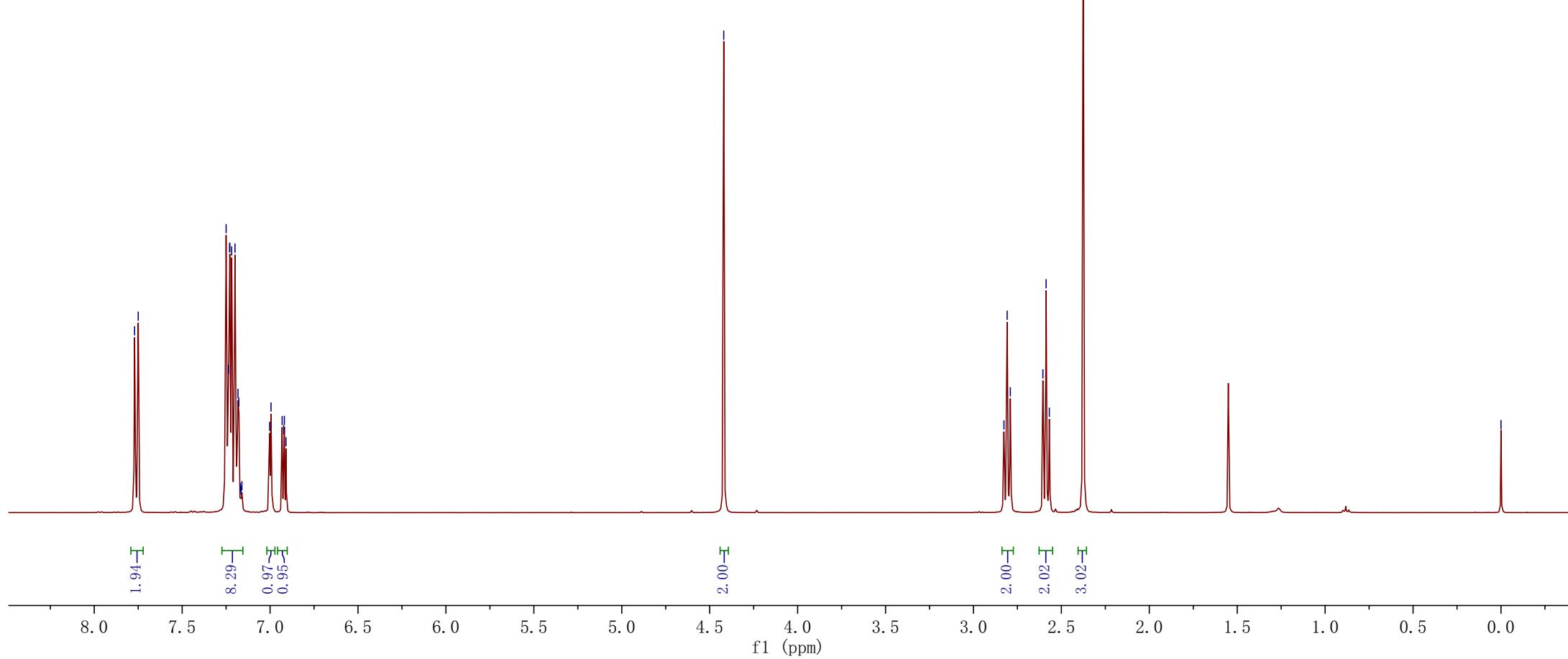
Field strength: 400 MHz



**1x**

{ { } }

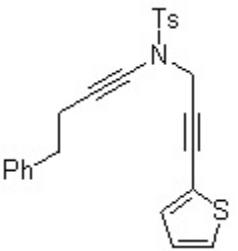
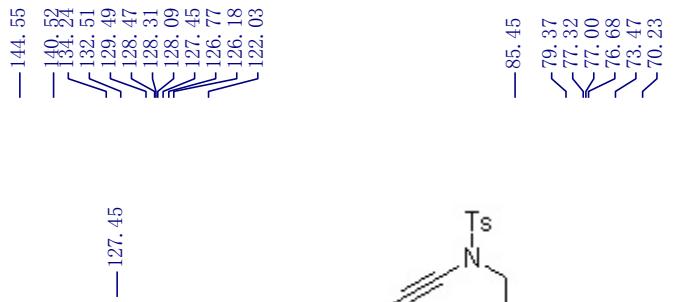
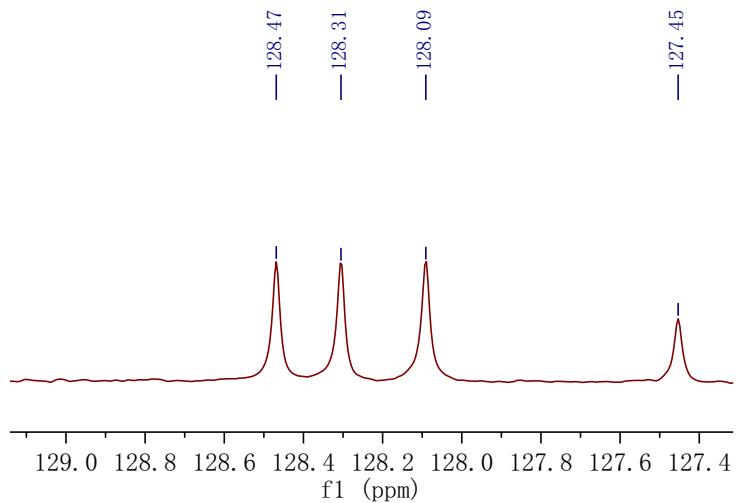
{ { } }



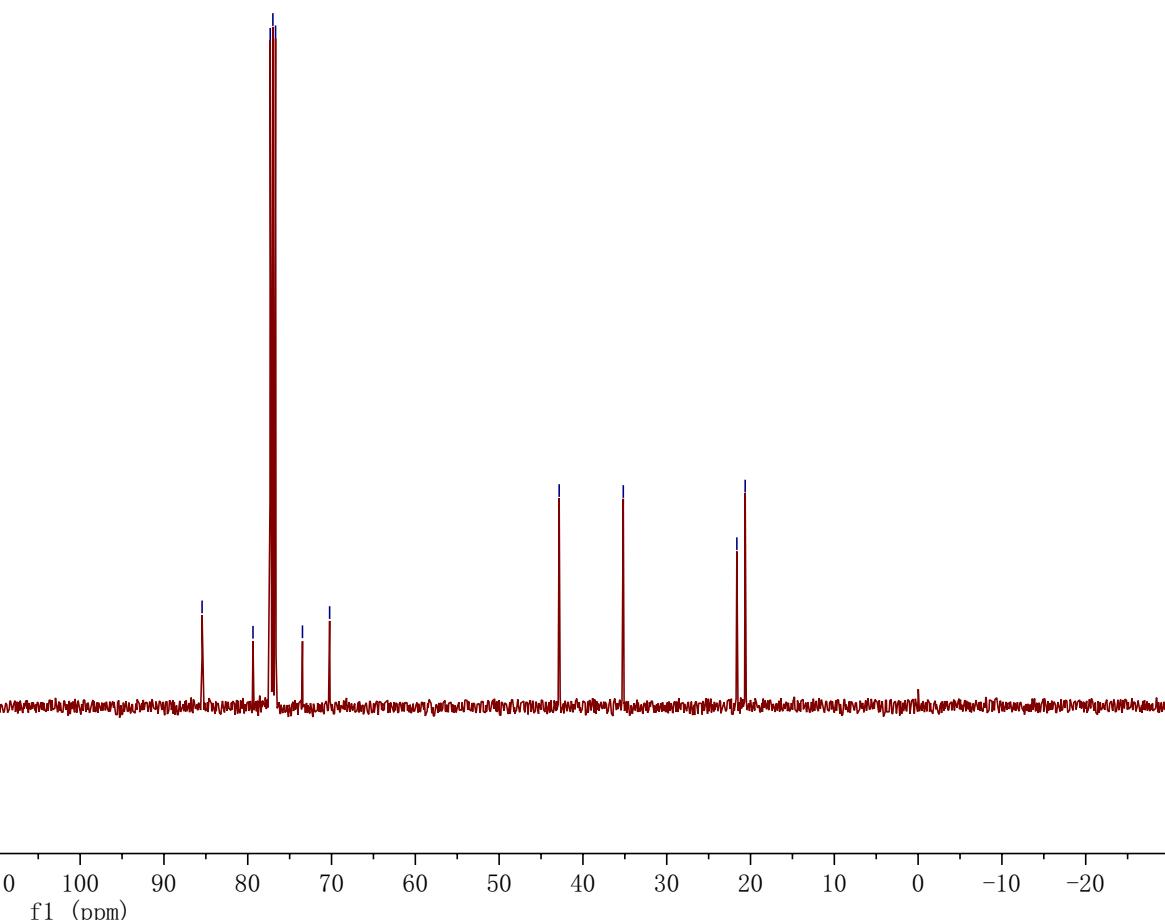
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**1x**



> 7.792

7.228  
7.207  
7.098  
7.076  
7.048  
7.028  
6.784  
6.762

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

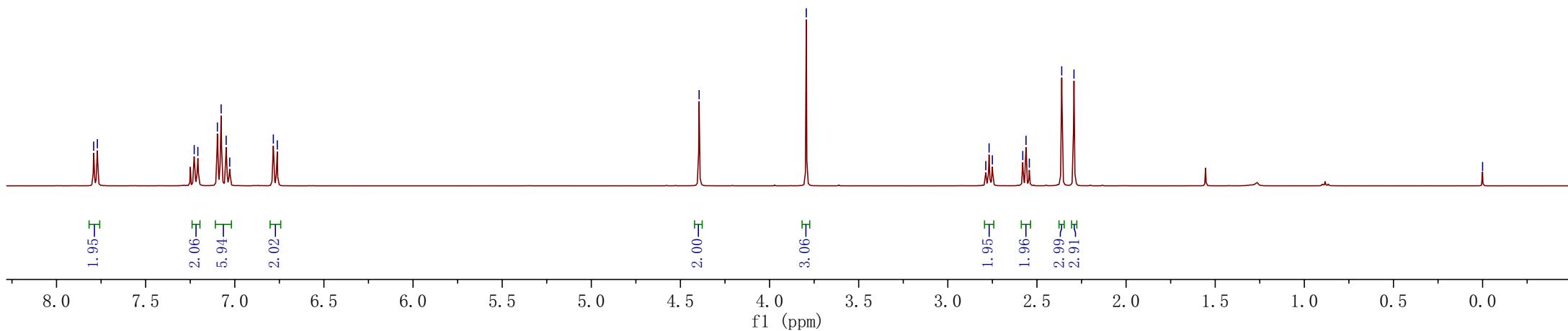
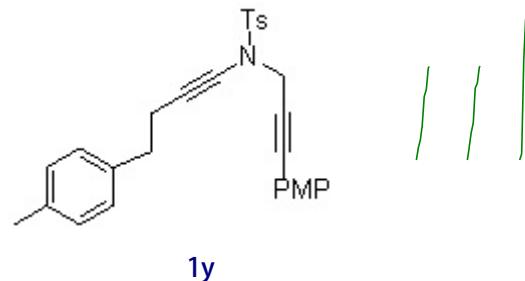
Field strength: 400 MHz

-4.395

-3.794

2.787  
2.768  
2.750  
2.579  
2.561  
2.543  
2.361  
2.292

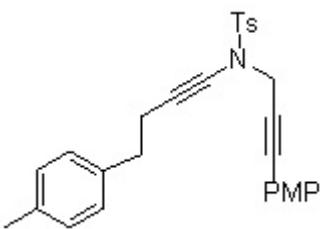
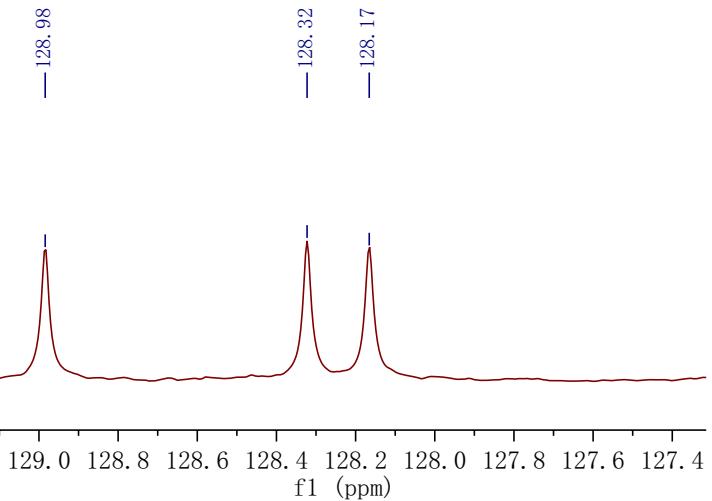
-0.000



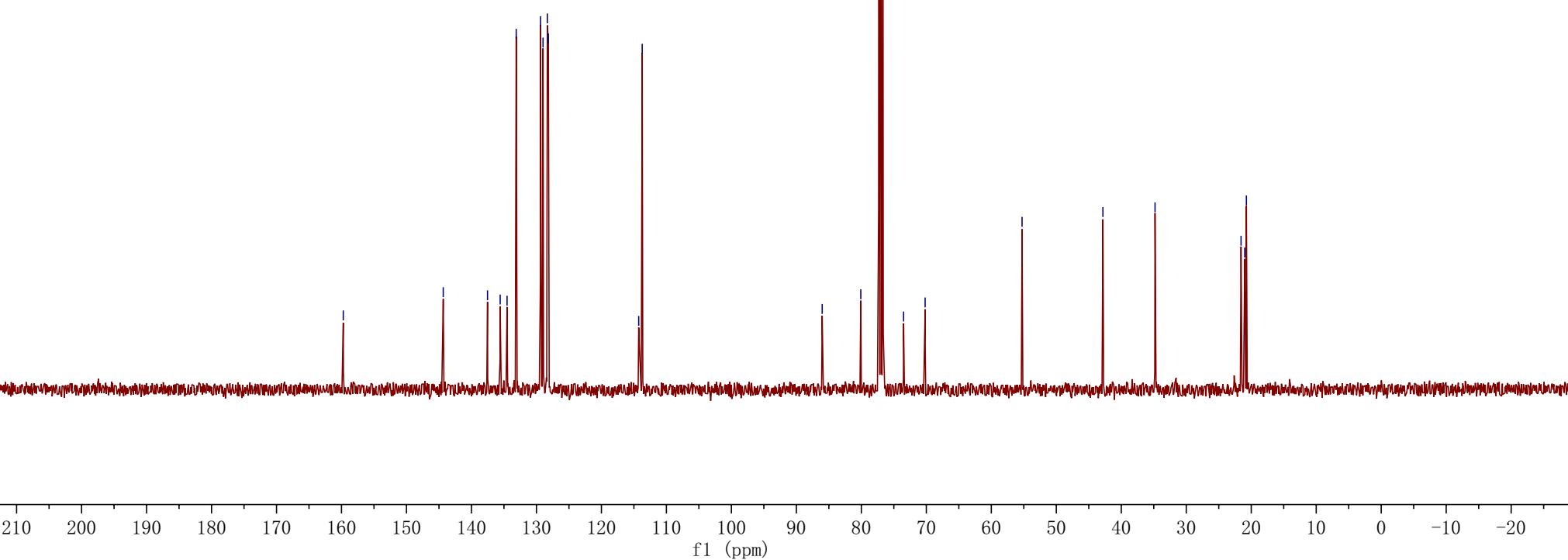
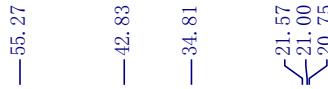
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



$1\text{y}$



7.766  
7.745  
7.229  
7.209  
7.149  
7.135  
7.128  
7.093  
7.072  
6.887  
6.866  
6.844  
6.791  
6.769

—4.394

—3.796

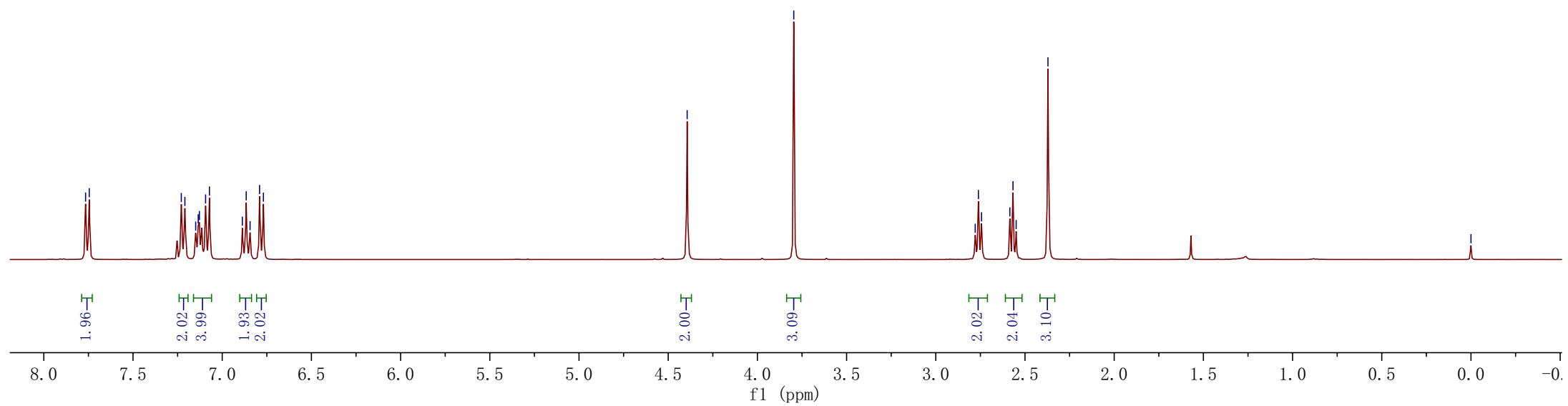
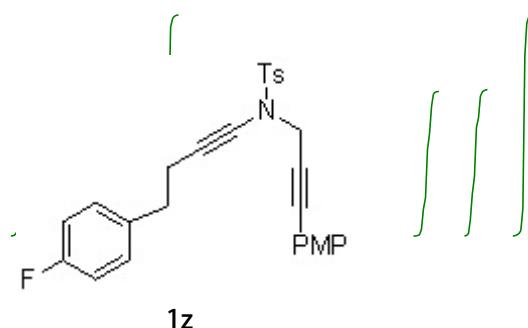
2.779  
2.761  
2.744  
2.385  
2.367  
2.349  
2.371

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

$\sim 162.64$   
 $\sim 160.22$   
 $\sim 159.78$

$-144.44$   
136.11  
134.48  
133.09  
129.96  
129.88  
129.39  
128.10

115.07  
114.86  
114.14  
113.76

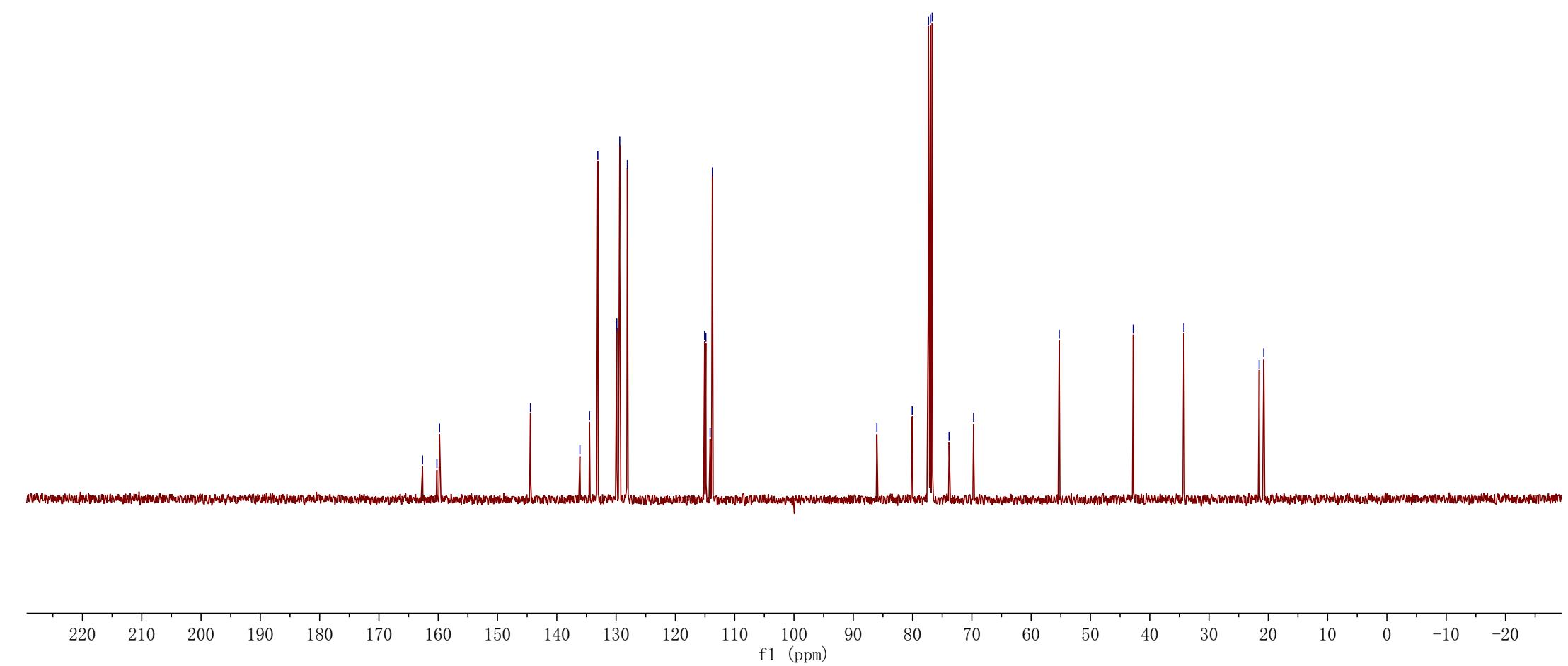
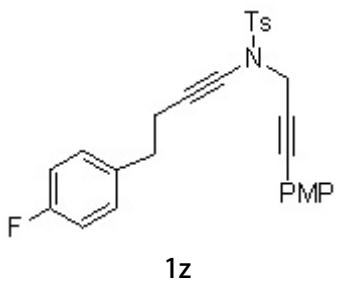
-86.02  
80.05  
77.32  
77.00  
76.68  
73.84  
69.70

-55.27

-42.78

-34.25

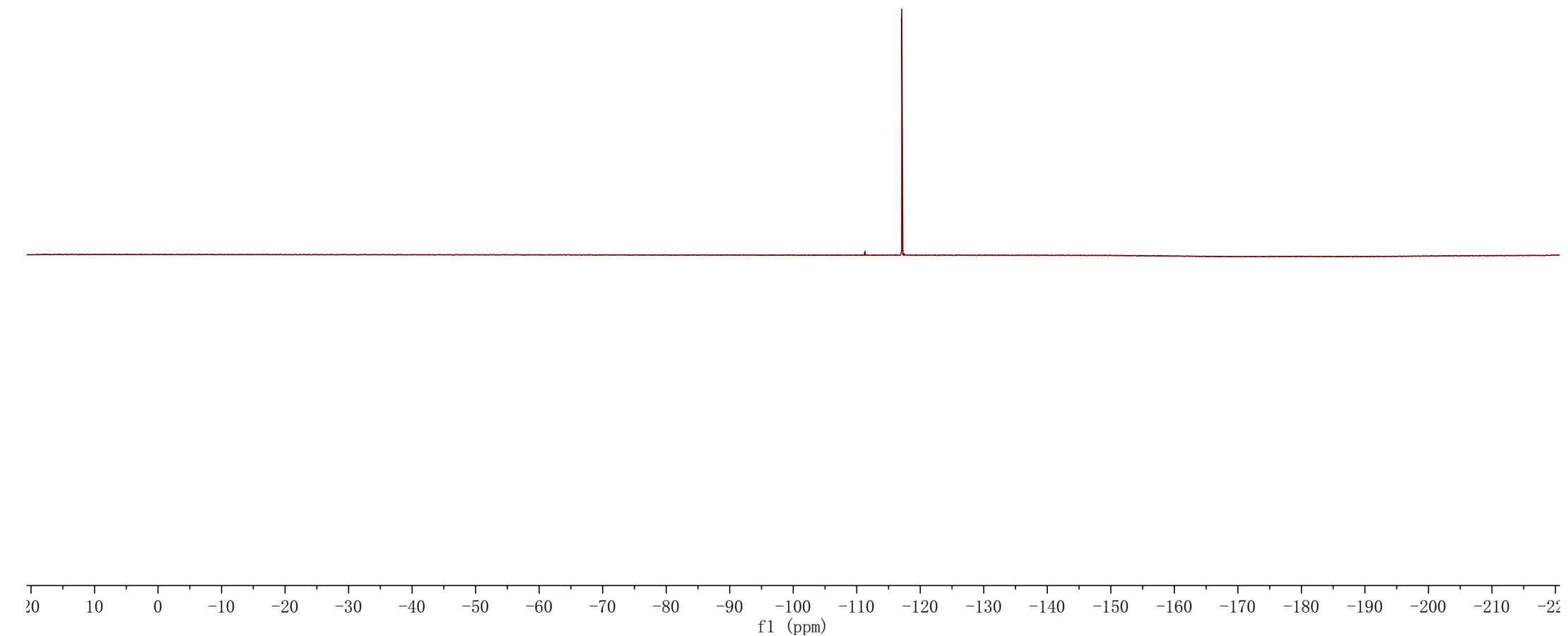
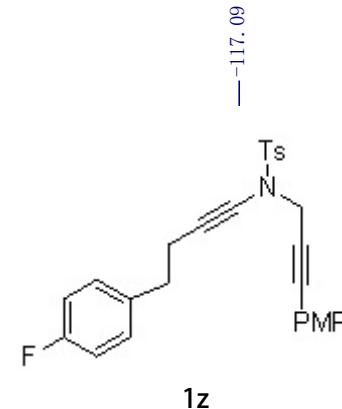
21.54  
20.76



Analysis:  $^{19}\text{F}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz



<7.750  
<7.729  
7.304  
7.284  
7.231  
7.210  
7.081  
7.066  
7.060  
7.046  
6.797  
<6.775

-4.391

-3.800

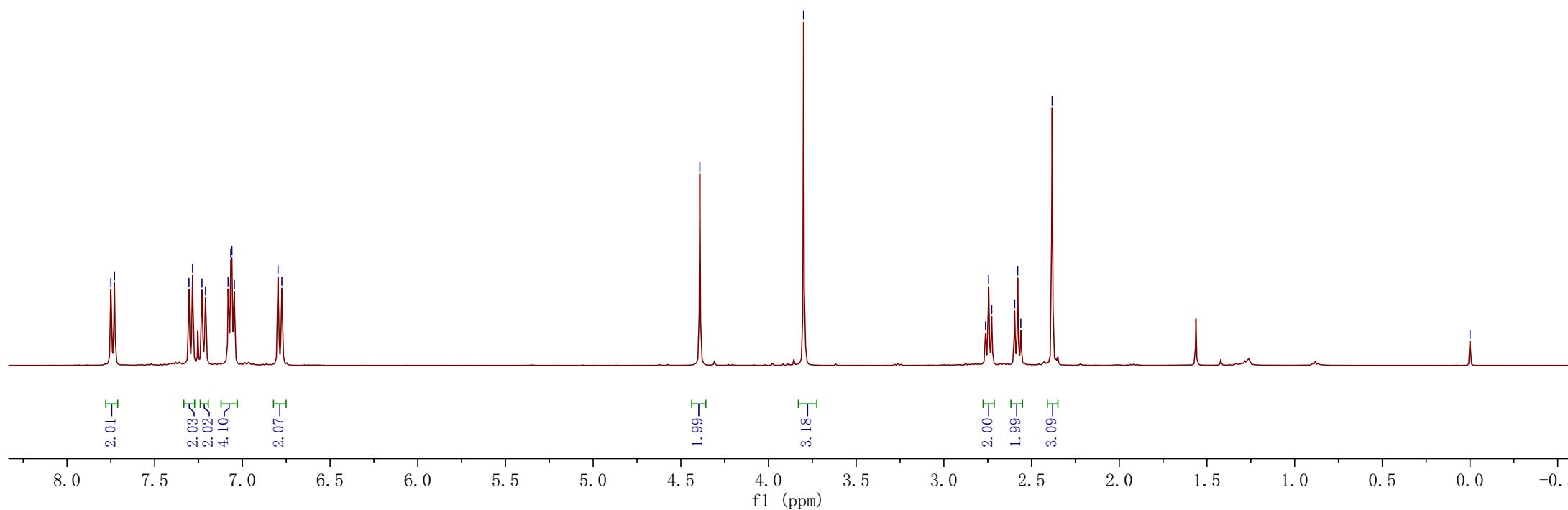
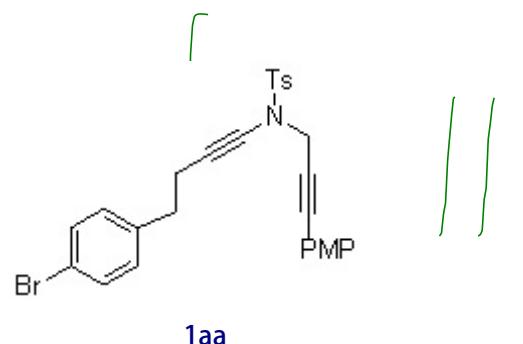
2.762  
2.745  
2.727  
2.596  
2.579  
2.561  
2.383

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

—159.79

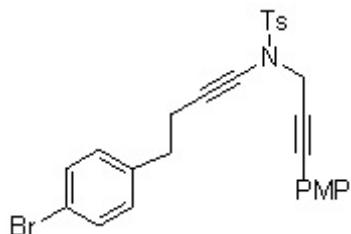
—144.47  
—139.42  
—134.54  
—133.10  
—131.30  
—130.31  
—129.43  
—128.08

—86.05  
—80.03  
—77.32  
—77.00  
—76.68  
—73.94  
—69.52

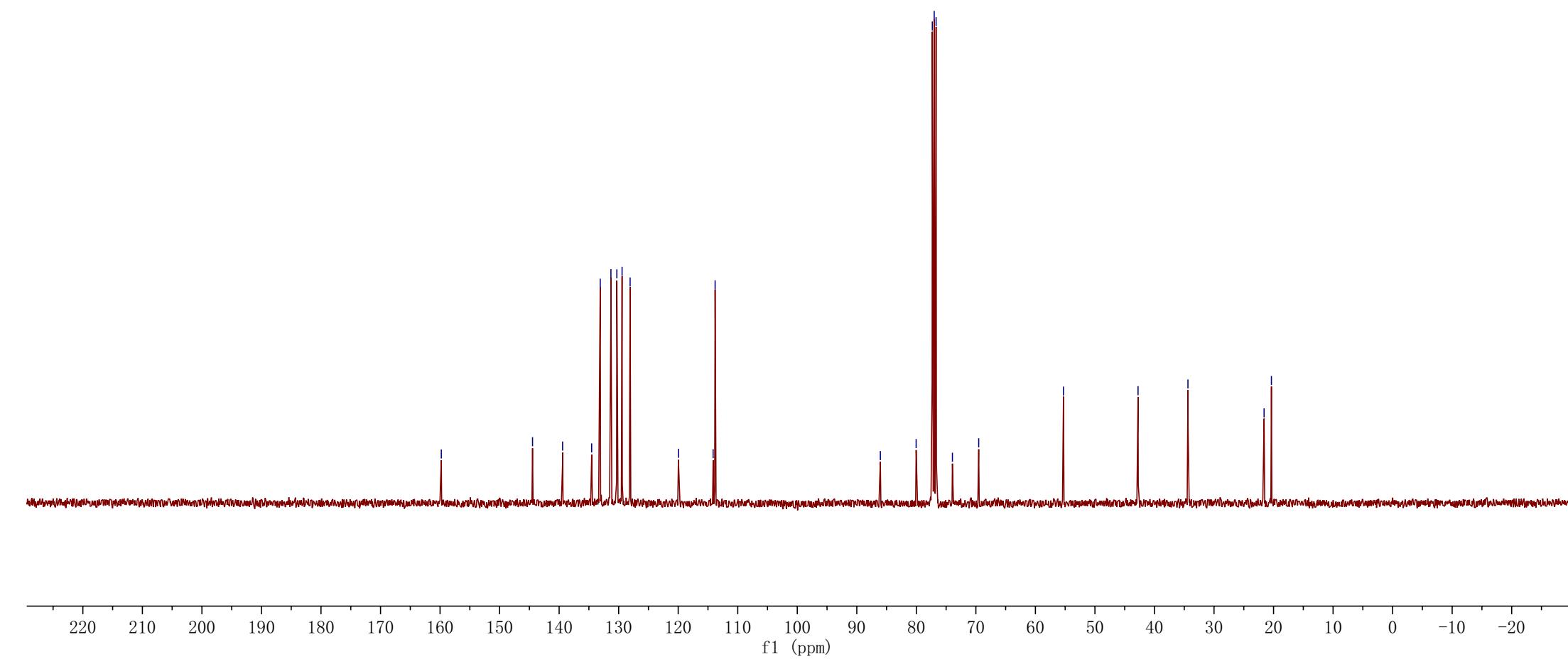
—55.29

—42.76  
—34.38

—21.59  
—20.36



1aa

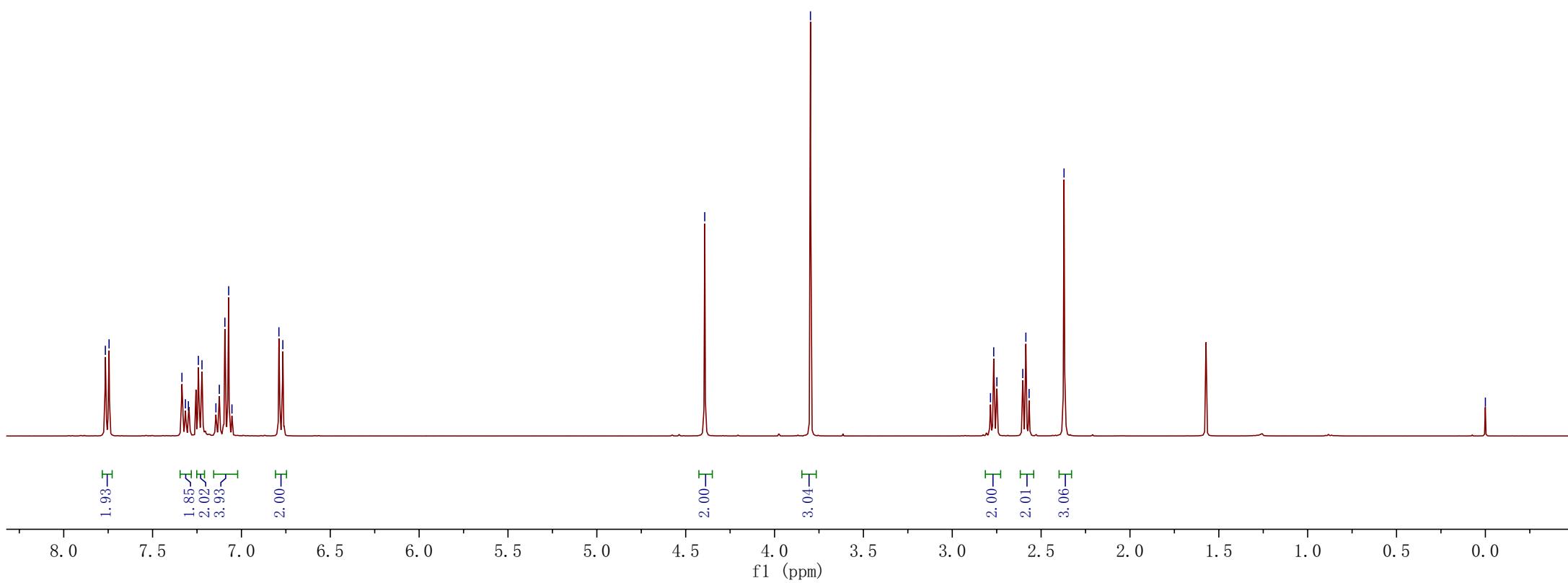
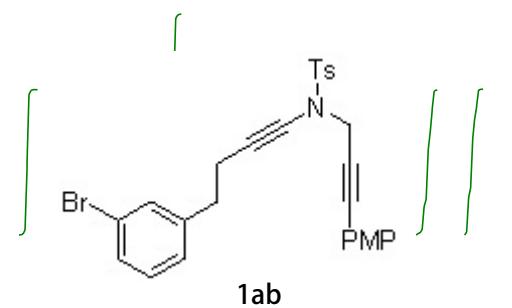


7.766  
7.745  
7.335  
7.315  
7.298  
7.242  
7.222  
7.144  
7.124  
7.093  
7.072  
7.053  
6.789  
6.767

Analysis:  $^1\text{H}$  NMR  
Solvent:  $\text{CDCl}_3$   
Field strength: 400 MHz

—4.393  
—3.798  
2.785  
2.767  
2.749  
2.603  
2.586  
2.568  
2.371

—0.000



— 159.75

— 144.45  
— 142.79  
134.42  
133.11  
131.46  
129.88  
129.43  
129.32  
128.10  
127.24  
122.28  
114.19  
113.75

— 86.09  
— 79.98  
— 77.32  
— 77.00  
— 76.68  
— 73.97  
— 69.50

— 55.28

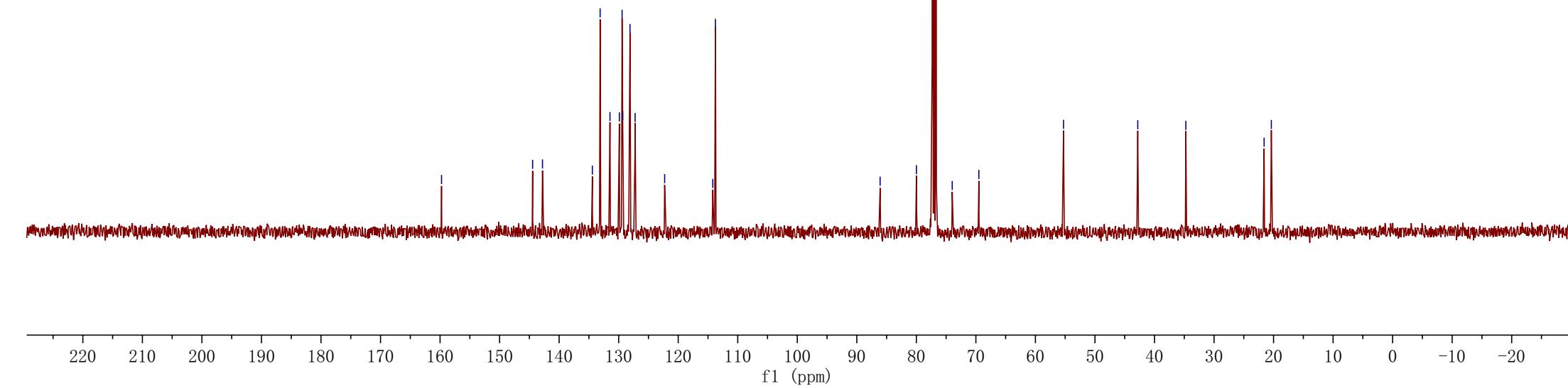
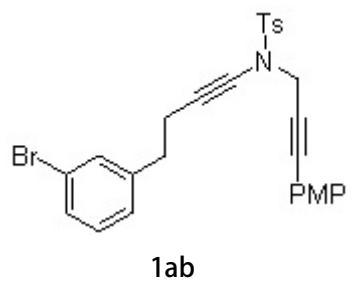
— 42.81  
— 34.73

— 21.58  
— 20.37

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.570  
7.549  
7.247  
7.226  
7.212  
7.196  
7.176  
7.162  
7.155  
7.146  
7.139  
7.104  
7.084  
7.041  
7.020  
6.775  
6.753

4.284  
4.203  
4.184  
4.166

-3.770

3.011  
2.992

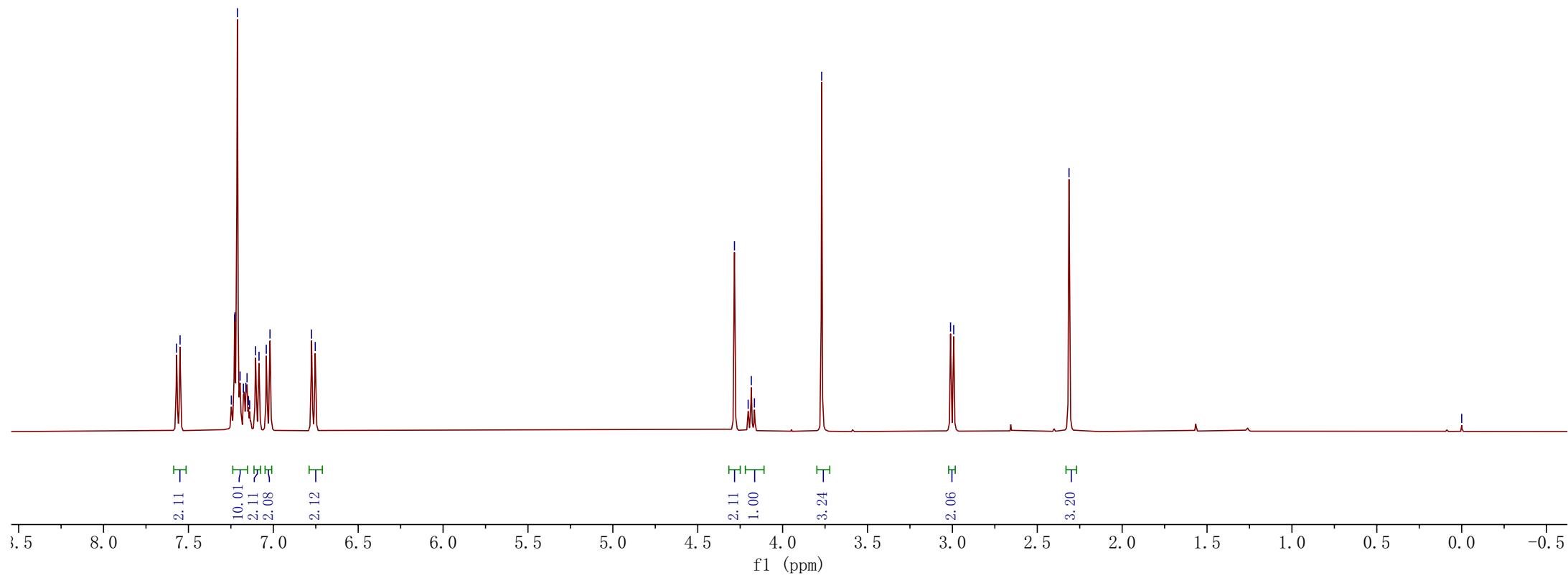
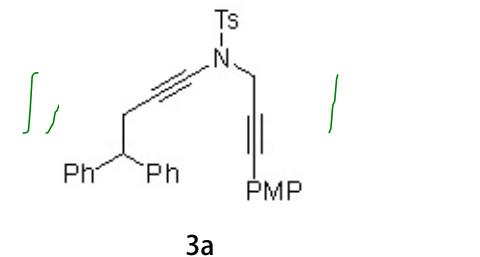
-2.313

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

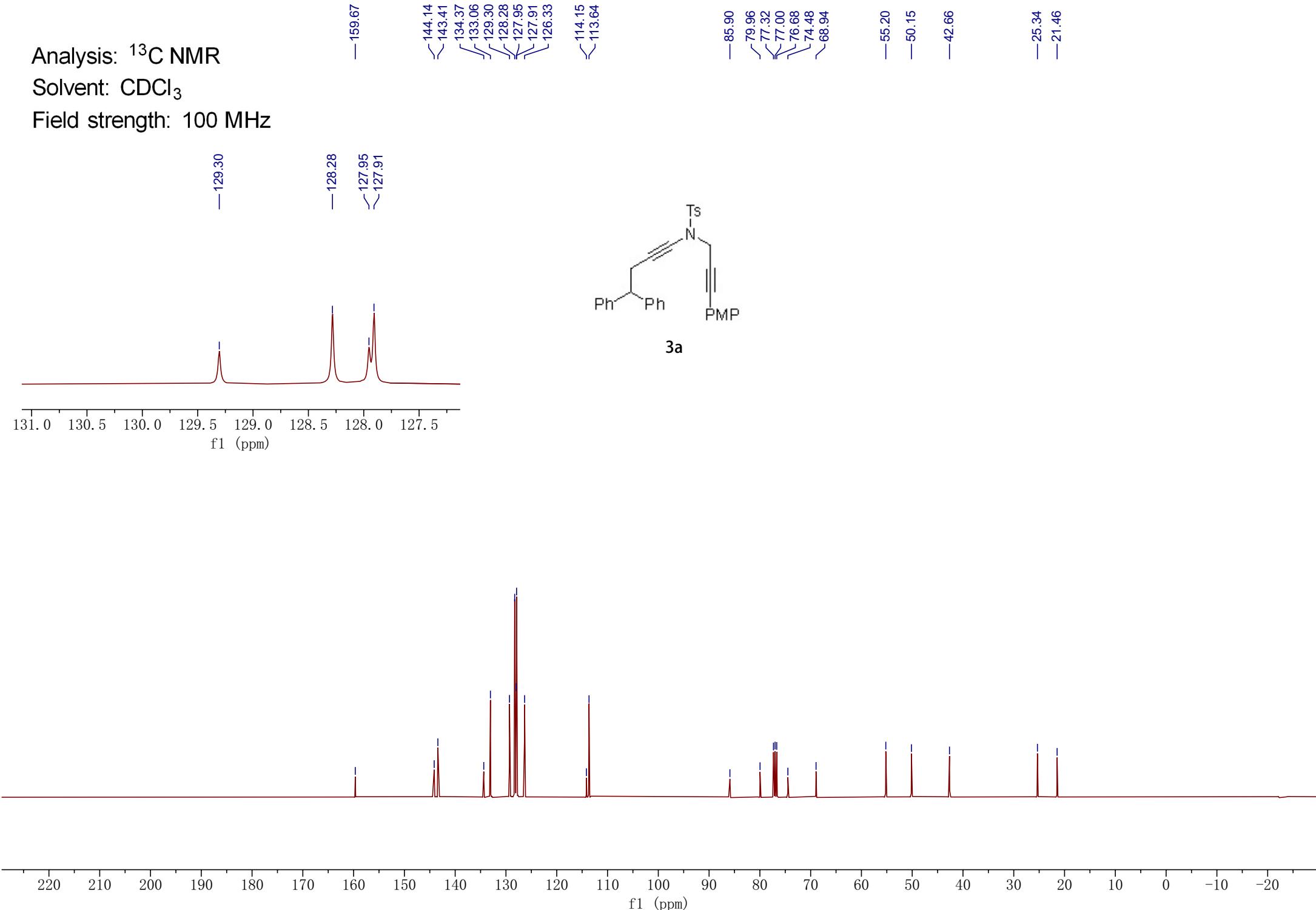
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.603  
7.585  
7.252  
7.236  
7.223  
7.218  
7.206  
7.181  
7.177  
7.164  
7.151  
7.063  
7.046

4.287  
4.208  
4.193  
4.178  
6.780  
6.762  
6.750  
6.732  
~3.783  
~3.738

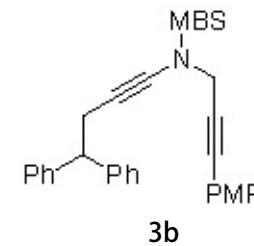
~3.018  
~3.003

-0.000

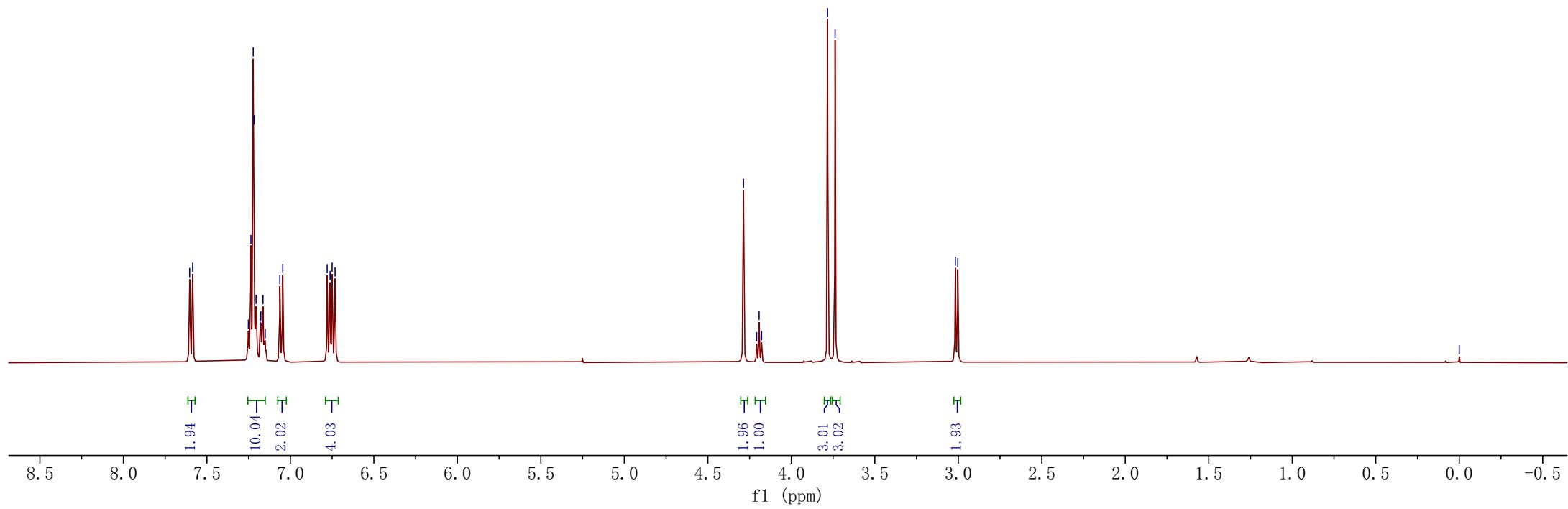
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz



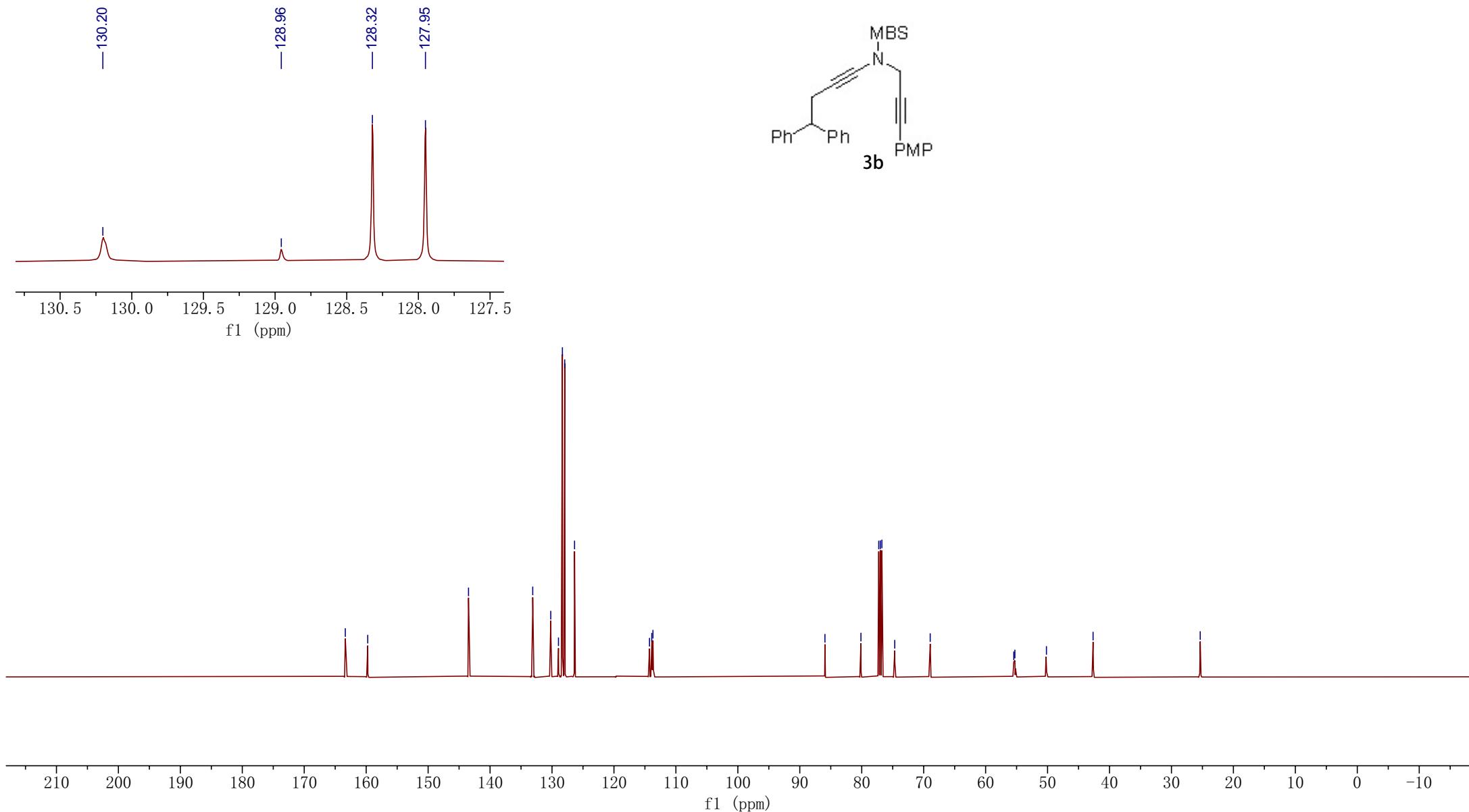
**3b**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



—0.000

3.032

3.013

3.817

4.181

4.200

4.219

4.332

6.821

7.006

7.028

7.193

7.211

7.237

7.224

7.483

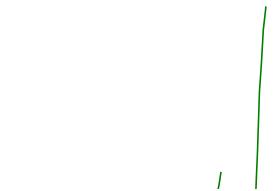
7.462

7.412

7.391

7.273

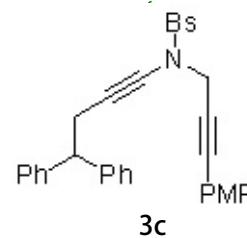
7.253



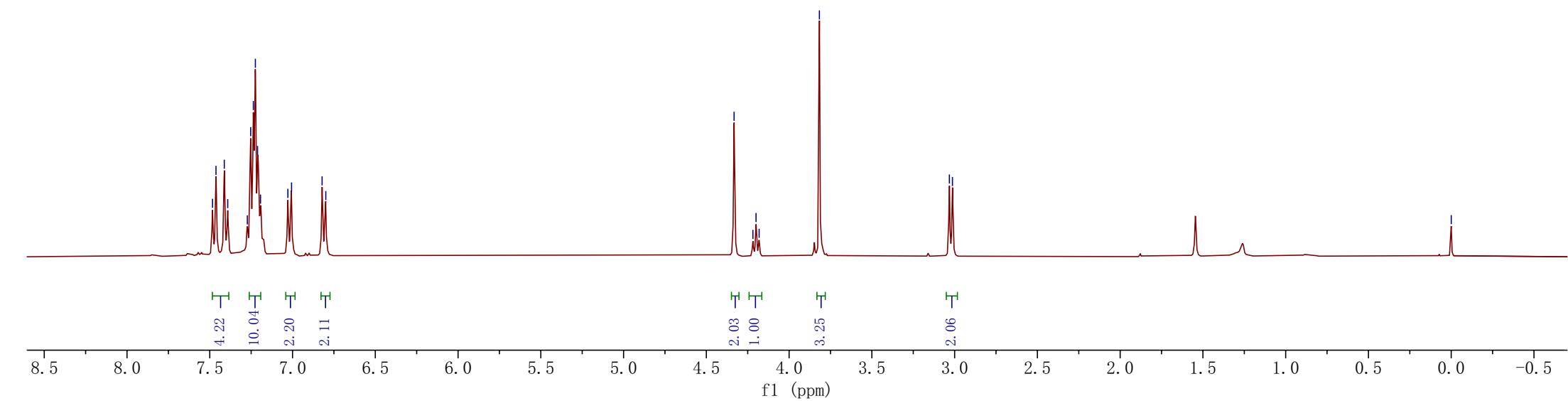
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



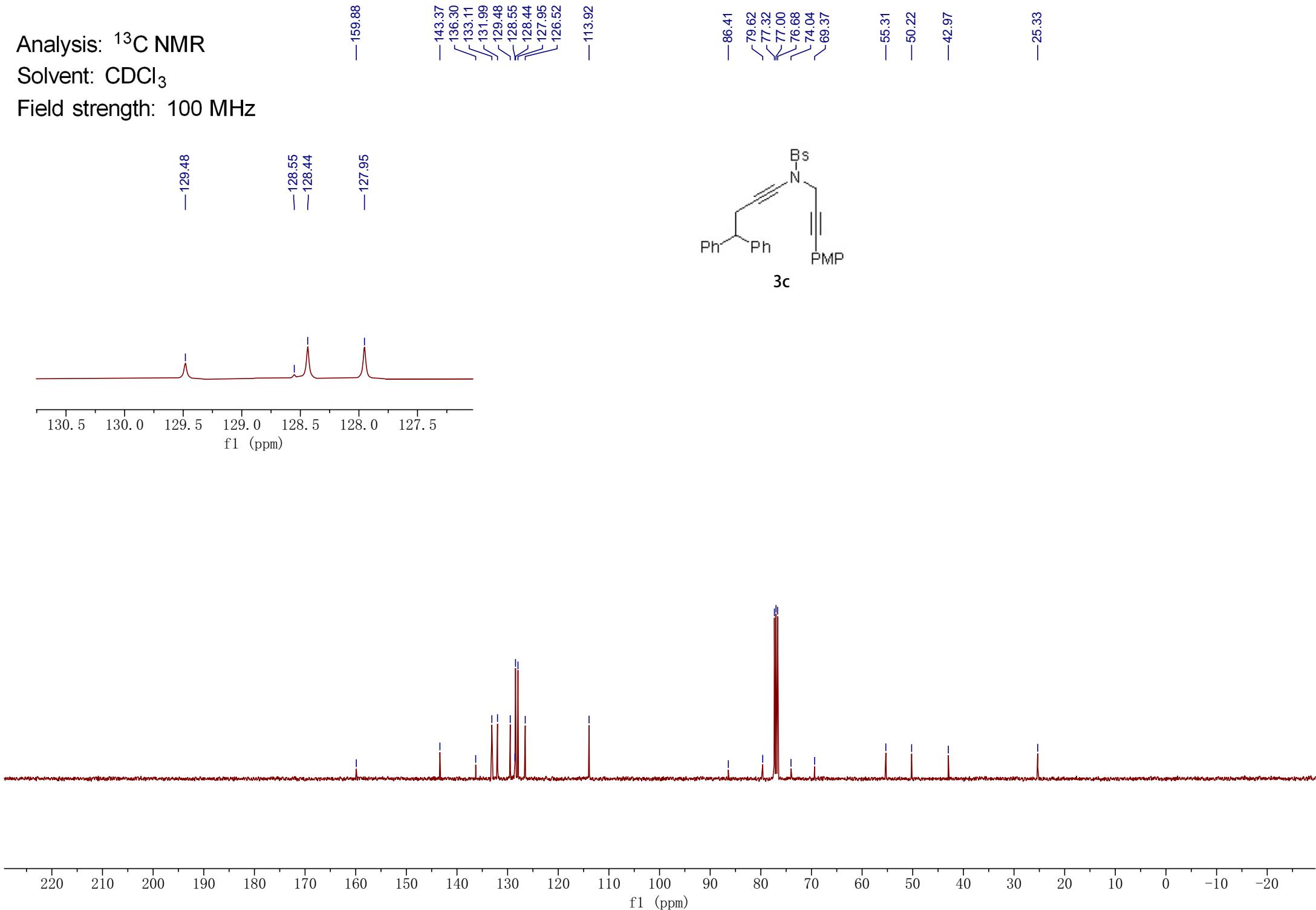
Sample: Compound 3c



Analysis:  $^{13}\text{C}$  NMR

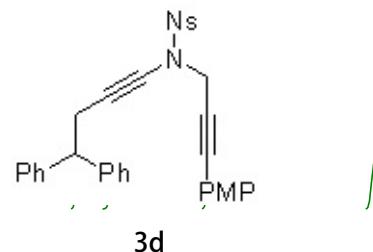
Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



8.003  
7.985  
7.737  
7.719  
7.277  
7.262  
7.234  
7.220  
7.198  
7.184  
7.184  
6.974  
6.956  
6.759  
6.742

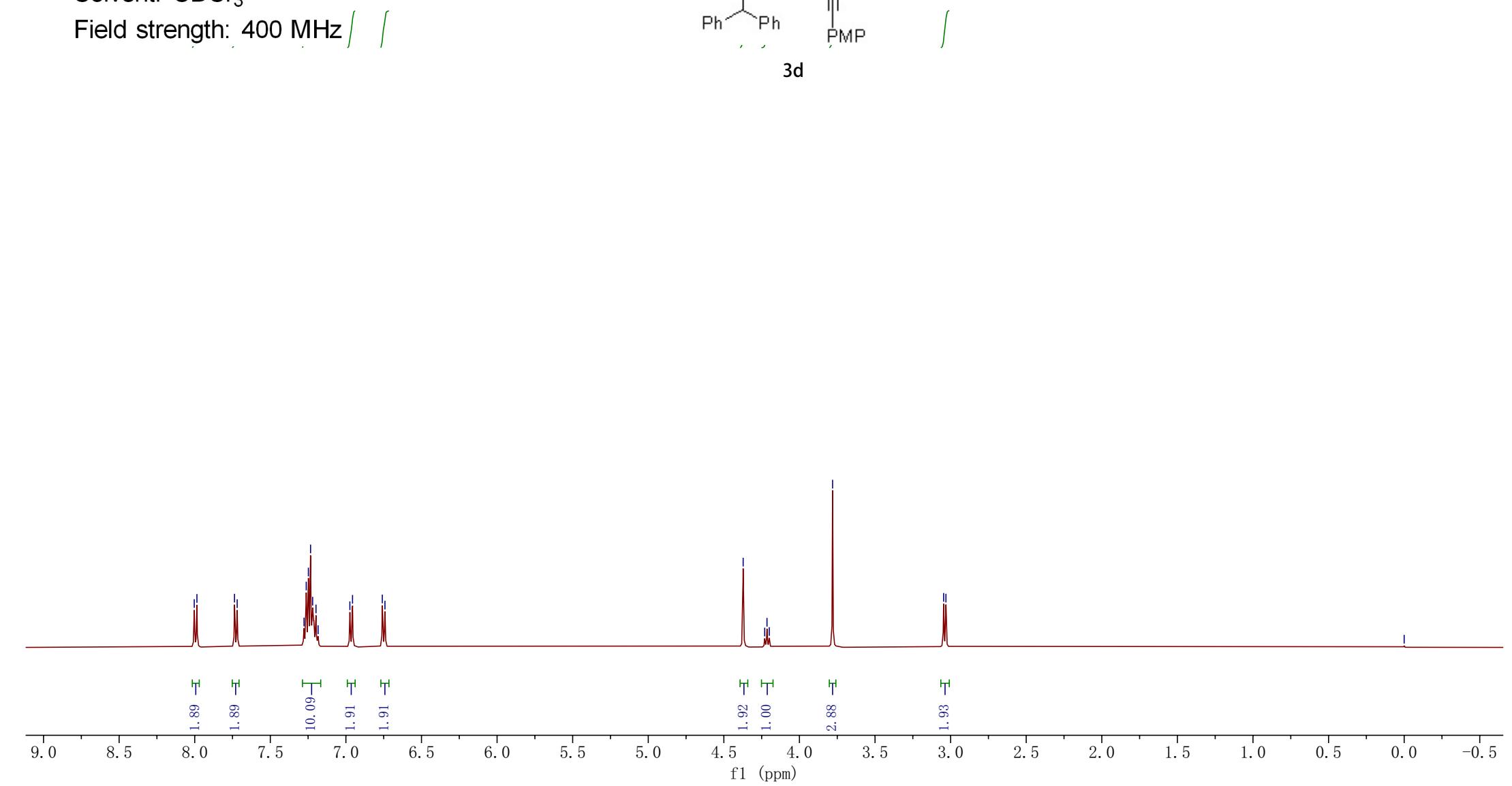
4.372  
4.230  
4.215  
4.200  
—3.781  
—3.046  
—3.031



Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

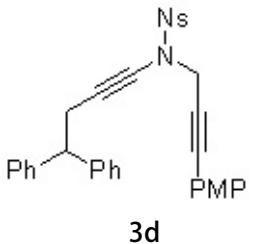
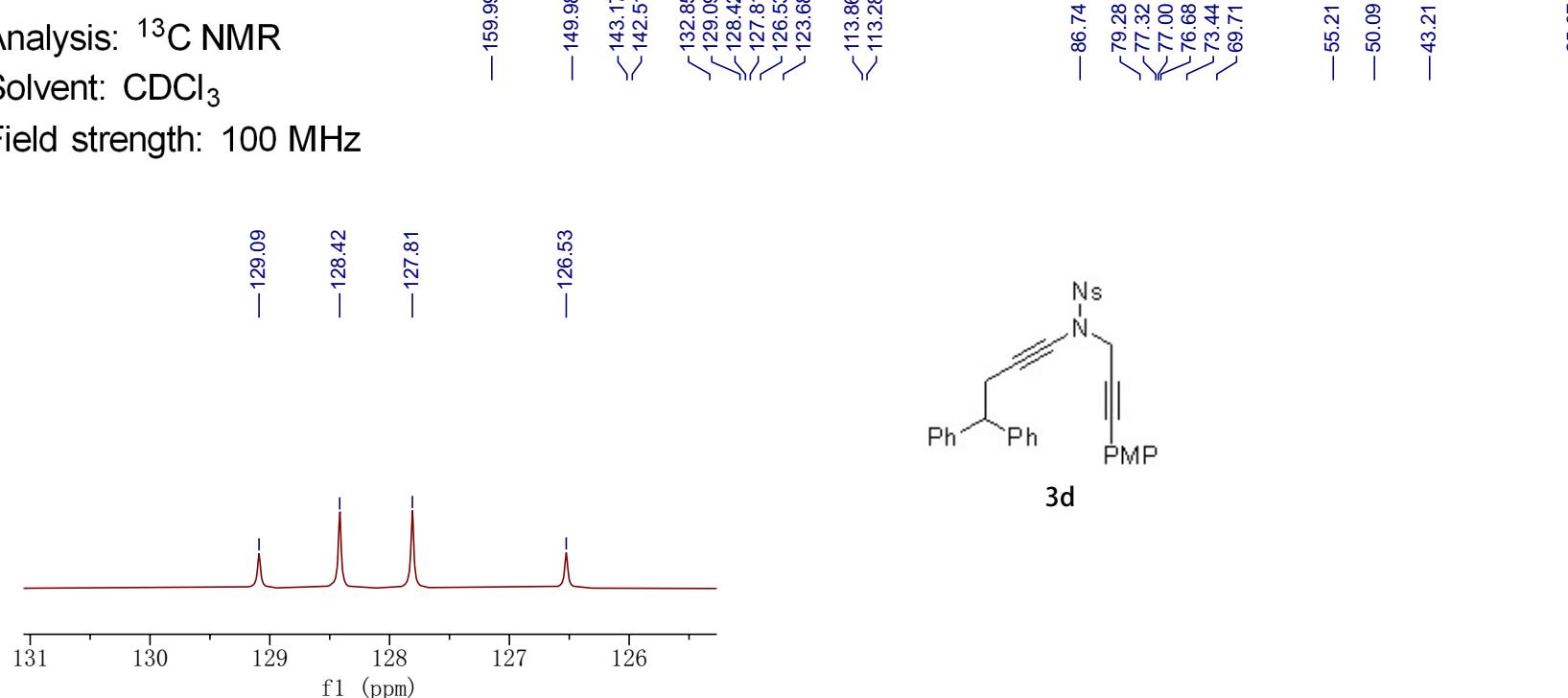


—0.000

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**3d**

8.380  
8.380  
7.847  
7.829  
7.810  
7.744  
7.726  
7.660  
7.656  
7.643  
7.639  
7.622  
7.608  
7.558  
7.542  
7.528  
7.194  
7.186  
7.167  
7.155  
7.147  
7.138  
7.130  
7.121  
6.744  
6.740  
6.731  
6.727  
6.607  
6.601  
6.597  
6.588  
6.584

4.365  
4.193  
4.178  
4.163

—3.750

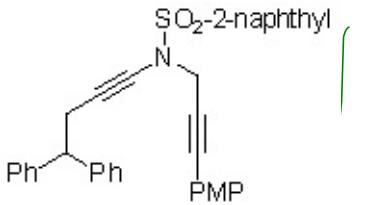
—3.017  
—3.003

—0.000

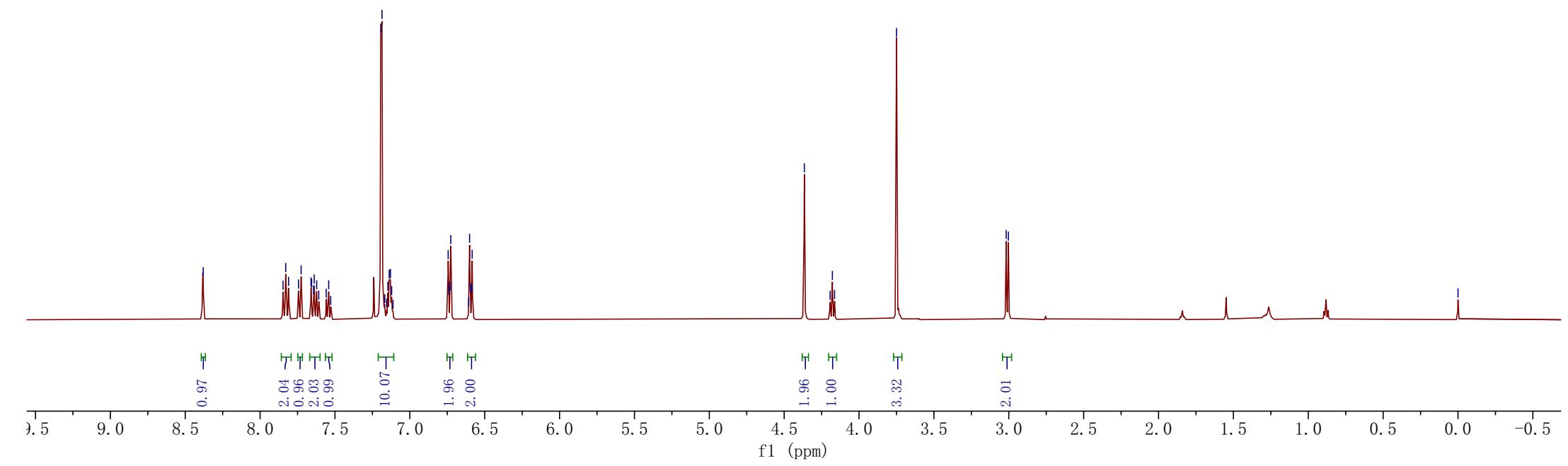
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz /



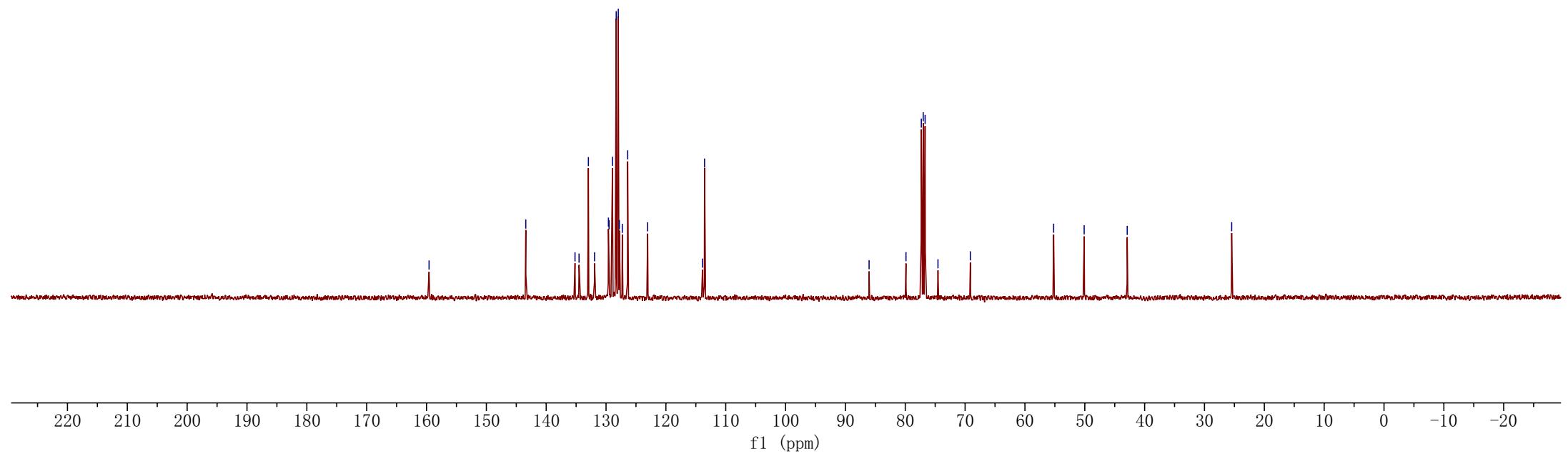
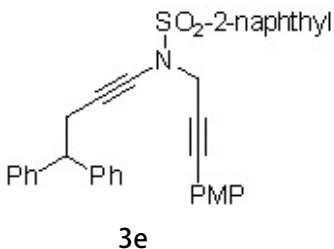
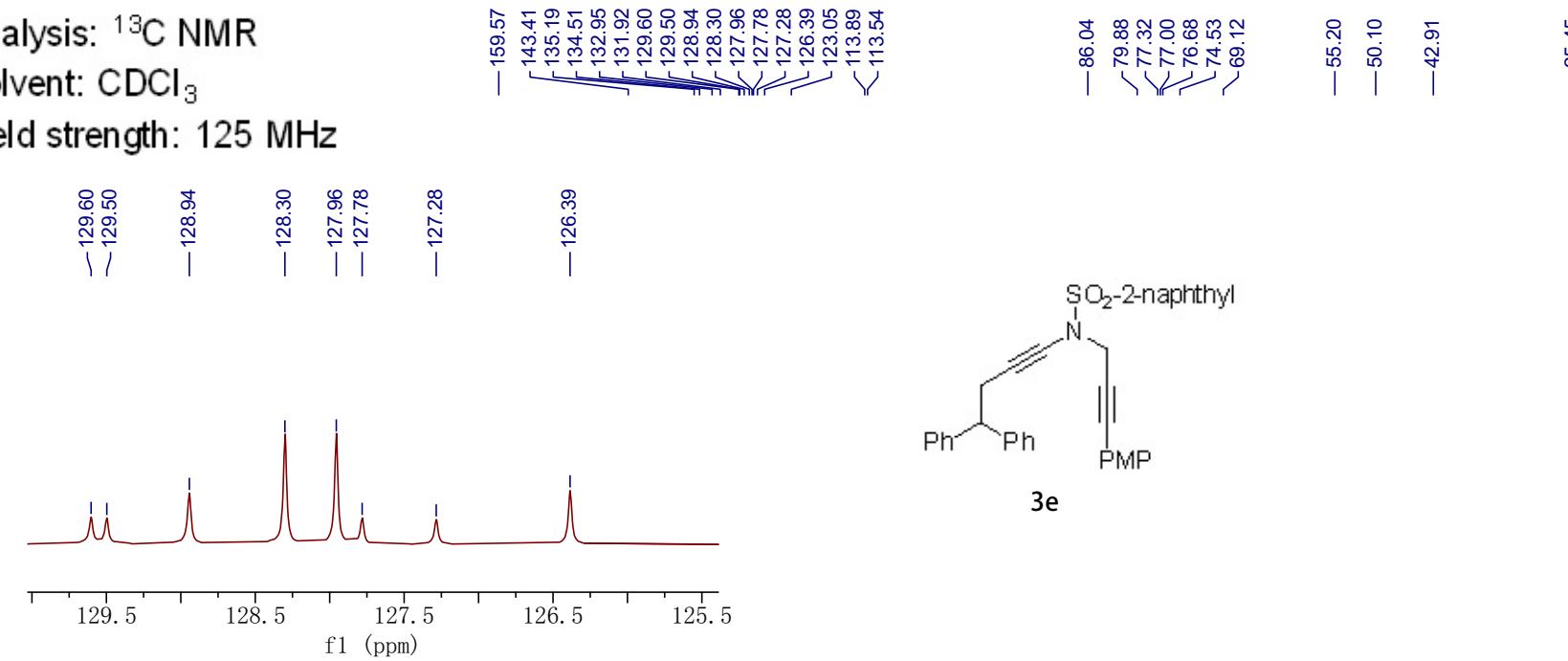
3e



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



<7.572  
<7.551  
7.255  
7.237  
7.221  
7.201  
7.186  
7.181  
7.172  
7.164  
7.155  
7.148  
7.112  
7.092  
7.035  
7.028  
7.023  
7.011  
7.006  
6.999  
6.776  
6.769  
6.763  
6.752  
6.747  
6.740

4.292  
4.210  
4.191  
4.173  
4.041  
4.023  
4.006  
3.988

<3.018  
<3.000

-2.326

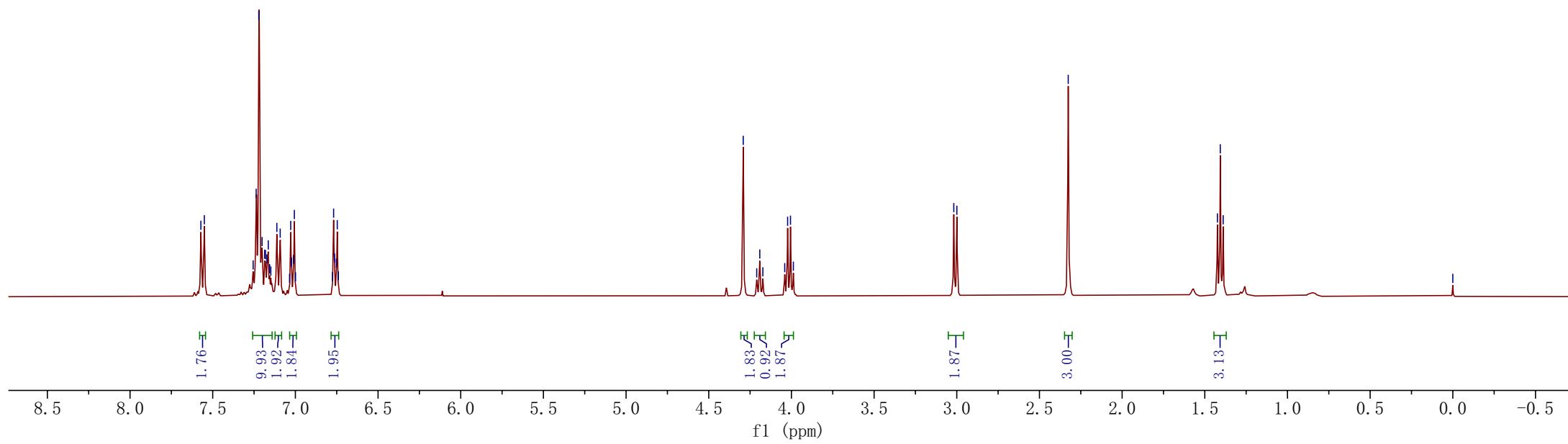
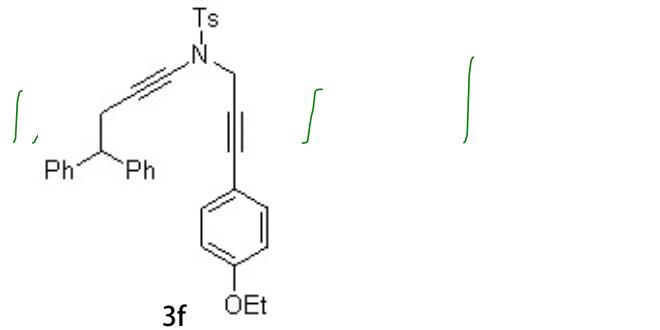
1.424  
1.406  
1.389

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

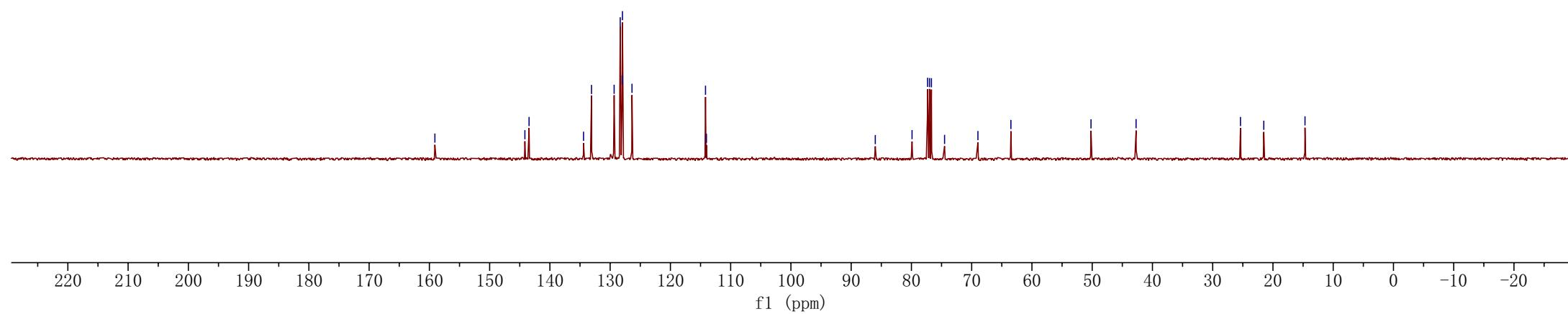
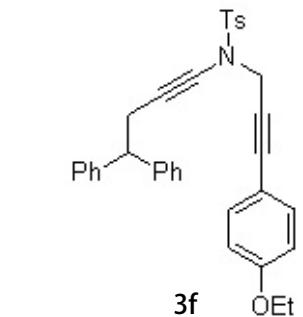
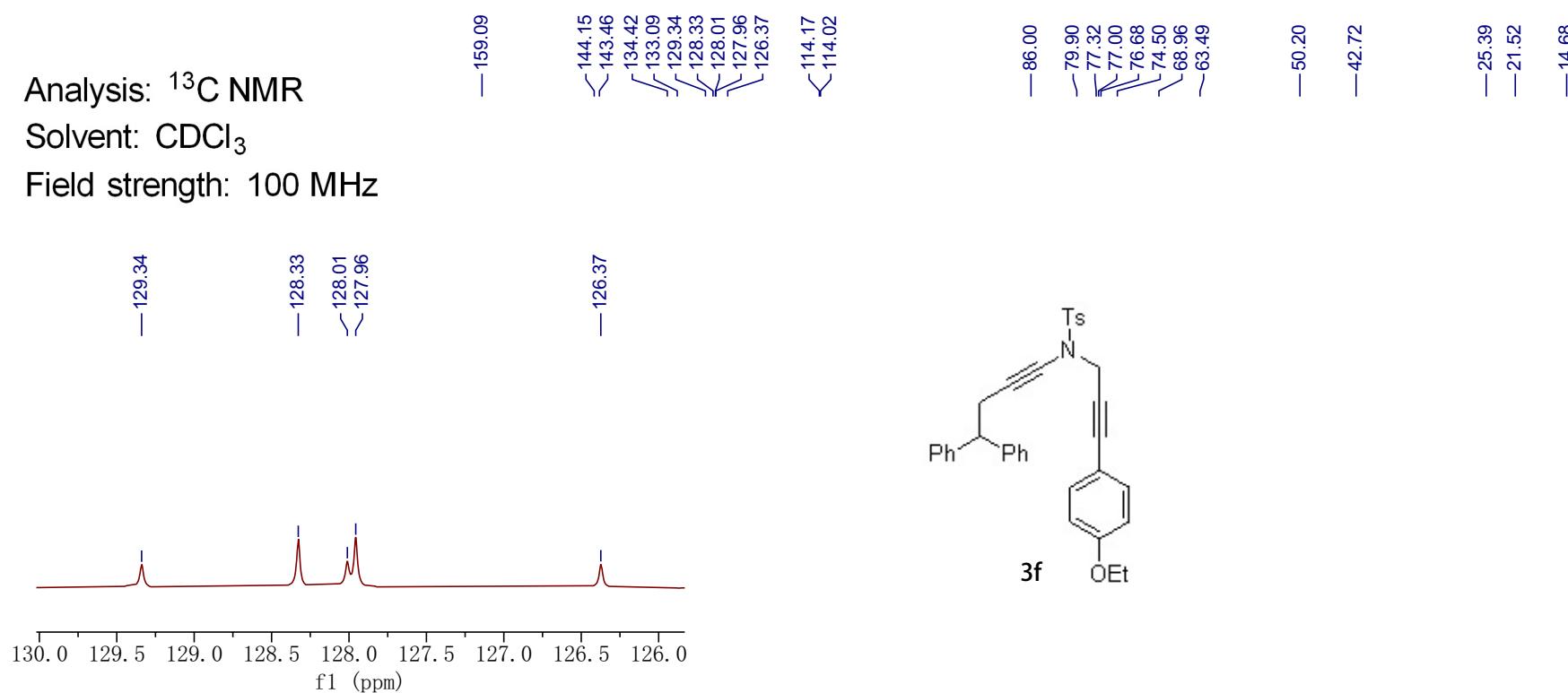
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.569  
7.548  
7.423  
7.402  
7.382  
7.363  
7.343  
7.325  
7.253  
7.235  
7.218  
7.200  
7.182  
7.177  
7.168  
7.160  
7.152  
7.144  
7.106  
7.085  
7.031  
7.009  
6.853  
6.830

—5.059

4.290  
4.209  
4.190  
4.172

3.017  
2.999

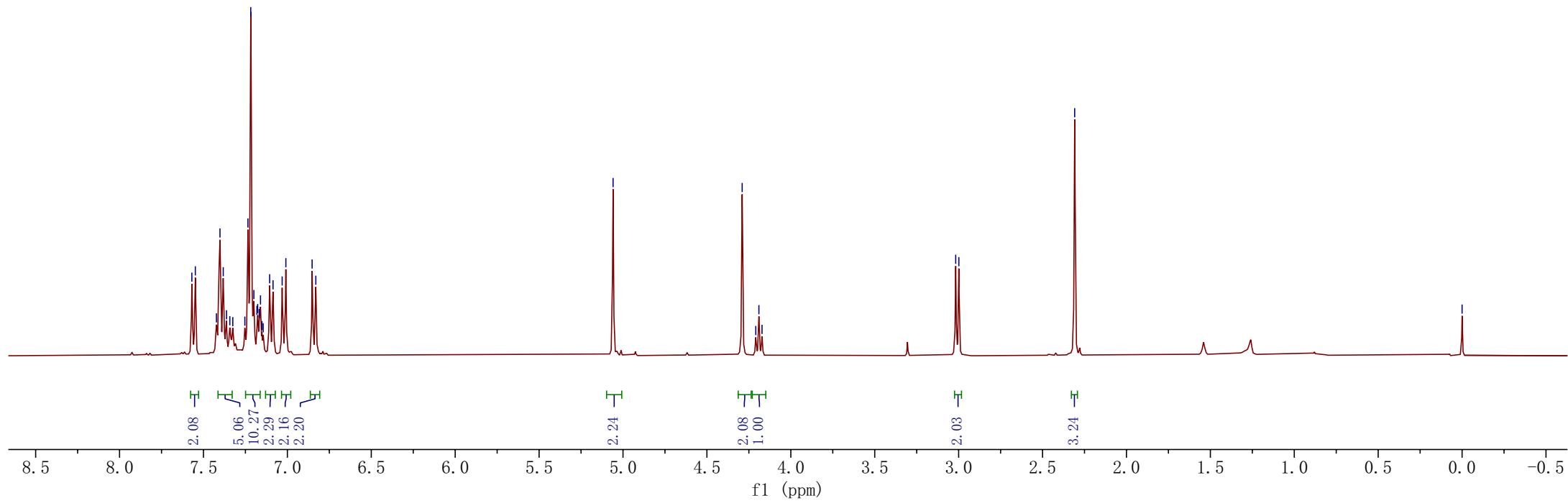
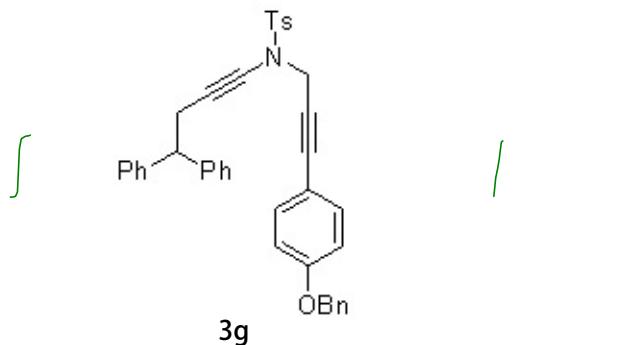
—2.309

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

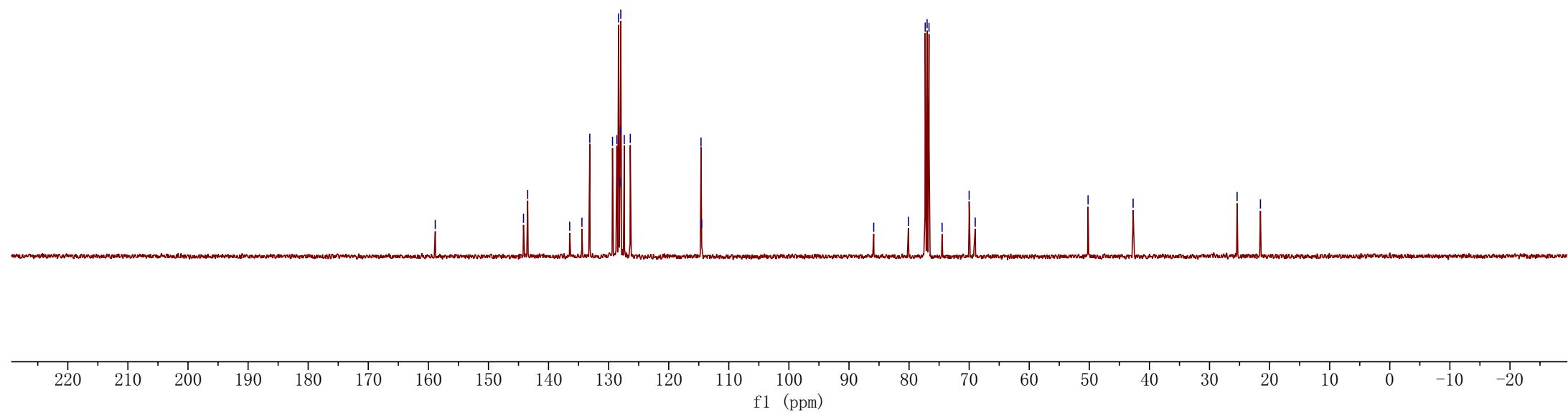
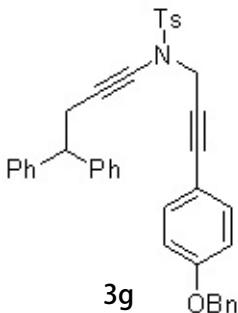
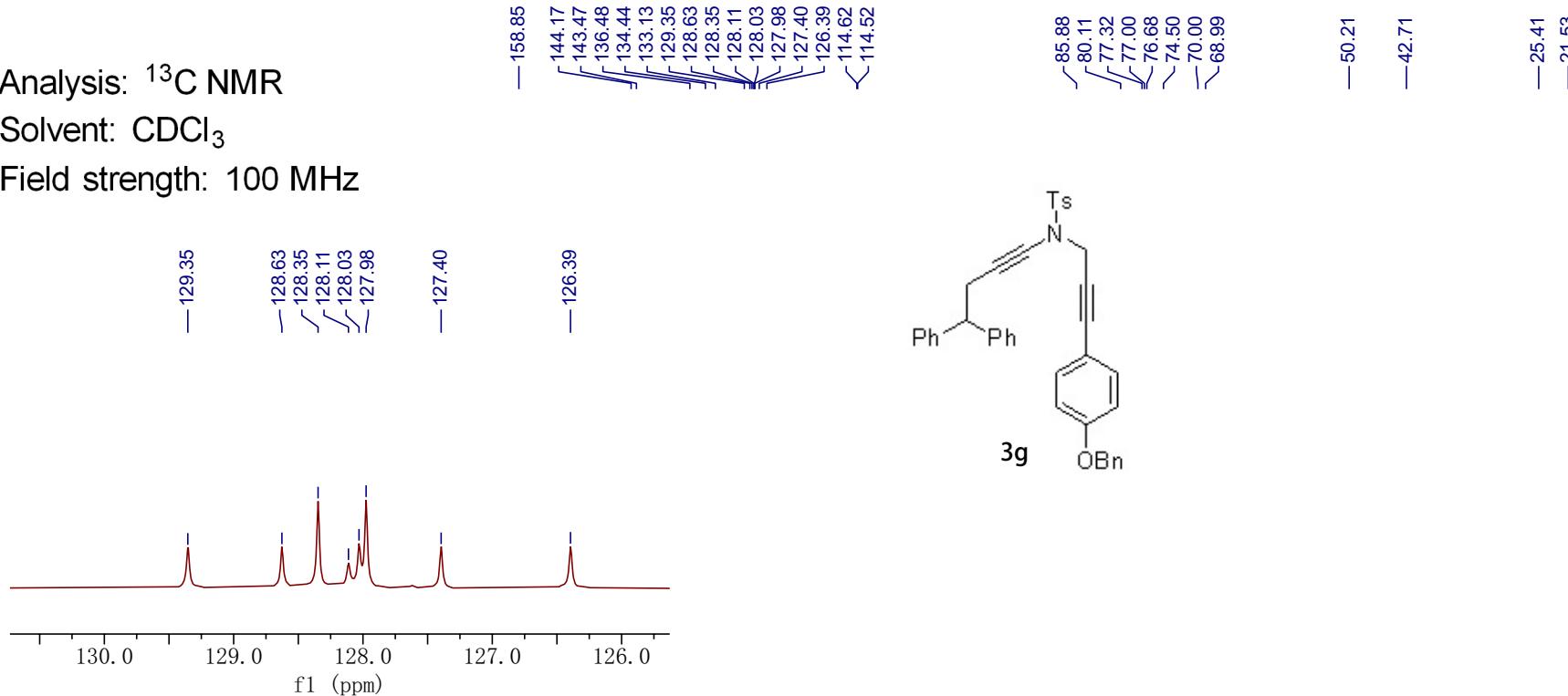
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

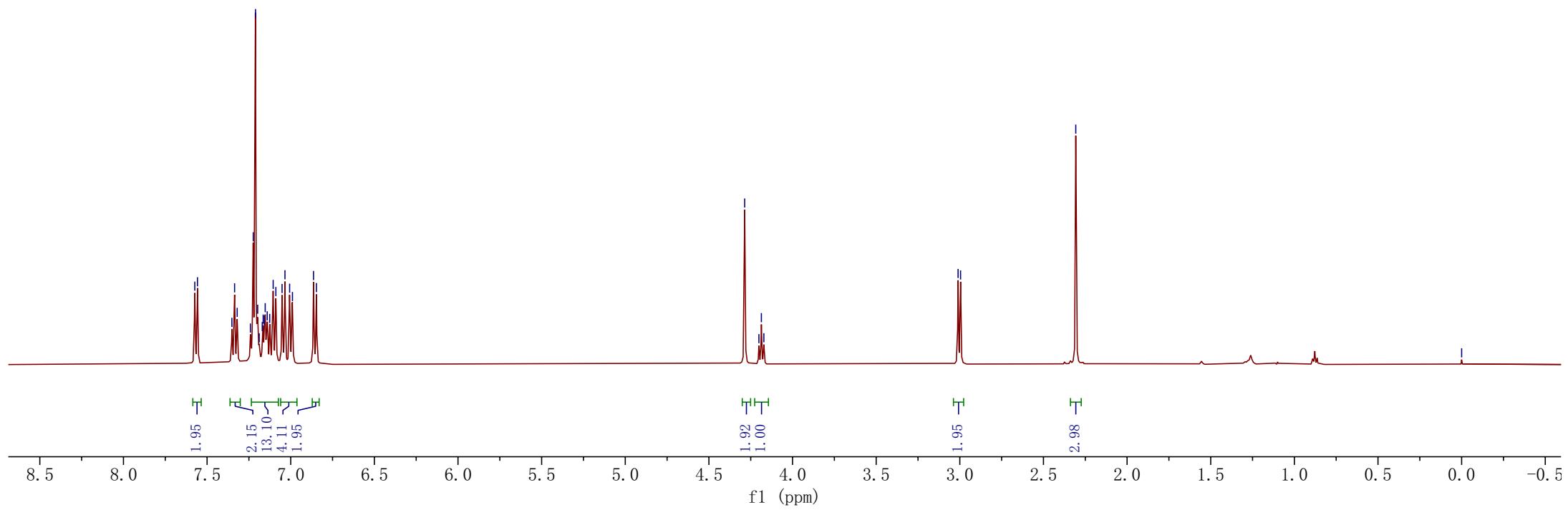
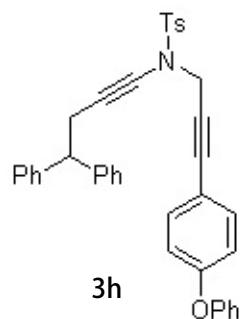




Analysis: <sup>1</sup>H NMR

Solvent: CDCl<sub>3</sub>

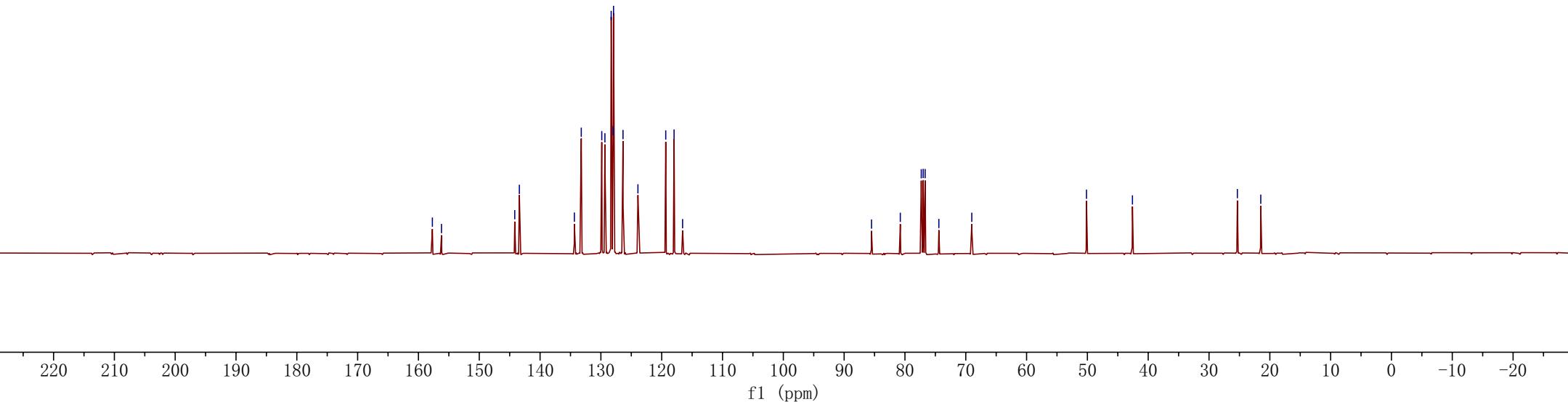
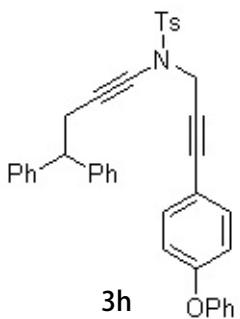
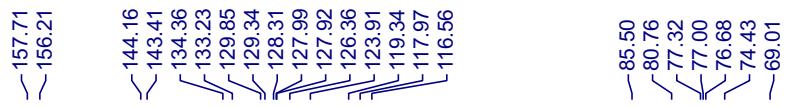
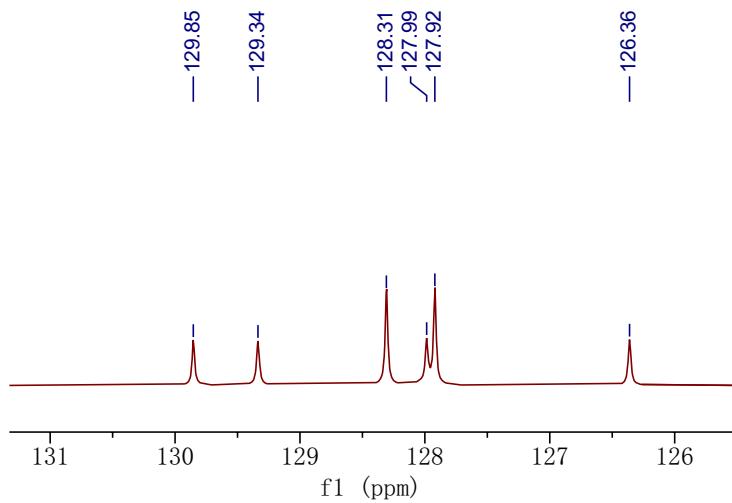
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



7.573  
7.553  
7.253  
7.232  
7.217  
7.202  
7.183  
7.176  
7.169  
7.162  
7.153  
7.146  
7.109  
7.089  
6.990  
6.974  
6.968  
6.723  
6.701

4.290  
4.211  
4.193  
4.174

3.020  
3.001

-2.325

-0.982

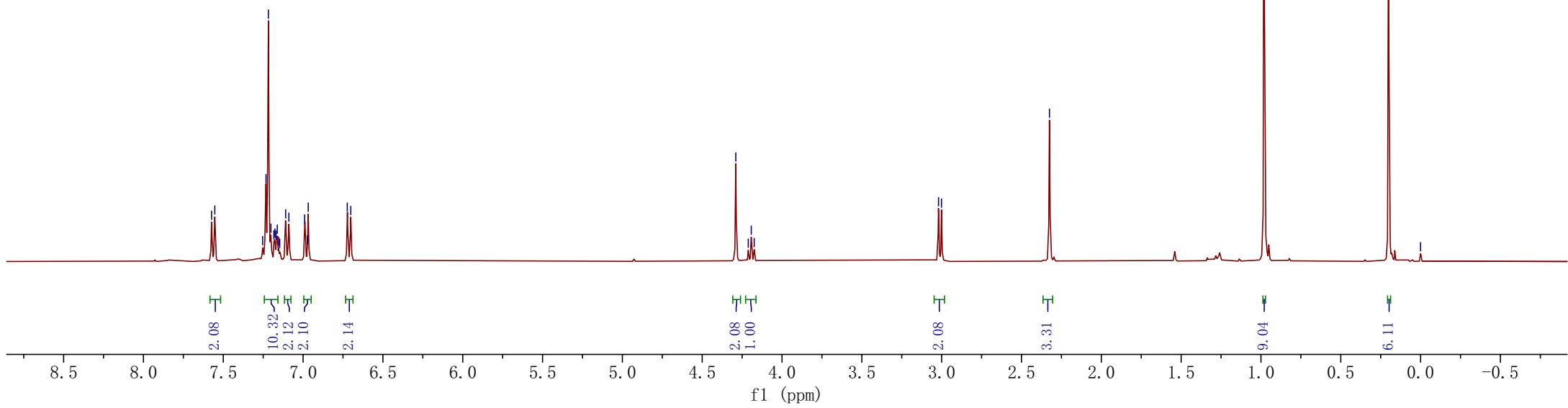
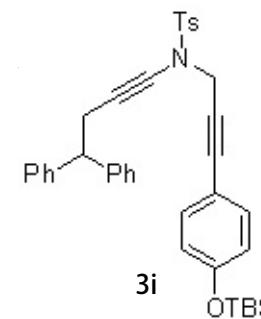
-0.201

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

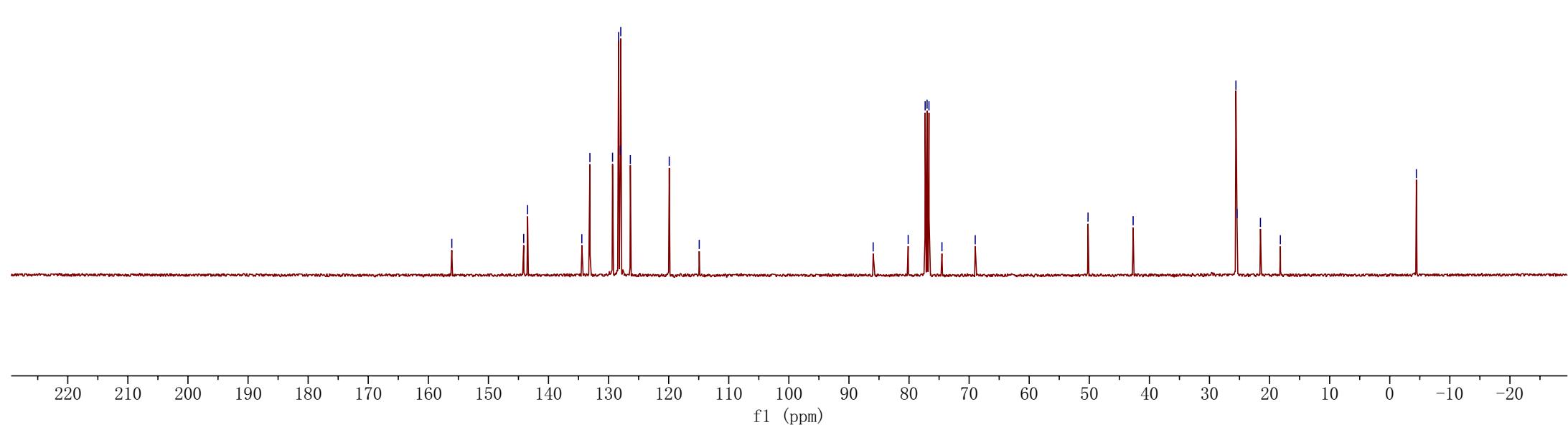
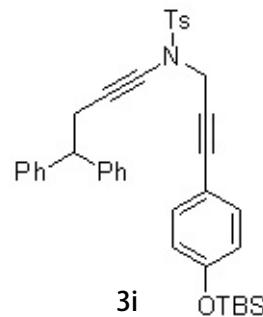
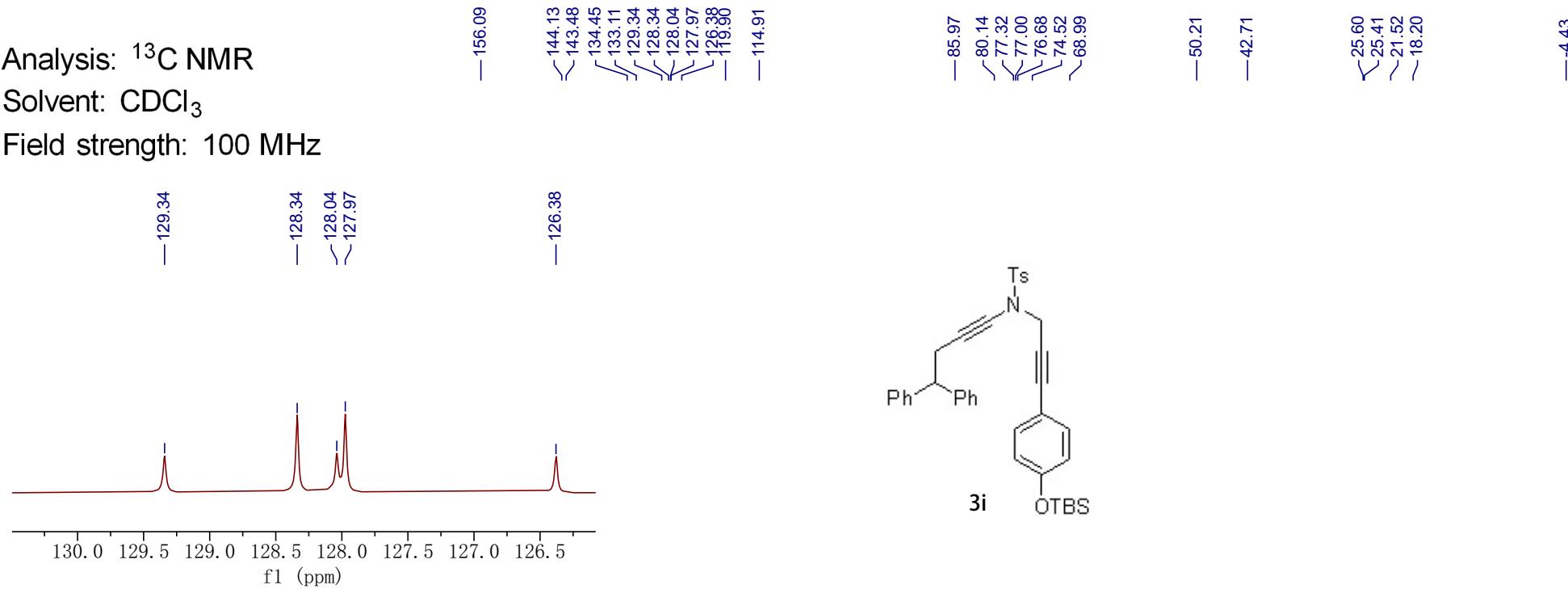
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



—0.000

<7.572  
<7.551  
7.262  
7.248  
7.226  
<7.219  
7.203  
<7.192  
7.186  
7.171  
7.154  
7.117  
7.096  
7.004  
6.983

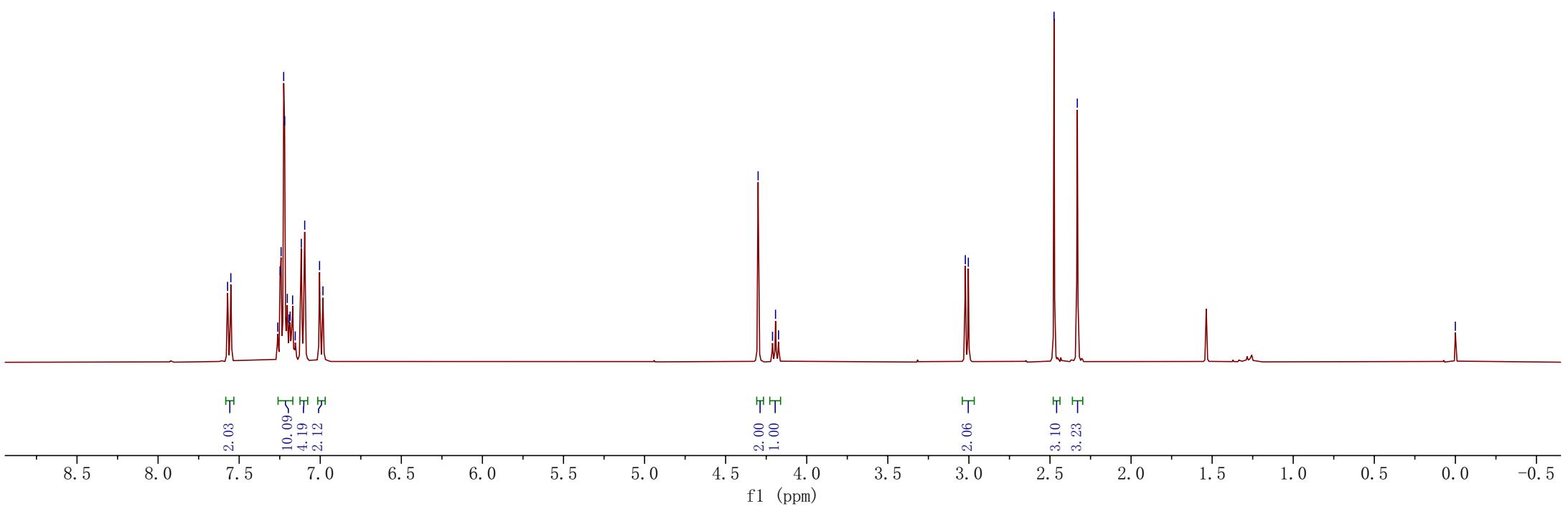
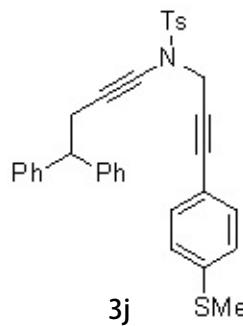
<3.022  
<3.004

—2.475  
—2.332

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

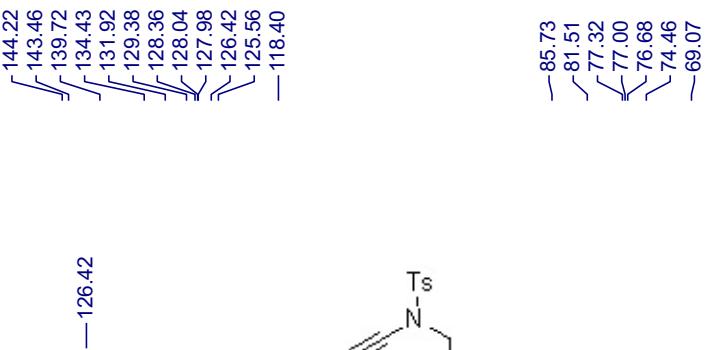
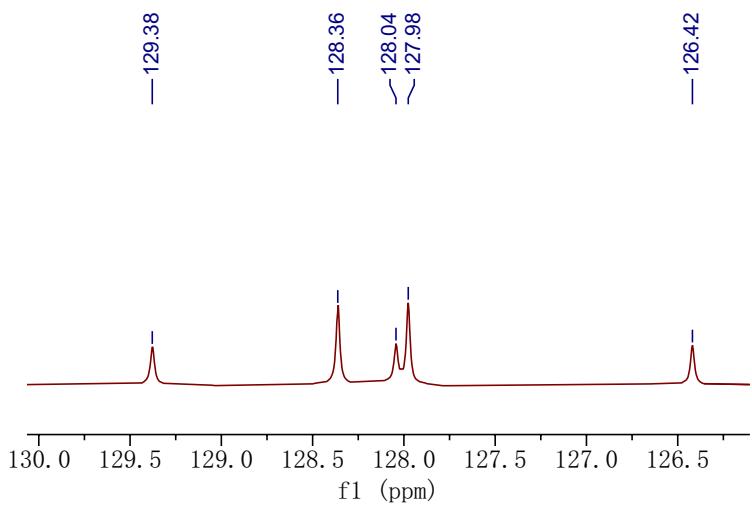
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

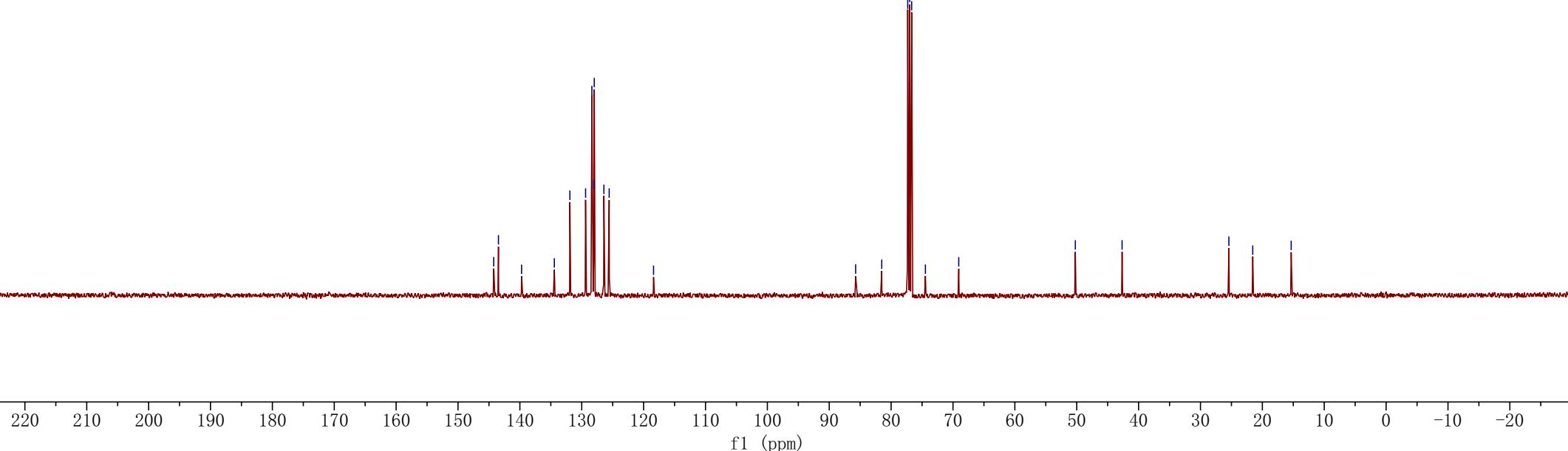
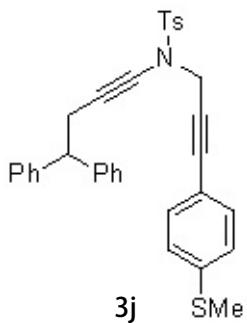
Field strength: 100 MHz



— 85.73  
— 81.51  
— 77.32  
— 77.00  
— 76.68  
— 74.46  
— 69.07

— 50.23  
— 42.67

— 25.41  
— 21.55  
— 15.34



— 0.000

2.337

2.326

3.021

3.002

4.302

4.212

4.194

4.175

7.571

7.550

7.260

7.242

7.225

7.219

7.203

7.190

7.185

7.168

7.160

7.152

7.115

7.094

7.067

7.046

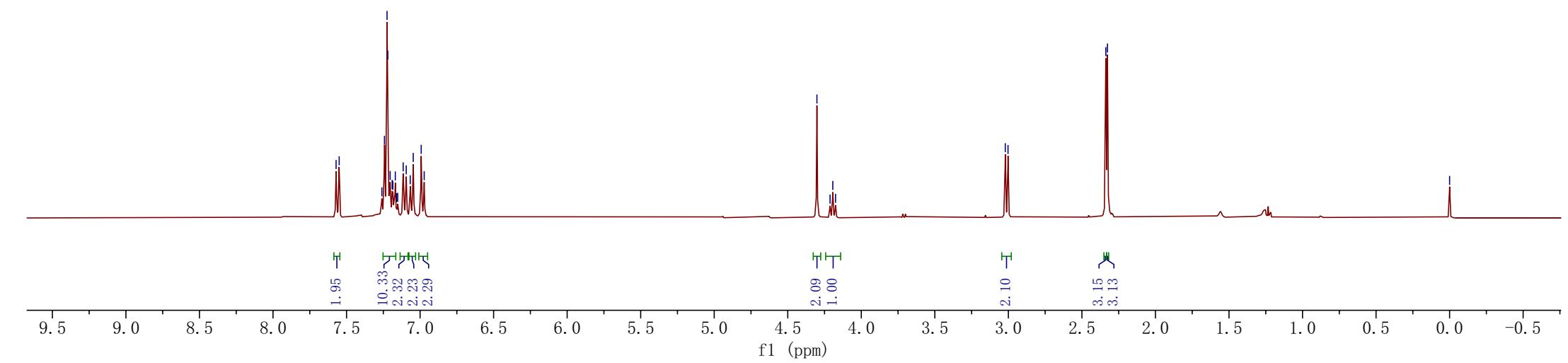
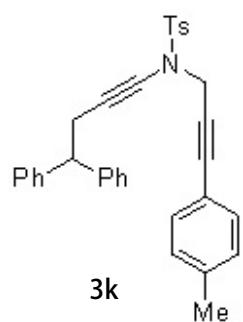
6.992

6.972

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

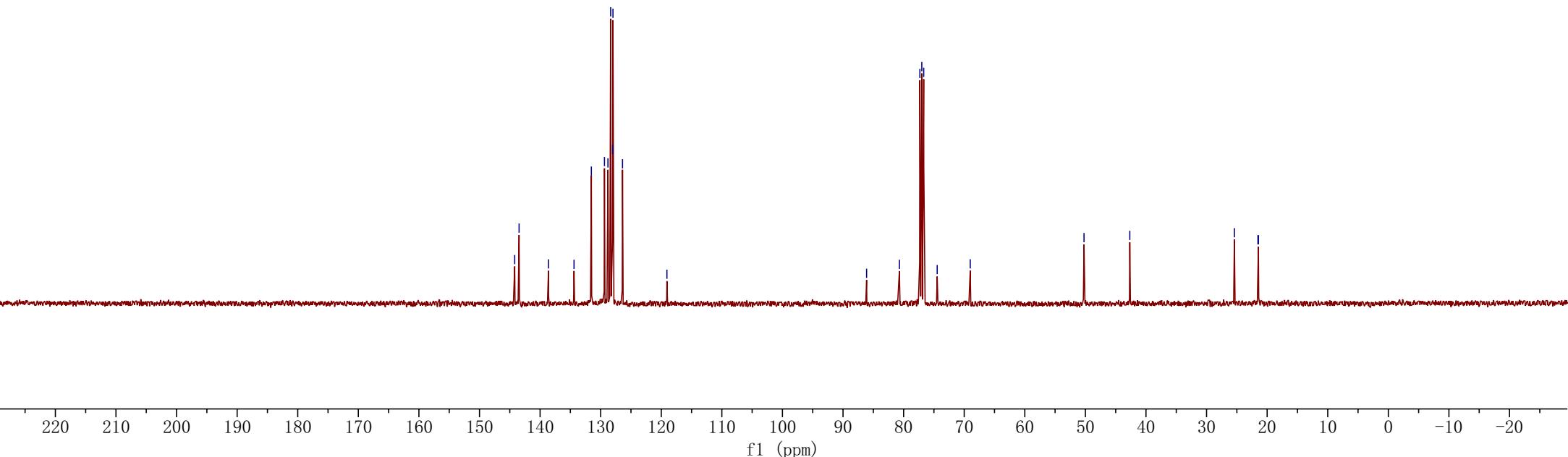
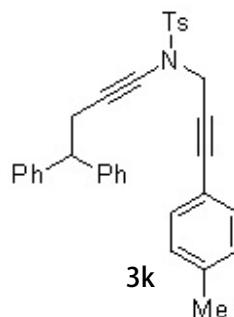
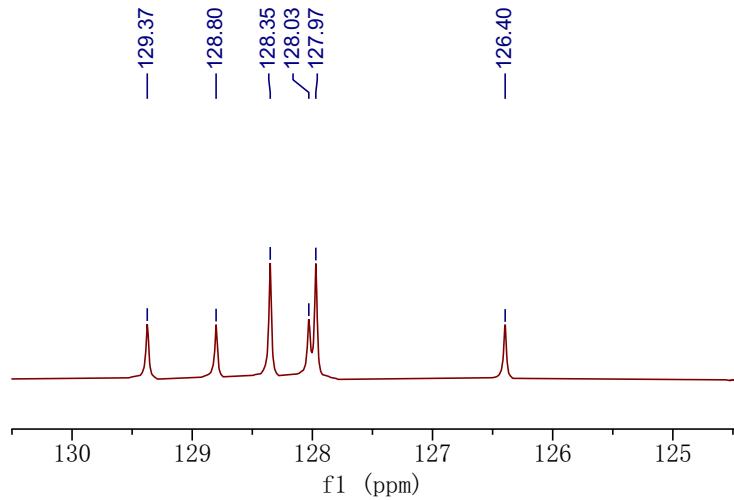
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.575  
7.554  
7.287  
7.269  
7.255  
7.237  
7.232  
7.215  
7.199  
7.178  
7.174  
7.165  
7.157  
7.149  
7.142  
7.104  
7.085  
7.068  
7.064

4.302  
4.212  
4.193  
4.175

3.021  
3.003

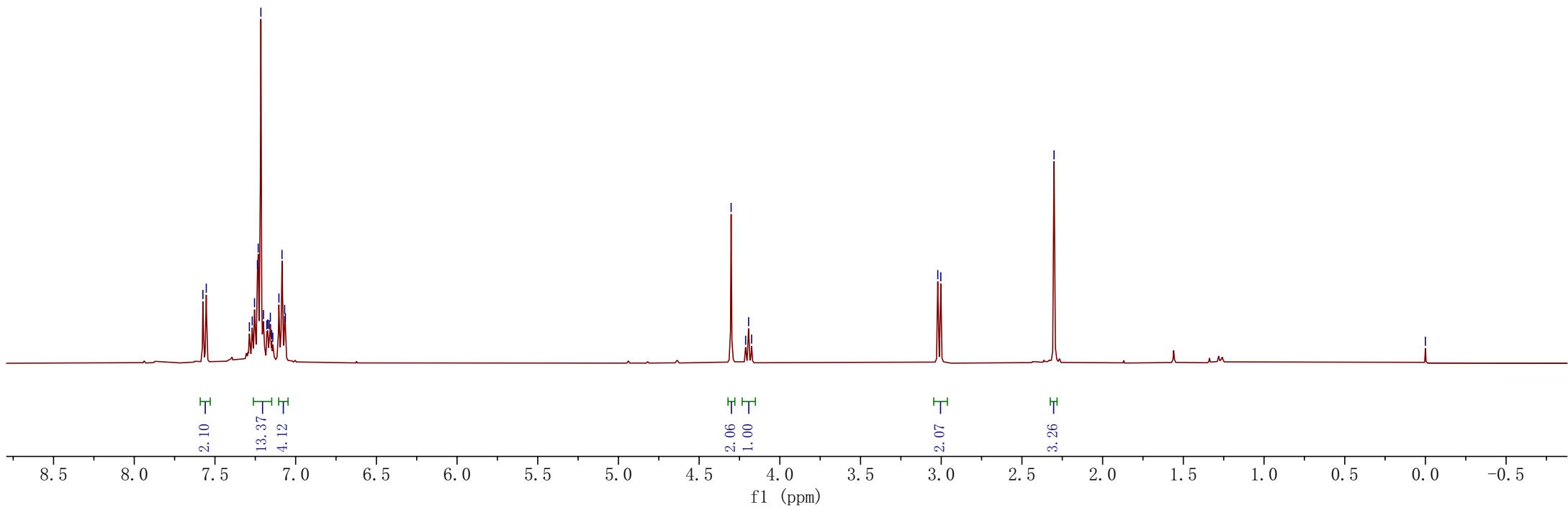
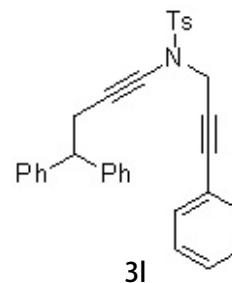
-2.301

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

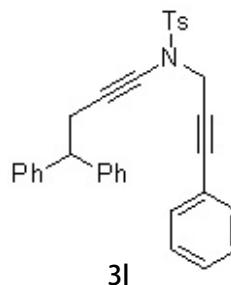
— 129.35  
— 128.44  
— 128.32  
— 128.02  
— 127.99  
— 127.92

— 144.23  
— 143.41  
— 134.33  
— 131.59  
— 129.35  
— 128.44  
— 128.32  
— 128.02  
— 127.99  
— 127.92  
— 126.37  
— 122.08

— 85.94  
— 81.38  
— 77.32  
— 77.00  
— 76.68  
— 74.41  
— 69.01

— 50.18  
— 42.57

— 25.35  
— 21.46



130.0 129.5 129.0 128.5 128.0 127.5 127.0

f1 (ppm)

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

f1 (ppm)

7.570  
7.549  
7.256  
7.238  
7.220  
7.202  
7.177  
7.156  
7.137  
7.122  
7.101  
6.861  
6.856  
6.840  
6.836  
6.697  
6.678  
6.644

4.302  
4.211  
4.192  
4.174

-3.762

3.021  
3.002

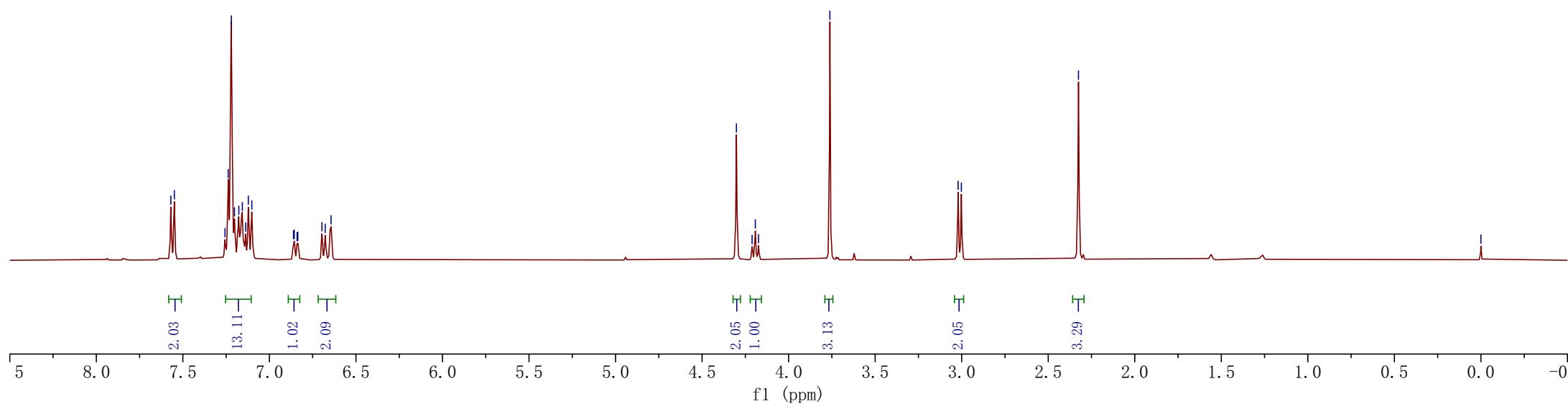
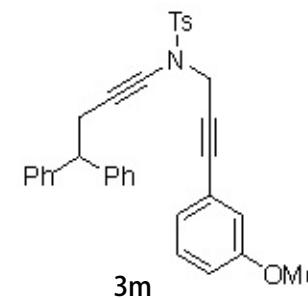
-2.325

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

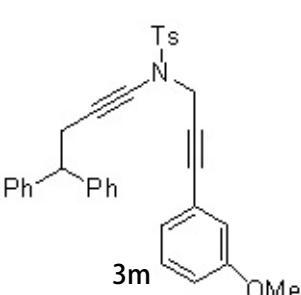
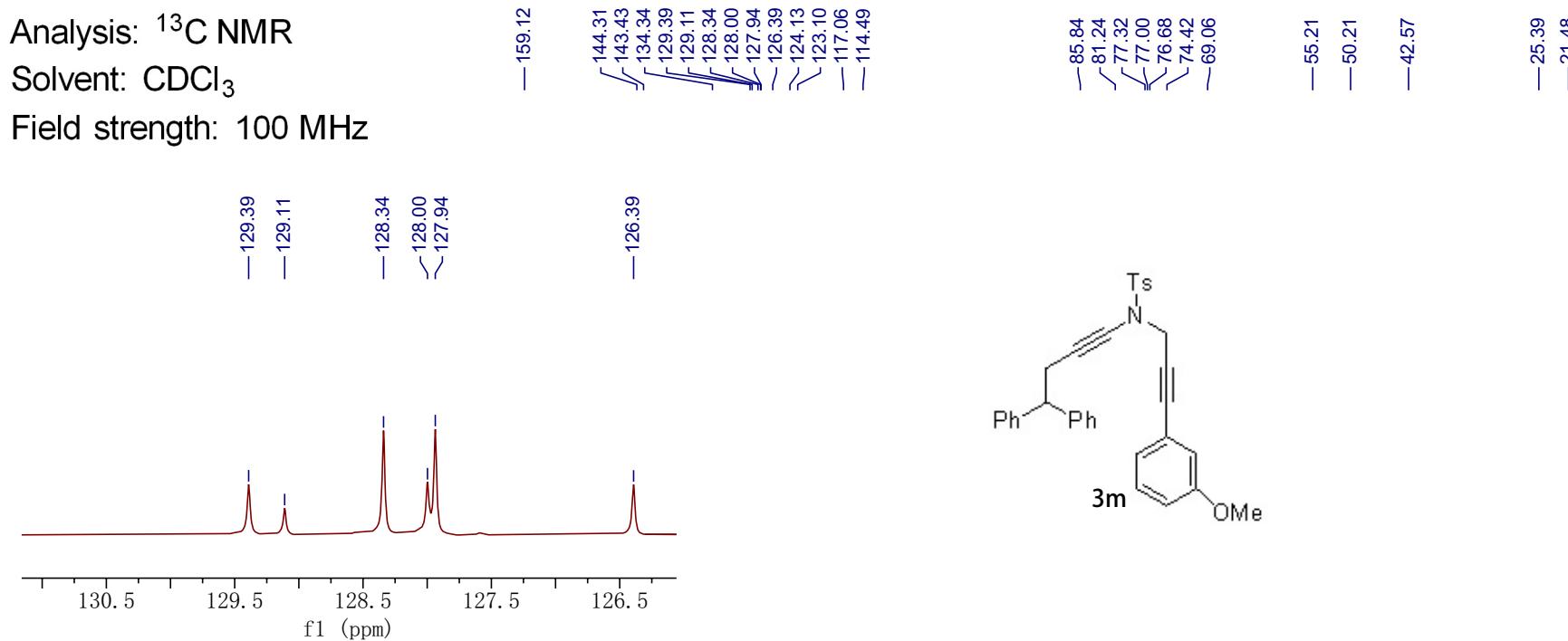
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



f1 (ppm)

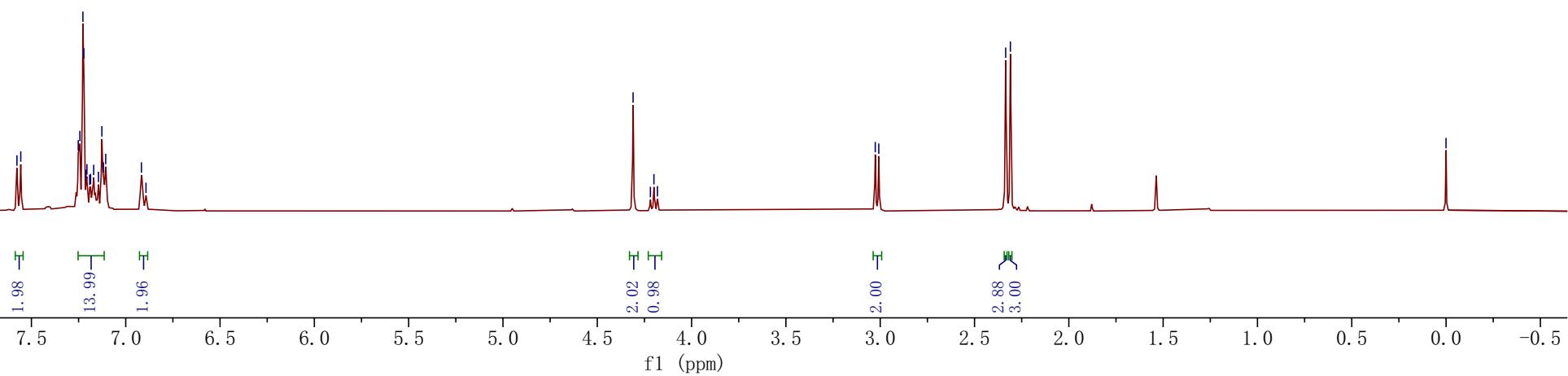
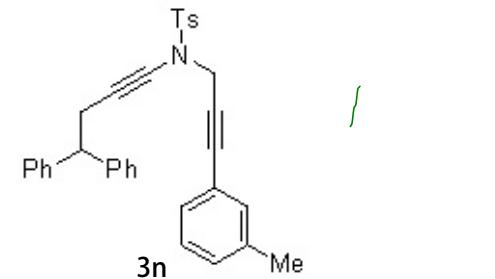
7.577  
7.556  
7.252  
7.243  
7.227  
7.222  
7.210  
7.206  
7.191  
7.186  
7.170  
7.145  
7.126  
7.118  
7.106  
6.917  
6.893

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

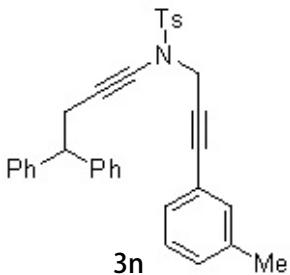
— 129.39  
— 129.36  
— 128.78  
— 128.37  
— 128.07  
— 127.98

— 144.18  
— 143.48  
— 137.69  
— 134.45  
— 132.16  
— 129.39  
— 129.36  
— 128.78  
— 128.37  
— 128.07  
— 127.98  
— 126.41  
— 121.98

— 86.13  
— 81.03  
— 77.32  
— 77.00  
— 76.68  
— 74.46  
— 69.04

— 50.25  
— 42.65

— 25.43  
— 21.55  
— 21.20



130.0 129.5 129.0 128.5 128.0 127.5 127.0  
f1 (ppm)

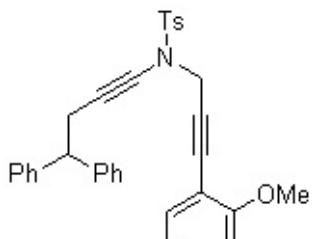
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20  
f1 (ppm)



Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

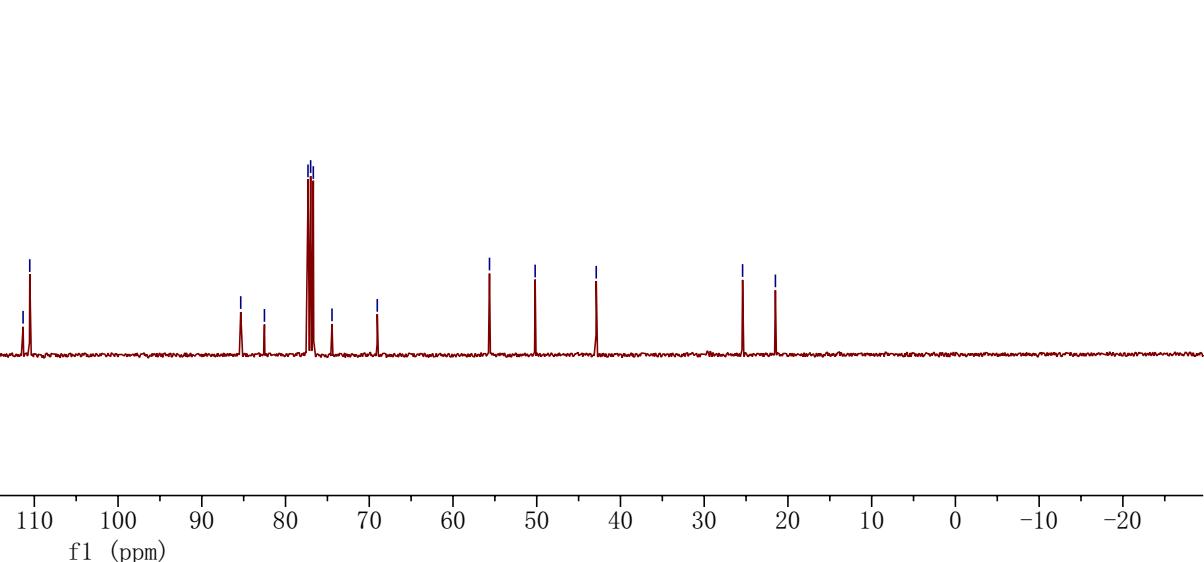
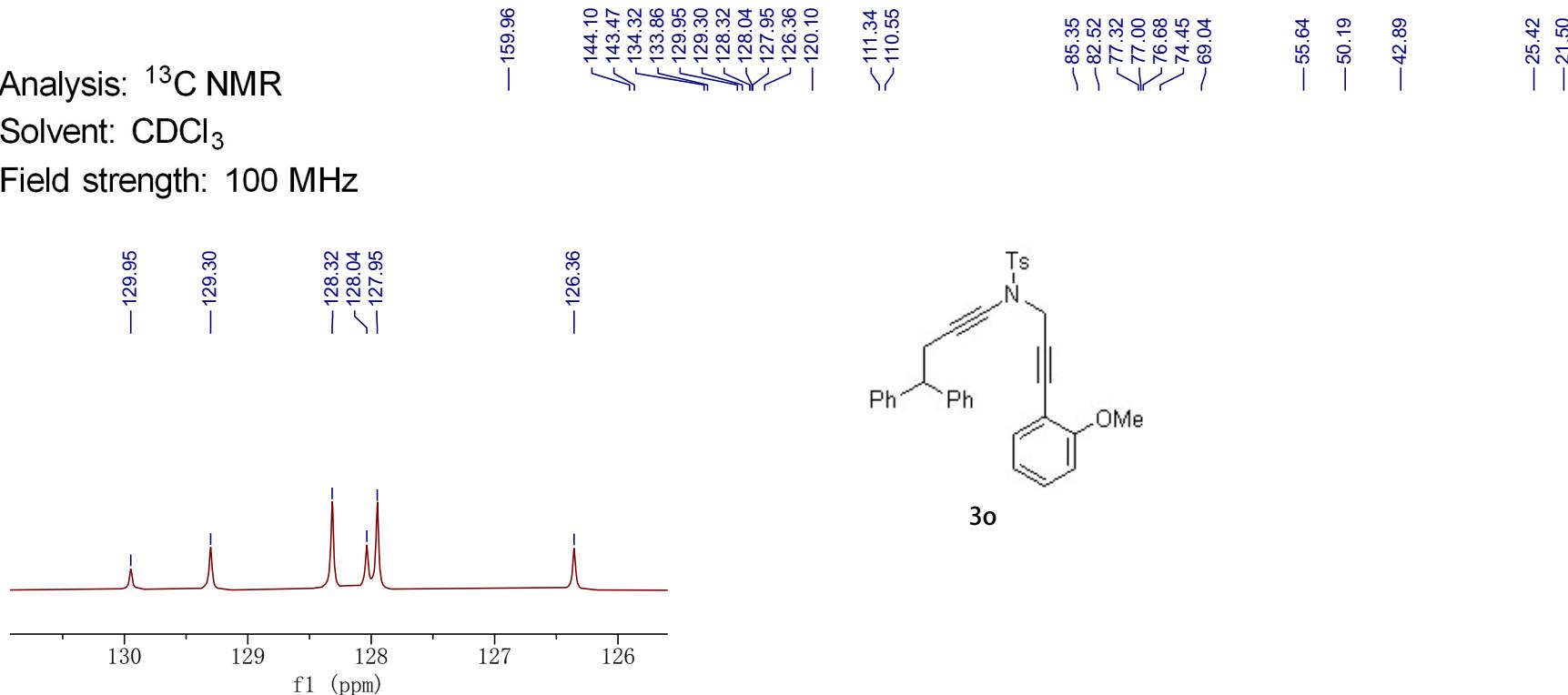
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.540  
7.520  
7.267  
7.246  
7.232  
7.221  
7.204  
7.191  
7.170  
7.137  
7.118  
7.076  
7.056

4.356  
4.213  
4.194  
4.175

3.021  
3.002

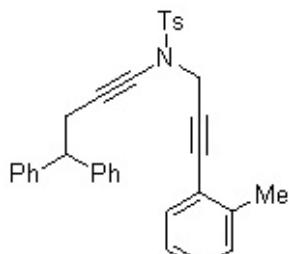
2.273  
2.159

-0.000

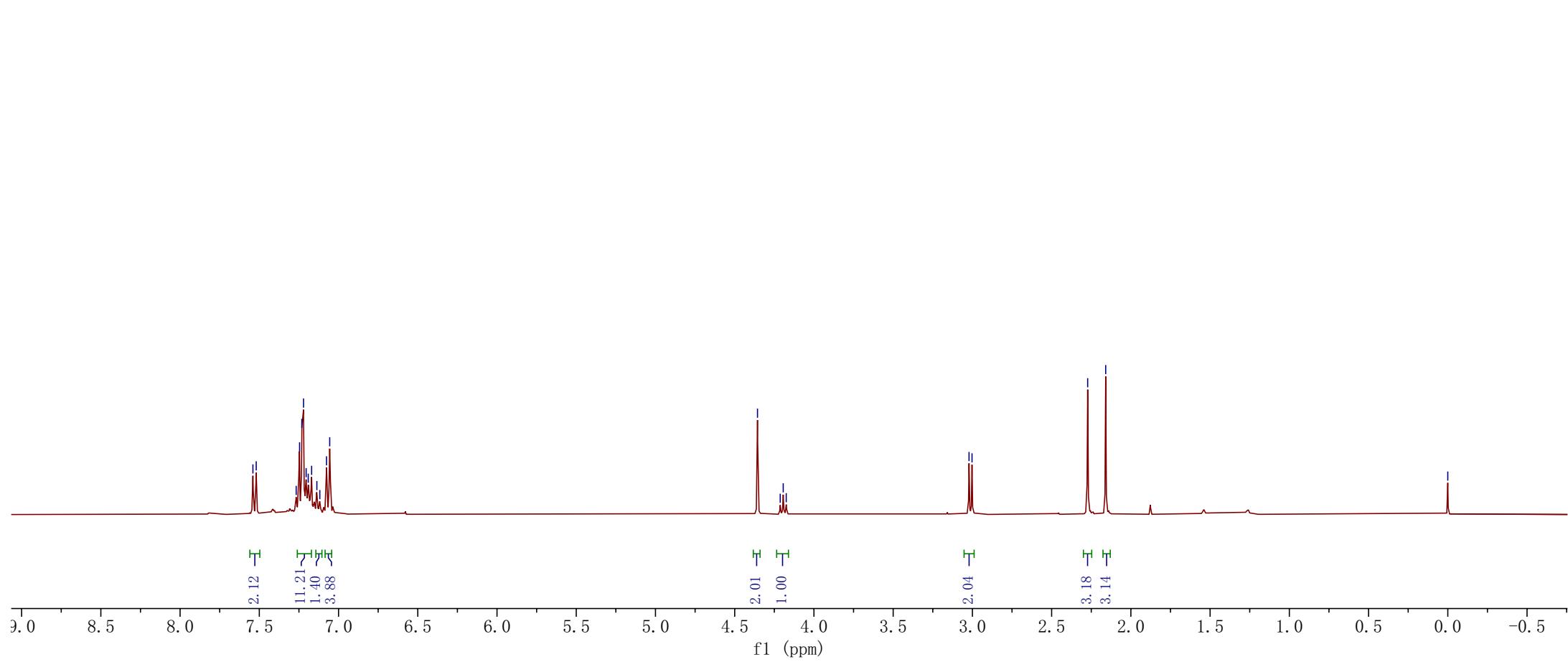
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



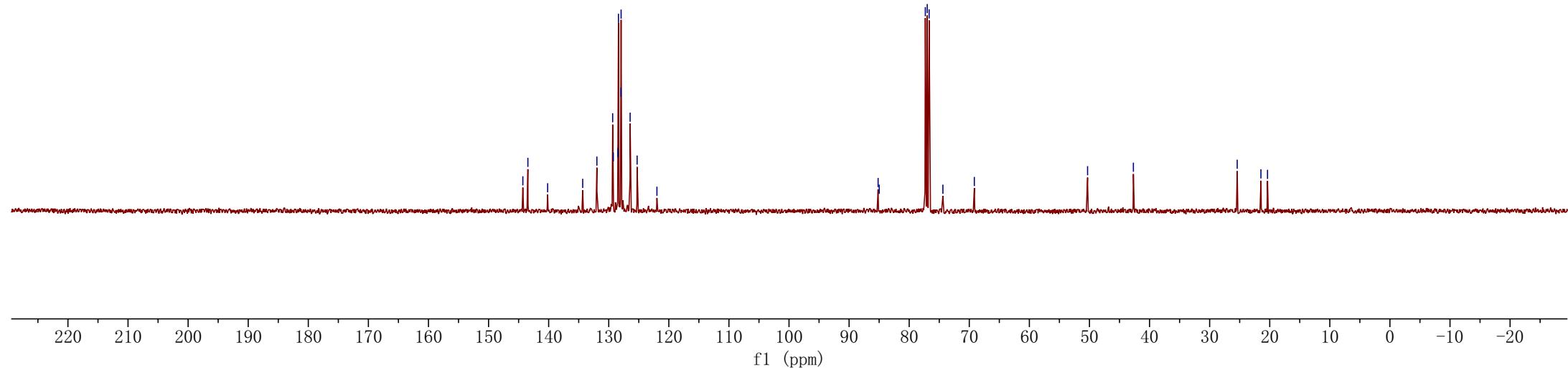
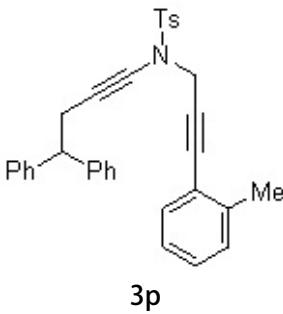
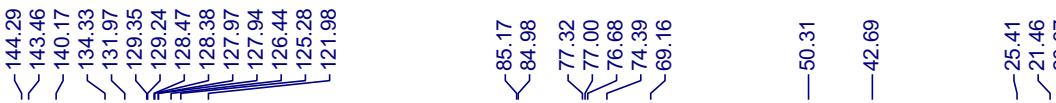
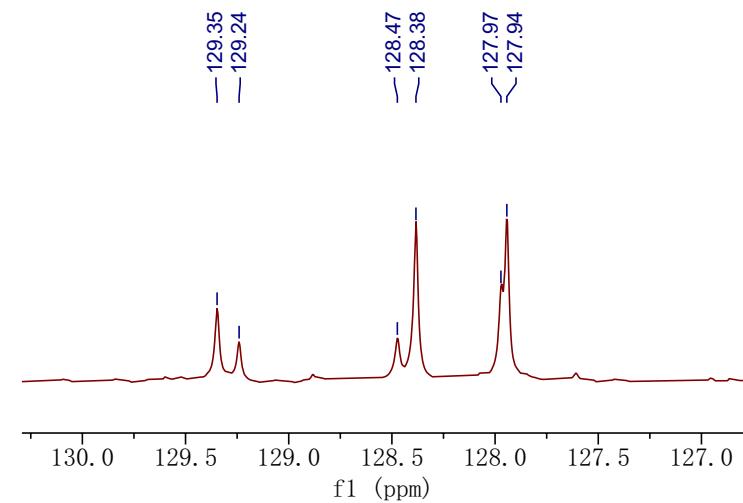
3p



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

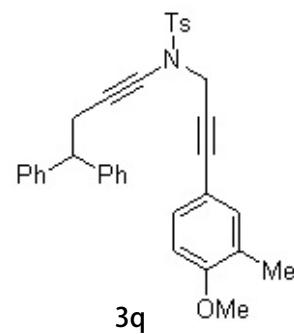




Analysis: <sup>1</sup>H NMR

Solvent: CDCl<sub>3</sub>

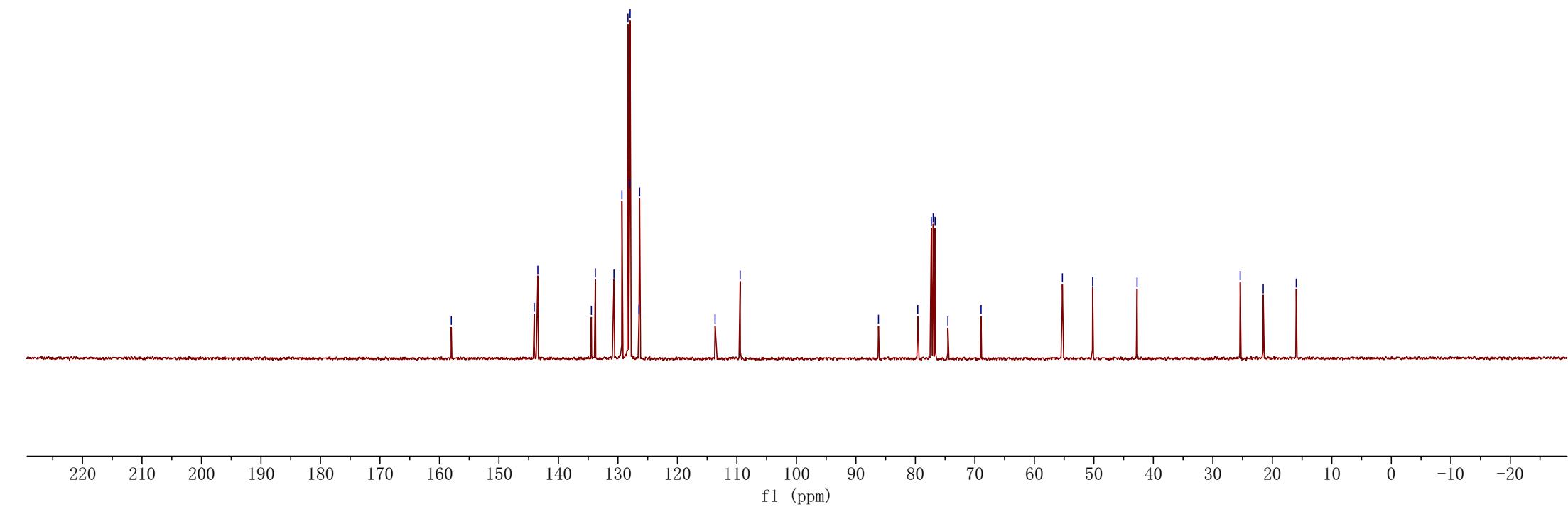
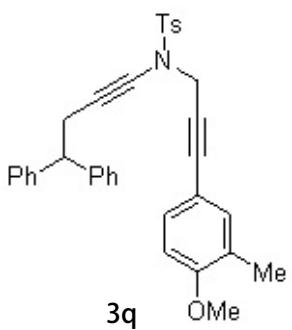
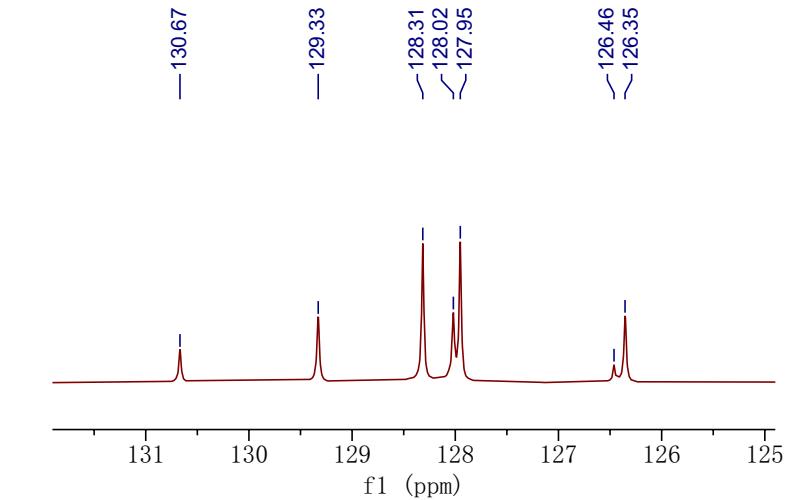
Field strength: 400 MHz



## Analysis: $^{13}\text{C}$ NMR

Solvent: CDCl<sub>3</sub>

Field strength: 100 MHz



7.578  
7.558  
7.260  
7.247  
7.225  
7.205  
7.188  
7.183  
7.167  
7.132  
7.112  
6.742  
6.704

4.305  
4.211  
4.193  
4.174  
3.878  
3.823

3.020  
3.001

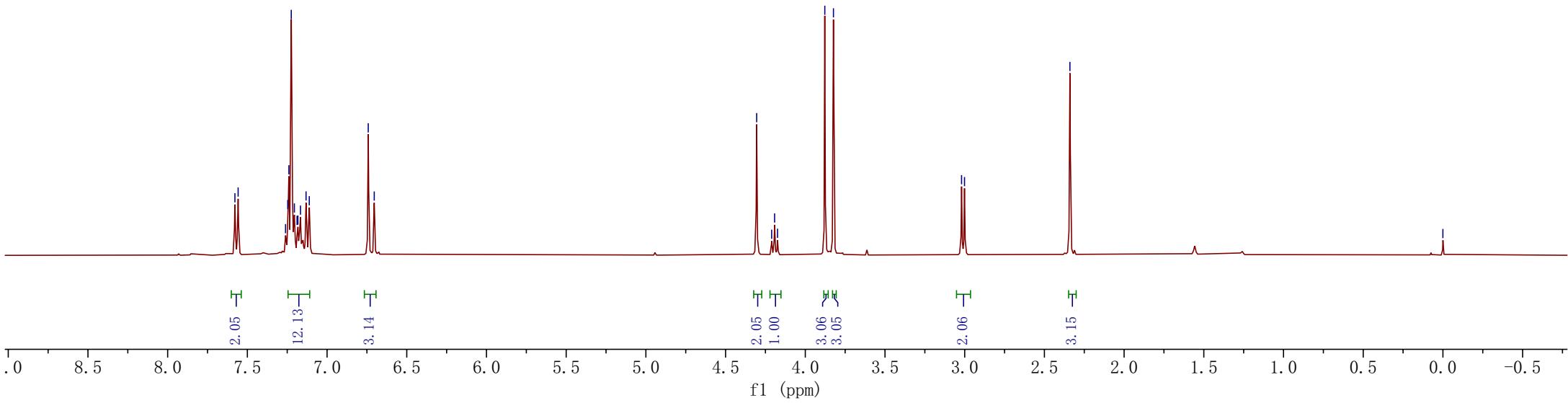
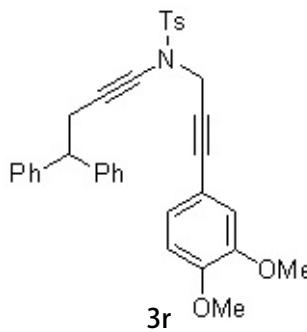
-2.340

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

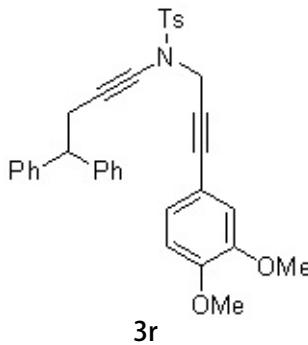
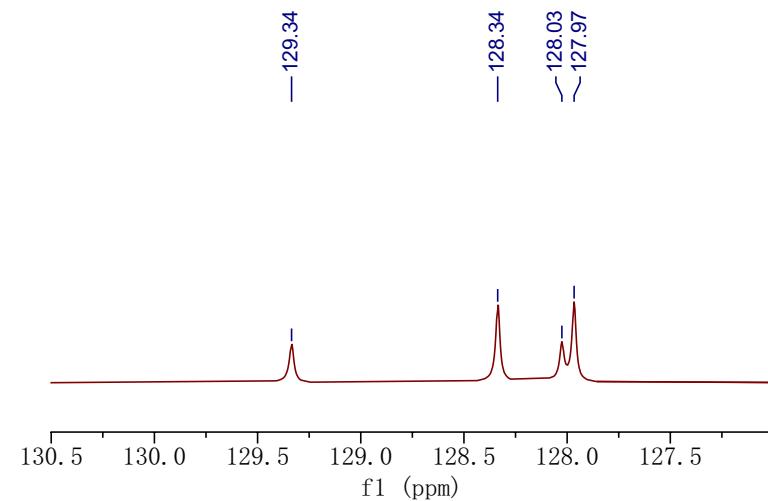
Field strength: 400 MHz



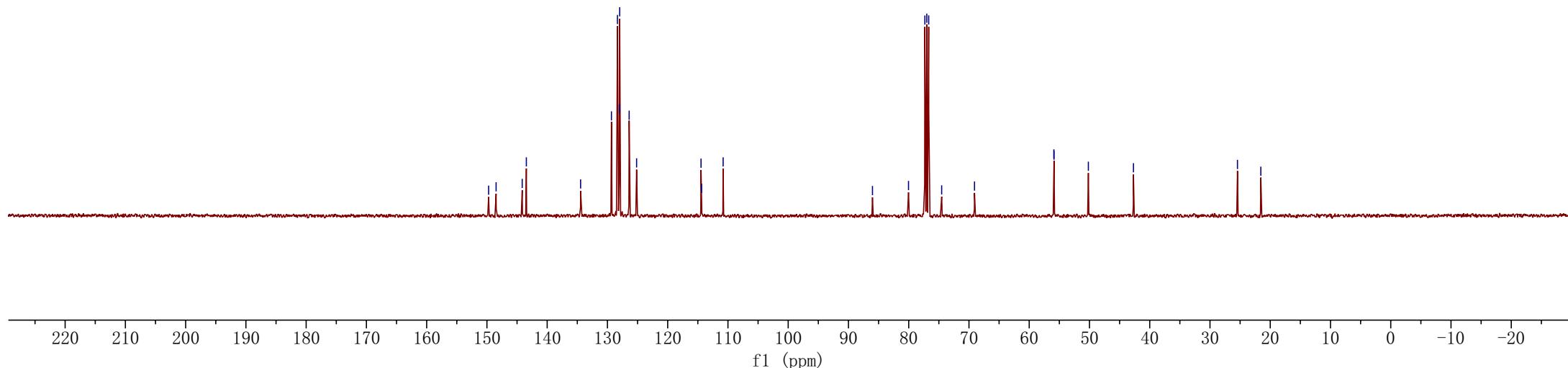
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**3r**

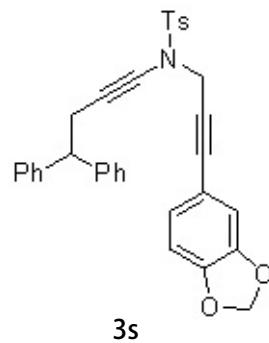




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

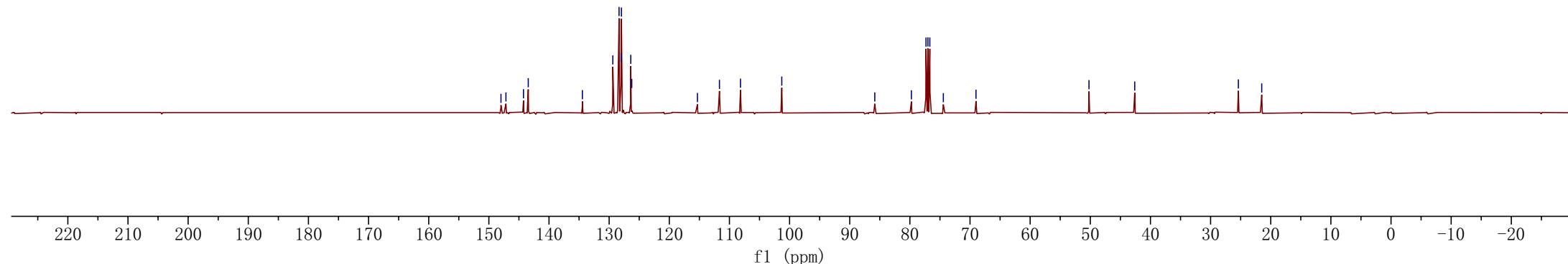
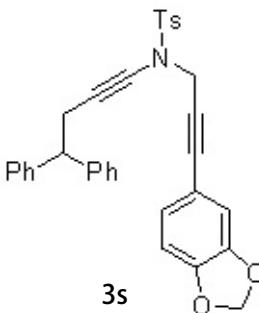
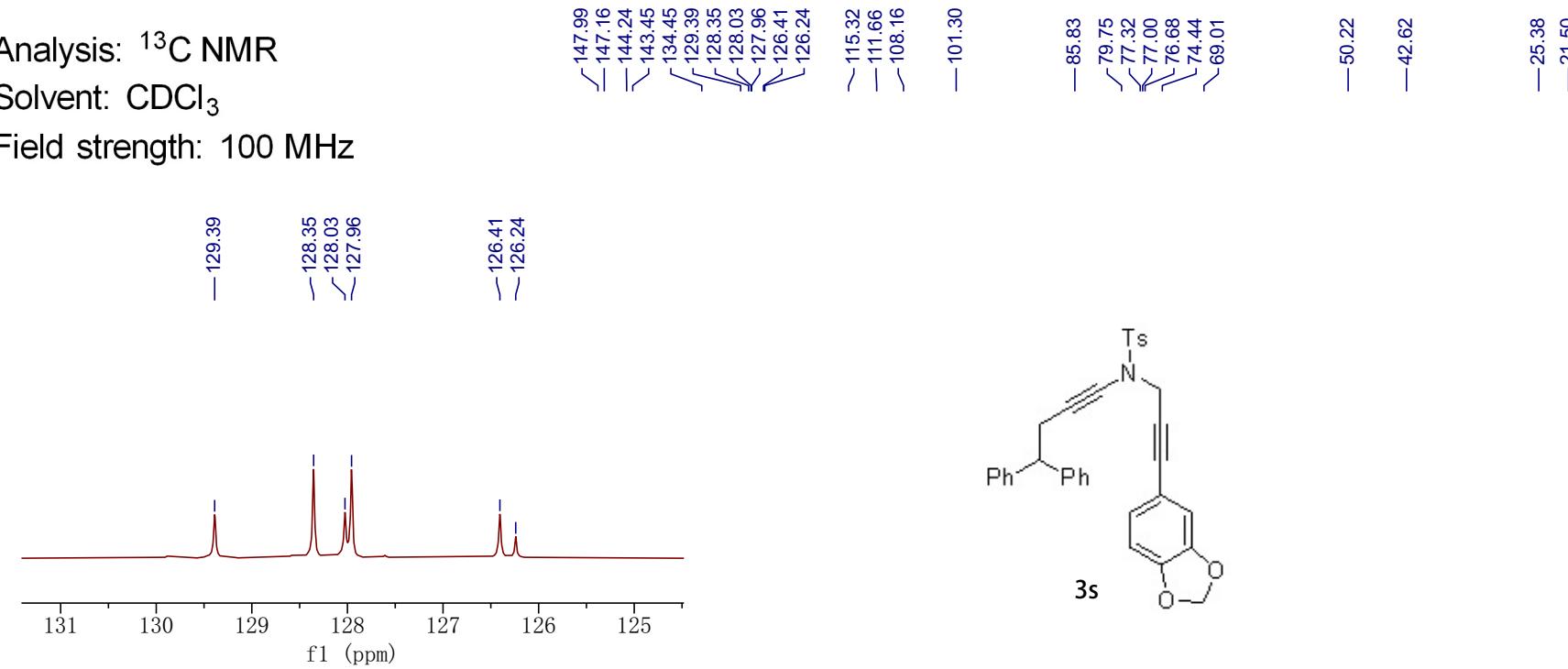
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

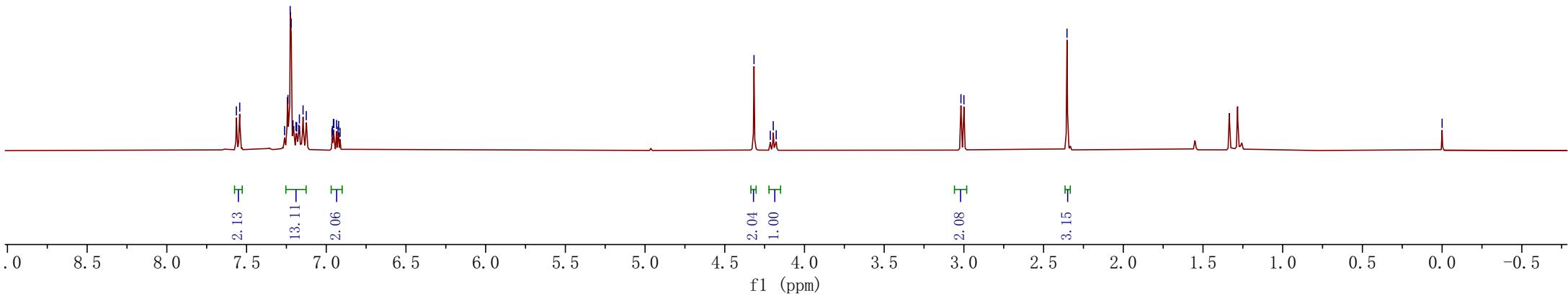
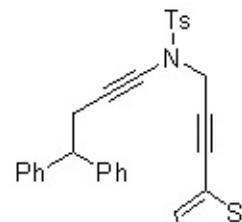




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

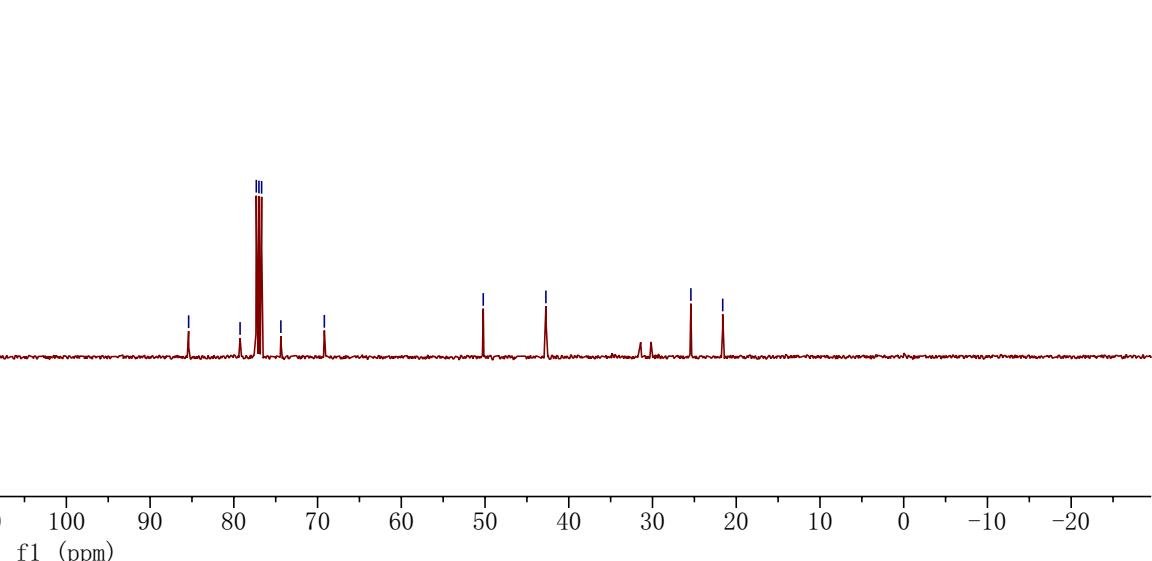
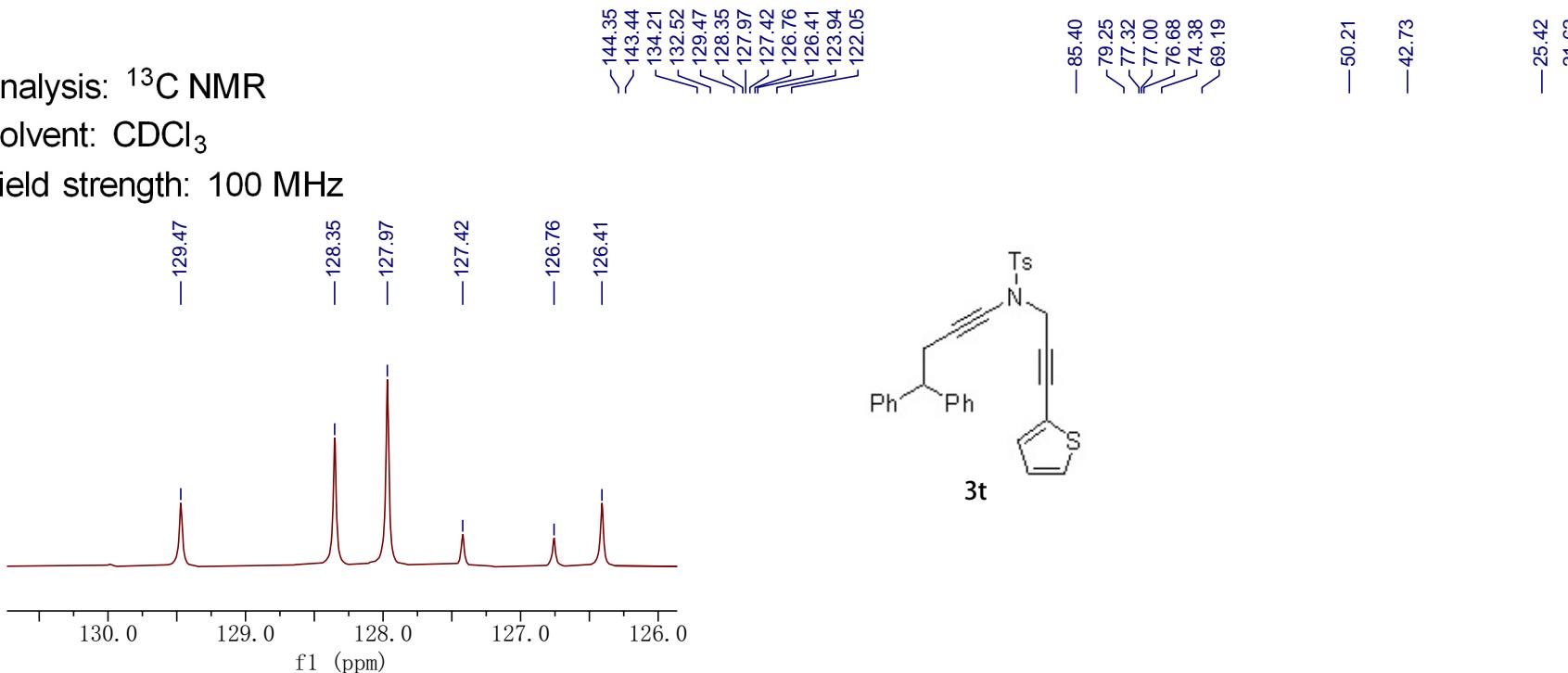
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.584  
7.564  
7.108  
7.103  
7.088  
7.044  
7.038  
7.024  
7.015  
6.782  
6.760

4.302  
4.146  
4.127  
4.109

3.801

2.978  
2.960

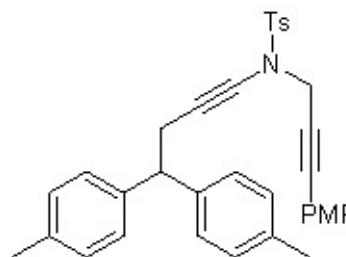
2.331  
2.275

-0.000

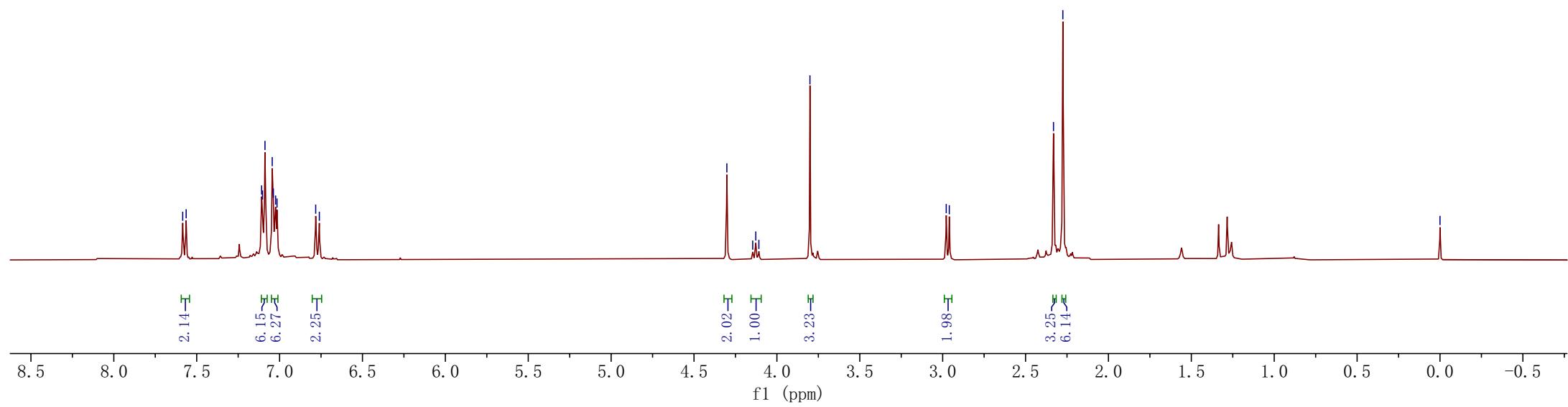
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



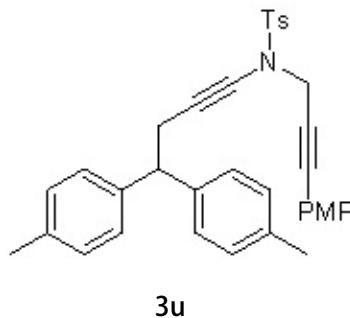
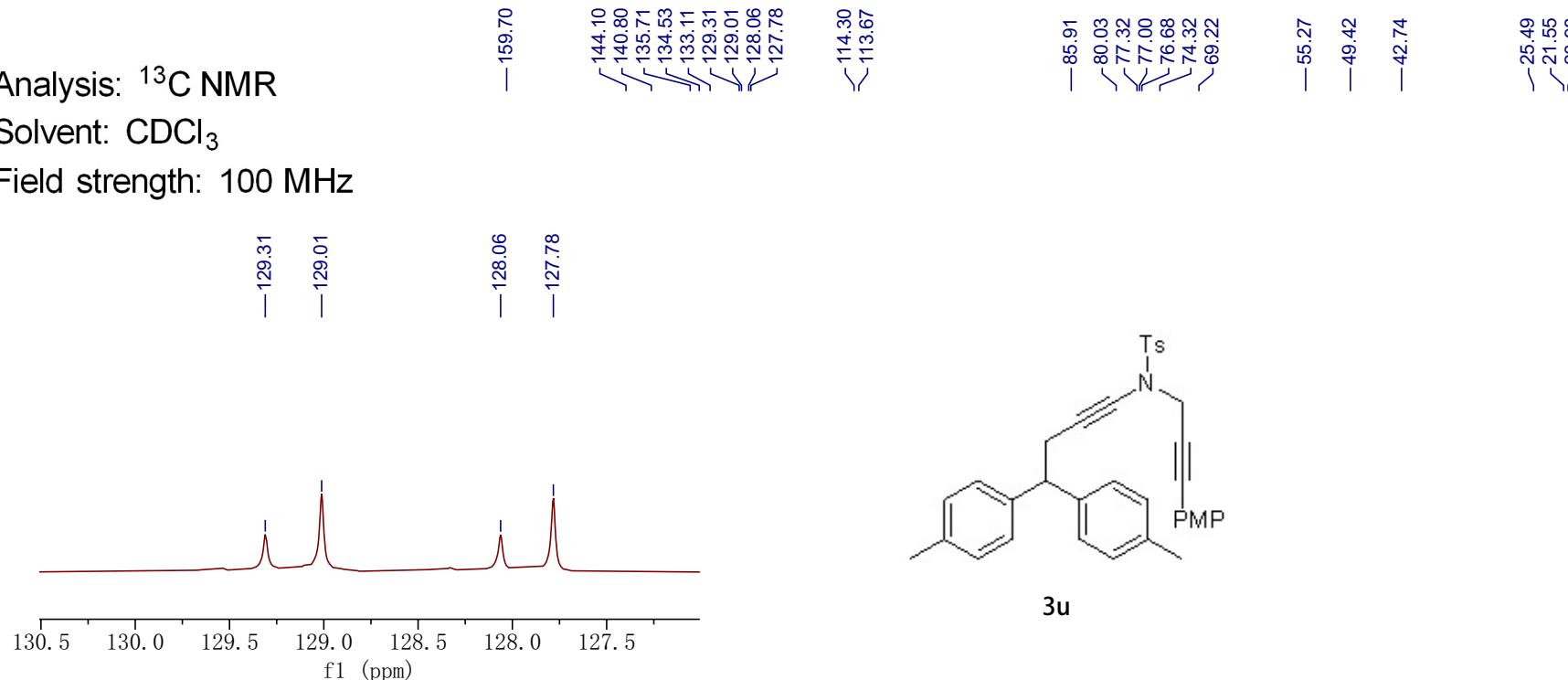
**3u**



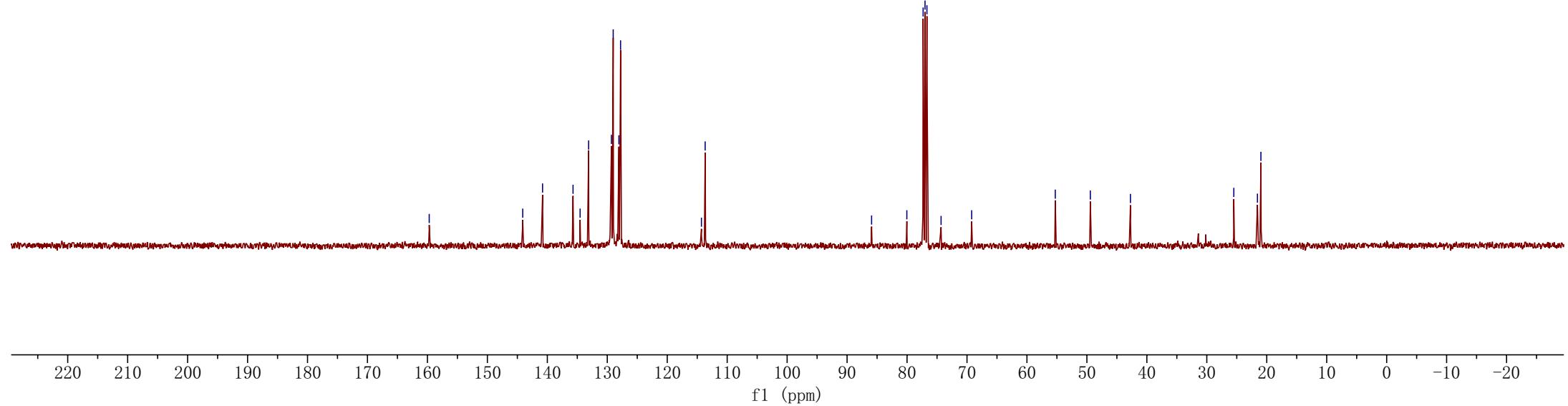
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**3u**

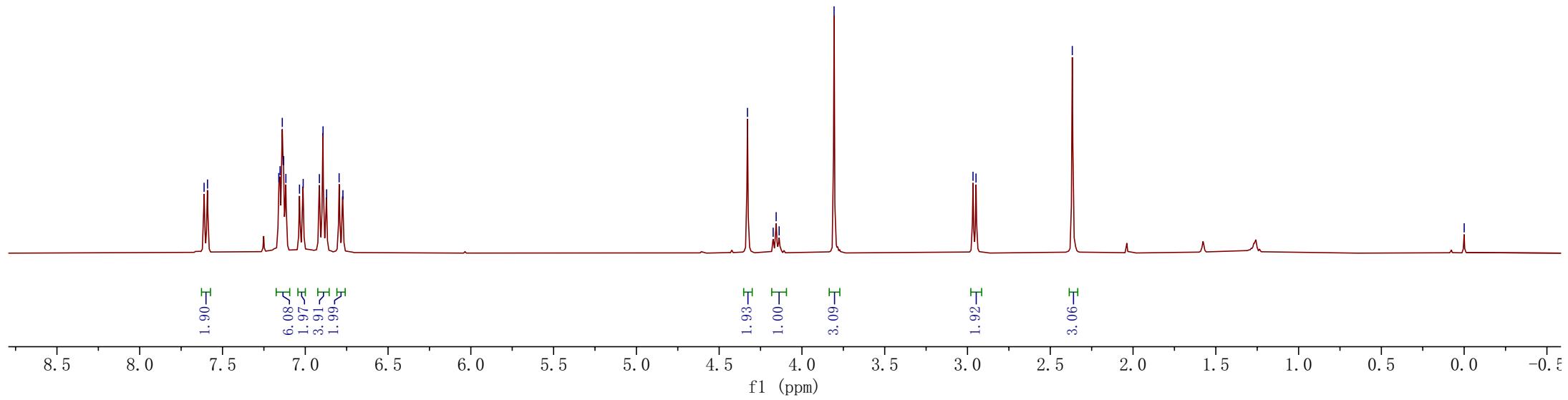
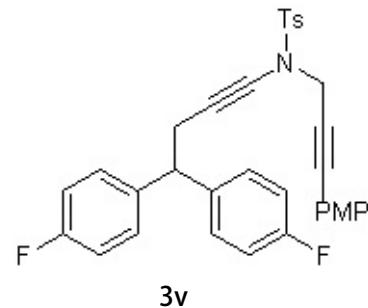




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 115.26  
— 115.05

— 114.06  
— 113.76

— 162.68  
— 160.25  
— 159.81

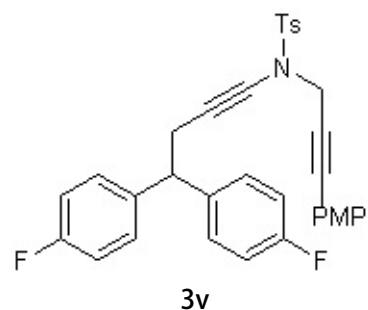
— 144.40  
— 138.96  
— 138.93  
— 134.48  
— 133.07  
— 129.43  
— 129.38  
— 129.35  
— 127.98

— 115.26  
— 115.05  
— 114.06  
— 113.76

— 85.97  
— 79.95  
— 77.32  
— 77.00  
— 76.68  
— 74.87  
— 68.44

— 55.28  
— 48.51  
— 42.67

— 25.69  
— 21.52



$3\mathbf{v}$

116 115 114 113 112 111

f1 (ppm)

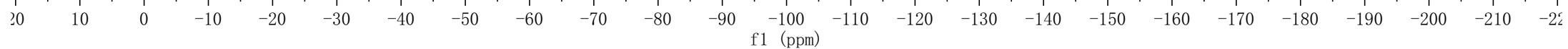
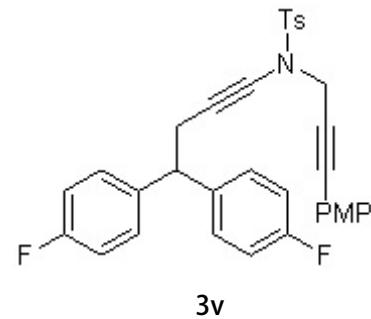
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

f1 (ppm)

Analysis:  $^{19}\text{F}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz



7.599  
7.579  
7.185  
7.163  
7.141  
7.111  
7.089  
7.015  
6.993  
6.802  
6.780

4.333  
4.157  
4.139  
4.121

-3.810

2.970  
2.952

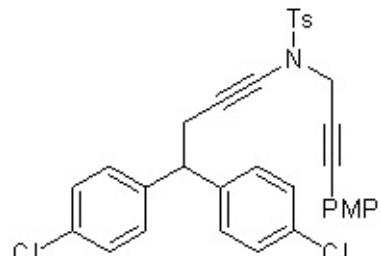
-2.380

-0.000

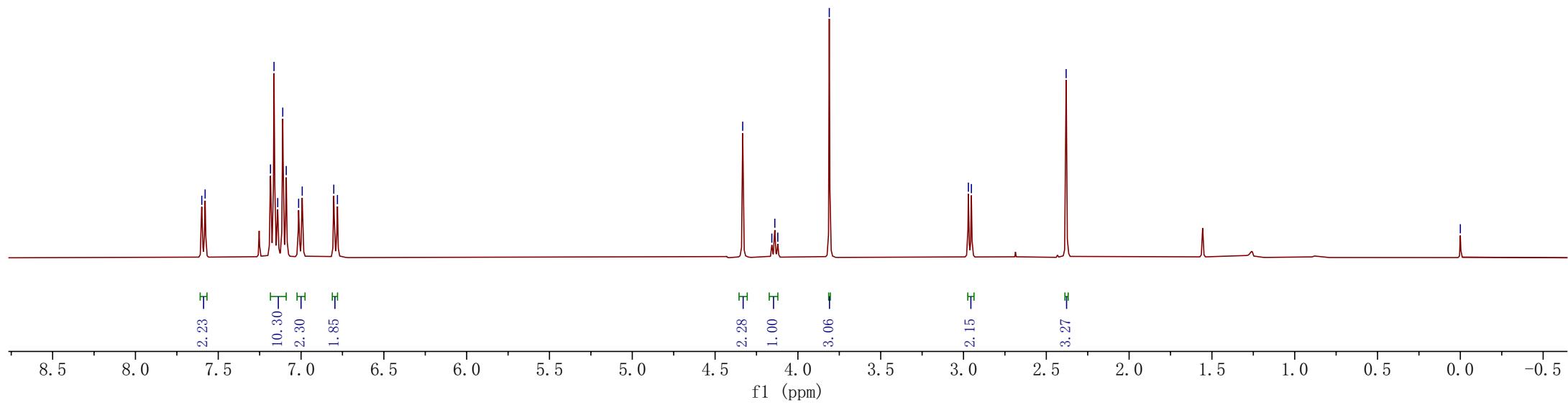
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



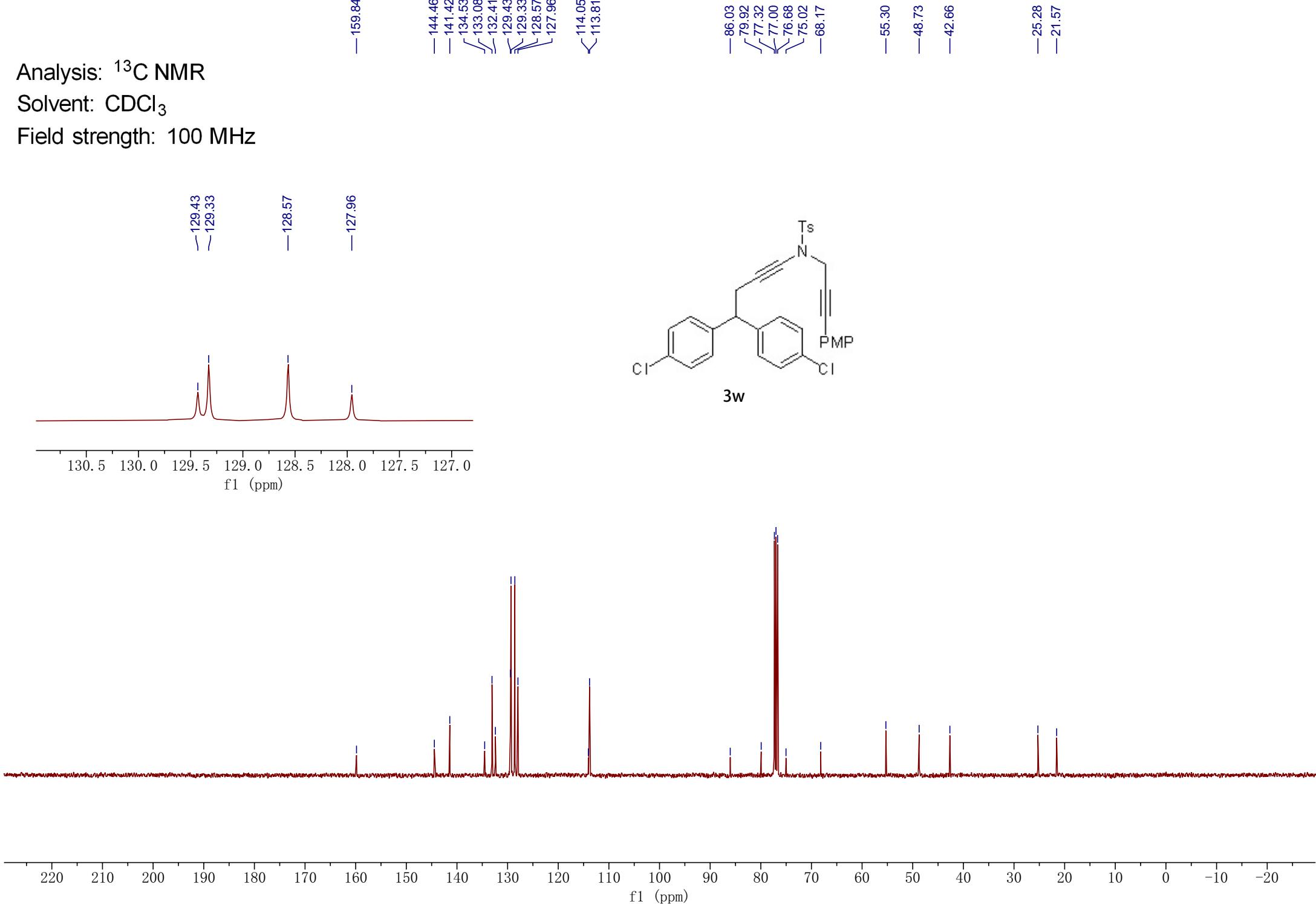
**3w**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

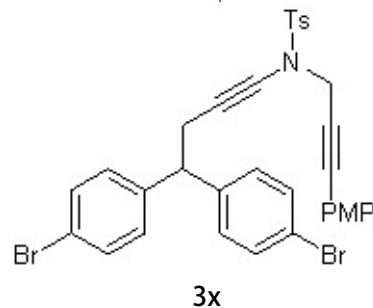


<7.598  
<7.577  
<7.334  
<7.313  
<7.166  
<7.146  
<7.054  
<7.033  
<7.009  
<6.988  
<6.807  
<6.785

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

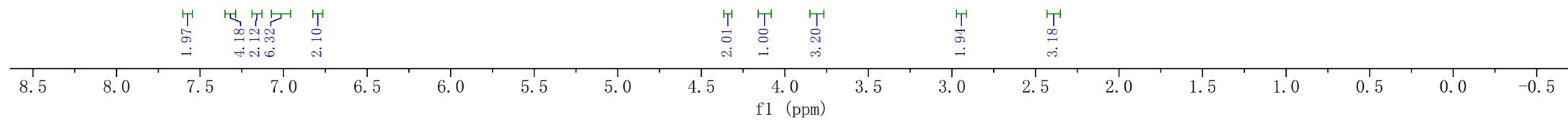


**3x**

1.97 -T  
4.18 -T  
2.12 -T  
6.32 -T  
2.10 -T

-4.333  
<4.128  
<4.110  
<4.092  
-3.813  
-2.967  
<2.949  
-2.389

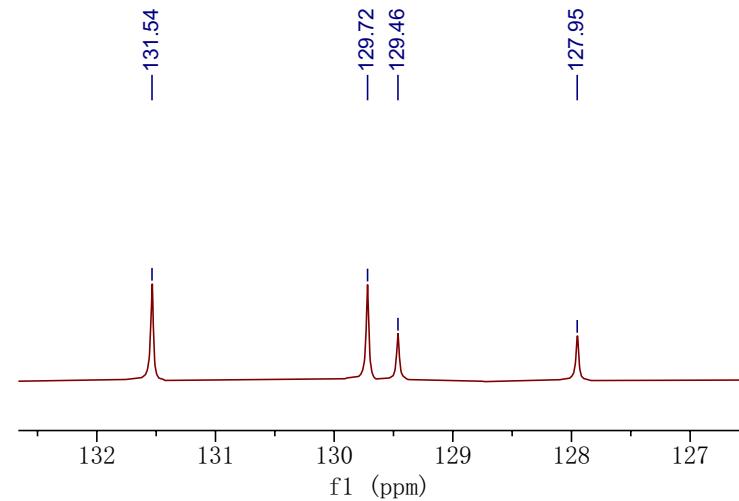
-0.000



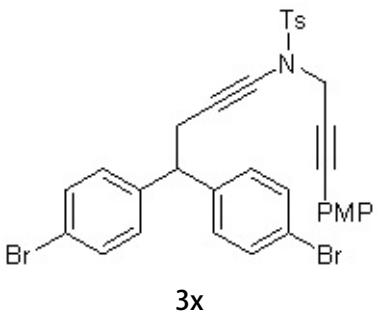
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



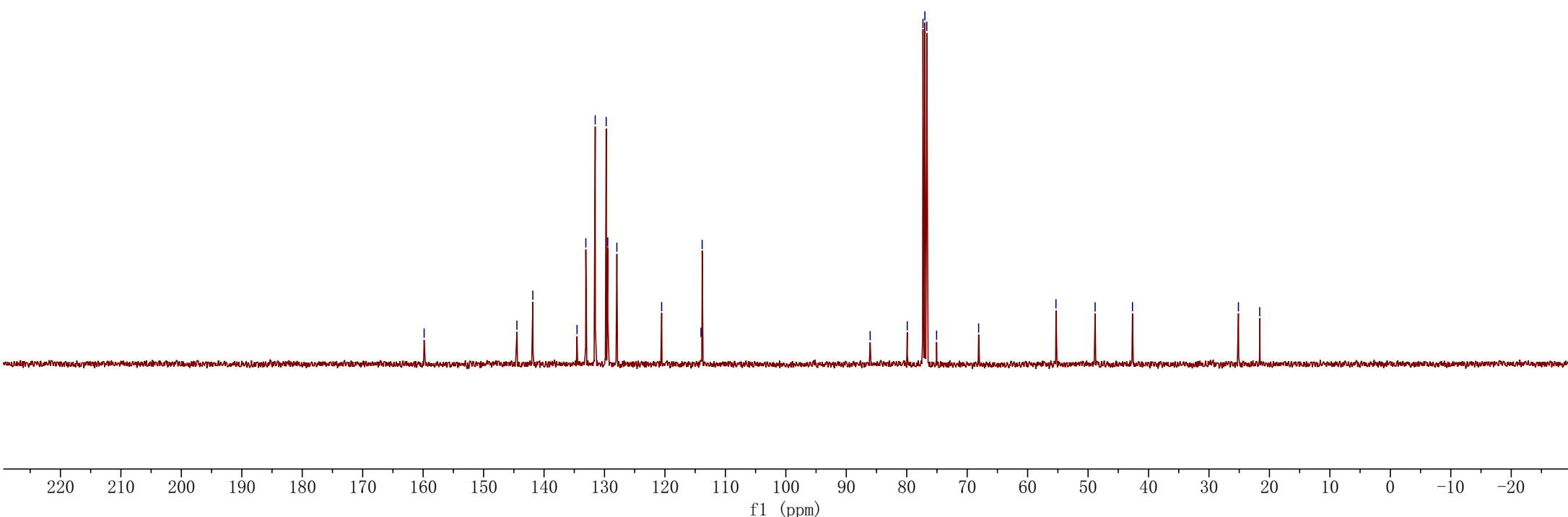
—144.48  
—141.85  
—134.54  
—133.09  
—131.54  
—129.72  
—129.46  
—127.95  
—120.55

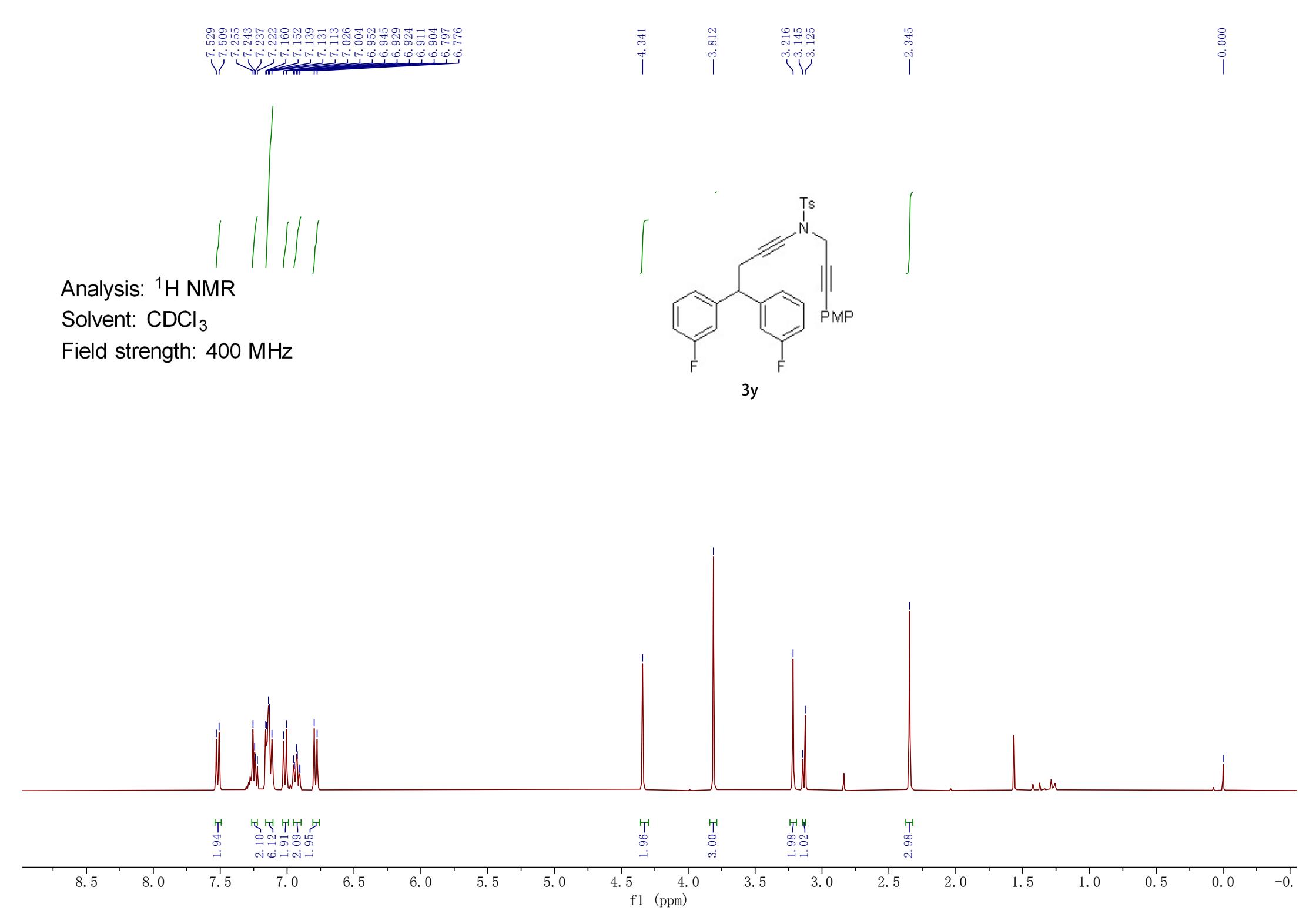


**3x**

—114.04  
—113.84  
—86.05  
—79.92  
—77.32  
—77.00  
—76.68  
—75.06  
—68.11

—55.31  
—48.84  
—42.66  
—25.13  
—21.61

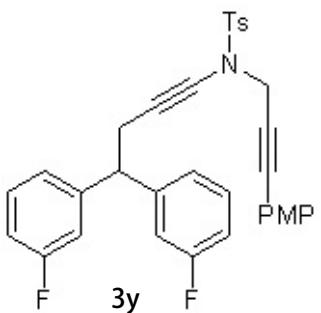
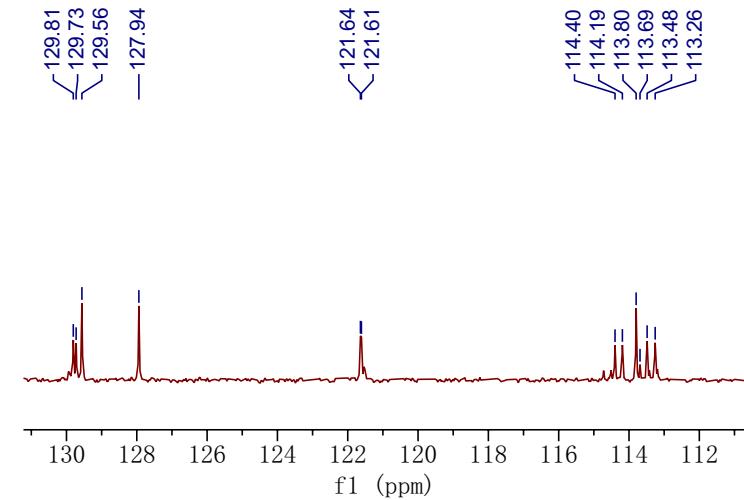




Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

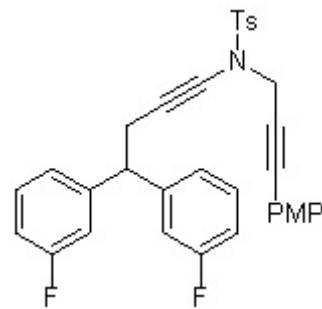
Field strength: 100 MHz



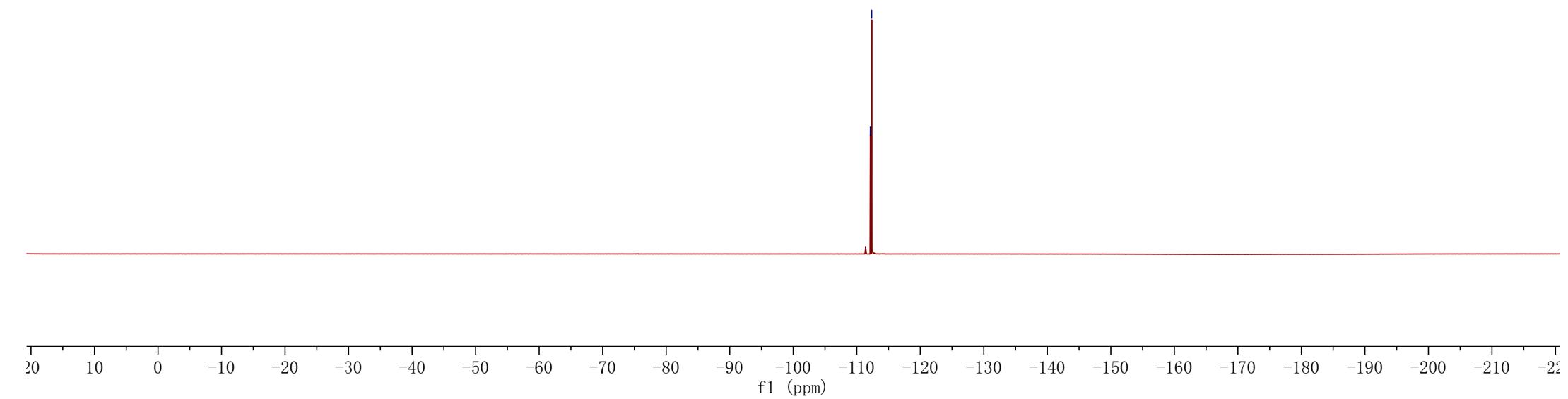
Analysis:  $^{19}\text{F}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz



3y



7.767  
7.747  
7.246  
7.227  
7.212  
7.205  
7.194  
7.173  
7.166  
7.160  
7.156  
7.089  
7.067  
6.782  
6.760

-4.387

-3.794

2.961  
2.944  
2.927  
2.909  
2.619  
2.604  
2.578  
2.562  
2.530  
2.511  
2.488  
2.470  
2.362

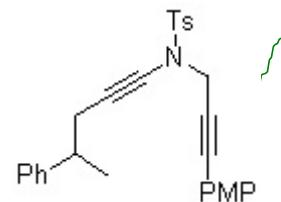
1.321  
1.304

0.000

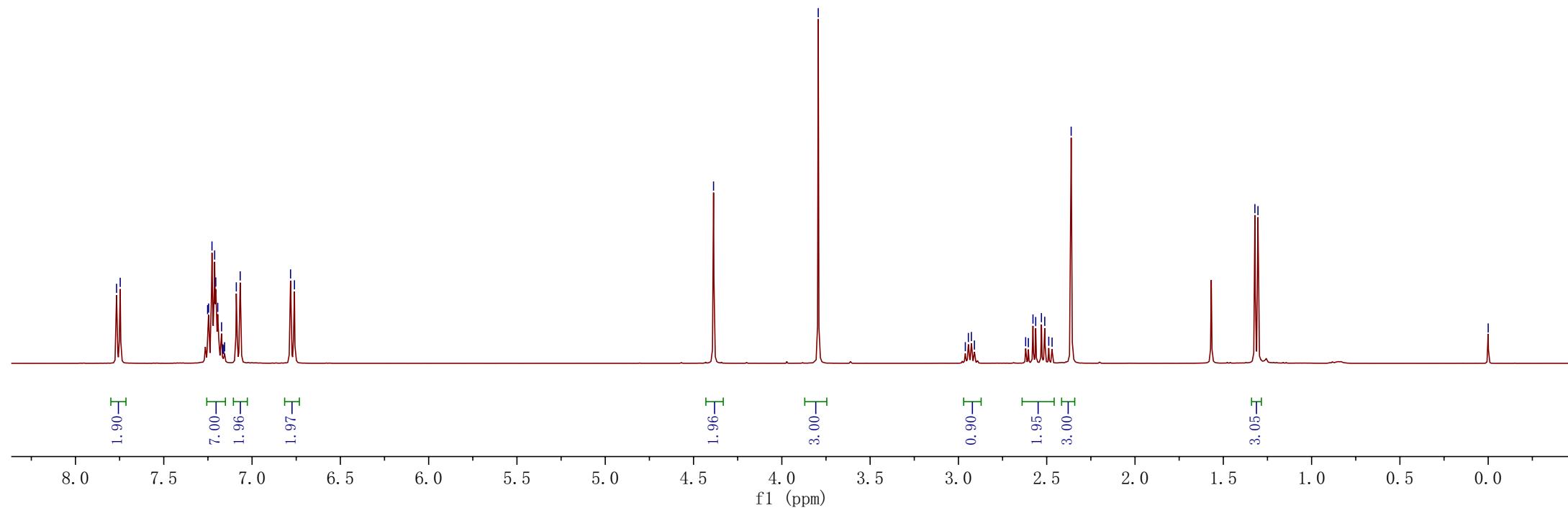
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



$3z$

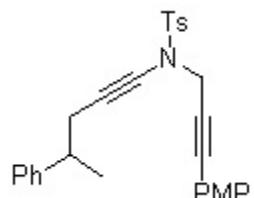


Analysis:  $^{13}\text{C}$  NMR

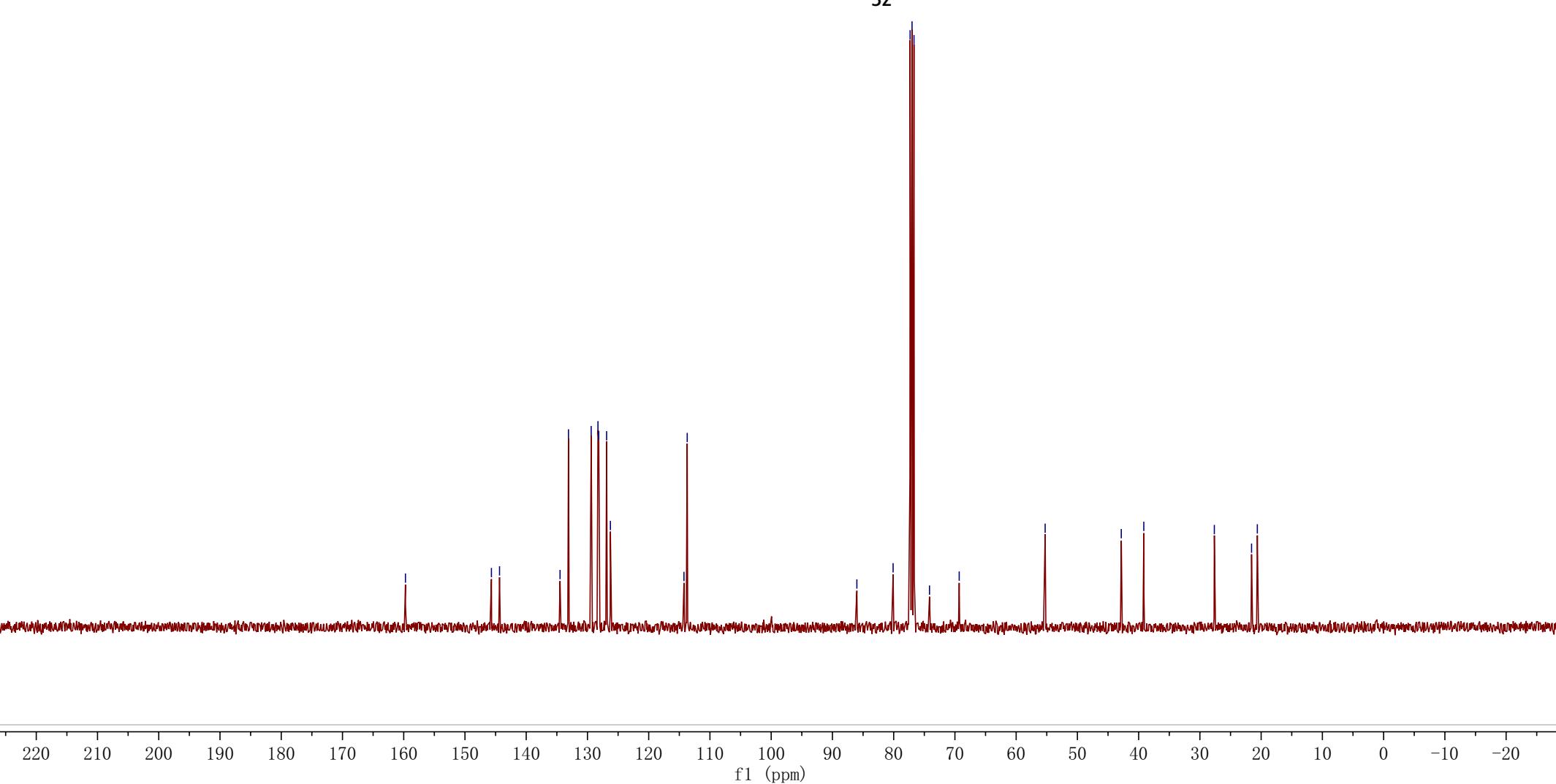
Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 159.72  
— 145.68  
— 144.36  
— 134.48  
— 133.10  
— 129.39  
— 128.29  
— 128.15  
— 126.87  
— 126.25  
— 114.24  
— 113.71  
— 86.01  
— 80.09  
— 77.32  
— 77.00  
— 76.68  
— 74.15  
— 69.30  
— 55.27  
— 42.84  
— 39.16  
— 27.64  
— 21.56  
— 20.62



**3z**



<7.619

<7.243

<7.226

<7.003

<6.999

<6.989

<6.985

<6.807

<6.623

<6.617

<6.613

<6.603

<6.599

<6.593

<6.531

<6.527

<6.269

<6.256

<6.251

<6.246

<6.242

<6.238

<6.233

<6.158

<6.139

<6.126

<6.121

<6.107

<6.088

<4.701

<4.684

-3.733

<2.735

<2.725

<2.718

<2.716

<2.706

<2.697

<2.688

<2.661

<2.653

<2.640

<2.629

<2.620

<2.610

<2.603

<2.599

<2.593

<2.585

<2.427

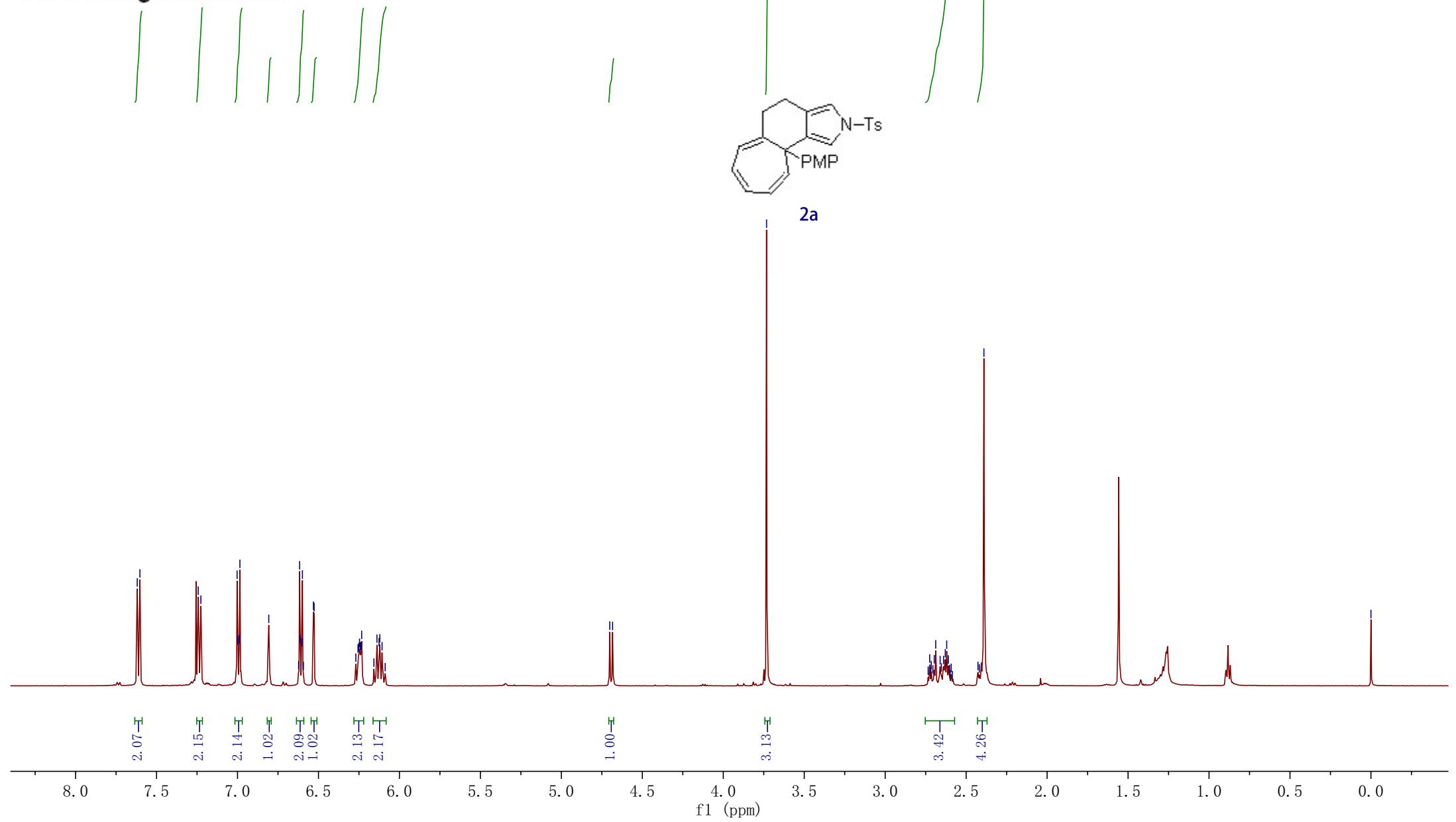
<2.419

<2.390

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125MHz

—157.42  
—144.46

136.39  
135.76  
134.75  
129.77  
129.05  
128.03  
127.38  
126.65  
125.13  
124.90  
124.19  
117.78  
115.12  
112.22  
106.87

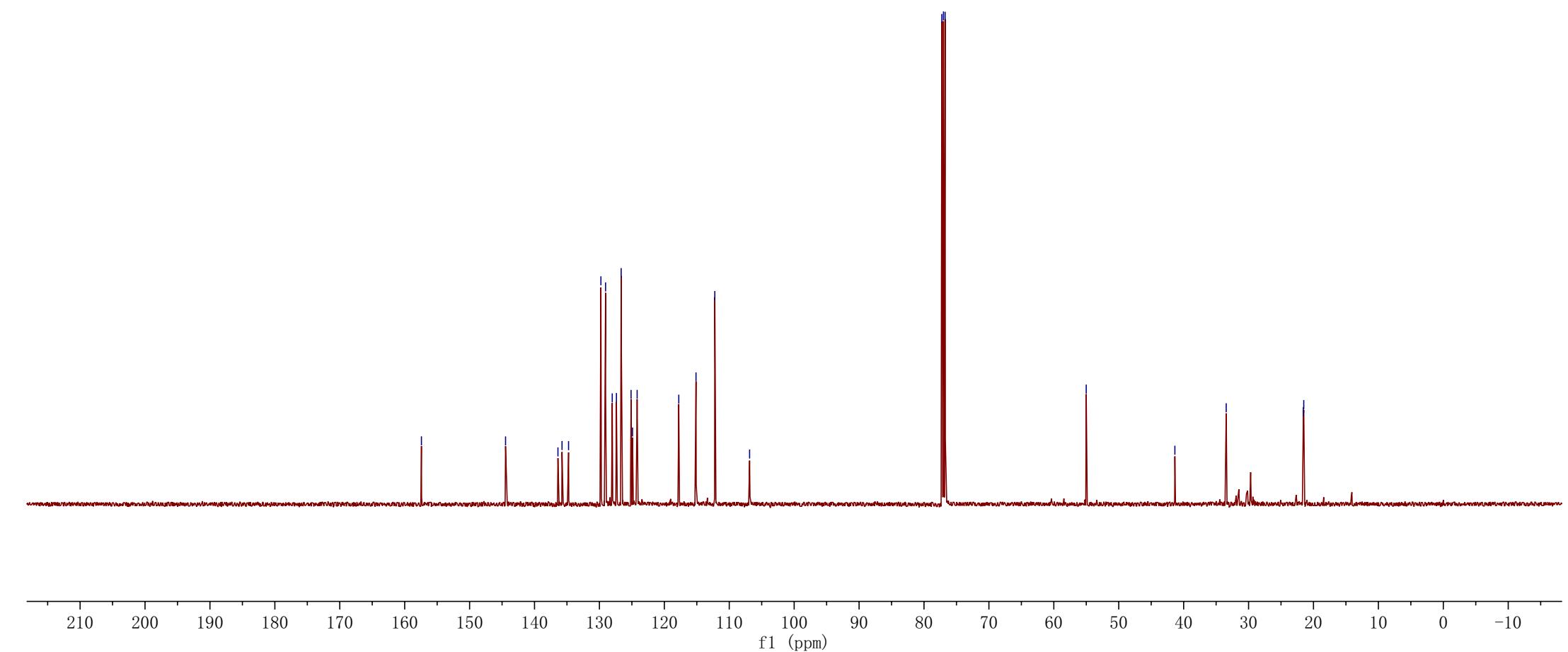
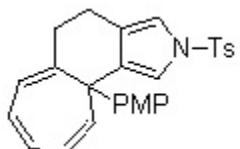
77.25  
77.00  
76.75

—55.01

—41.35

—33.44

21.56  
21.50



<7.049  
<7.032  
—6.819  
<6.631  
<6.614  
<6.479  
<6.475  
<6.292  
<6.283  
<6.177  
<6.158  
<6.148  
<6.134  
<6.115

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

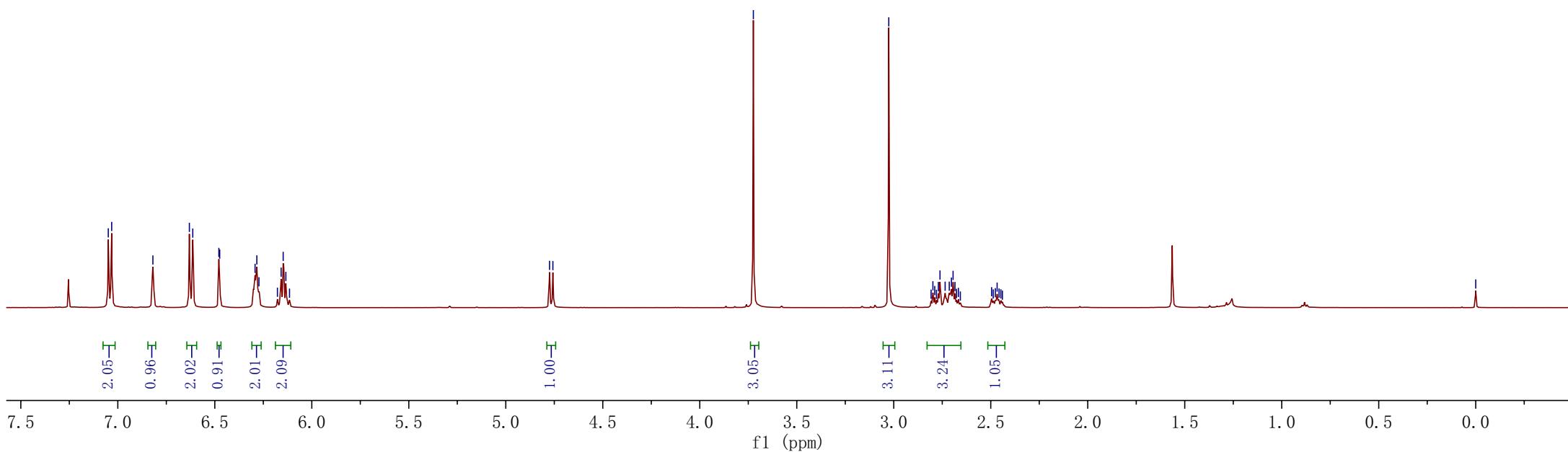
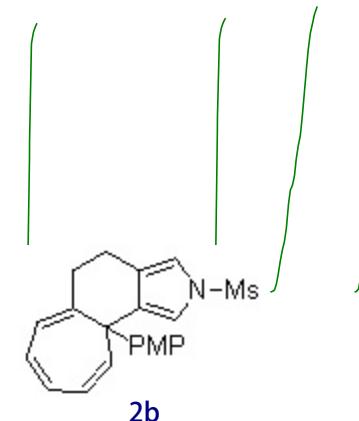
Field strength: 500 MHz

<4.774  
—4.757

—3.724

—3.026  
—2.808  
—2.798  
—2.789  
—2.780  
—2.770  
—2.762  
—2.735  
—2.714  
—2.703  
—2.694  
—2.684  
—2.677  
—2.667  
—2.657  
—2.496  
—2.487  
—2.476  
—2.467  
—2.457  
—2.448  
—2.440

—0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125MHz

— 157.48

— 135.78  
— 134.62  
— 129.10  
— 128.07  
— 127.43  
— 125.15  
— 124.69  
— 124.27  
— 117.33  
— 114.93  
— 114.79  
— 112.28  
— 106.62

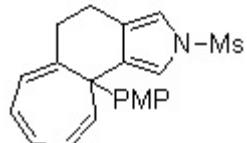
— 77.25  
— 77.00  
— 76.75

— 55.00

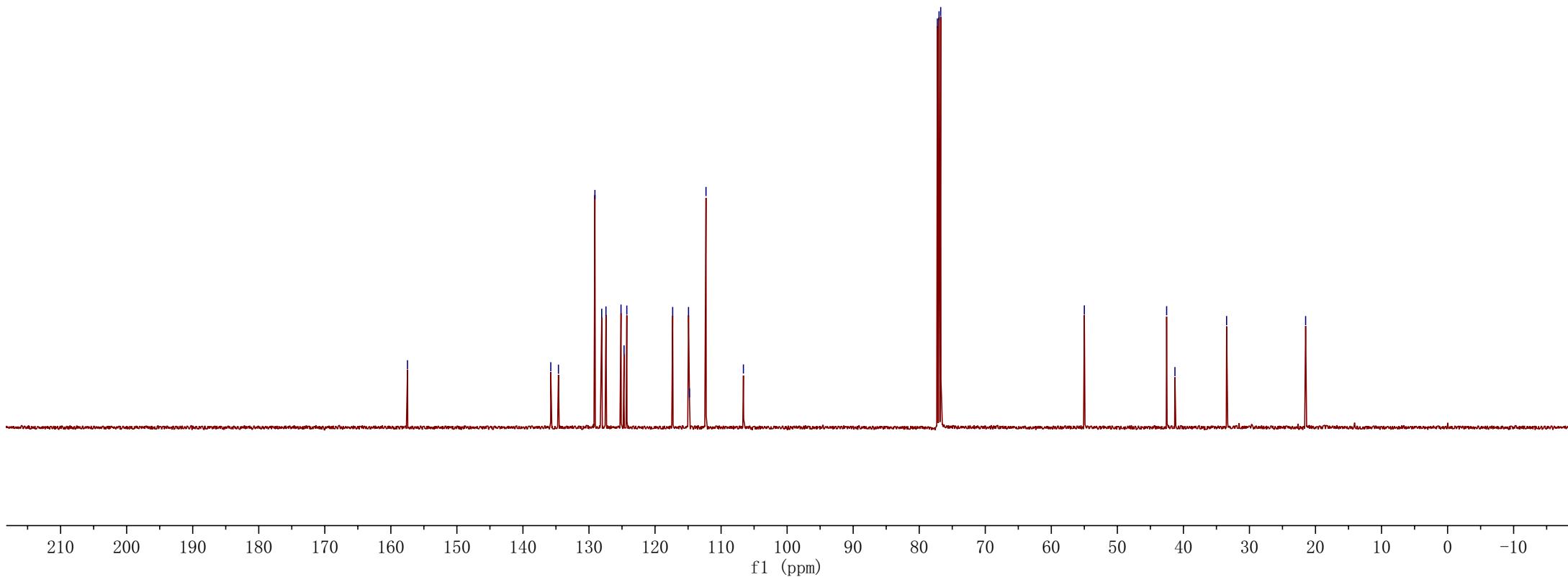
— 42.54  
— 41.28

— 33.46

— 21.50



2b



<7.041  
<7.019  
-6.801  
-6.620  
-6.599  
-6.463  
-6.459  
-6.305  
-6.294  
-6.282  
-6.189  
-6.166  
-6.152  
-6.137  
-6.113

<4.818  
<4.796

-3.712  
-3.150  
-3.132  
-3.113  
-3.095  
-2.809  
-2.799  
-2.787  
-2.762  
-2.736  
-2.711  
-2.697  
-2.684  
-2.500  
-2.474  
-2.466  
-2.456  
-2.443

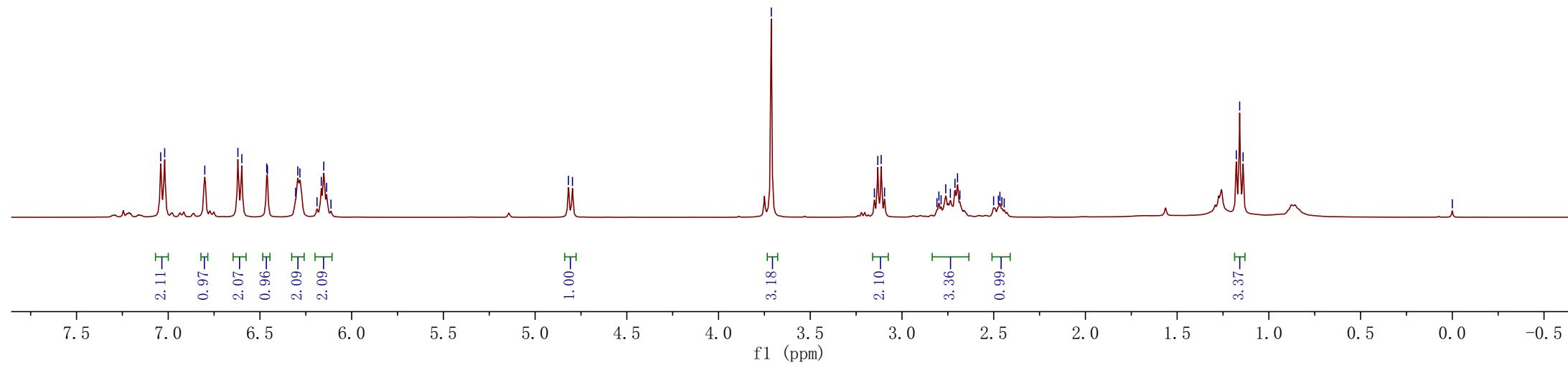
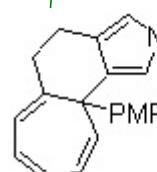
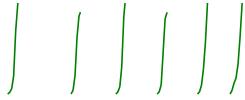
<1.177  
<1.159  
<1.141

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

—157.41

135.36  
134.80  
128.92  
128.15  
127.49  
125.16  
124.30  
124.13  
117.82  
116.70  
115.31  
112.22  
108.29

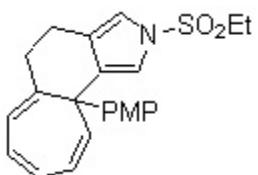
77.32  
77.00  
76.68

—54.97  
—49.89

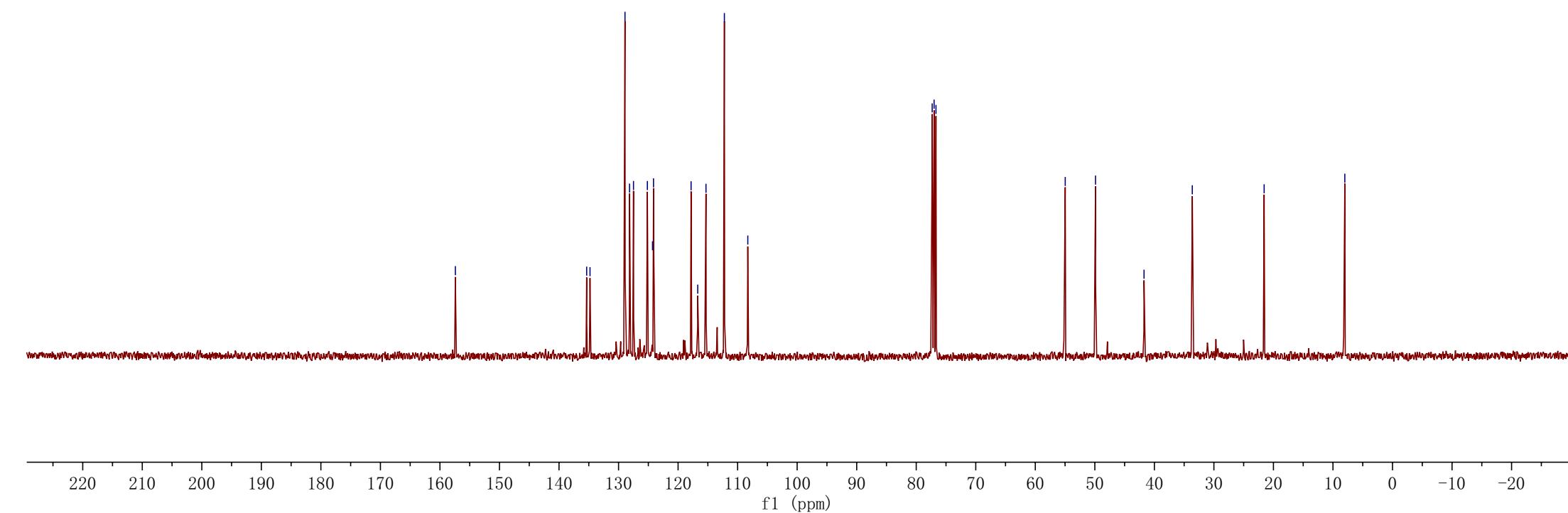
—41.73  
—33.63

—21.56

—8.01



2c



<7.616  
 <7.596  
 <7.235  
 <7.214  
 6.987  
 6.966  
 -6.805  
 6.604  
 6.583  
 6.533  
 6.528  
 6.264  
 6.242  
 6.225  
 6.153  
 6.130  
 6.114  
 6.097  
 6.073

<4.694  
 <4.672

3.966  
 3.948  
 3.931  
 3.913

2.735  
 2.724  
 2.712  
 2.684  
 2.656  
 2.630  
 2.615  
 2.602  
 <2.422

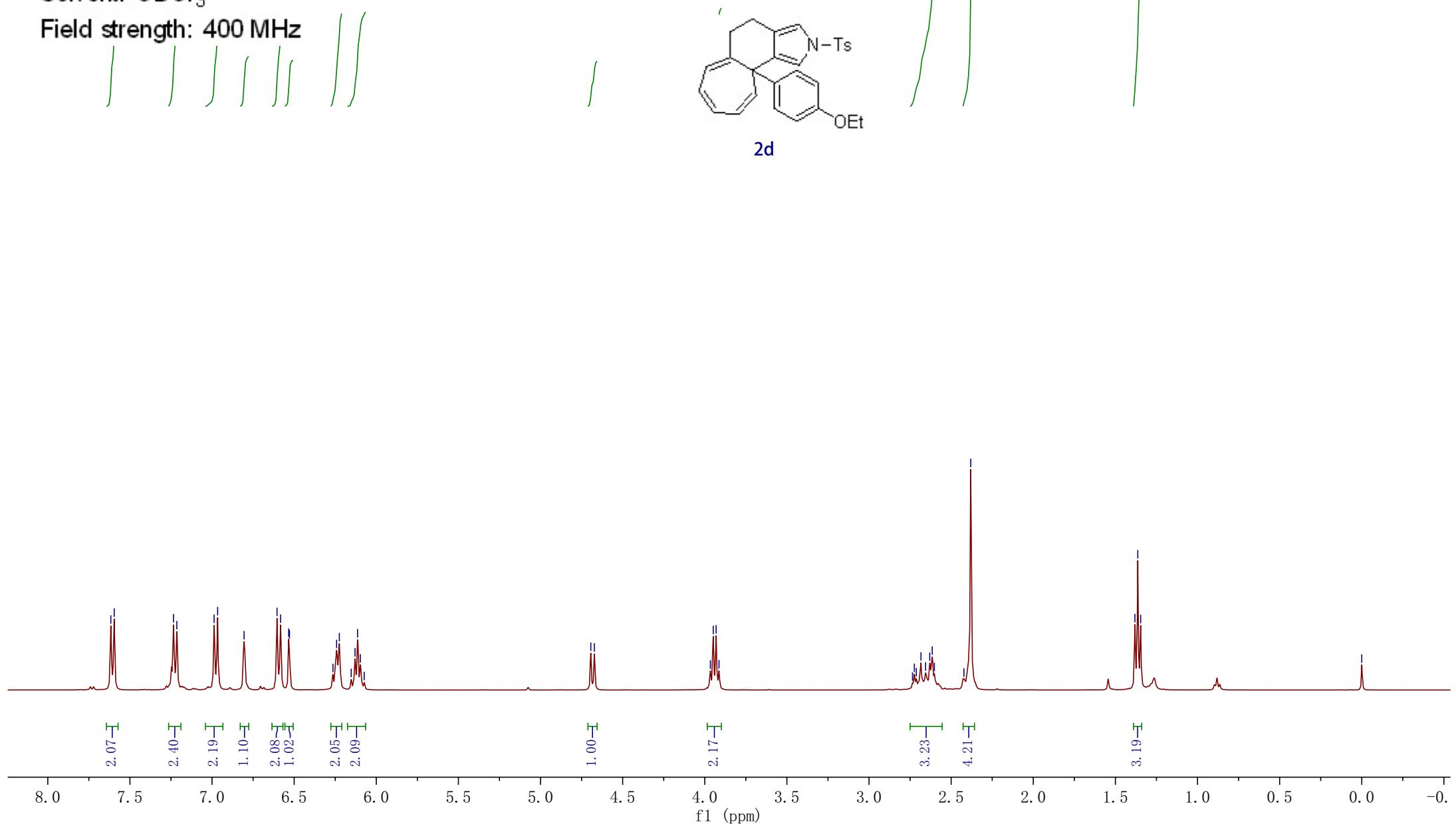
1.381  
 1.364  
 1.346

-0.000

**Analysis:  $^1\text{H}$  NMR**

**Solvent:**  $\text{CDCl}_3$

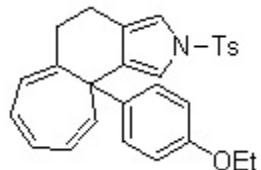
**Field strength:** 400 MHz



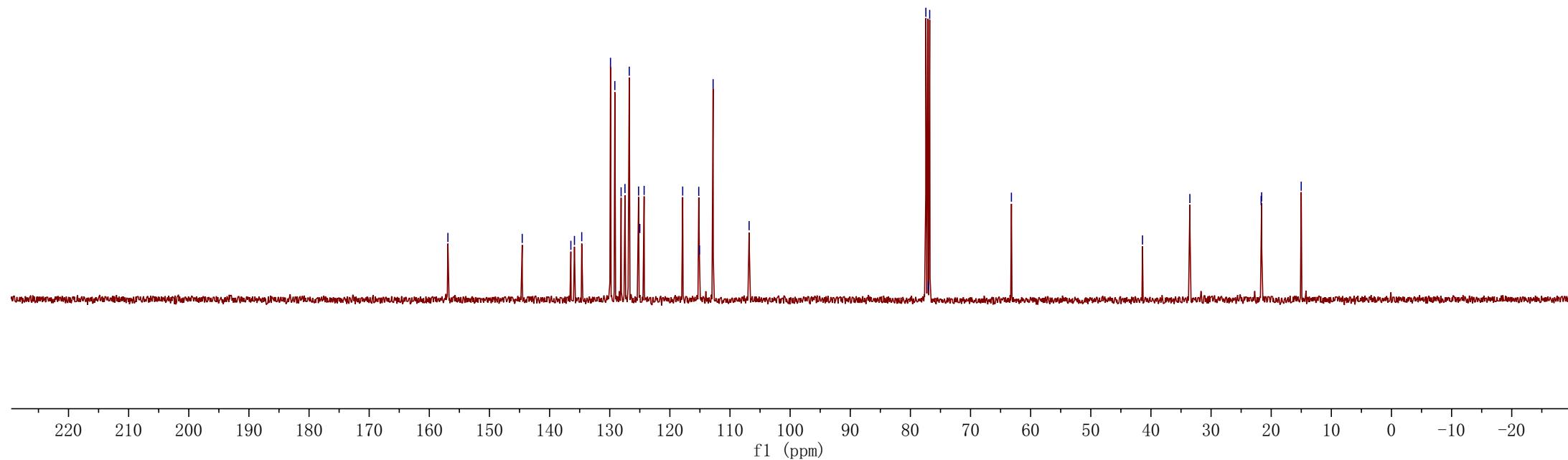
Analysis:  $^{13}\text{C}$  NMR

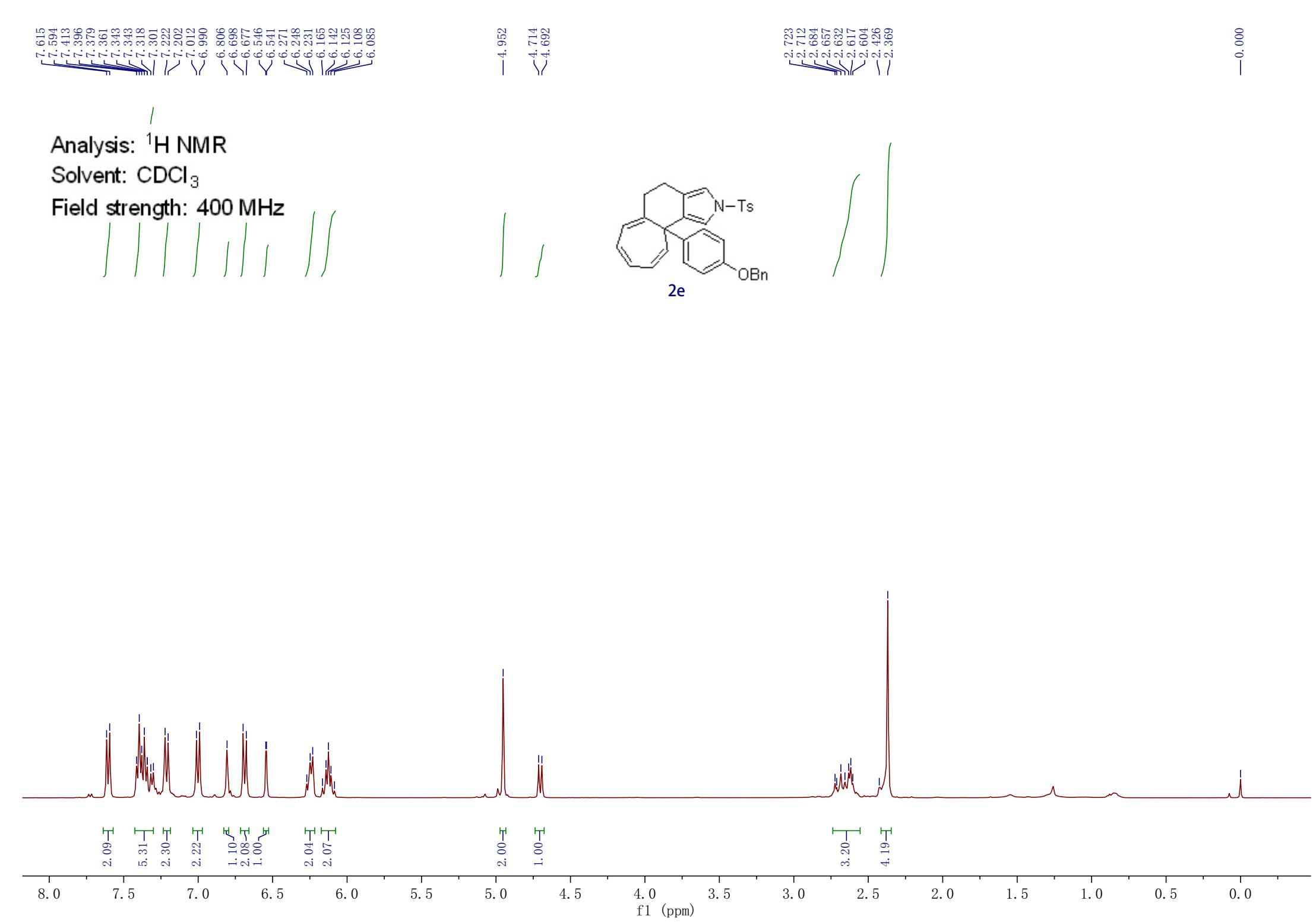
Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**2d**

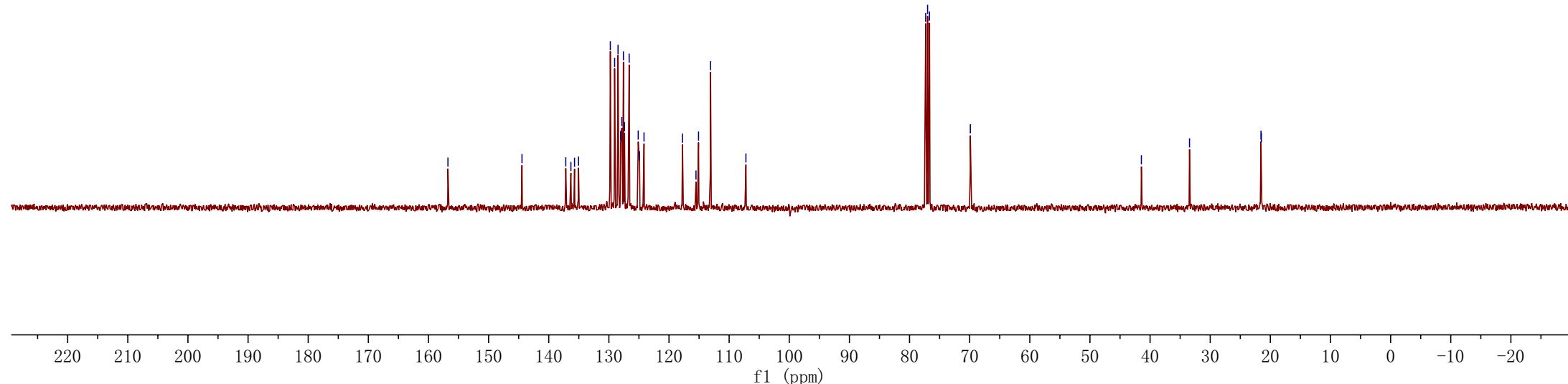
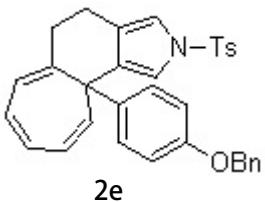
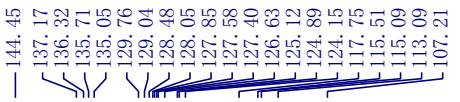
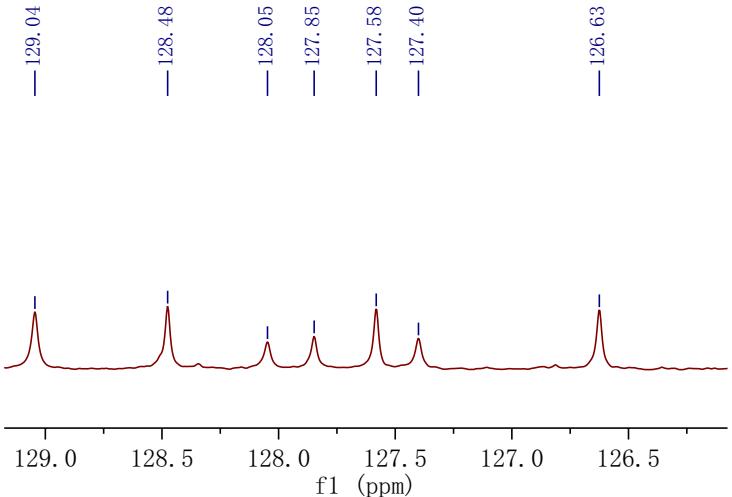




Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.461  
<7.440  
<7.060  
<6.781  
<6.759  
<6.660  
<6.391  
<6.385  
<6.369  
<6.108  
<6.086  
<6.069  
<5.991  
<5.967  
<5.950  
<5.932  
<5.908

<4.584  
<4.563

2.587  
2.576  
2.564  
2.552  
2.535  
2.525  
2.506  
2.479  
2.472  
2.459  
2.282  
2.279  
2.273  
2.269  
2.252  
2.243  
2.231  
2.205

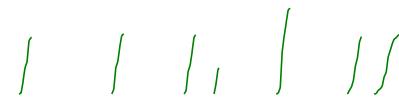
-0.797

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

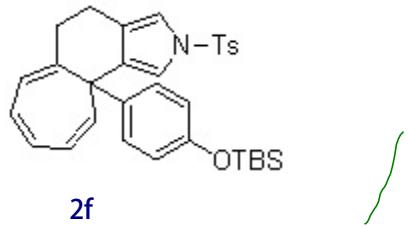
Field strength: 400 MHz



0.94

f1 (ppm)

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



6.22

9.00

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

—153.31

—144.45

136.32  
135.77  
135.44  
129.76  
128.97  
128.10  
127.46  
126.63  
125.07  
124.92  
124.07  
118.25  
117.75  
116.40  
115.03  
108.11

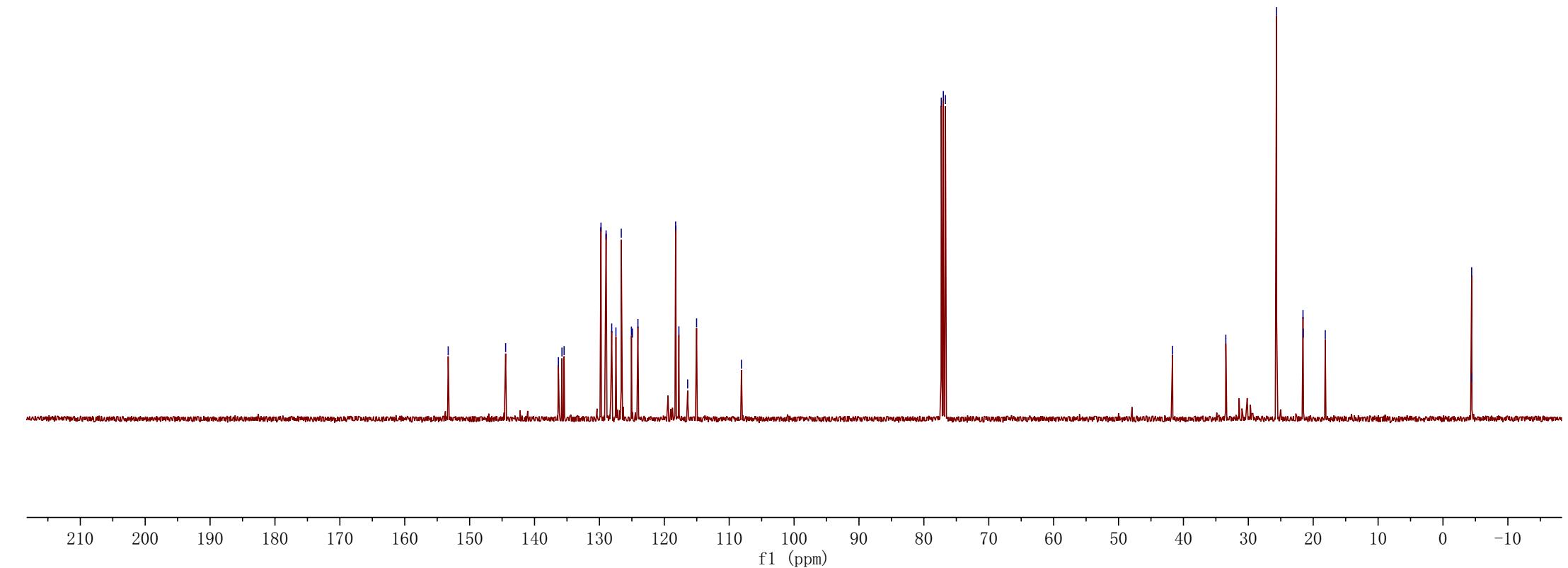
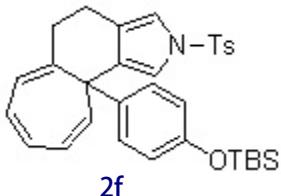
77.32  
77.00  
76.68

—41.68

—33.47

—25.65  
—21.57  
—21.54  
—18.14

—4.42  
—4.45



7.743  
7.723  
7.314  
7.294  
7.273  
7.264  
7.244  
7.201  
7.190  
7.179  
7.132  
7.123  
7.111  
7.079  
7.061  
7.053  
7.047  
6.966  
6.947  
6.905  
6.854  
6.832  
6.808  
6.786

—5.100

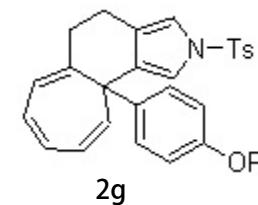
2.910  
2.900  
2.891  
2.869  
2.860  
2.794  
2.788  
2.763  
2.755  
2.731  
2.721  
2.612  
2.577  
2.533  
2.522  
2.514  
2.500  
2.490  
2.481  
2.362

—0.000

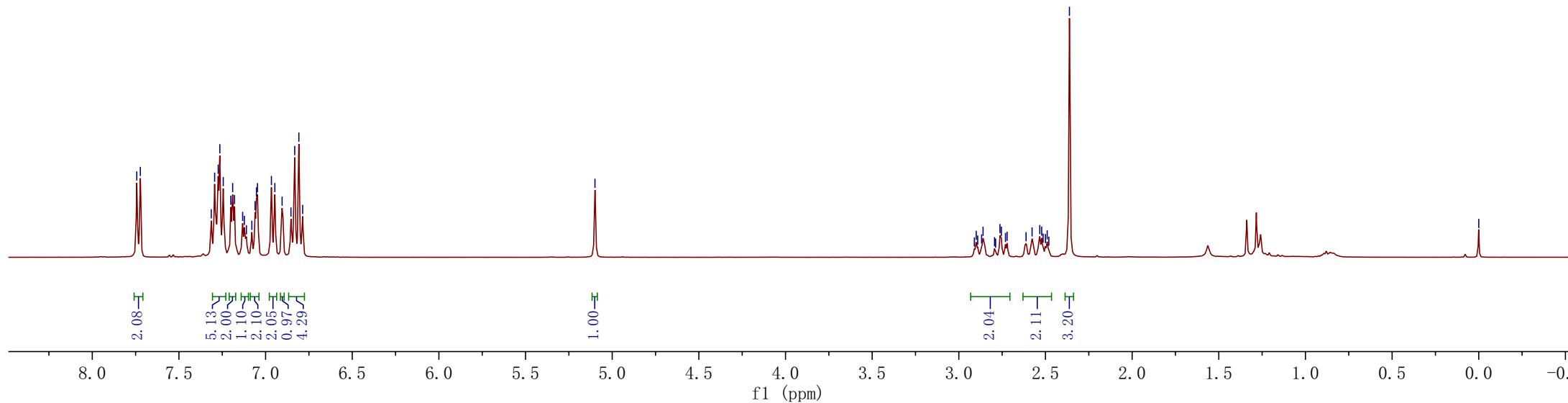
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



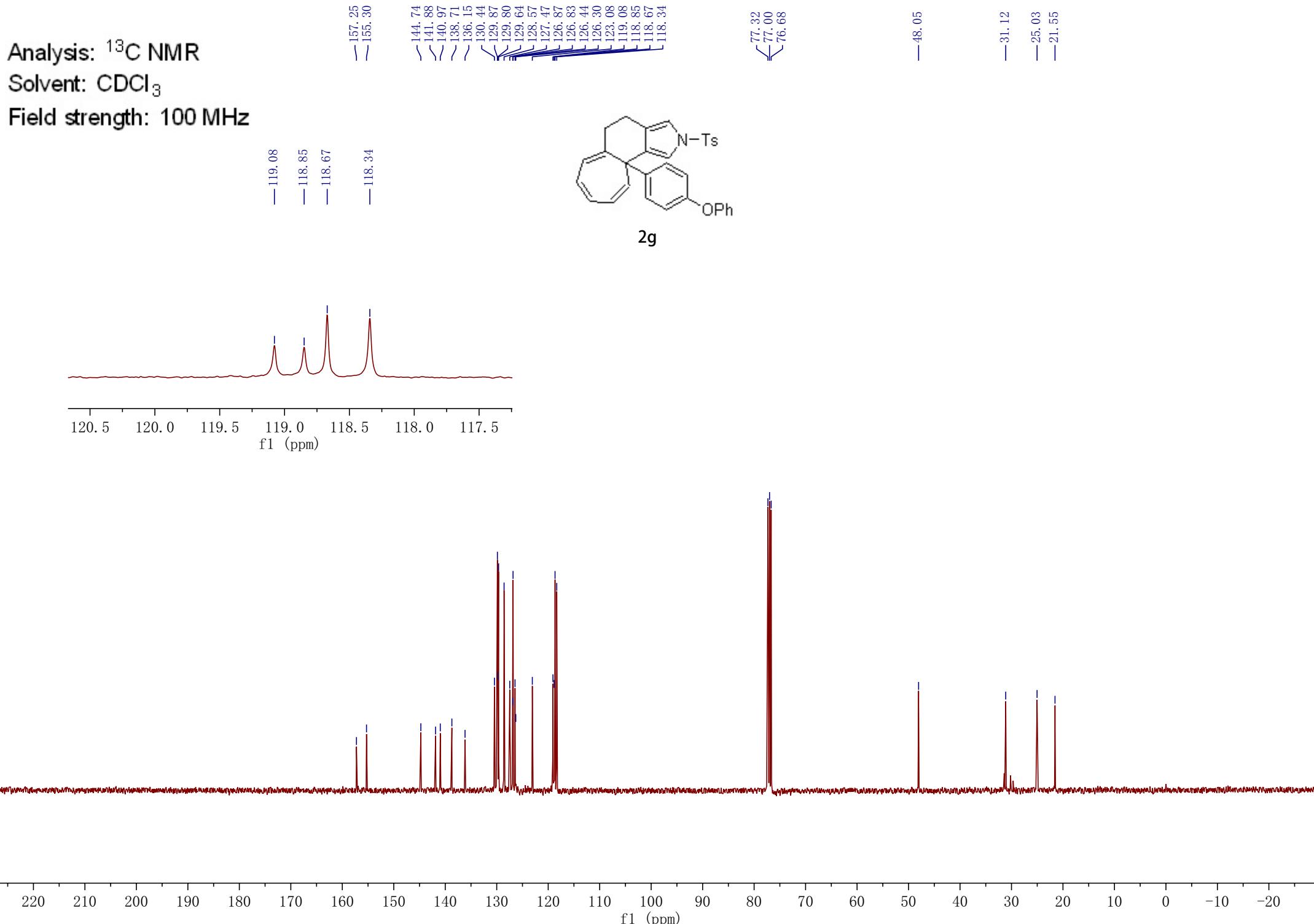
2g



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.616

<7.595

<7.240

<7.220

<7.220

<6.979

<6.959

<6.959

<6.872

<6.853

<6.798

<6.798

<6.558

<6.553

<6.284

<6.269

<6.252

<6.180

<6.157

<6.141

<6.123

<6.099

<4.807

<4.785

<2.754

<2.729

<2.702

<2.690

<2.656

<2.641

<2.628

<2.448

<2.440

<2.424

<2.408

<2.390

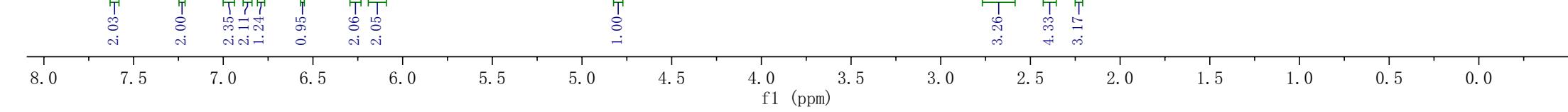
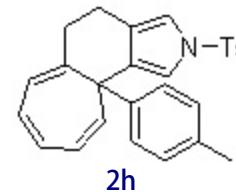
<2.234

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

f1 (ppm)

<7.620  
<7.599  
<7.245  
<7.225  
≤7.004  
≤6.984  
≤6.898  
≤6.878  
≤6.803  
≤6.583  
≤6.578  
≤6.296  
≤6.282  
≤6.265  
≤6.192  
≤6.168  
≤6.151  
≤6.133  
≤6.109

<4.851  
<4.829

2.764  
2.752  
2.740  
2.730  
2.719  
2.713  
2.703  
2.680  
2.670  
2.655  
2.642  
2.642  
2.578  
2.559  
2.540  
2.521  
2.458  
2.453  
2.436  
2.424  
2.417  
2.395

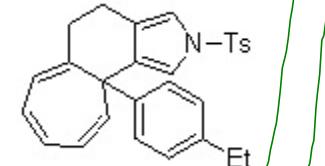
1.201  
1.182  
1.163

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



**2i**

2.02  
2.09  
2.31  
2.21  
1.10  
0.98  
2.05  
2.10

1.00

3.19  
2.39  
4.47

3.32

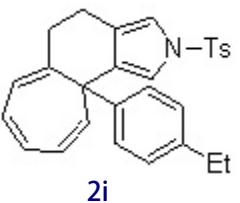
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

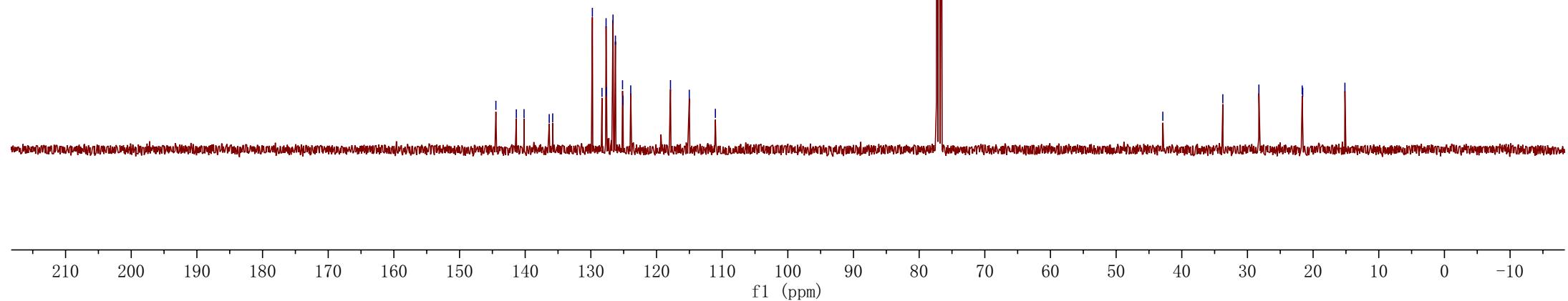
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**2i**



>7.629

<7.242

>7.221

>6.945

>6.923

>6.793

<6.577

>6.571

>6.470

>6.448

>6.257

>6.240

>6.221

>6.165

>6.142

>6.129

>6.114

>6.092

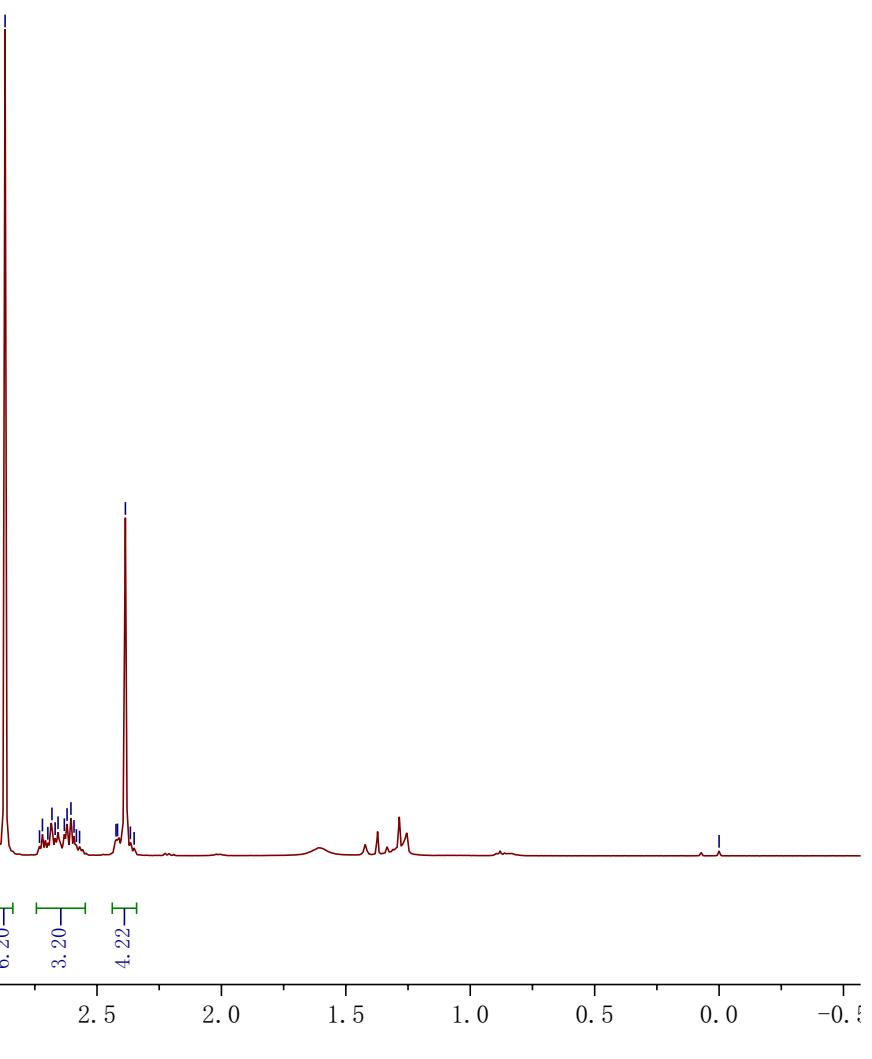
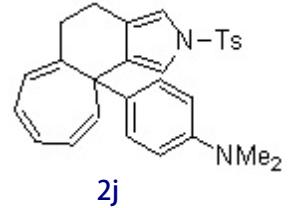
<4.671

>4.650

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



-0.000

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

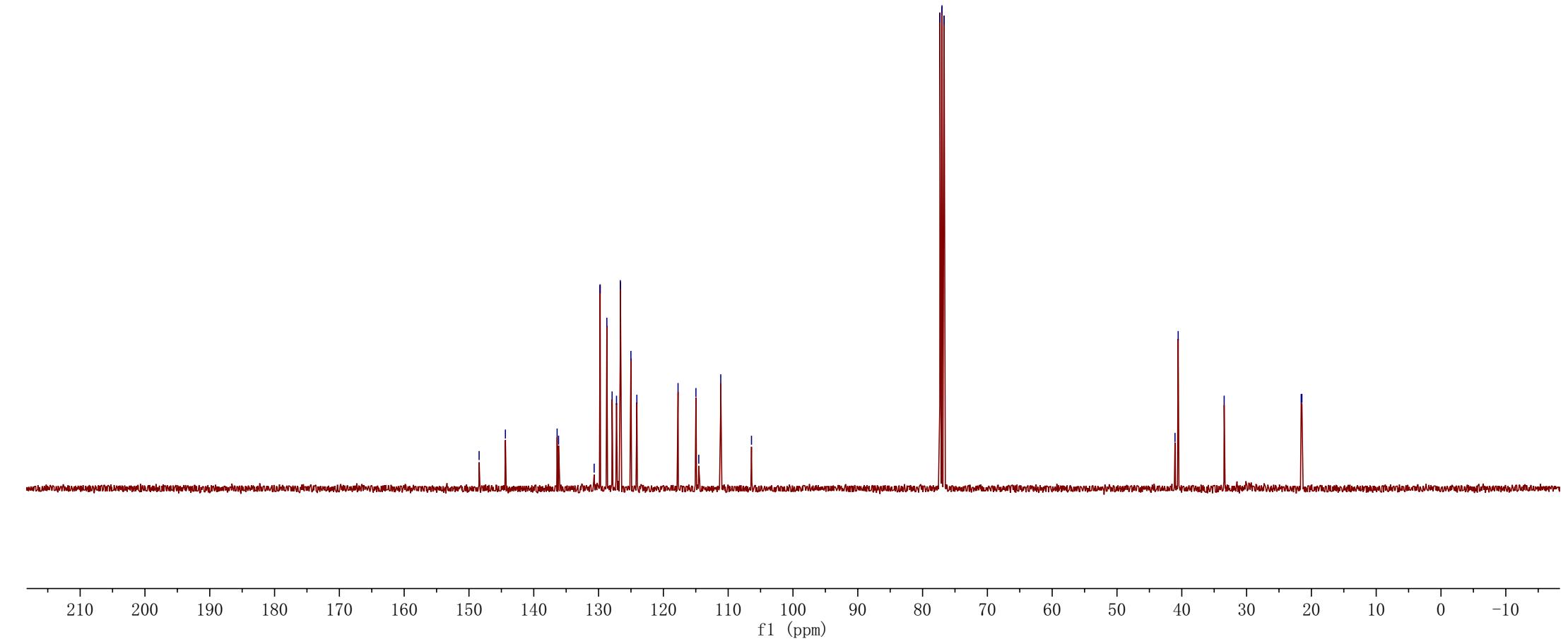
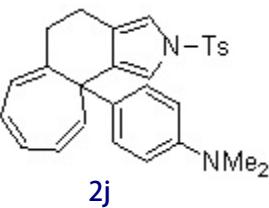
-148.43  
-144.38  
136.40  
136.17  
136.17  
130.68  
129.76  
128.72  
127.91  
127.23  
126.64  
125.01  
124.09  
117.73  
114.98  
114.54  
-111.15  
-106.40

77.32  
77.00  
76.68

41.05  
40.56

21.58  
21.47

-33.46



7.614  
7.593  
7.296  
7.279  
7.237  
7.221  
7.202  
7.184  
6.851  
6.830  
6.776  
6.588  
6.583  
6.473  
6.451  
6.227  
6.205  
6.189  
6.167  
6.144  
6.131  
6.116  
6.092

4.694  
4.672  
4.538

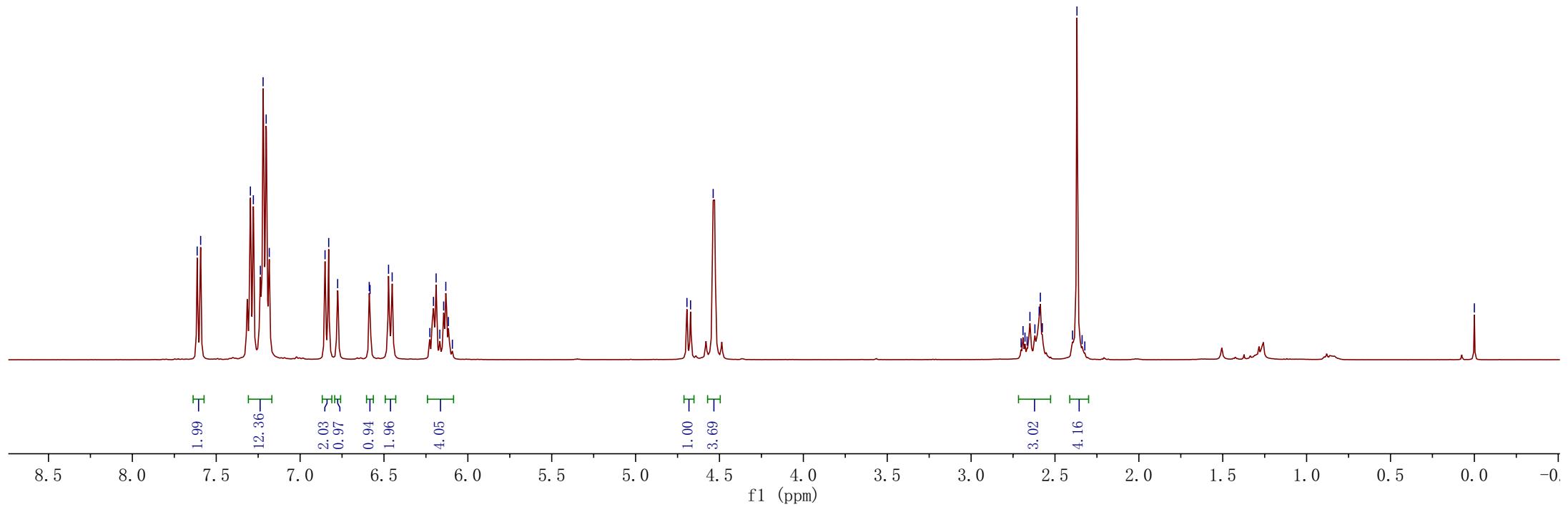
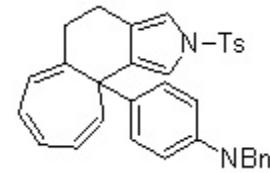
2.702  
2.691  
2.679  
2.666  
2.649  
2.620  
2.594  
2.587  
2.575  
2.395  
2.369  
2.338  
2.322

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

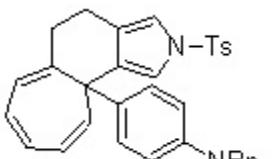
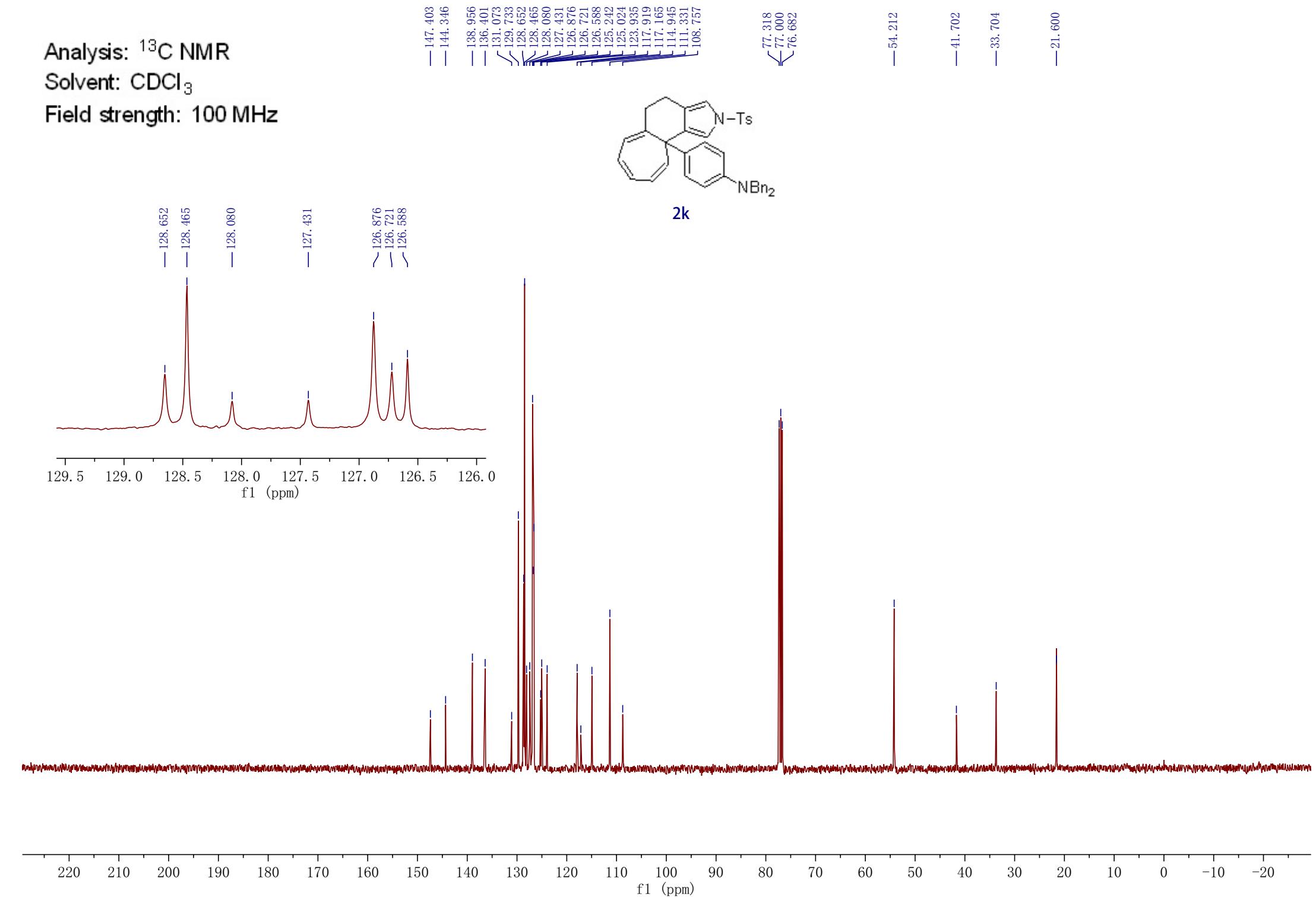
Field strength: 400 MHz

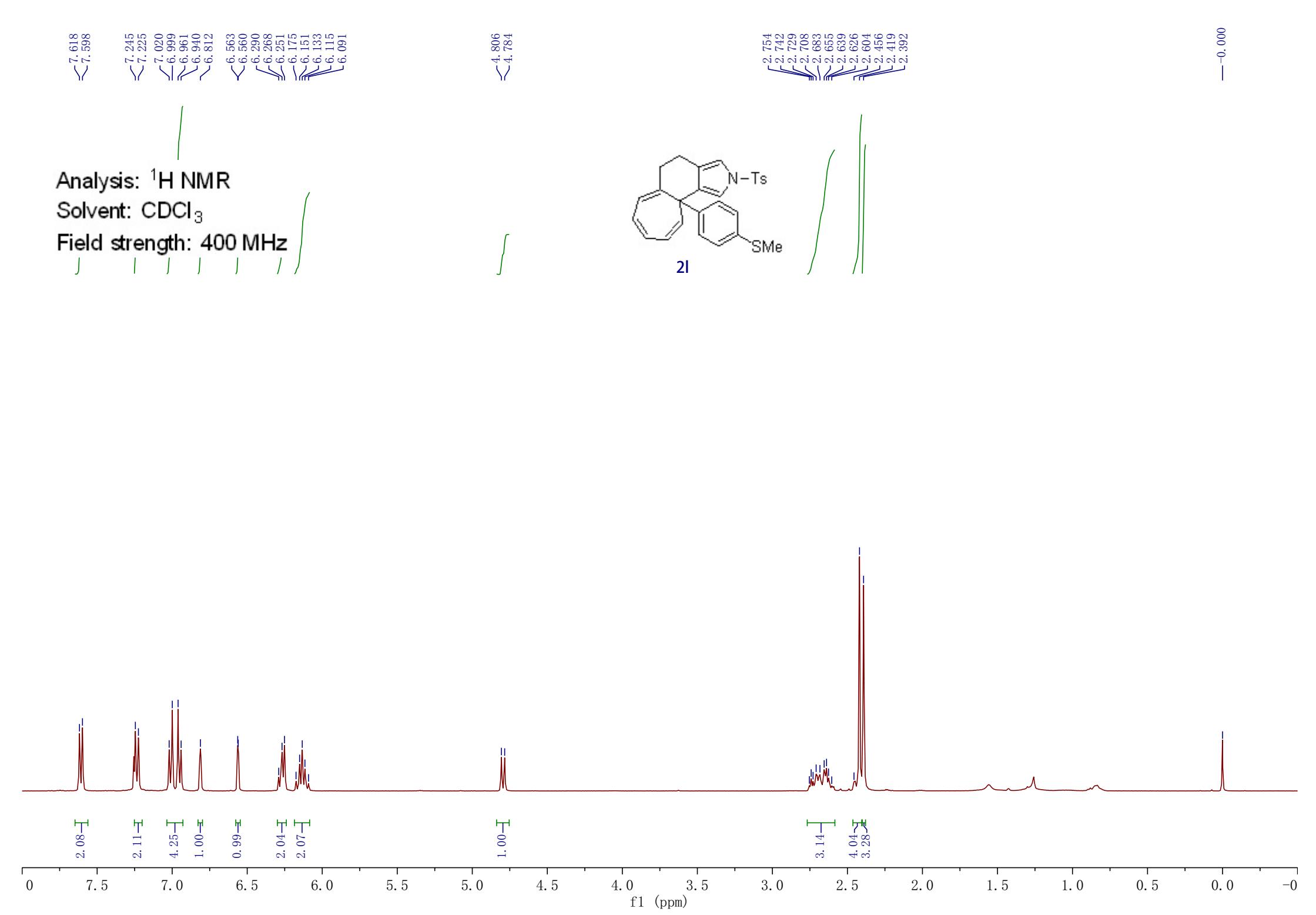


Analysis:  $^{13}\text{C}$  NMR

Solvent: CDCl<sub>3</sub>

Field strength: 100 MHz





Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

144.53  
140.09  
136.30  
135.29  
135.09  
129.80  
128.43  
128.34  
127.65  
126.66  
125.23  
124.91  
124.04  
117.85  
117.76  
115.15  
— 109.54

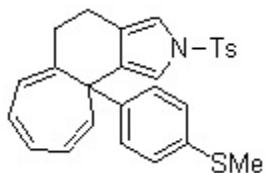
77.32  
77.00  
76.68

— 42.45

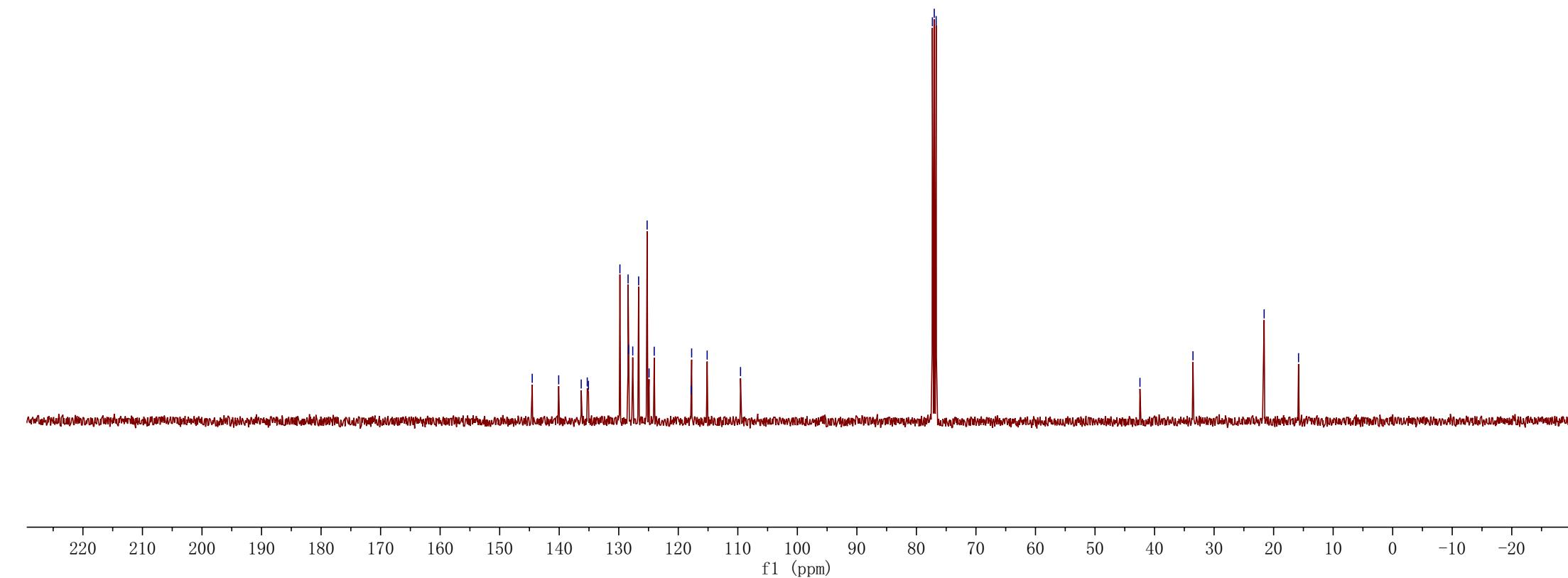
— 33.55

— 21.59

— 15.81



**2l**



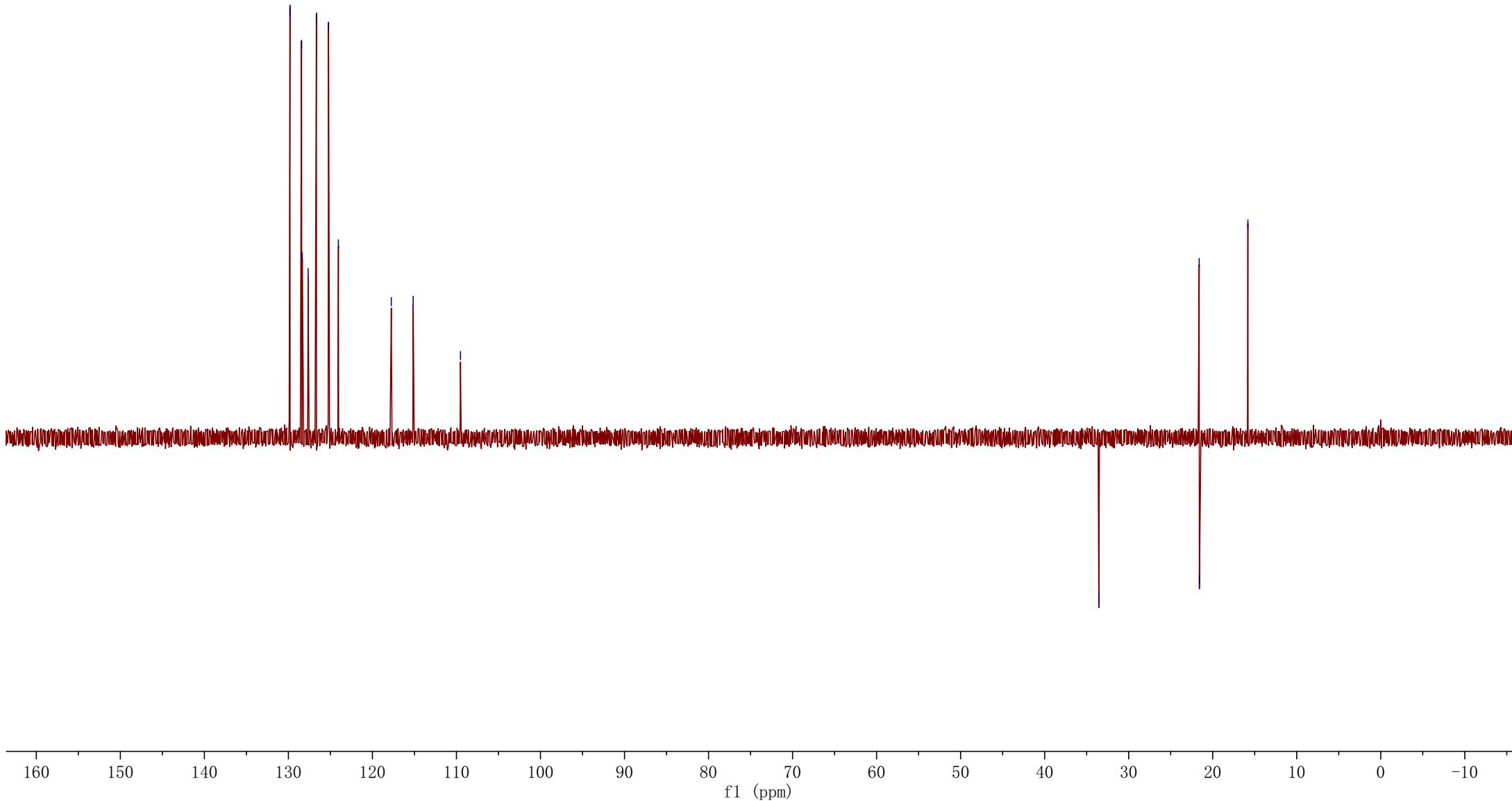
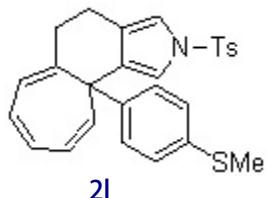
129.82  
128.44  
128.35  
127.65  
126.67  
125.22  
124.05  
— 117.76  
— 115.15  
— 109.52

— 33.55  
— 21.61  
— 21.59  
— 15.81

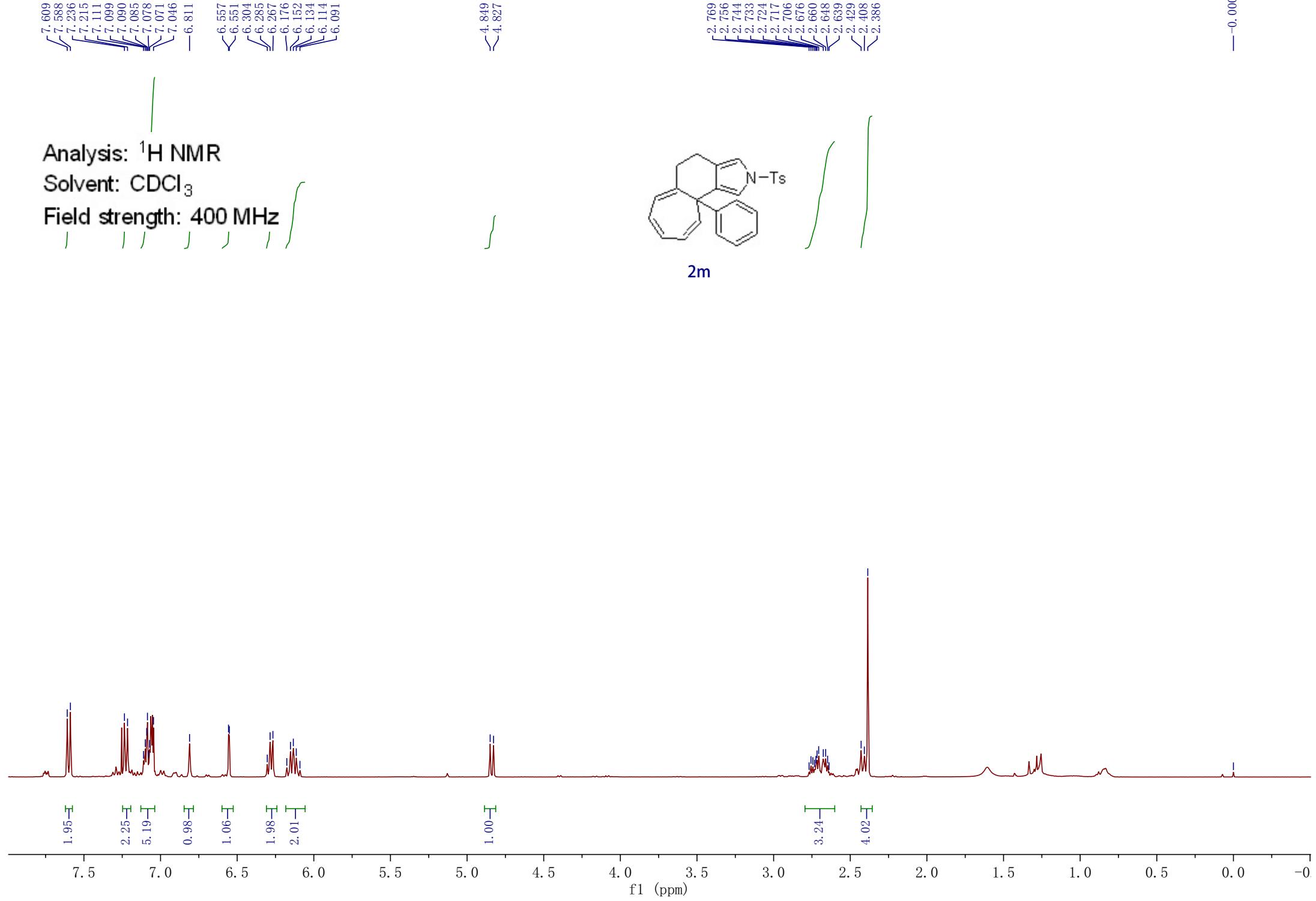
Analysis:  $^{13}\text{C}$  NMR DEPT135

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



—0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 129.78  
— 128.28  
— 127.91  
— 127.63  
— 126.81  
— 126.64  
— 125.78  
— 125.23  
— 125.02

— 144.50  
— 143.02

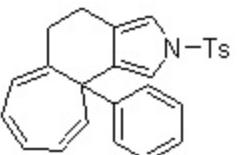
— 136.30  
— 135.47  
— 129.78  
— 128.28  
— 127.91  
— 127.63  
— 126.81  
— 126.64  
— 125.78  
— 125.23  
— 125.02

— 77.32  
— 77.00  
— 76.68

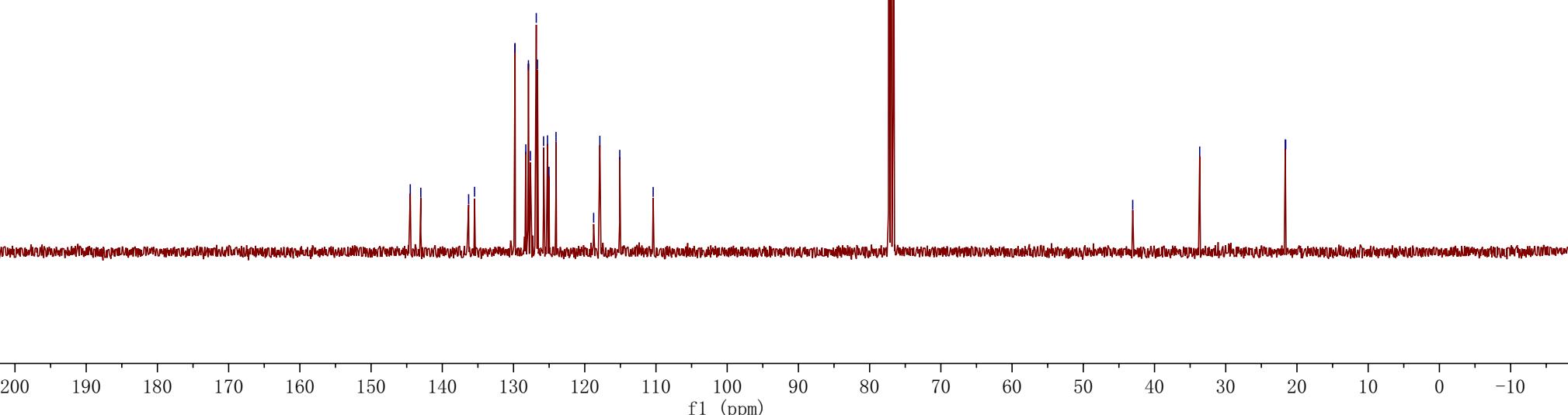
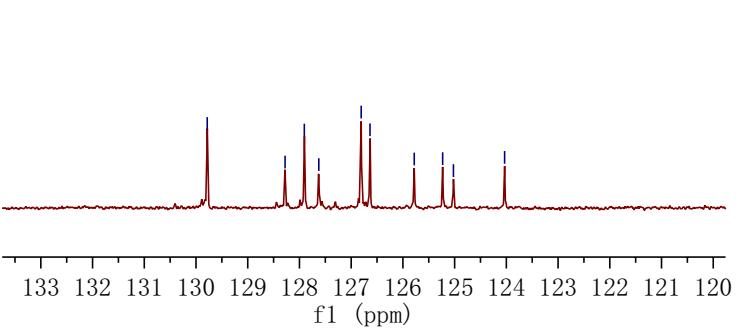
— 43.06

— 33.66

— 21.64  
— 21.58



2m



7.617  
7.597  
7.234  
7.214  
7.064  
7.049  
7.043  
7.029  
6.824  
6.757  
6.736  
6.736  
6.714  
6.519  
6.515  
6.283  
6.259  
6.242  
6.157  
6.133  
6.115  
6.096  
6.072

4.750  
4.729

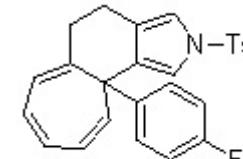
2.746  
2.735  
2.723  
2.694  
2.665  
2.641  
2.628  
2.614  
2.592  
2.442  
2.418  
2.407  
2.377

-0.000

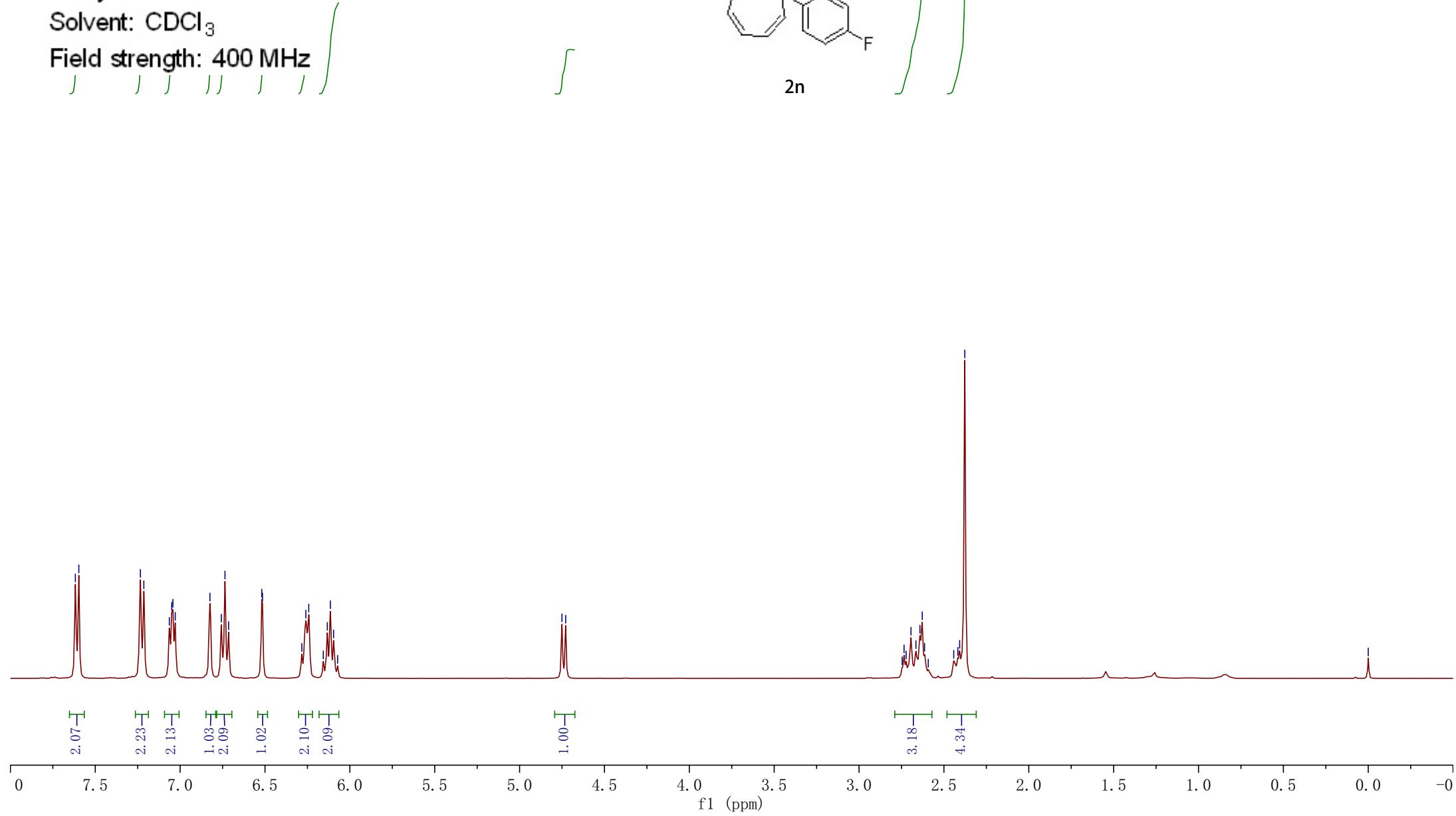
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



2n



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 129.78  
— 129.39  
— 128.19  
— 127.53  
— 126.64  
— 124.73  
— 124.21

— 144.57

— 162.04

— 159.62

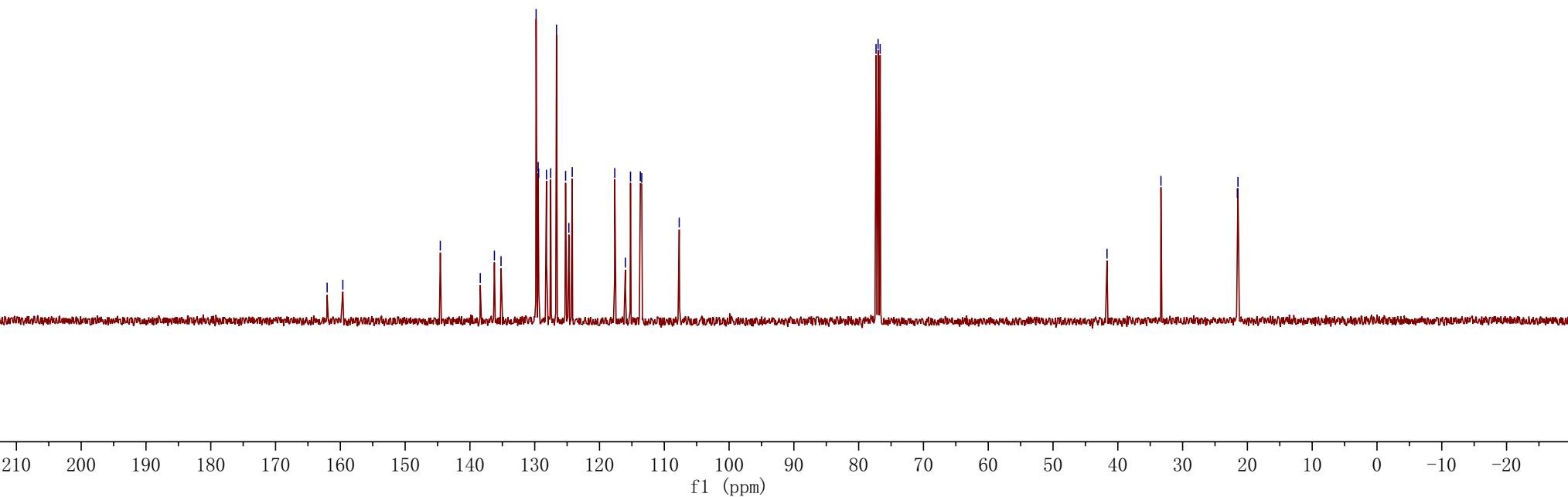
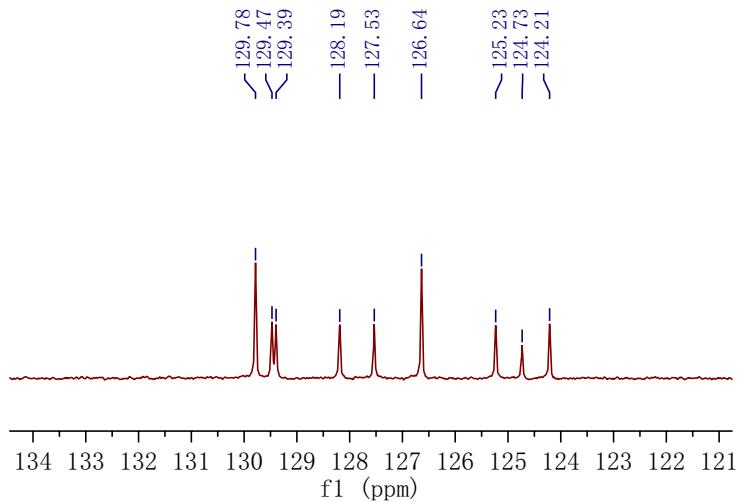
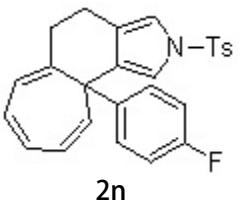
— 138.40  
— 136.22  
— 135.20  
— 129.78  
— 129.47  
— 129.39  
— 128.19  
— 127.53  
— 126.64  
— 125.23  
— 124.73  
— 124.21  
— 117.65  
— 116.01  
— 115.21  
— 113.69  
— 113.48  
— 107.70

— 77.32  
— 77.00  
— 76.68

— 41.67

— 33.34

— 21.55  
— 21.46

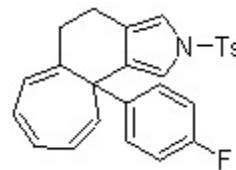


Analysis:  $^{13}\text{F}$  NMR

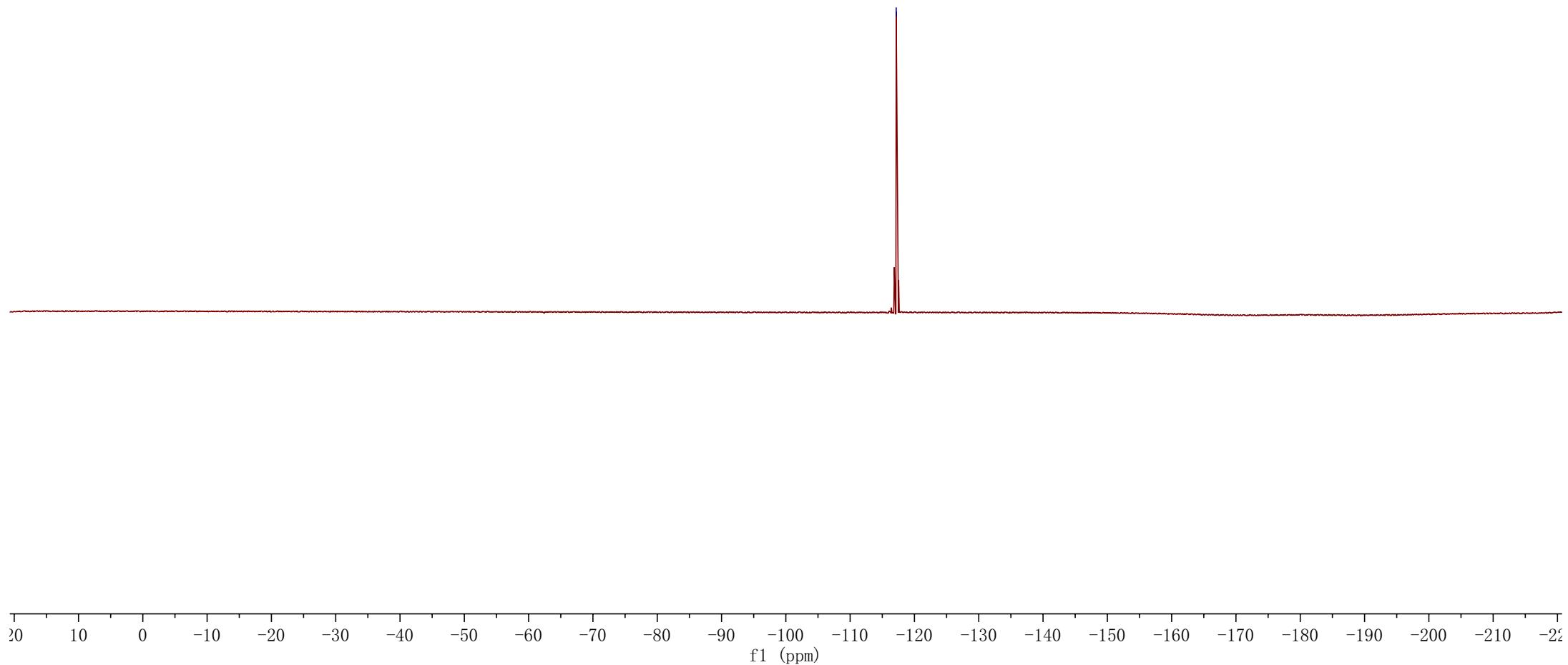
Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz

-117, 16



**2n**



<7.619

<7.242

<7.222

-7.021

-6.826

<6.543

<6.538

<6.299

<6.277

<6.260

<6.179

<6.155

<6.135

<6.117

<4.832

<4.810

2.754

2.742

2.729

2.708

2.703

2.692

2.680

2.656

2.642

2.627

2.458

2.451

2.425

2.409

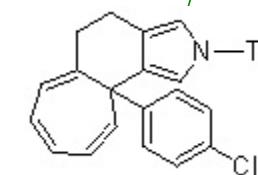
2.386

-0.000

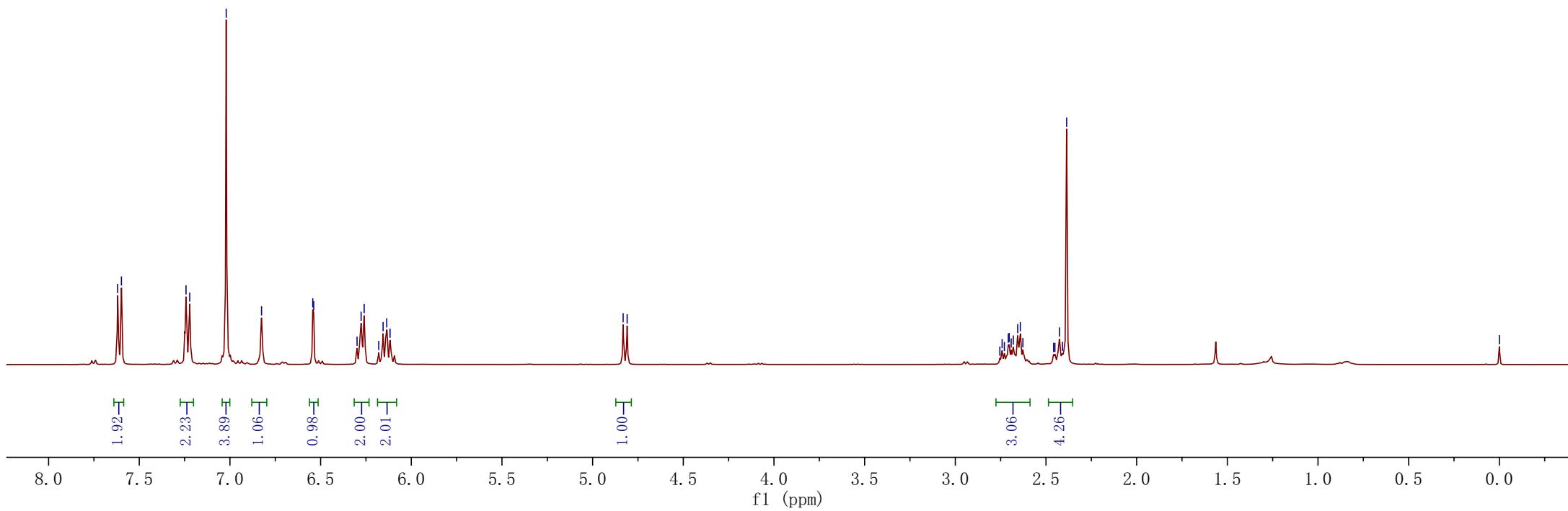
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



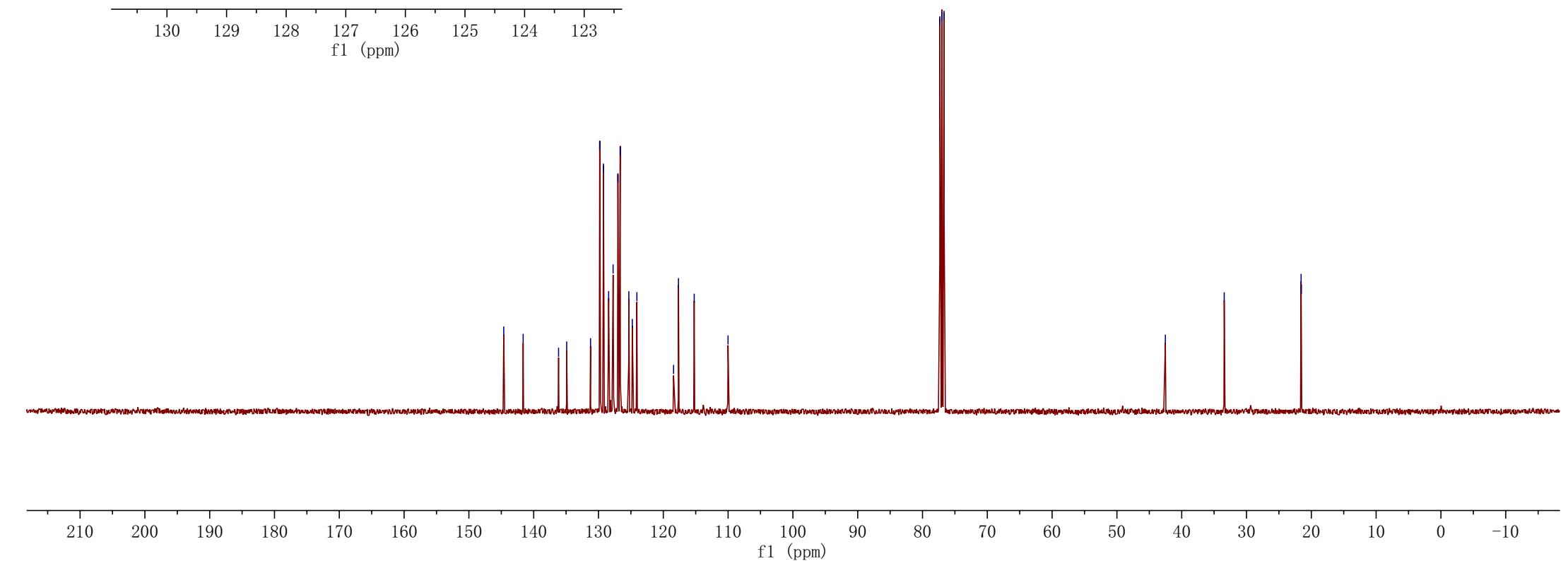
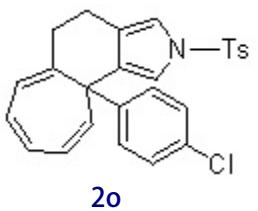
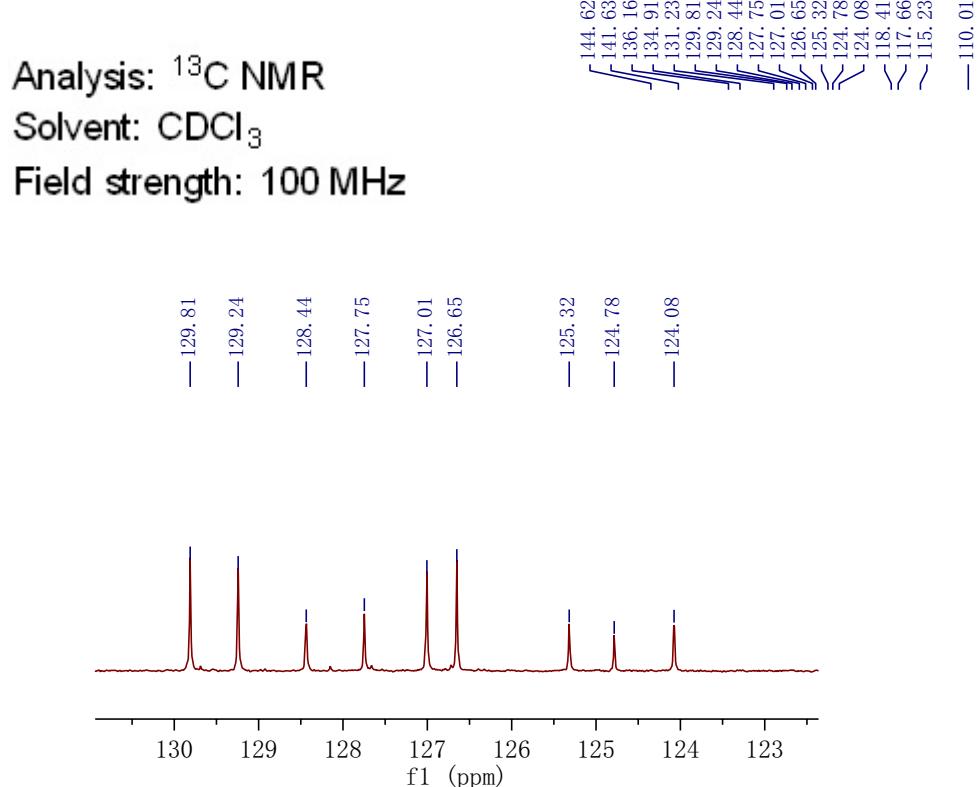
**2o**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



—0.000

7.618  
7.247  
7.226  
7.176  
7.155  
6.981  
6.960  
6.824

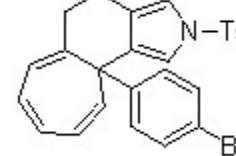
6.548  
6.543  
6.301  
6.279  
6.262  
6.184  
6.160  
6.140  
6.122  
6.097

4.844  
4.822

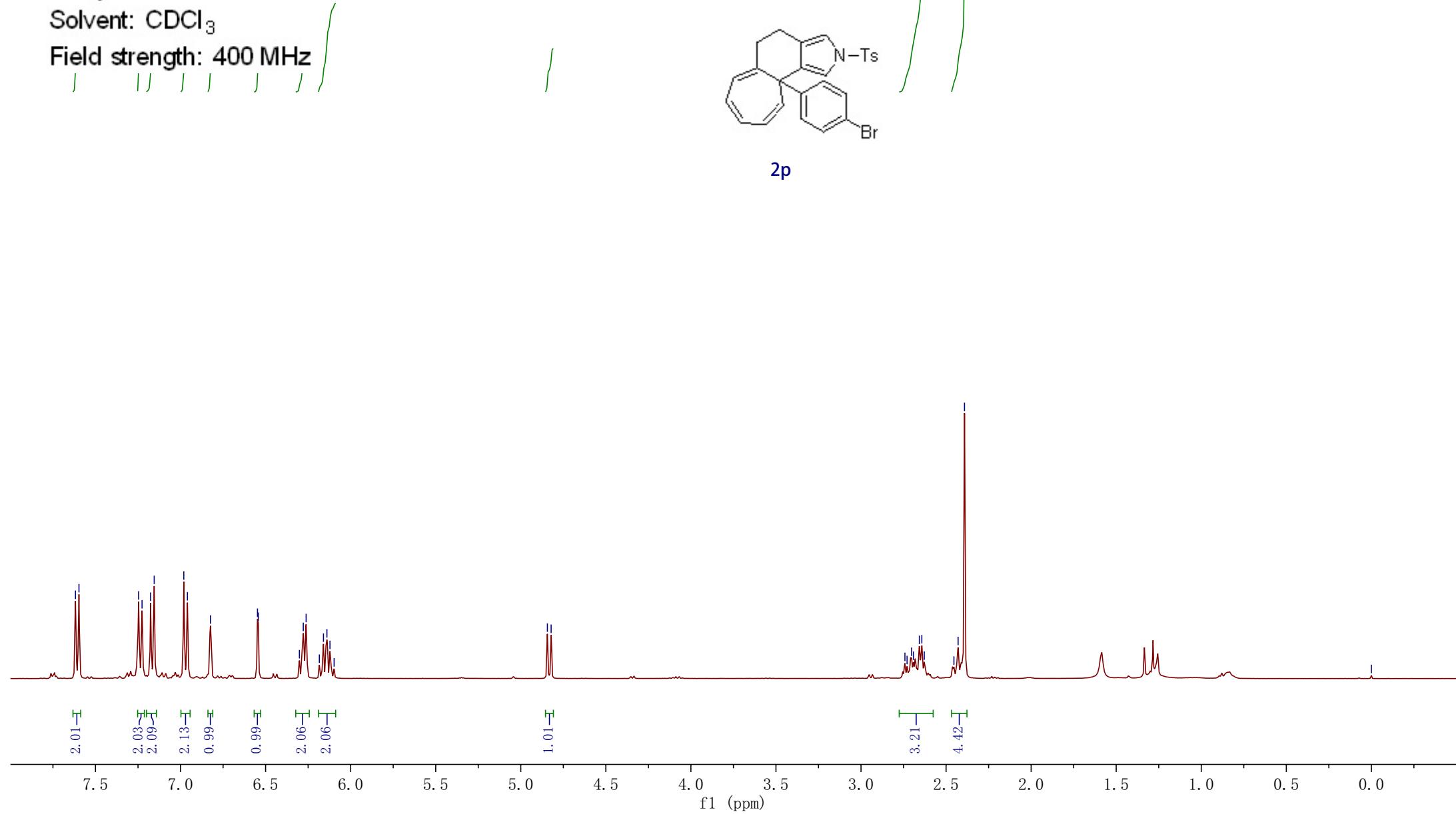
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



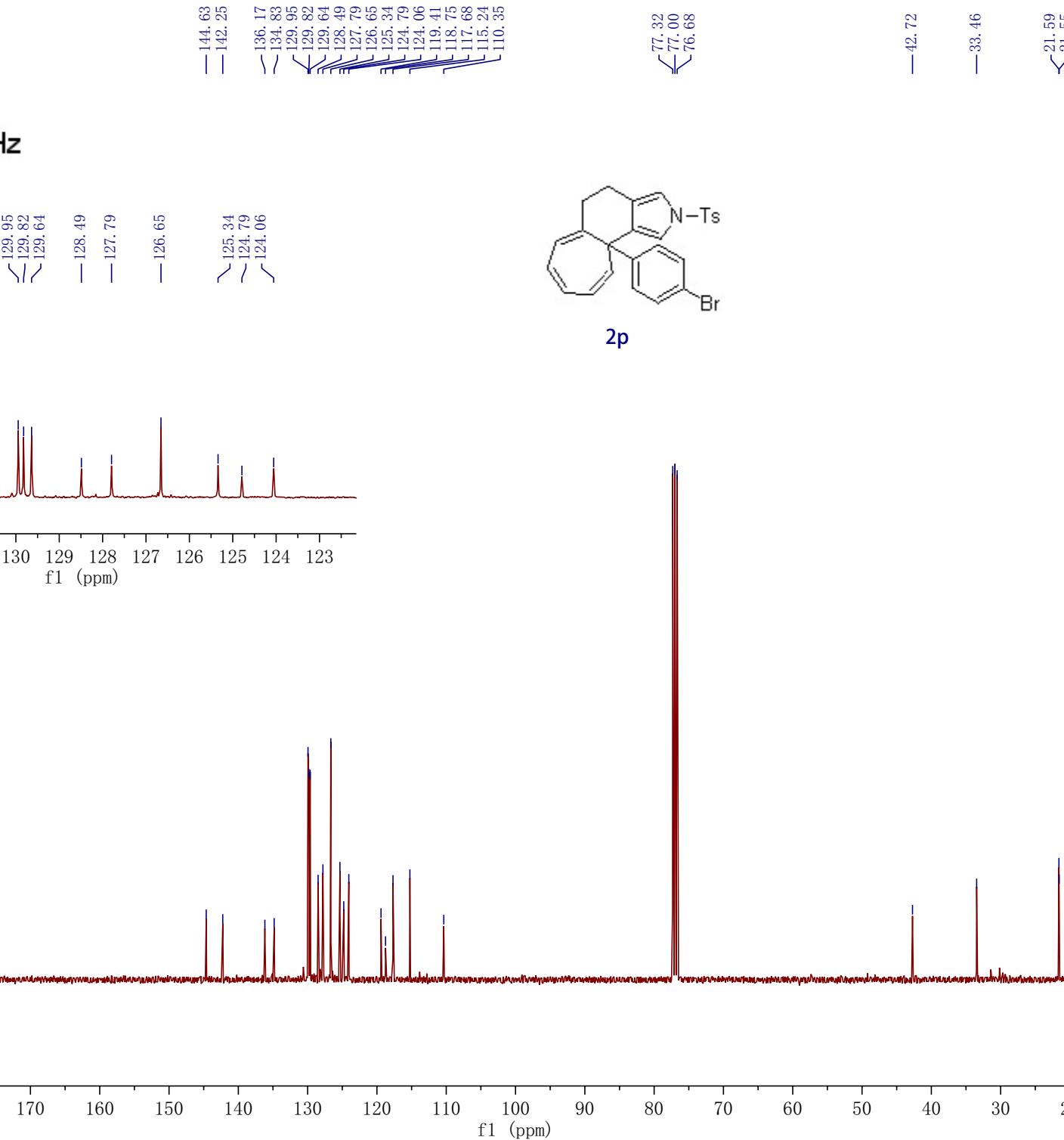
2p



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.738  
7.718  
7.599  
7.579

7.224  
7.204  
7.181  
7.161

6.831

6.540  
6.330  
6.307  
6.291  
6.178  
6.153  
6.137  
6.124  
6.107  
6.083

4.961  
4.939

3.855

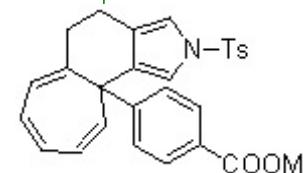
2.771  
2.757  
2.739  
2.725  
2.693  
2.679  
2.664  
2.480  
2.453  
2.431  
2.373

0.000

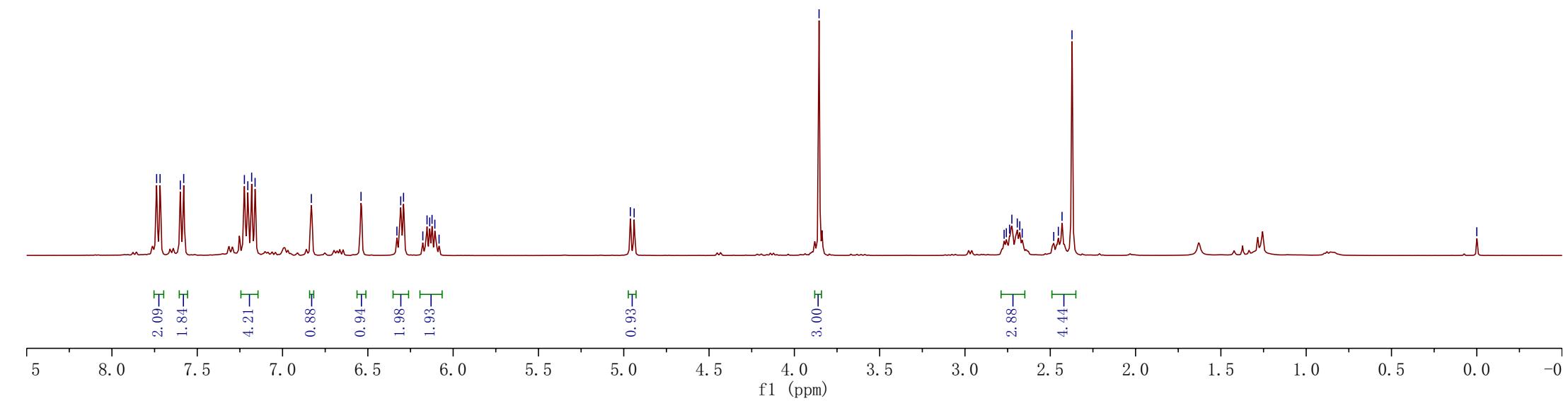
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



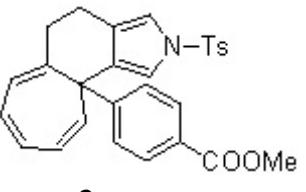
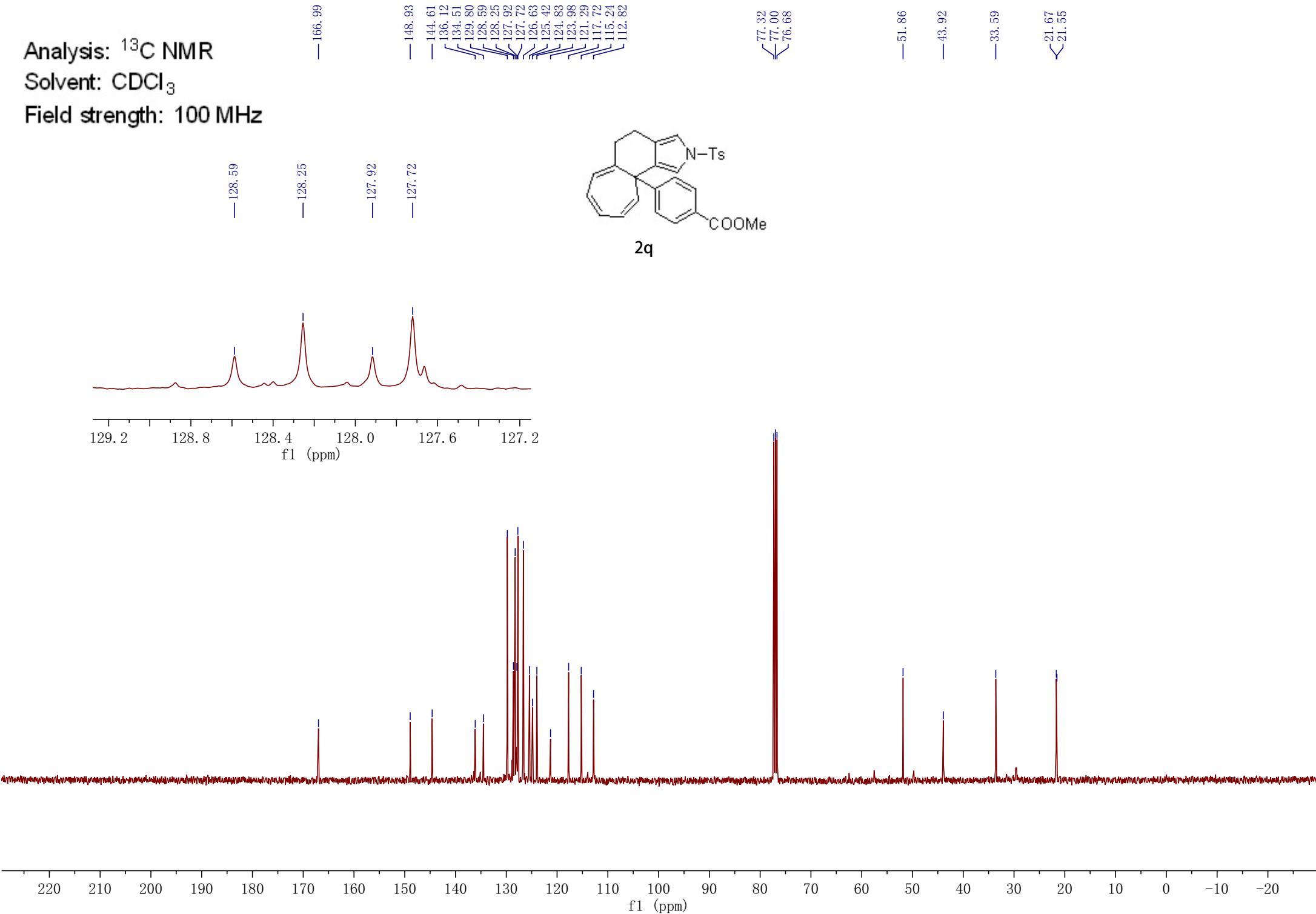
2q



Analysis:  $^{13}\text{C}$  NMR

Solvent: CDCl<sub>3</sub>

Field strength: 100 MHz



<7.616

7.234  
7.214  
7.001  
6.981  
6.962  
6.808  
6.701  
6.681  
6.651  
6.608  
6.580  
6.299  
6.287  
6.275  
6.222  
6.198  
6.177  
6.159  
6.135

Analysis:  $^1\text{H}$  NMR

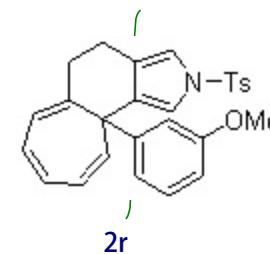
Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

<4.935

4.913

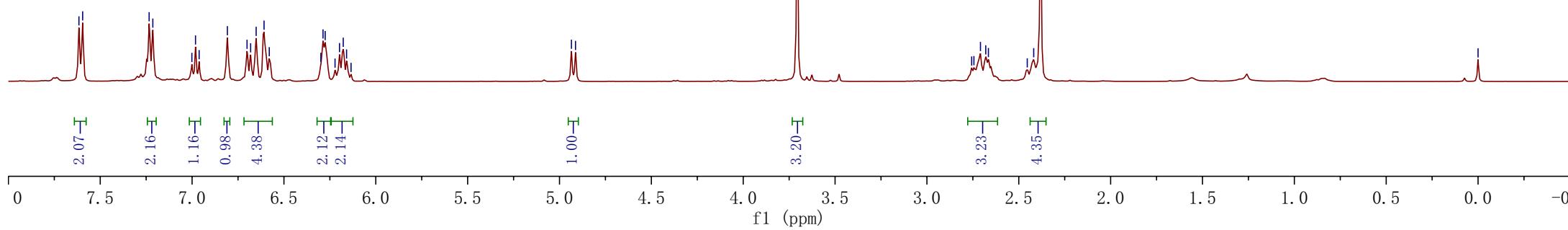
-3.706



2r

2.756  
2.744  
2.709  
2.680  
2.665  
2.454  
2.419  
2.382

-0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 158.16

— 145.03  
— 144.48

— 136.31  
— 135.41  
— 129.77  
— 128.52  
— 127.84  
— 127.65  
— 126.63  
— 125.29  
— 125.14  
— 123.86  
— 122.29  
— 120.55  
— 117.87  
— 115.04  
— 114.46  
— 113.82  
— 110.28

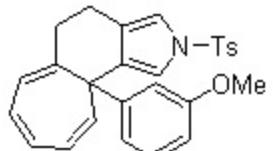
— 77.32  
— 77.00  
— 76.68

— 54.99

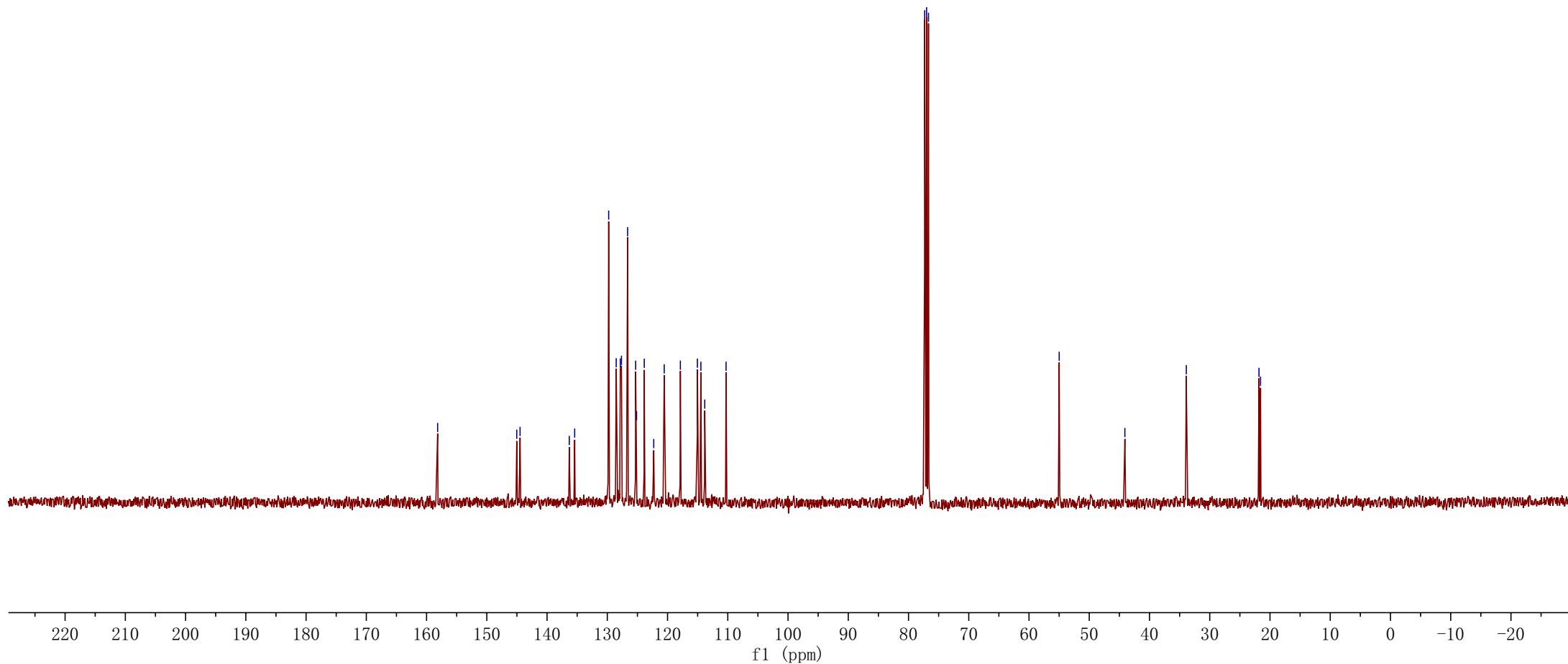
— 44.09

— 33.89

— 21.82  
— 21.57



2r



<7.607  
<7.587

7.227  
7.207  
6.961  
6.942  
6.924  
6.900  
6.865  
6.843  
6.803  
6.561  
6.556  
6.289  
6.253  
6.183  
6.159  
6.139  
6.120  
6.096

<4.846  
<4.824

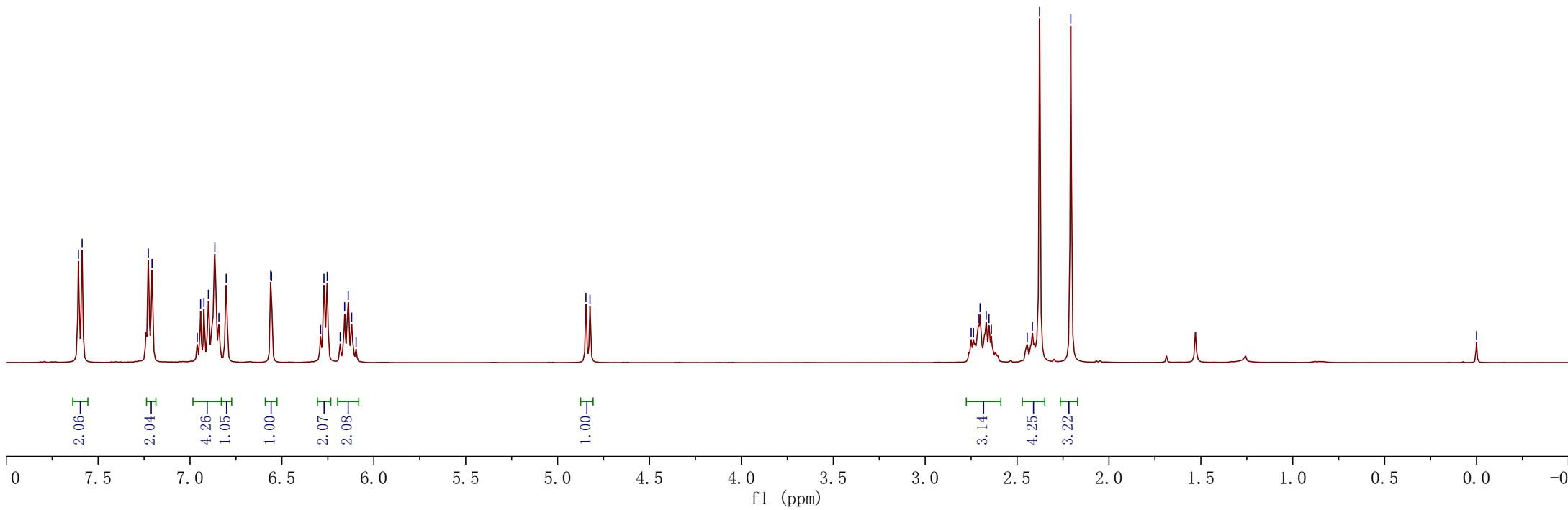
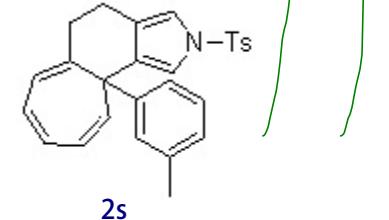
2.750  
2.737  
2.710  
2.701  
2.668  
2.653  
2.640  
2.445  
2.417  
2.377  
-2.208

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

$\nearrow^{136.35}$   
 $\searrow^{136.08}$

$\nearrow^{129.74}$   
 $\nearrow^{128.58}$   
 $\nearrow^{128.25}$   
 $\nearrow^{127.60}$   
 $\nearrow^{126.61}$   
 $\nearrow^{126.57}$   
 $\nearrow^{126.55}$   
 $\nearrow^{125.20}$   
 $\nearrow^{125.11}$   
 $\nearrow^{124.94}$   
 $\nearrow^{123.96}$

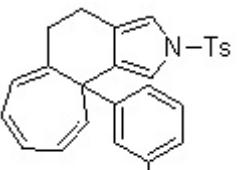
$\nearrow^{144.45}$   
 $\nearrow^{142.97}$   
 $\nearrow^{142.97}$   
 $\nearrow^{136.35}$   
 $\nearrow^{136.08}$   
 $\nearrow^{135.68}$   
 $\nearrow^{129.74}$   
 $\nearrow^{128.58}$   
 $\nearrow^{128.25}$   
 $\nearrow^{127.60}$   
 $\nearrow^{126.61}$   
 $\nearrow^{126.57}$   
 $\nearrow^{126.55}$   
 $\nearrow^{125.20}$   
 $\nearrow^{125.11}$   
 $\nearrow^{124.94}$   
 $\nearrow^{123.96}$

$\nearrow^{77.32}$   
 $\nearrow^{77.00}$   
 $\nearrow^{76.68}$

$\nearrow^{-43.24}$

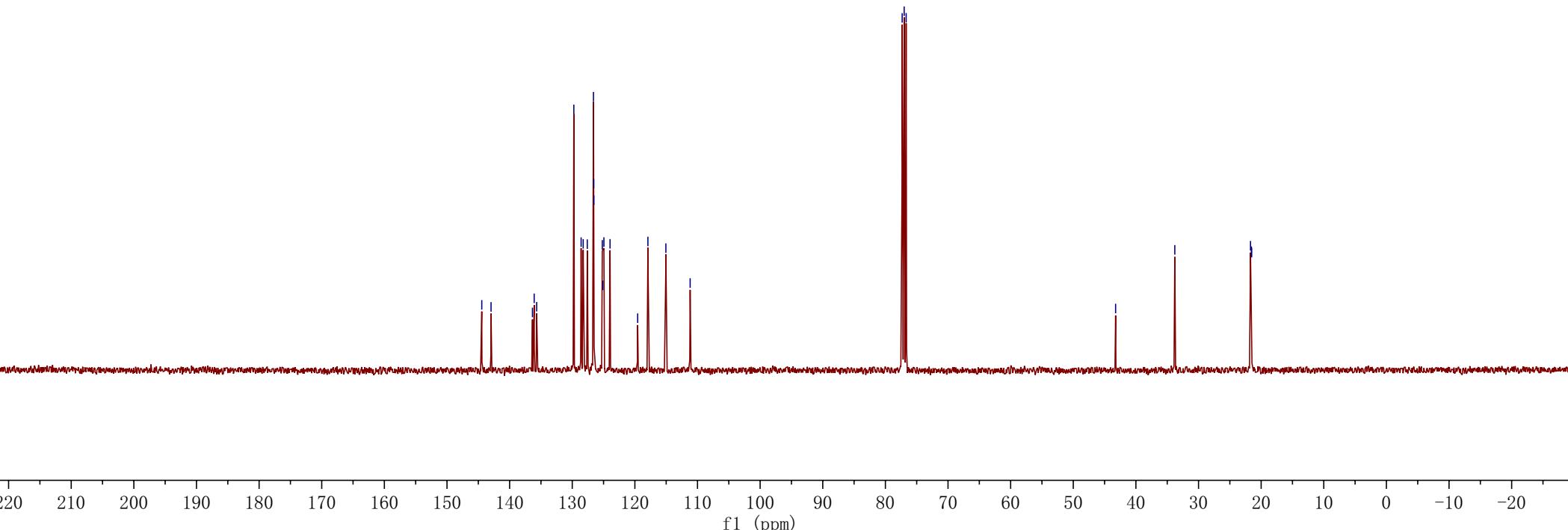
$\nearrow^{-33.79}$

$\nearrow^{21.70}$   
 $\nearrow^{21.56}$   
 $\nearrow^{21.52}$



2s

138 136 134 132 130 128 126 124 122  
f1 (ppm)



<7.620  
<7.600  
7.254  
7.232  
7.181  
7.162  
<7.056  
<7.036  
6.947  
6.928  
6.908  
6.824  
6.564  
6.559  
6.326  
6.303  
6.286  
6.222  
6.198  
6.182  
6.169  
6.153  
6.128

4.898  
4.876

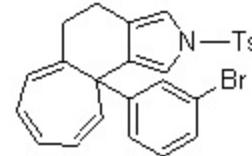
2.766  
2.754  
2.741  
2.722  
2.714  
2.703  
2.676  
2.661  
2.647  
2.625  
2.462  
2.456  
2.438  
2.429  
2.392

—0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



2t



4.22

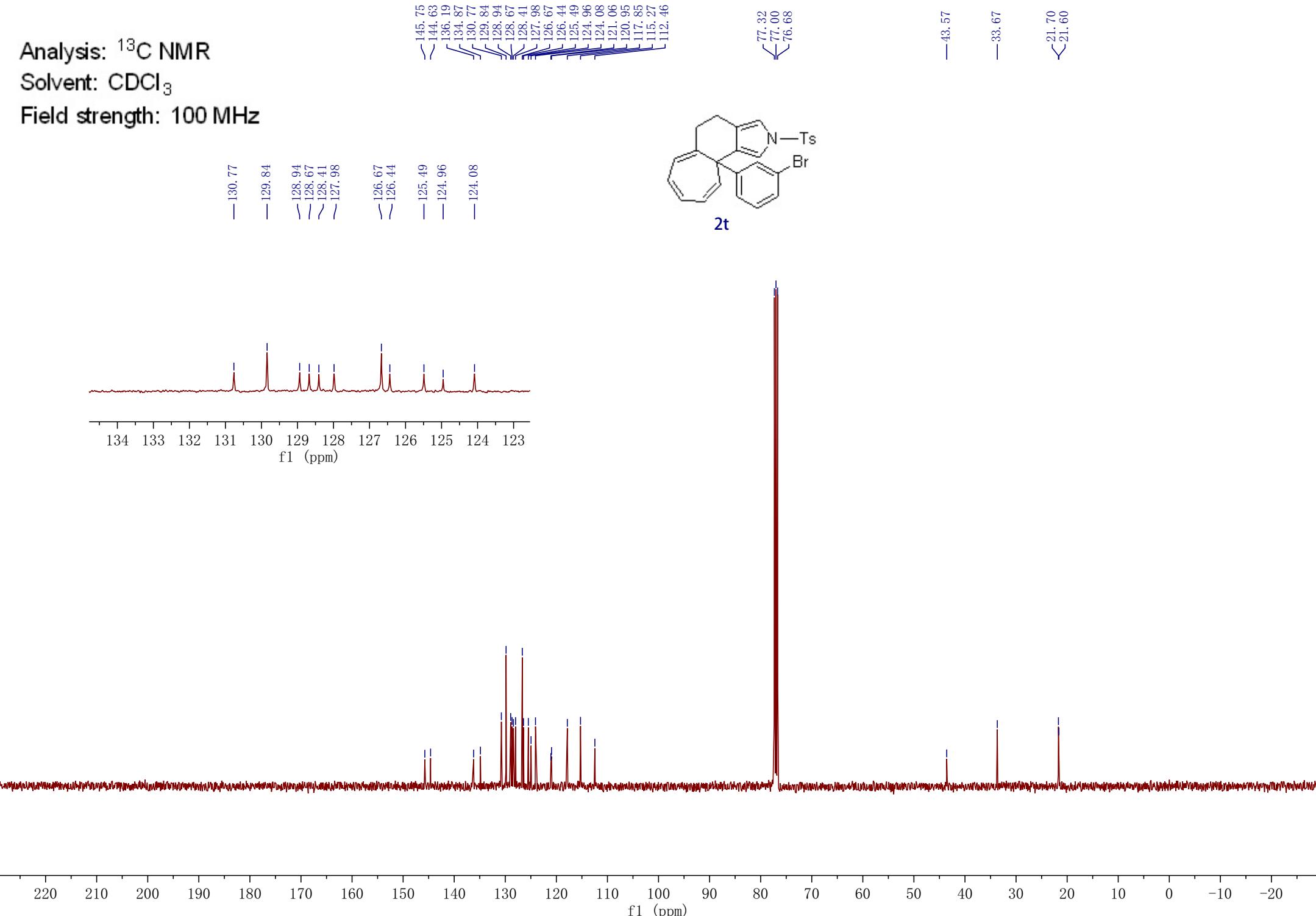
f1 (ppm)

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

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.624

<7.223

6.820

6.647

6.644

6.626

6.623

6.600

6.586

6.564

6.284

6.260

6.243

6.190

6.167

6.150

6.132

6.109

<4.766

<4.745

<3.802

<3.746

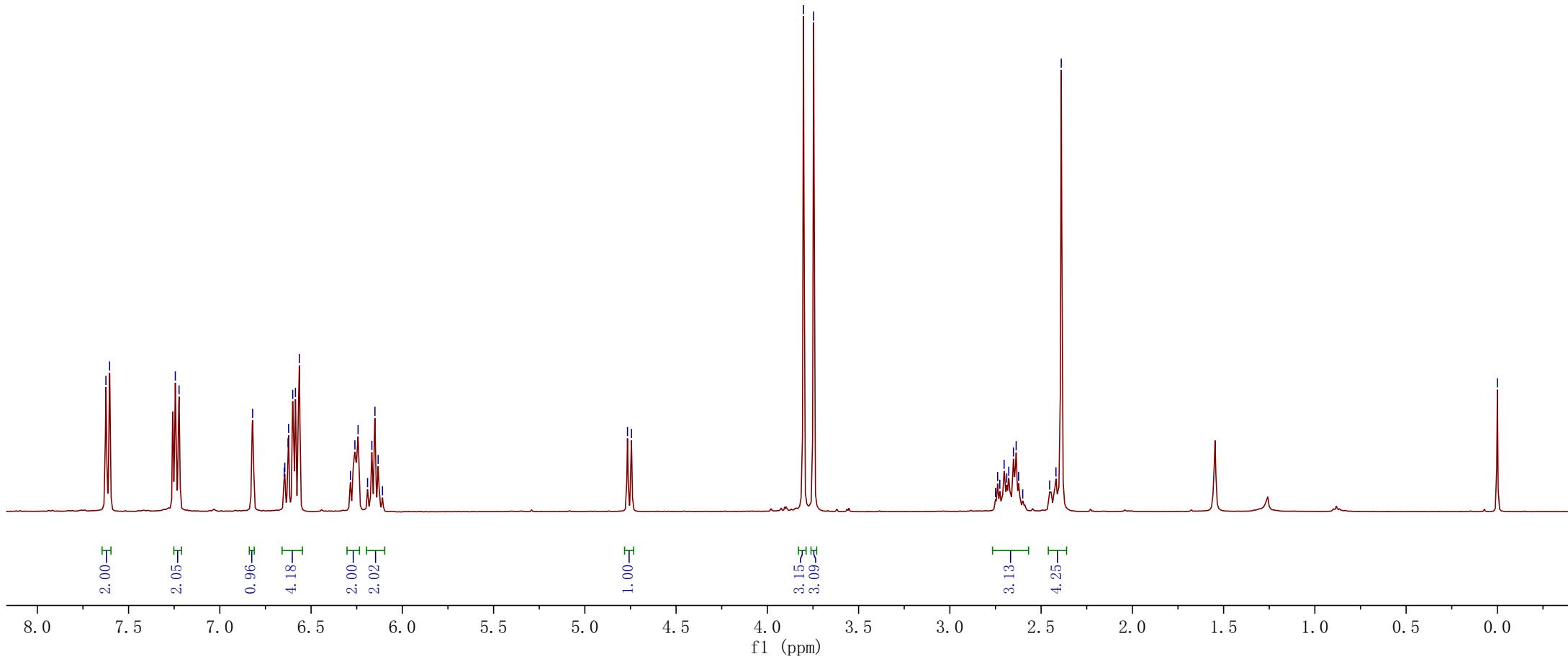
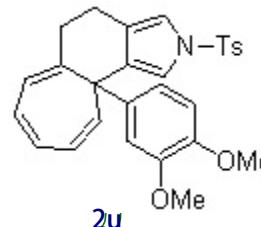
2.750  
2.738  
2.726  
2.703  
2.688  
2.677  
2.652  
2.637  
2.623  
2.601  
2.453  
2.419  
2.390

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

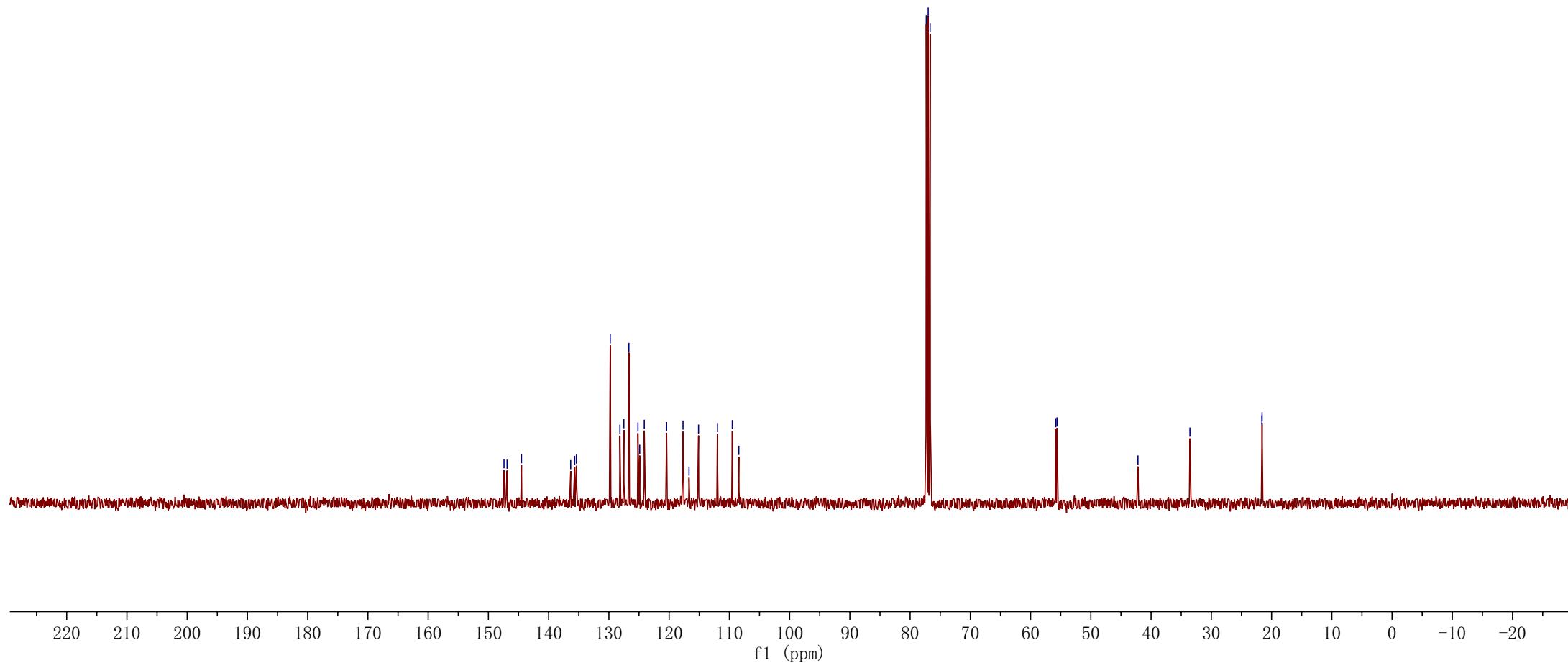
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.620

<7.242  
<7.221  
6.880  
6.875  
6.859  
6.854  
6.796  
6.537  
6.523  
6.502  
6.273  
6.254  
6.236  
6.182  
6.159  
6.142  
6.125  
6.101

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

<4.743

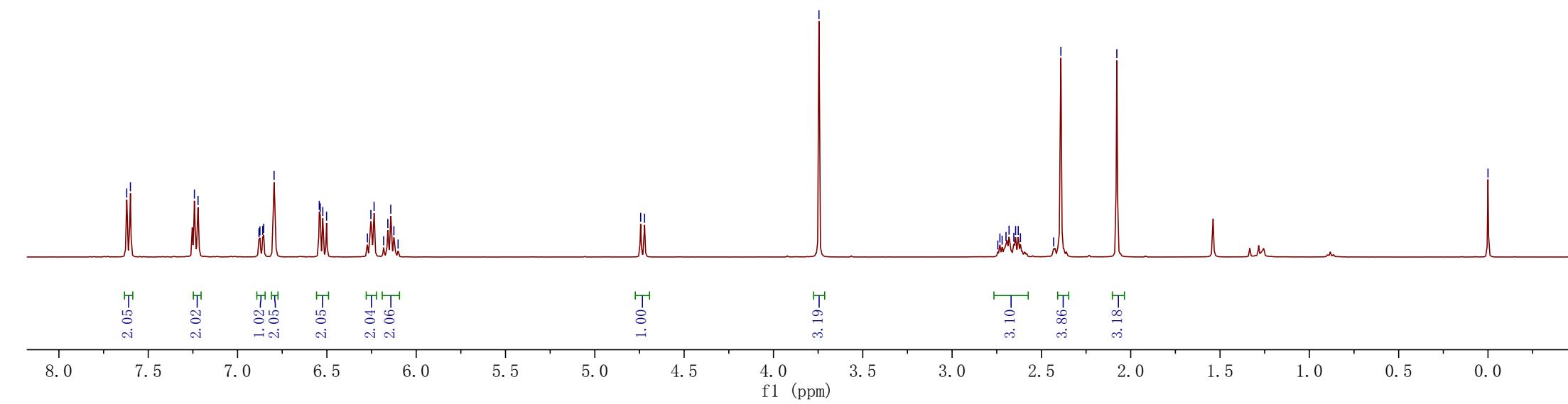
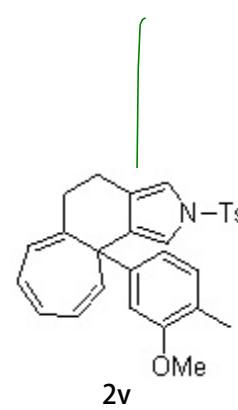
<4.721

-3.745

2.744  
2.732  
2.720  
2.698  
2.681  
2.654  
2.644  
2.630  
2.617  
2.431  
2.391

-2.078

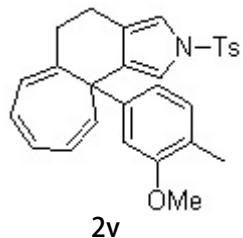
-0.000



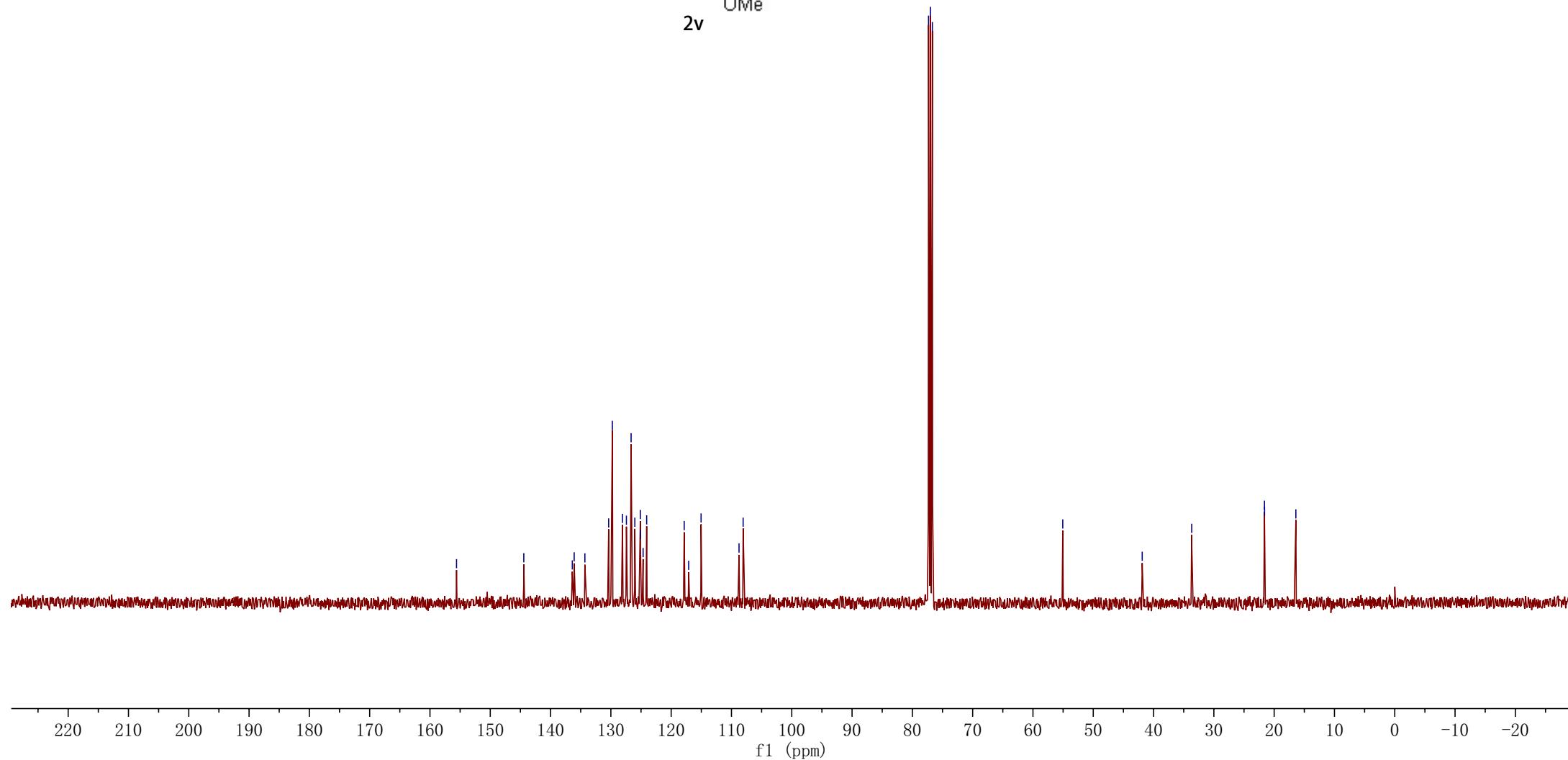
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



**2v**



<7.613

<7.622

<7.252

<7.232

<6.815

<6.580

<6.552

<6.523

<6.503

<6.254

<6.240

<6.206

<6.183

<6.168

<6.152

<5.858

<5.851

<4.739

<4.718

<2.727

<2.716

<2.692

<2.683

<2.652

<2.628

<2.618

<2.423

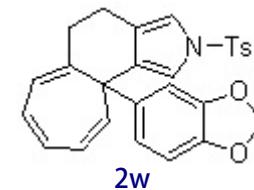
<2.389

<-0.000

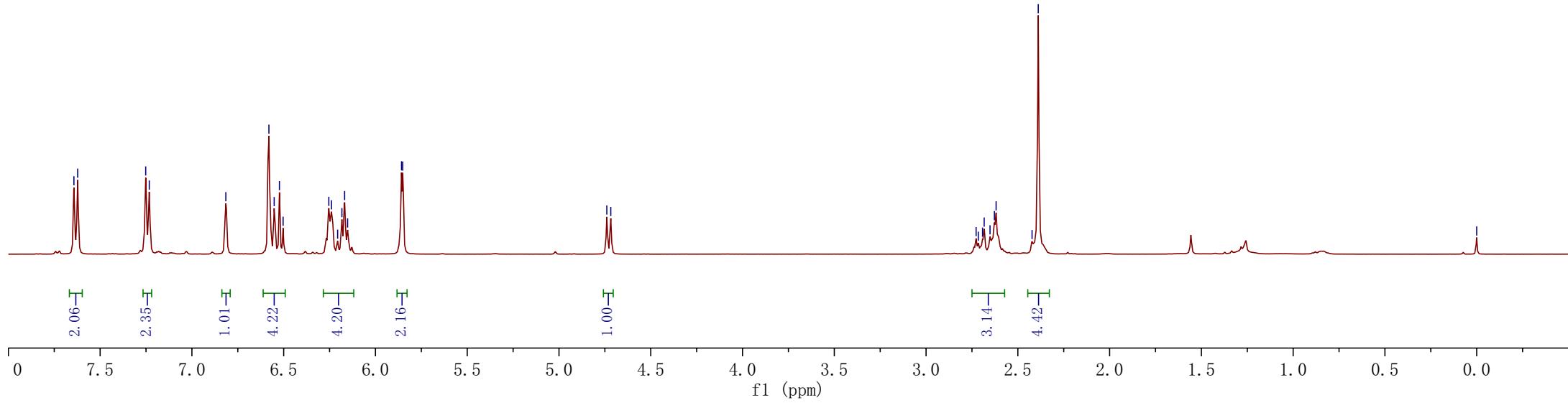
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



2w



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

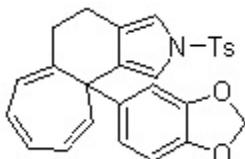
146.16  
145.30  
144.52  
136.81  
136.30  
135.49  
129.79  
128.20  
127.56  
126.67  
125.18  
124.86  
124.16  
121.08  
117.69  
117.02  
115.11  
108.87  
108.71  
106.69  
100.62

77.32  
77.00  
76.68

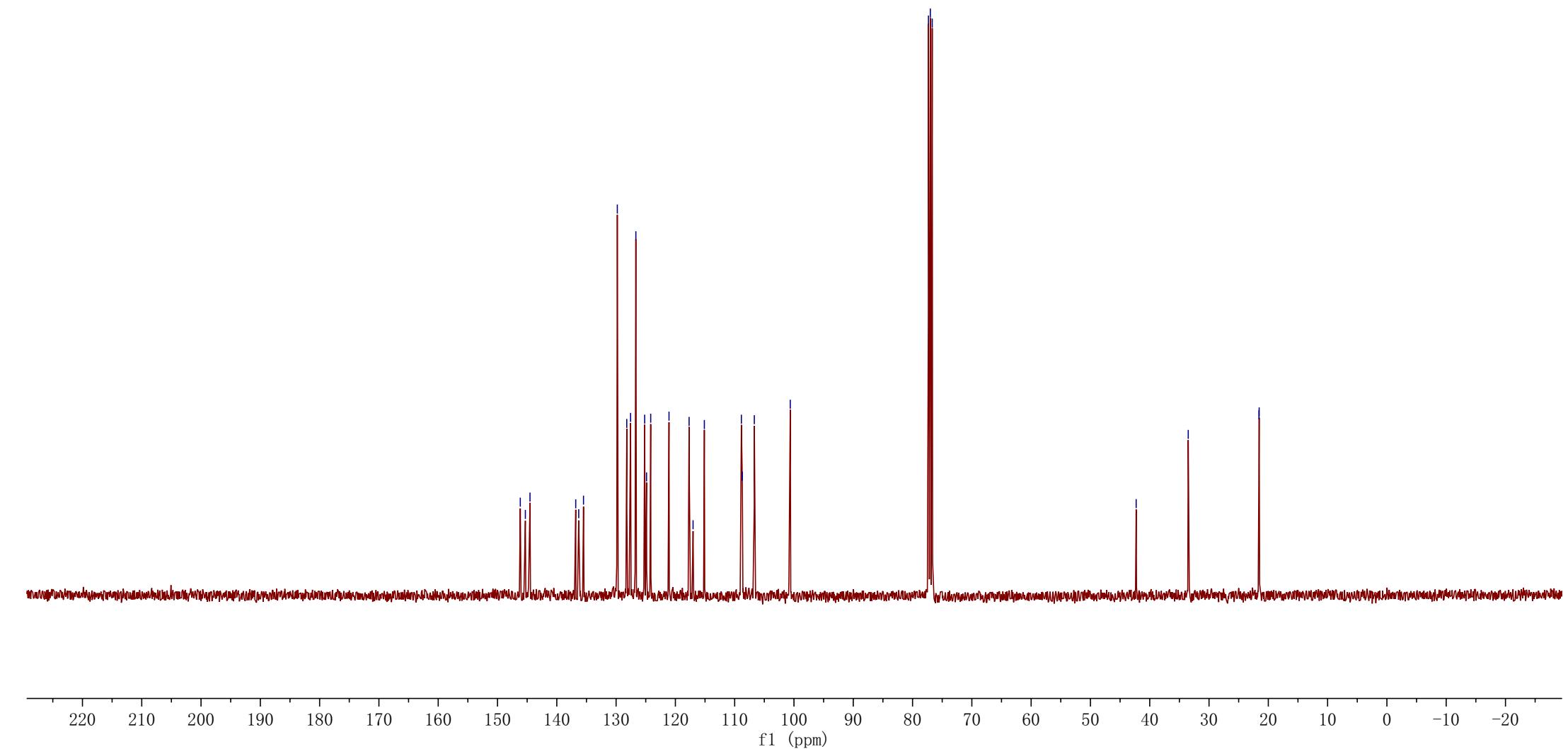
-42.29

-33.51

21.57  
21.54



**2w**



7.647  
7.626  
7.253  
7.233  
6.912  
6.900  
6.859  
6.853  
6.816  
6.676  
6.667  
6.655  
6.629  
6.623  
6.343  
6.330  
6.322  
6.308  
6.291  
6.270

-0.000

Analysis:  $^1\text{H}$  NMR

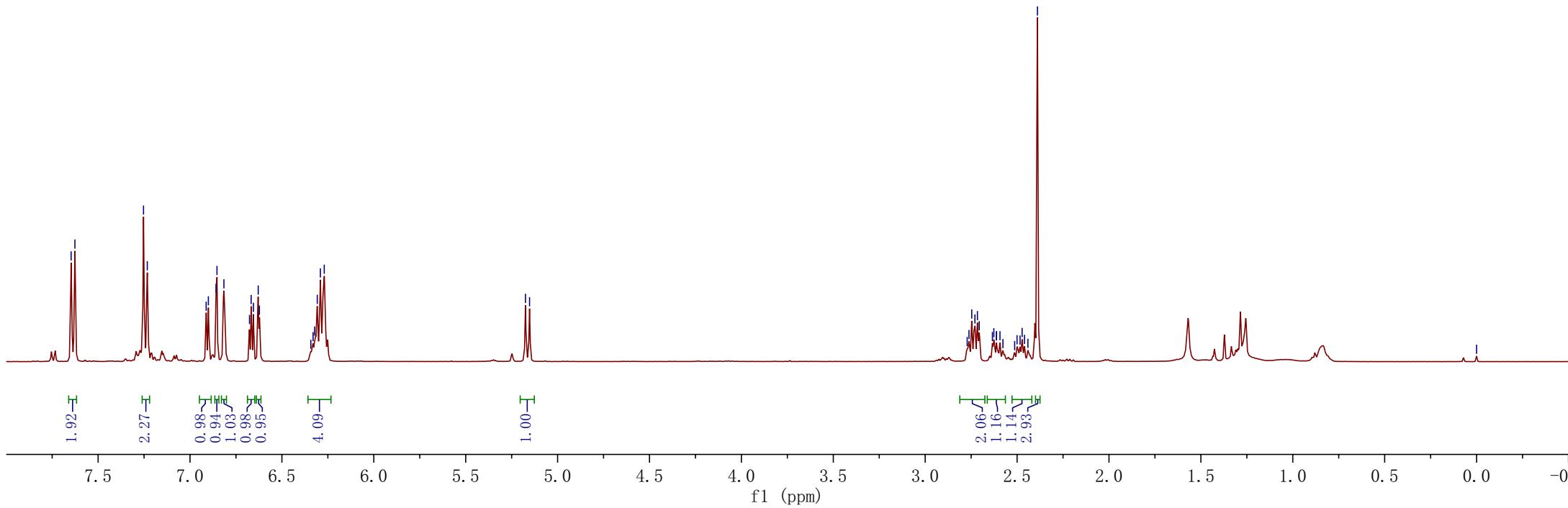
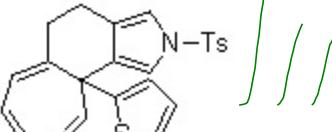
Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

| | | || || |

5.175  
5.153

2.772  
2.762  
2.747  
2.729  
2.716  
2.706  
2.634  
2.627  
2.612  
2.612  
2.593  
2.577  
2.513  
2.500  
2.484  
2.473  
2.460  
2.441  
2.389



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 128.40

— 126.64

— 125.85

— 125.21

— 125.14

— 124.76

— 124.09

— 148.57

— 144.56

— 136.29

— 135.36

— 129.82

— 129.11

— 128.40

— 126.64

— 125.85

— 125.21

— 125.14

— 124.76

— 124.09

— 122.12

— 119.11

— 117.88

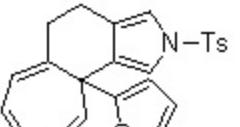
— 114.96

77.32  
77.00  
76.68

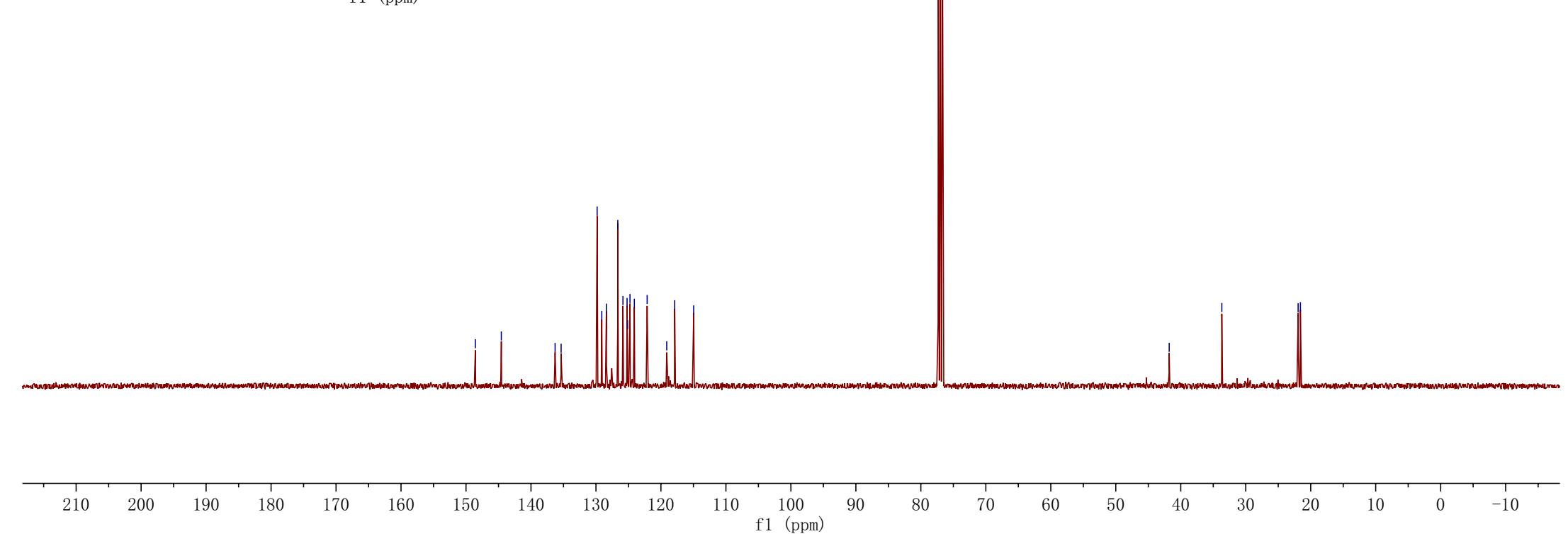
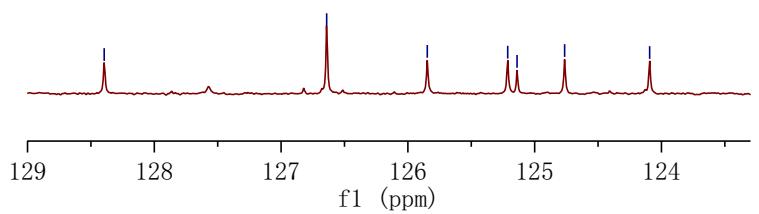
— 41.78

— 33.68

— 21.94  
— 21.58



**2x**



7.611  
7.591

7.228

7.208

6.989

6.968

-6.796

6.621

6.600

-6.471

6.087  
6.069  
6.001  
5.980  
5.821  
5.803

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



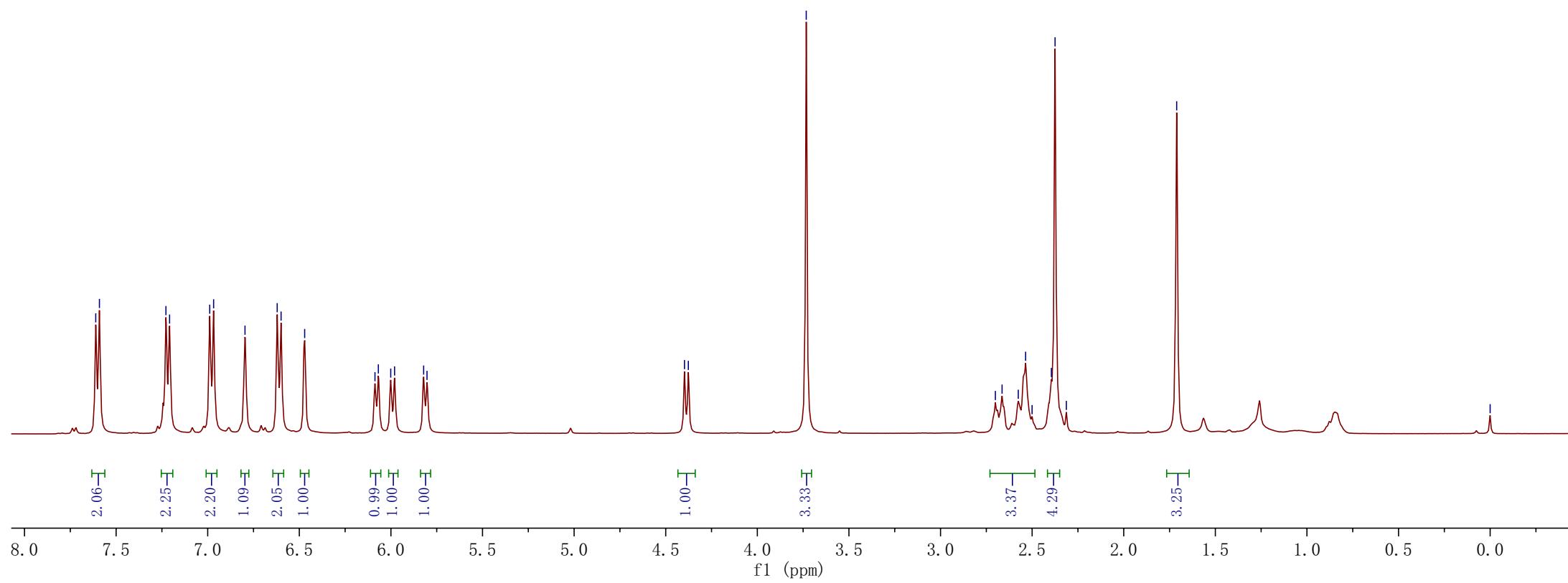
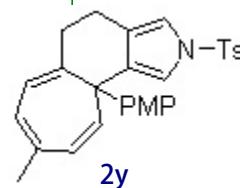
4.398  
4.377

3.733

2.701  
2.664  
2.576  
2.536  
2.500  
2.395  
2.375  
2.313

1.711

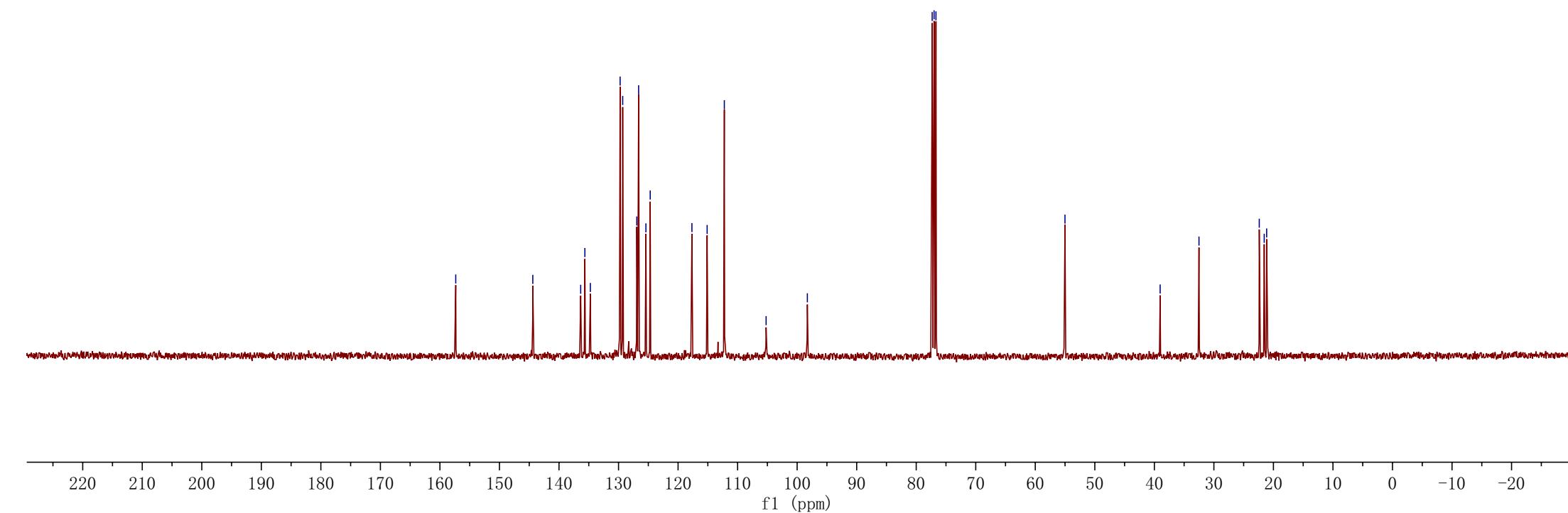
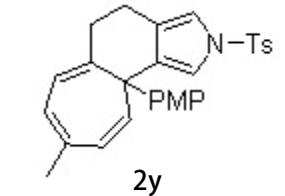
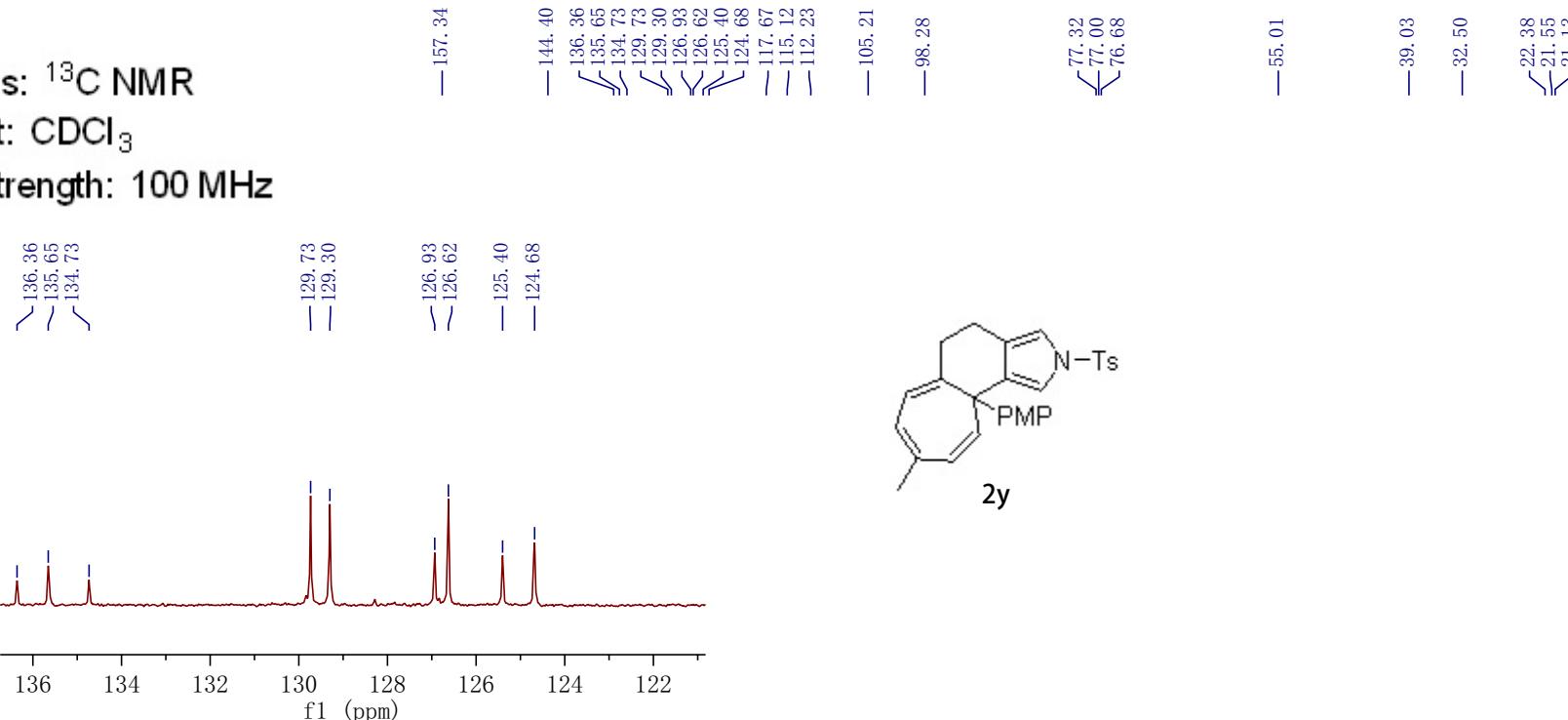
0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



<7.619

<7.236

<7.216

<7.025

<7.003

-6.814

<6.625

<6.604

<6.587

<6.583

<6.249

<6.232

<6.209

<6.189

<5.935

<5.916

<5.897

<5.879

5.162

<5.148

<5.137

<5.124

-3.726

2.749

<2.738

<2.719

<2.709

<2.684

<2.671

<2.656

<2.625

<2.416

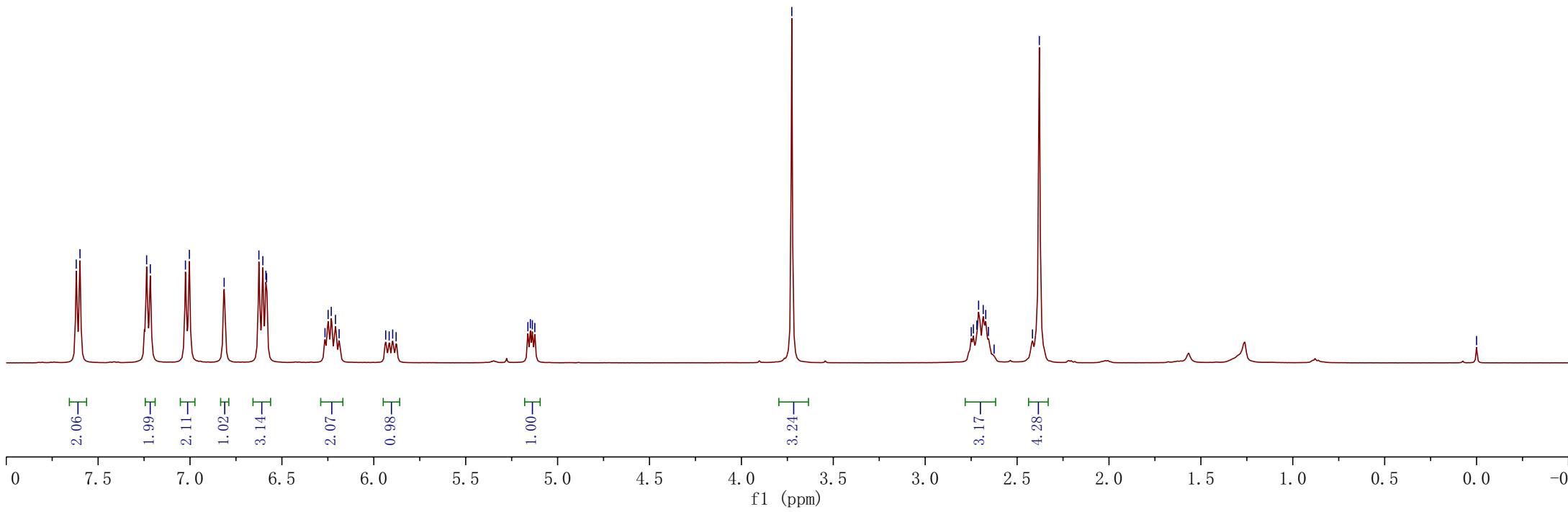
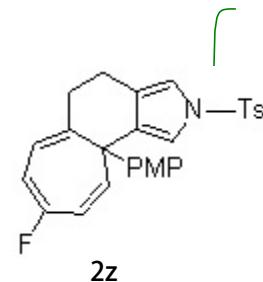
<2.379

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

136.23  
135.68  
135.43  
129.80  
128.07  
126.64  
125.09  
121.67  
121.57  
120.35  
120.23  
117.84  
116.99  
116.68  
115.07  
112.50  
111.82  
111.56  
144.58

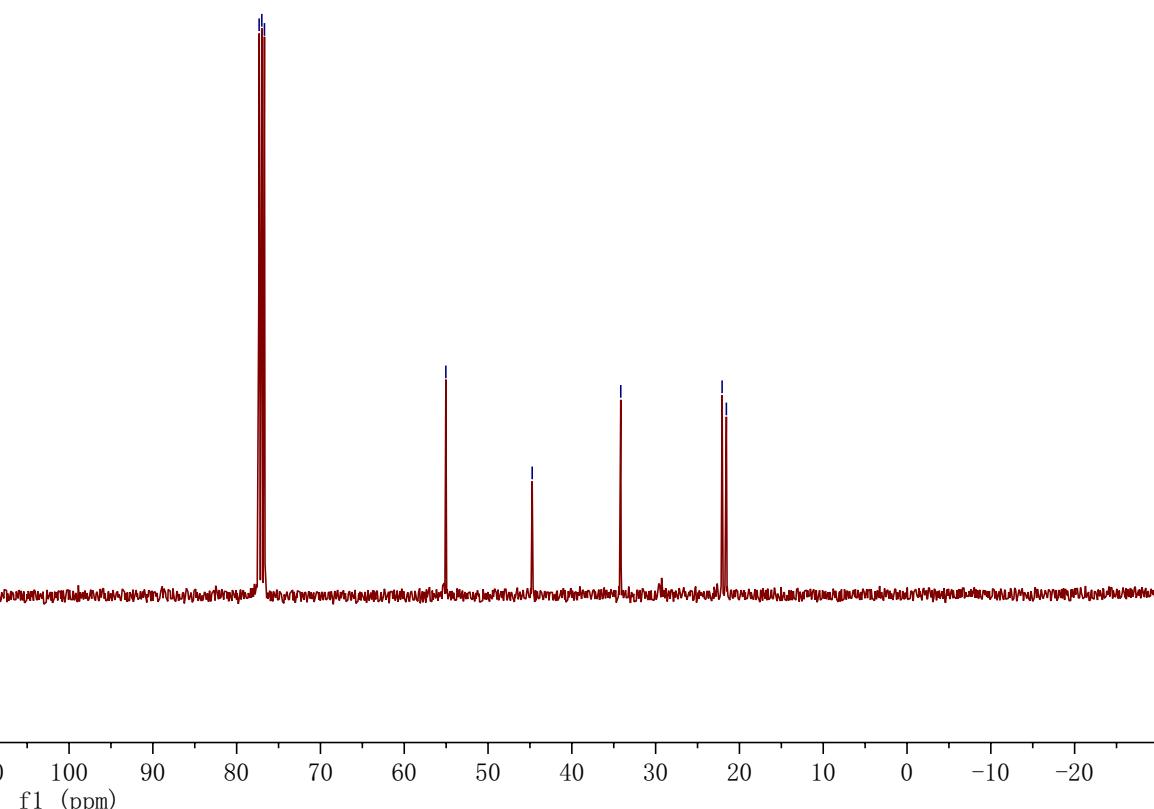
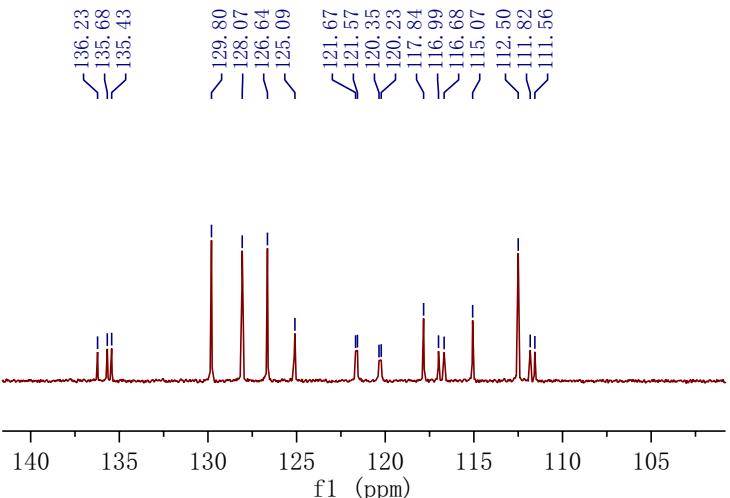
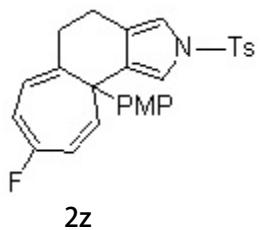
161.94  
159.51  
157.68

-55.04

-44.73

-34.16

22.07  
21.56

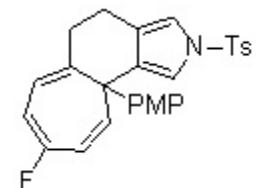


Analysis:  $^{13}\text{F}$  NMR

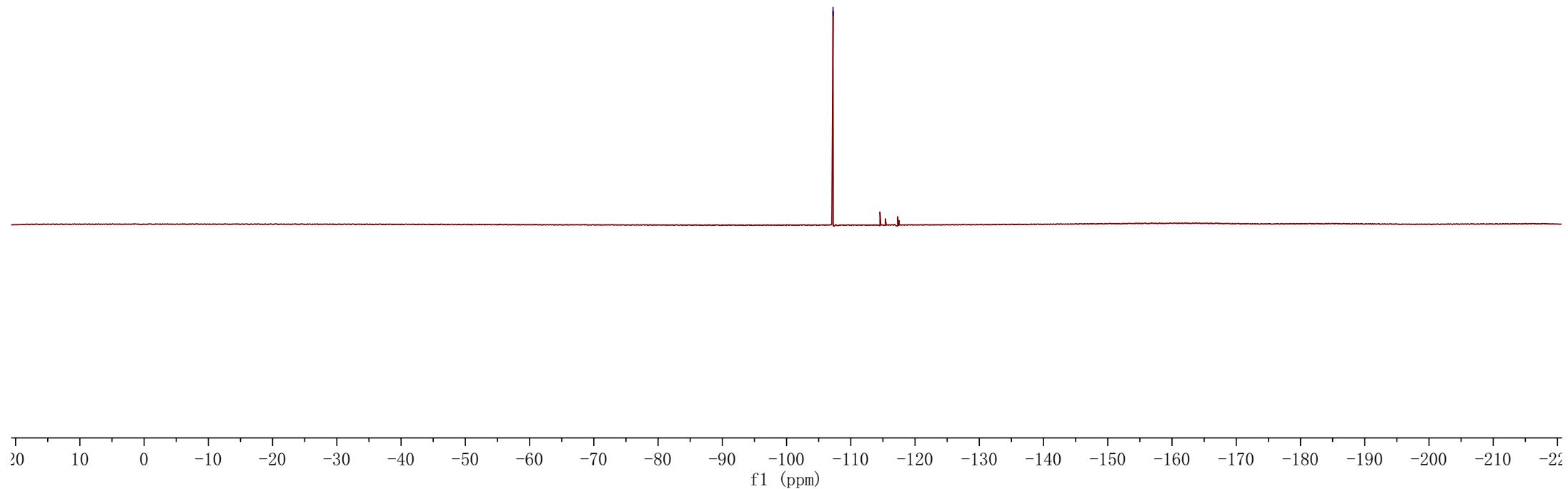
Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz

— -107.24



**2z**



<7.618

<7.240

<7.220

<6.977

<6.956

<6.917

<6.648

<6.626

<6.513

<6.508

<6.380

<6.358

<6.118

<6.099

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

<4.745

<4.721

3.745

2.759

2.747

2.735

2.723

2.711

2.699

2.640

2.629

2.615

2.604

2.431

2.416

2.402

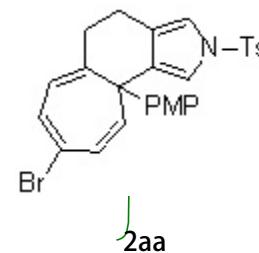
2.383

2.368

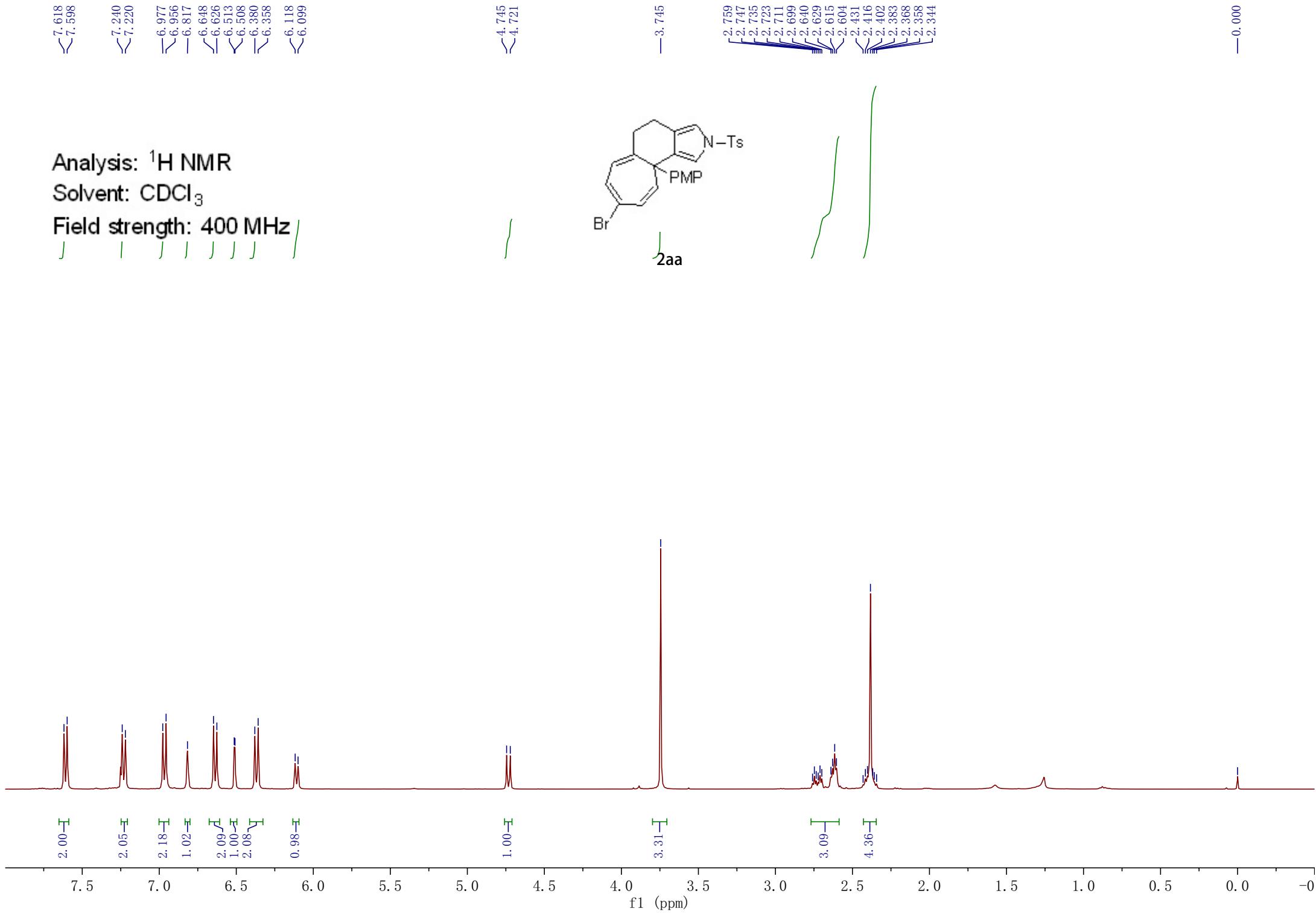
2.358

2.344

-0.000



2aa



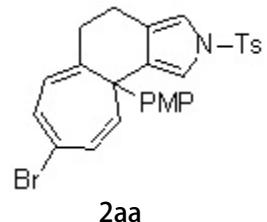
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

— 157.72

144.59  
136.21  
135.00  
134.32  
130.91  
129.81  
128.43  
127.68  
126.67  
124.56  
124.05  
121.42  
121.08  
117.89  
115.17  
112.55  
112.48



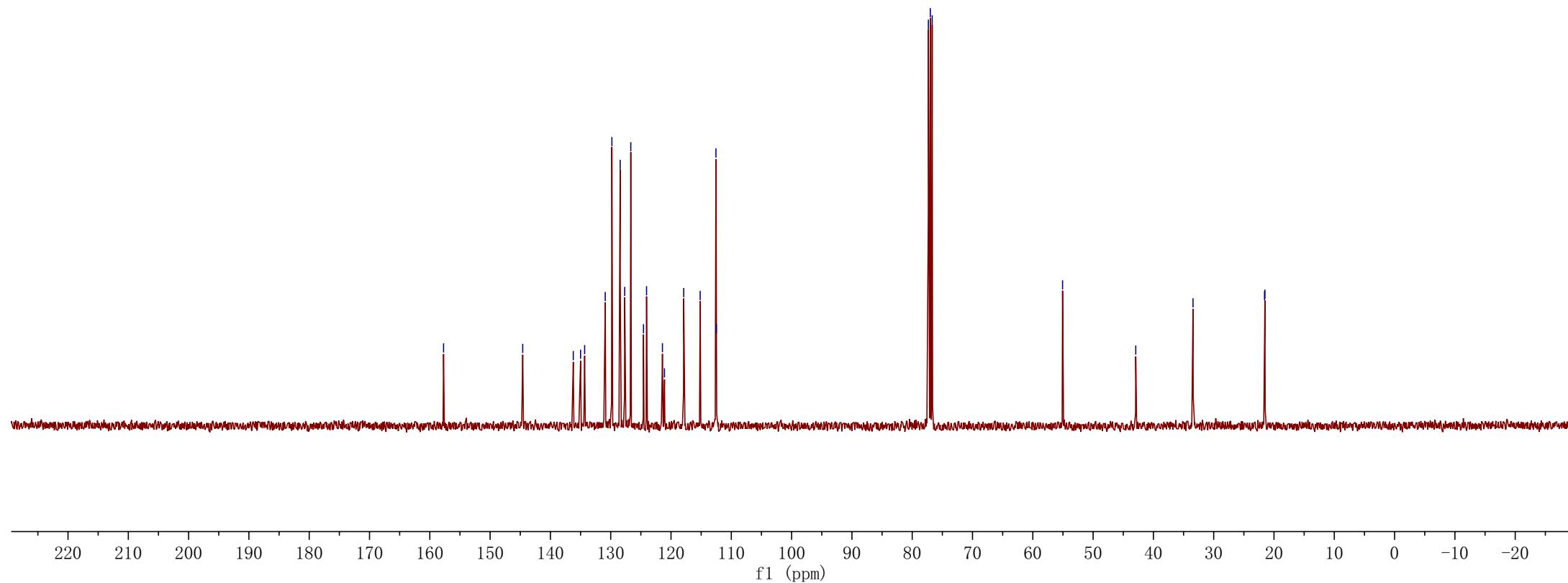
77.32  
77.00  
76.68

— 55.07

— 42.93

— 33.43

21.57  
21.50



7.647  
7.630  
7.270  
7.256  
7.240  
7.233  
7.199  
7.169  
7.139  
7.125  
7.033  
7.016  
6.826  
6.703  
6.686  
6.375  
6.370  
6.230  
6.214  
6.199  
5.827  
5.823  
5.816  
5.811  
5.806  
5.799  
5.794  
5.676  
5.658  
5.647  
5.632

3.757  
3.669  
3.660  
3.645  
3.635  
3.506  
3.492

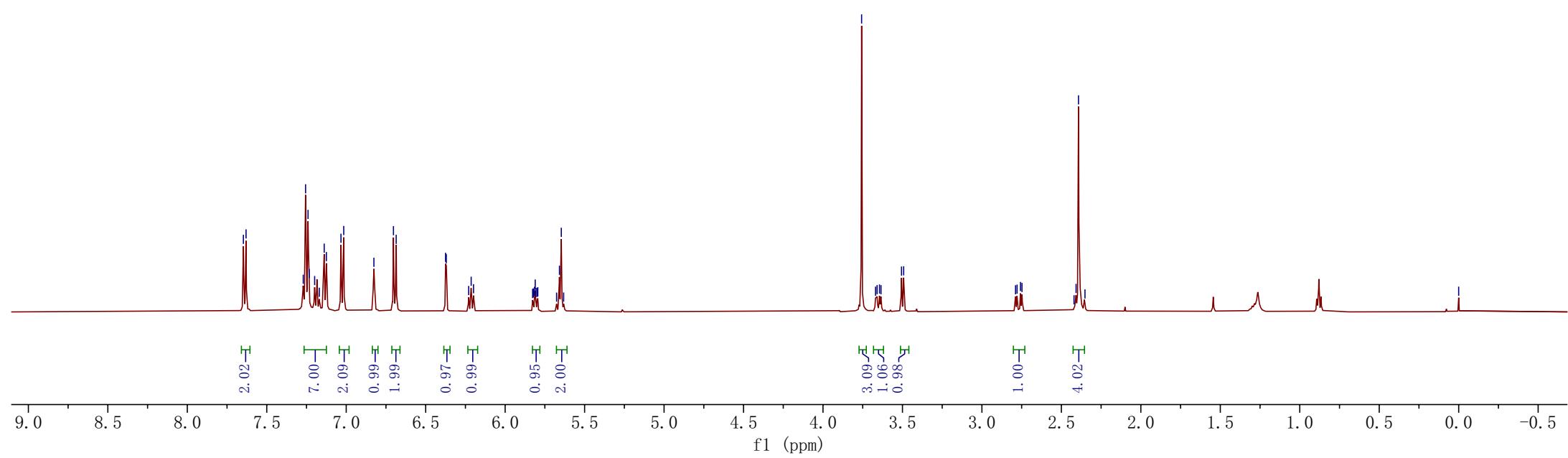
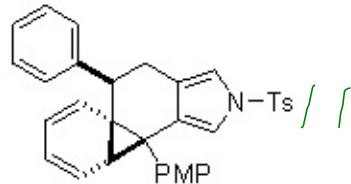
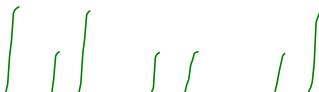
2.789  
2.779  
2.757  
2.748  
2.421  
2.408  
2.392  
2.352

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

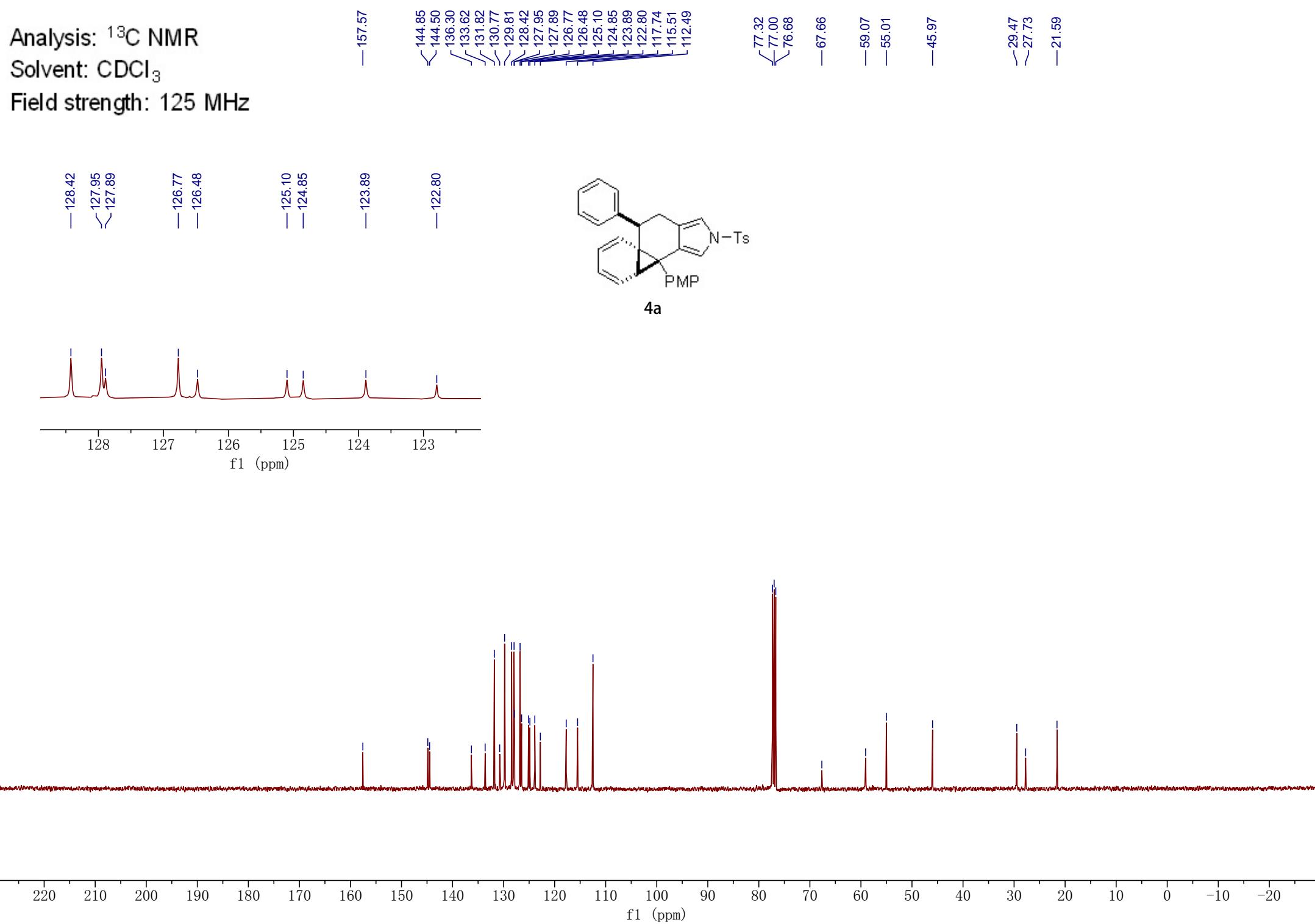
Field strength: 500 MHz

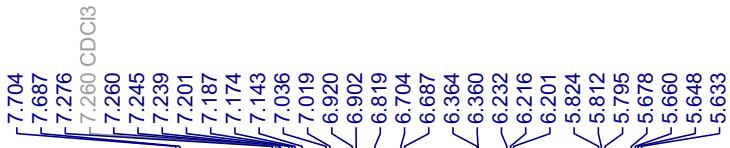


Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz

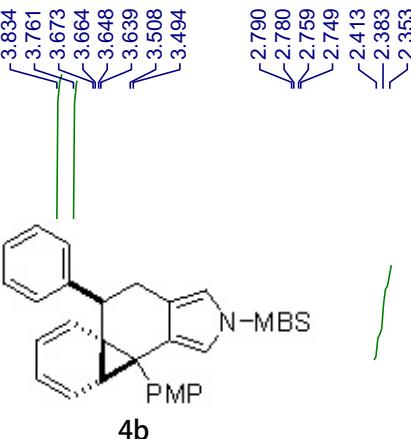




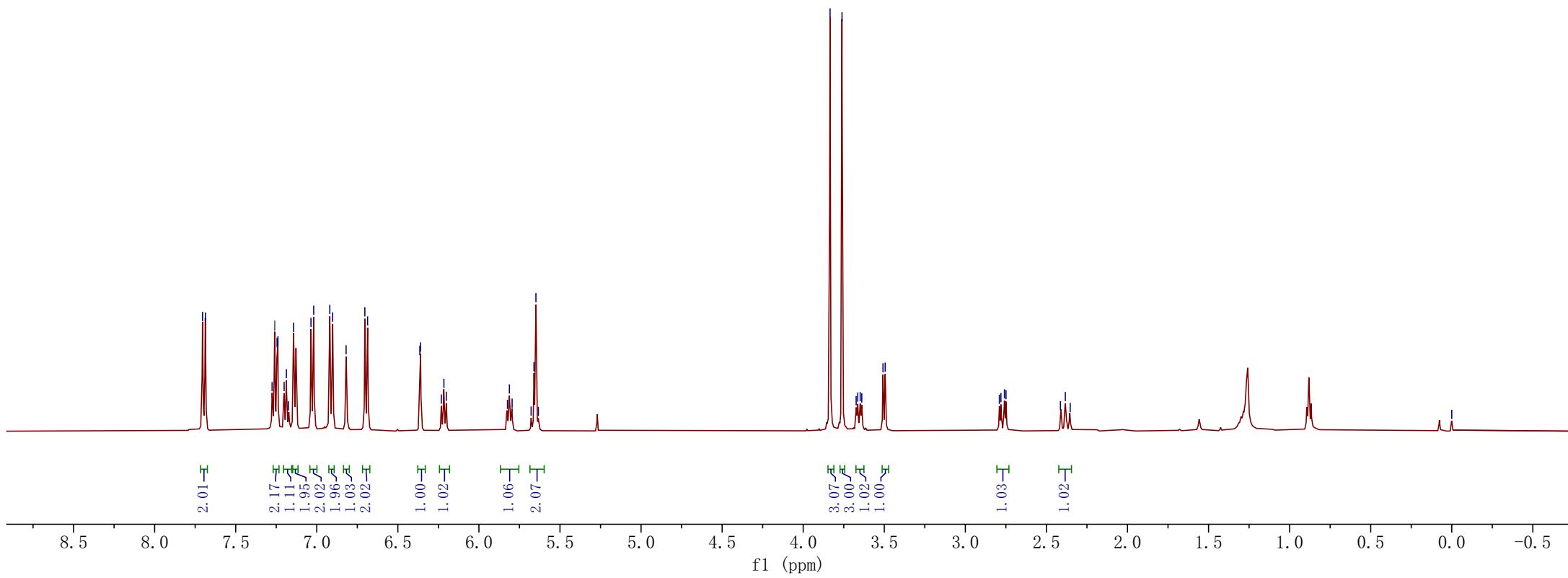
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz



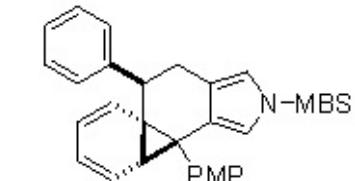
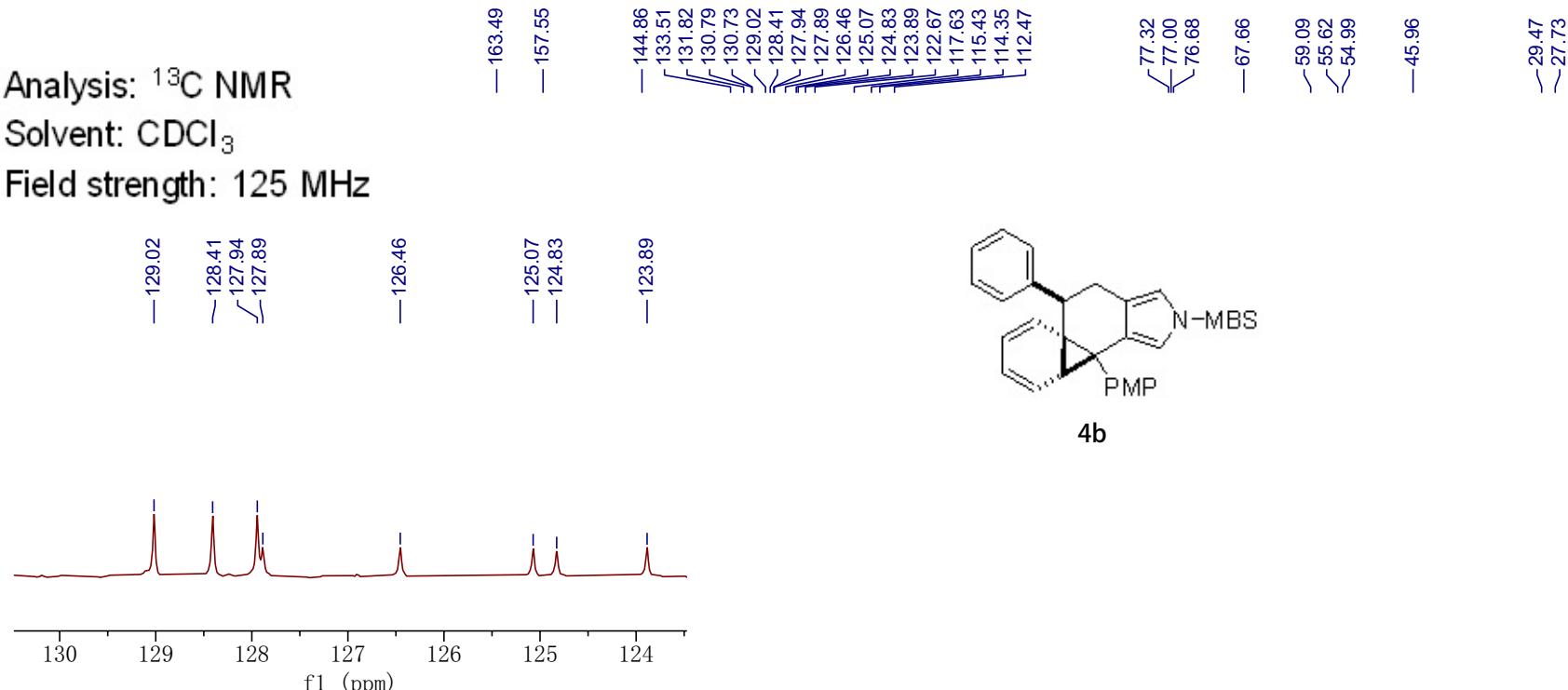
**4b**



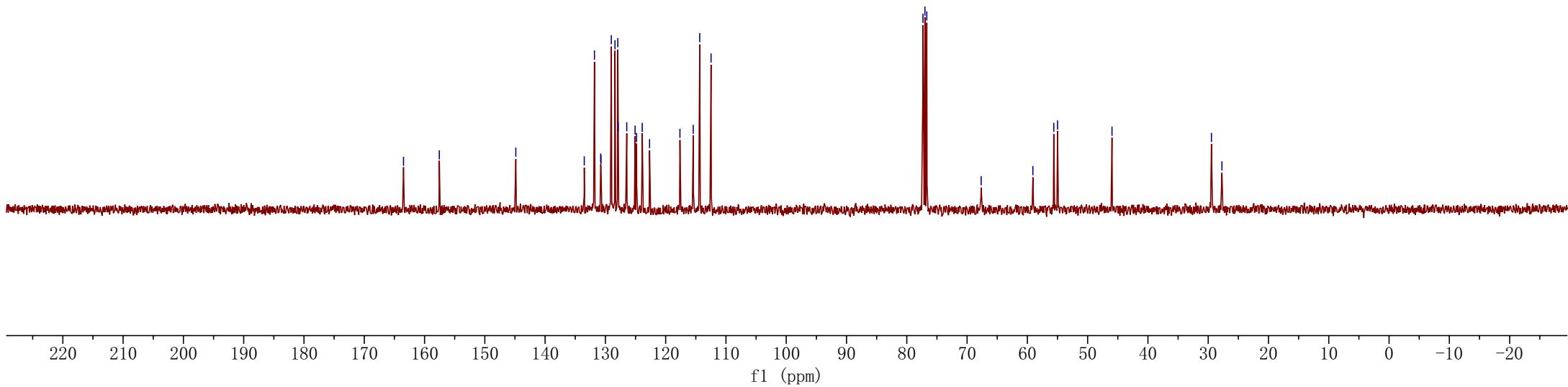
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



**4b**



7.602  
7.284  
7.267  
7.248  
7.214  
7.196  
7.178  
7.143  
7.126  
7.033  
7.011  
6.812  
6.713  
6.691  
6.345  
6.339  
6.245  
6.224  
6.207  
5.832  
5.818  
5.803  
5.687  
5.666  
5.652

3.770  
3.677  
3.664  
3.646  
3.633  
3.489  
3.472

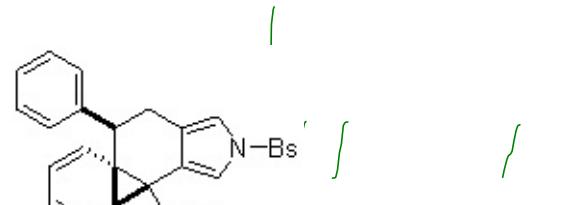
2.803  
2.790  
2.763  
2.751  
2.420  
2.389  
2.350

-0.000

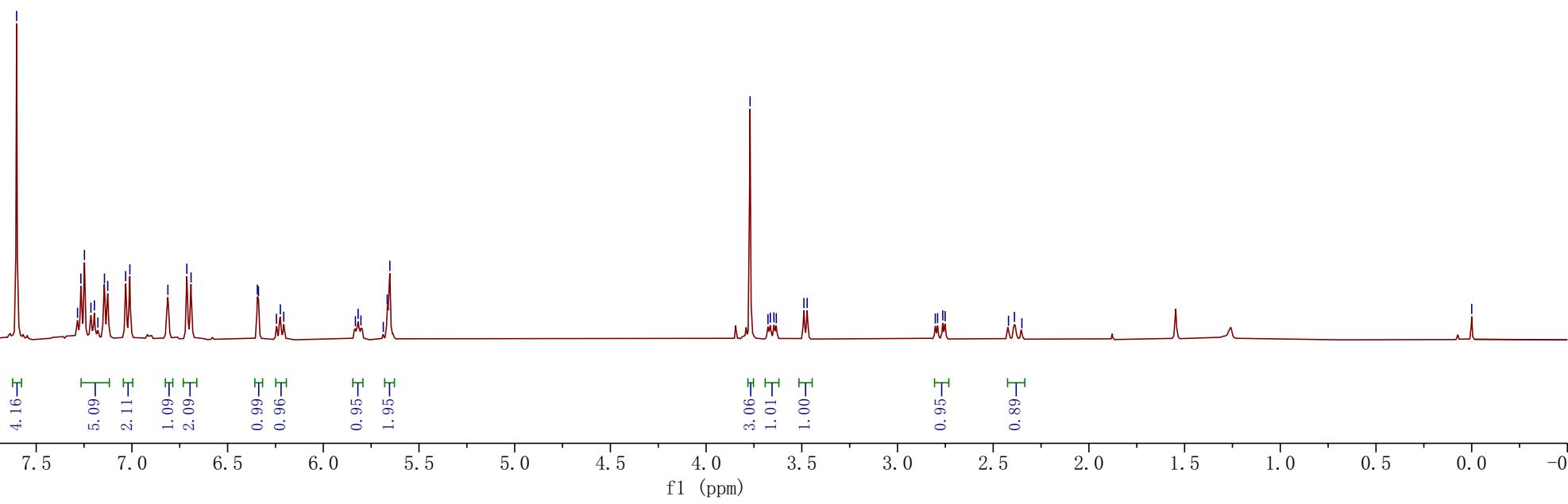
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



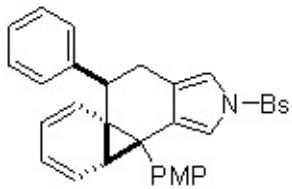
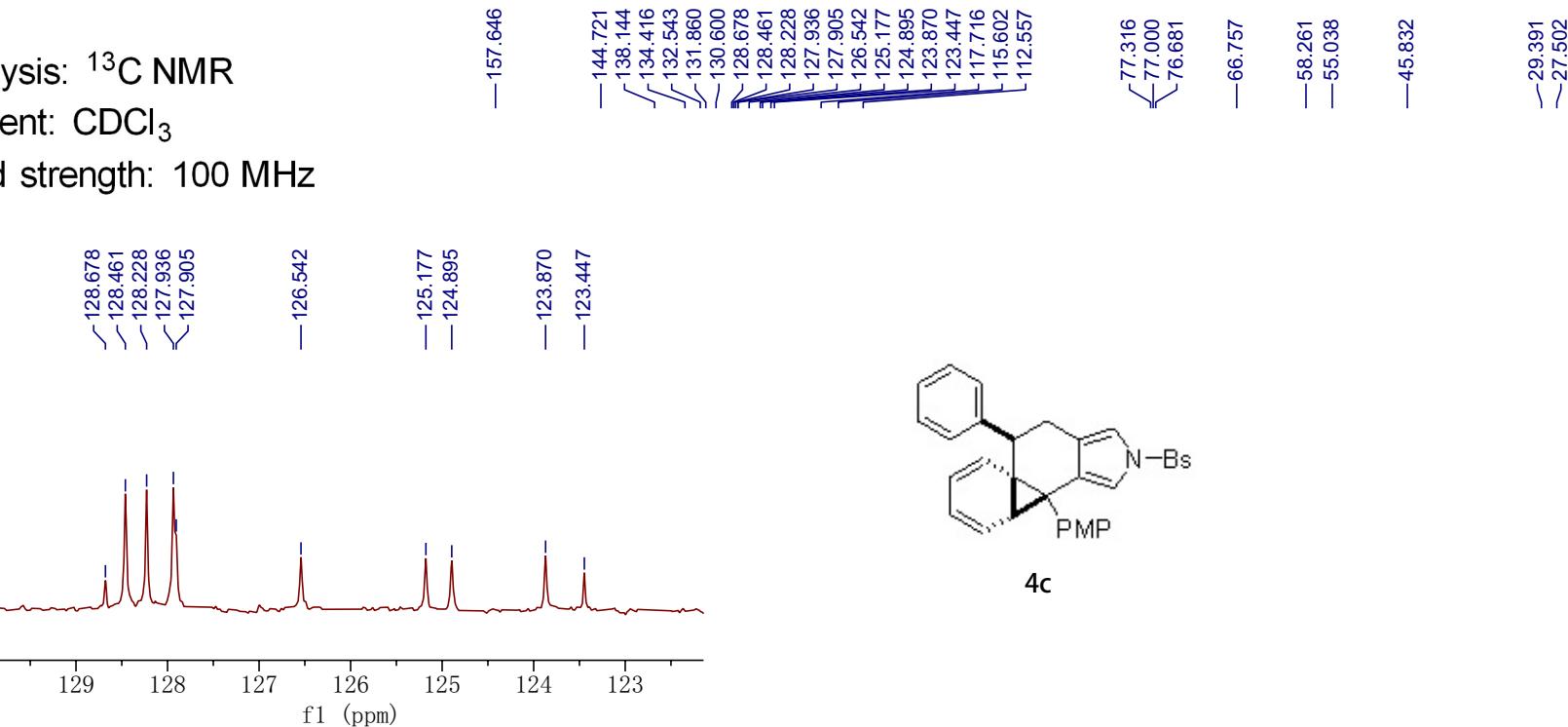
4c



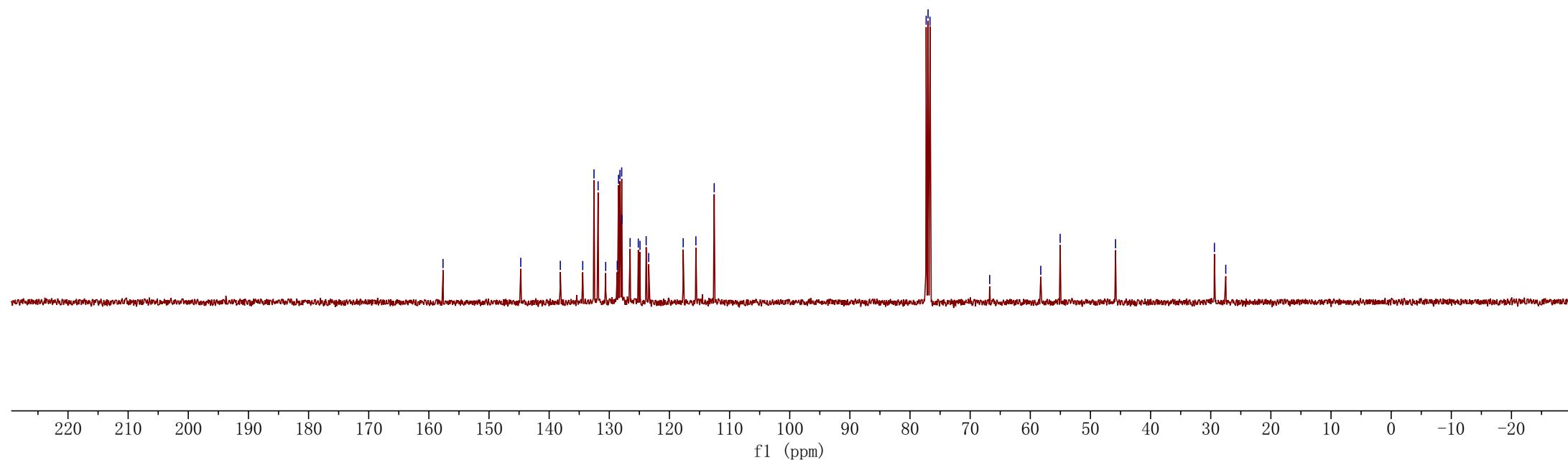
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



4c



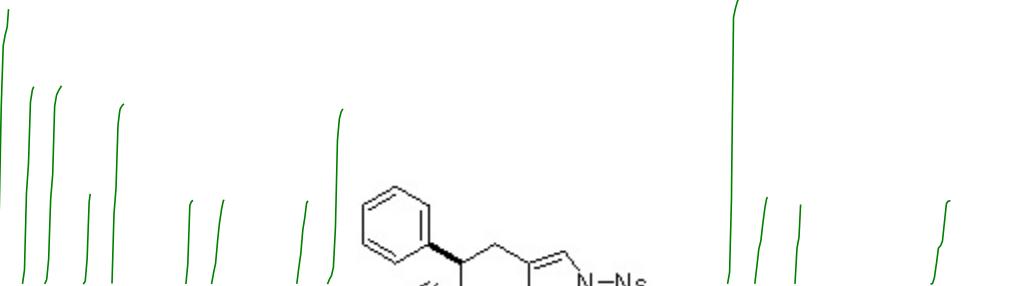
8.317  
8.312  
8.300  
8.295  
7.927  
7.922  
7.910  
7.905  
7.285  
7.268  
7.264  
7.257  
7.248  
7.217  
7.214  
7.199  
7.18  
7.136  
7.123  
7.118  
7.025  
7.020  
7.009  
7.003  
6.841  
6.721  
6.716  
6.705  
6.699  
6.365  
6.359  
6.244  
6.225  
6.206  
5.845  
5.840  
5.831  
5.825  
5.819  
5.809  
5.804  
5.693  
5.671  
5.661  
5.656  
5.638  
3.780  
3.665  
3.653  
3.635  
3.623  
3.473  
3.456  
2.815  
2.802  
2.775  
2.763  
2.434  
2.429  
2.403  
2.398  
2.395  
2.390  
2.364  
2.359

-0.000

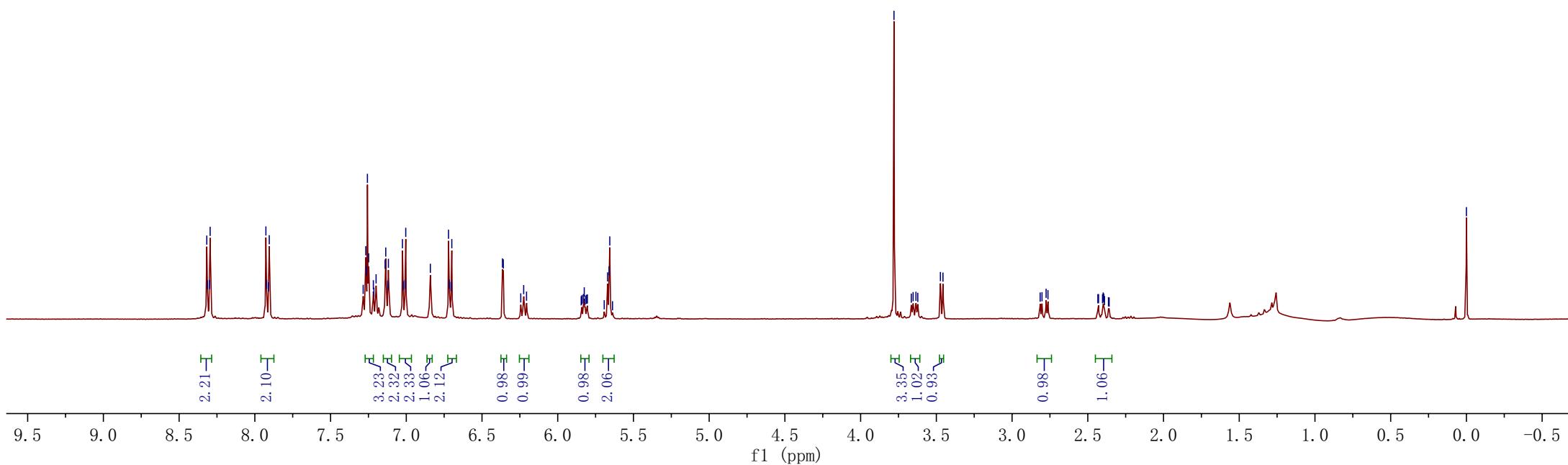
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



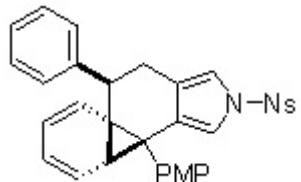
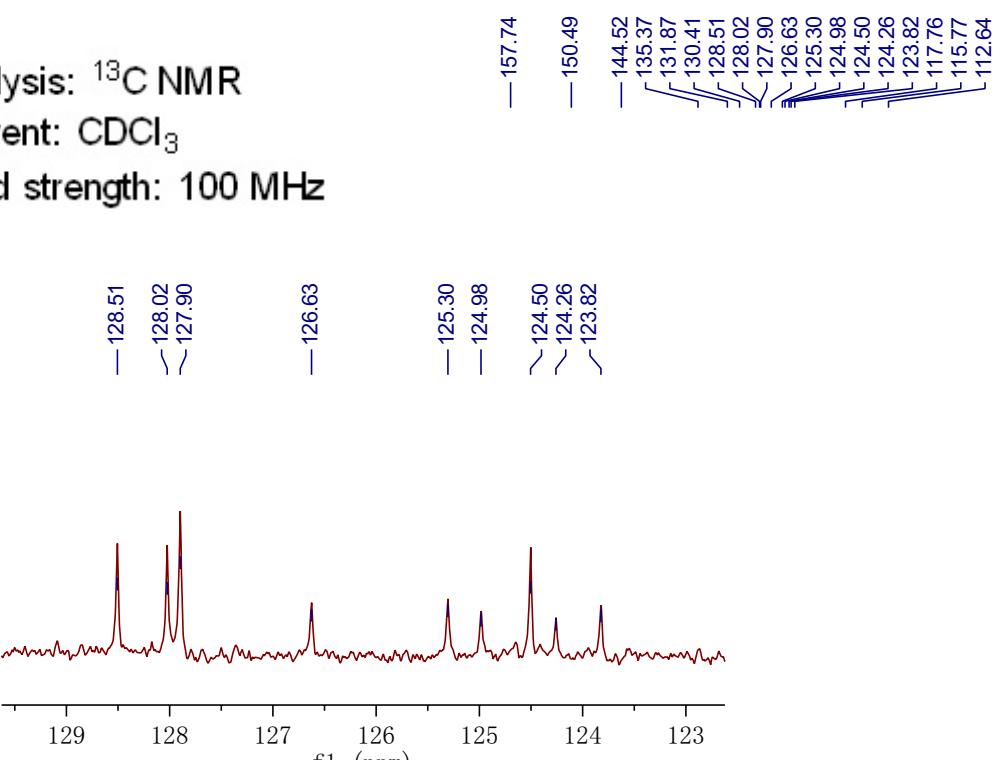
4d



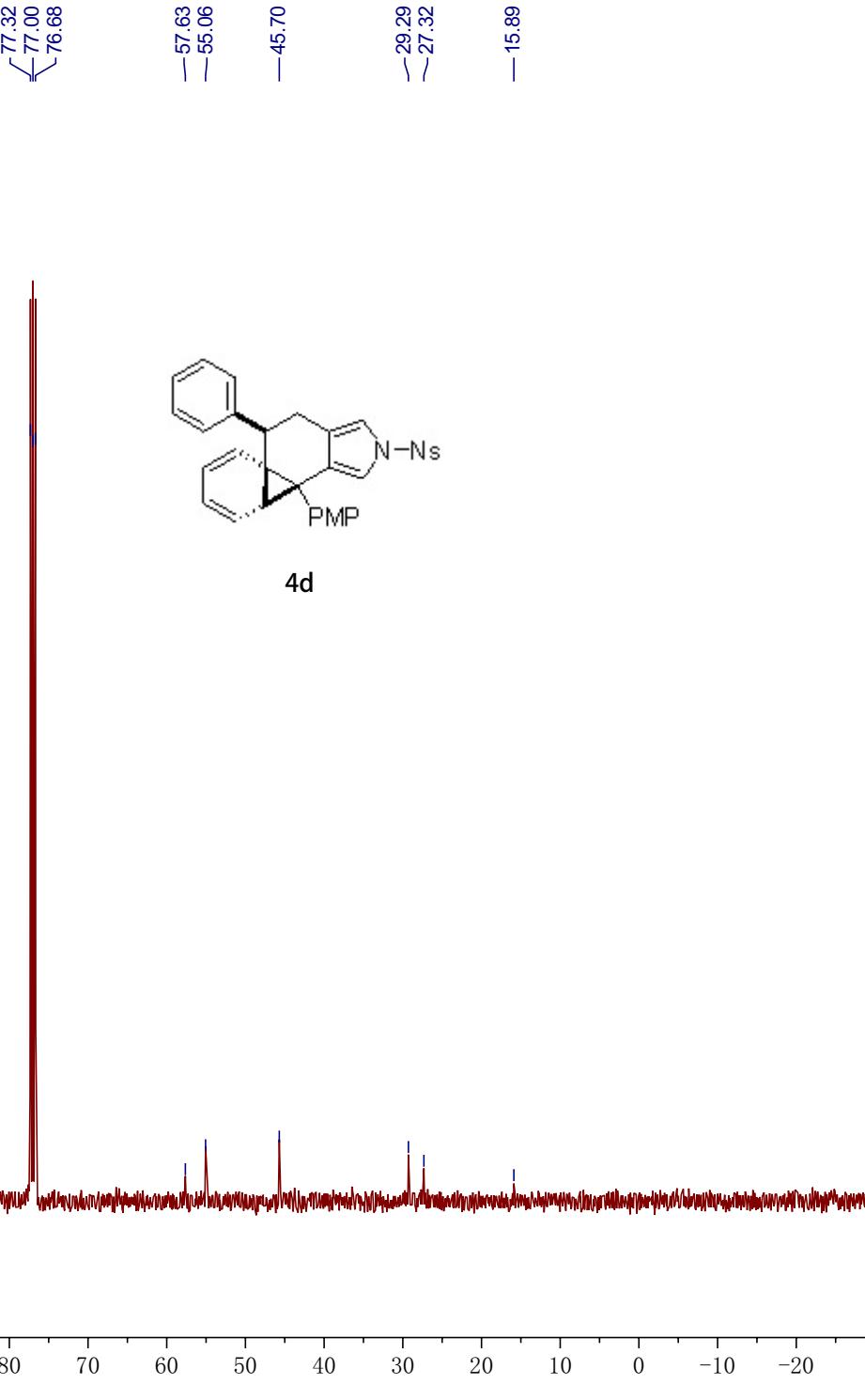
### Analysis: $^{13}\text{C}$ NMR

Solvent: CDCl<sub>3</sub>

Field strength: 100 MHz



4d



HJJ-02-94.1.A

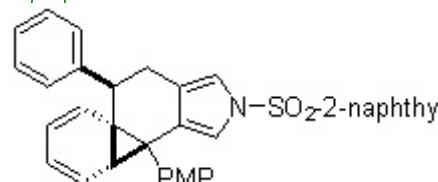
$$\begin{array}{r} 2.782 \\ 2.773 \\ 2.751 \\ 2.741 \\ \hline 2.397 \end{array}$$

600

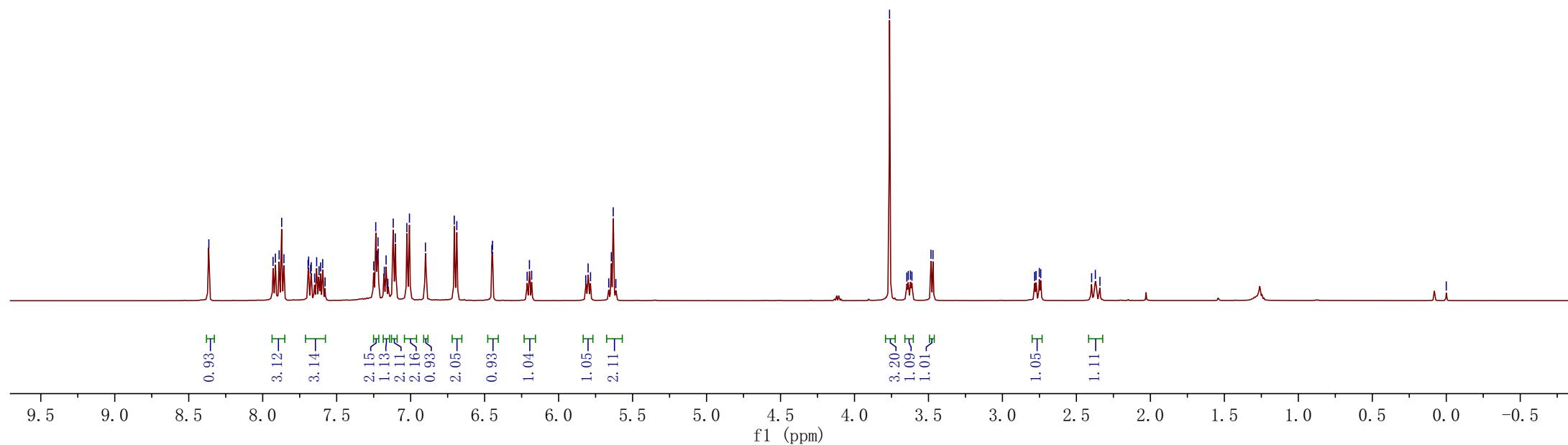
Analysis:  $^1\text{H}$  NMR

Solvent: CDCl<sub>3</sub>

Field strength: 500 MHz



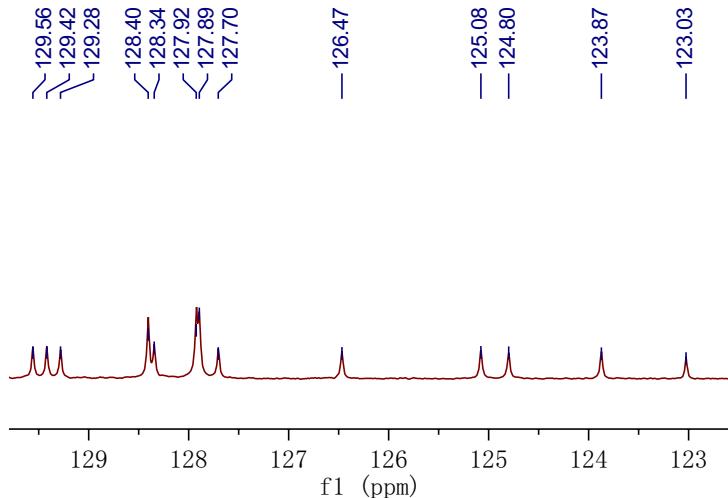
40



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.650  
7.630  
7.278  
7.261  
7.242  
7.206  
7.187  
7.140  
7.123  
7.018  
6.996  
6.822  
6.694  
6.672  
6.373  
6.368  
6.231  
6.211  
6.192  
5.826  
5.811  
5.790  
5.680  
5.658  
5.643  
5.624

4.009  
3.991  
3.974  
3.956  
3.670  
3.658  
3.639  
3.627  
3.507  
3.490

2.793  
2.781  
2.754  
2.742  
2.414  
2.402  
2.387  
2.380  
2.348  
2.344

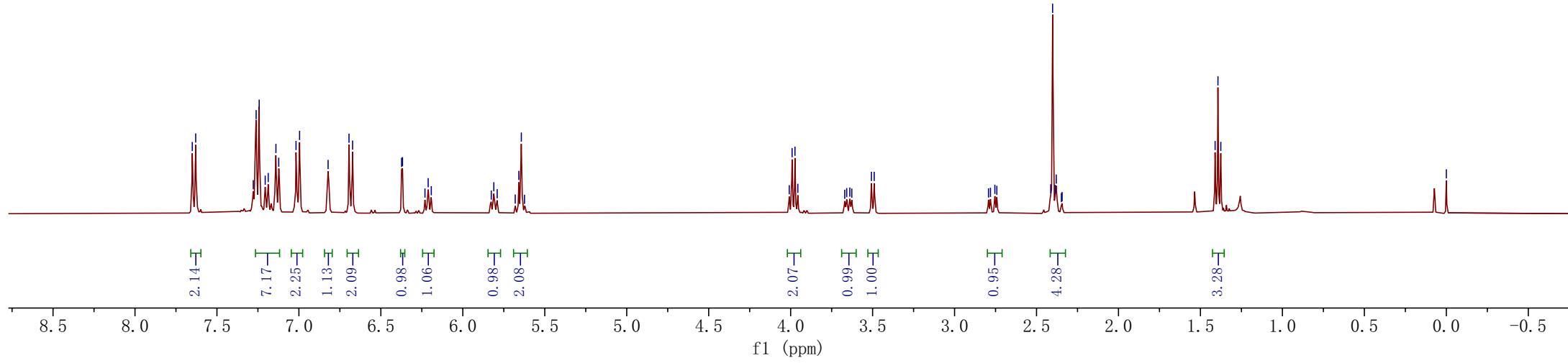
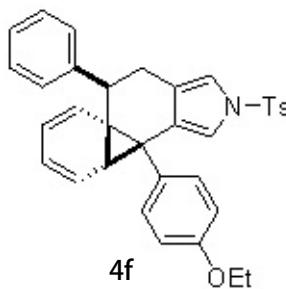
1.411  
1.393  
1.376

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

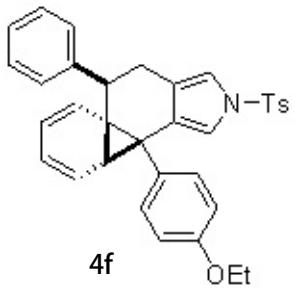
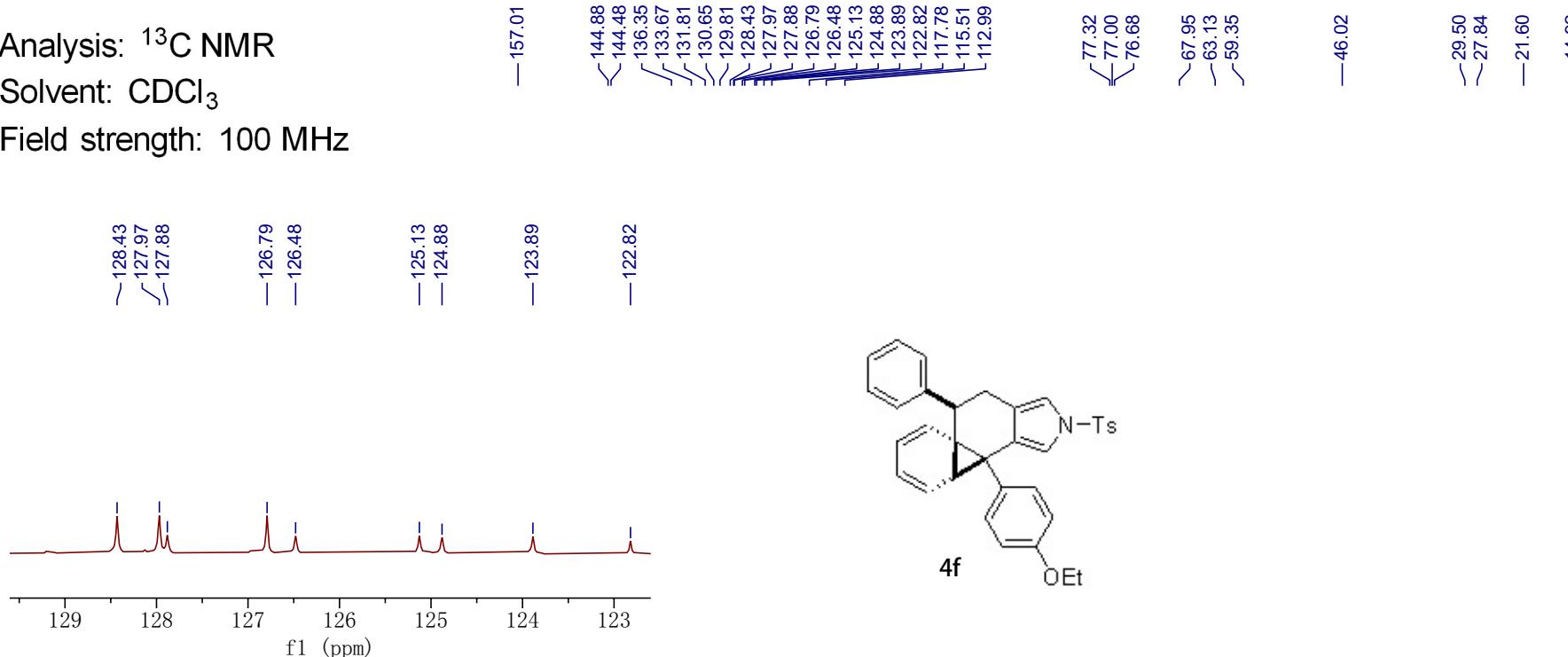
Field strength: 400 MHz



## Analysis: $^{13}\text{C}$ NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.651  
7.630  
7.446  
7.429  
7.400  
7.238  
7.363  
7.336  
7.318  
7.259  
7.207  
7.141  
7.124  
7.042  
7.020  
6.825  
6.790  
6.768  
6.384  
6.378  
6.239  
6.220  
6.202  
5.842  
5.826  
5.805  
5.694  
5.672  
5.656  
5.631

-4.998

3.674  
3.662  
3.643  
3.631  
3.525  
3.508

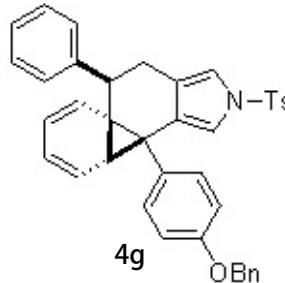
2.796  
2.784  
2.757  
2.745  
2.416  
2.398  
2.375  
2.347

-0.000

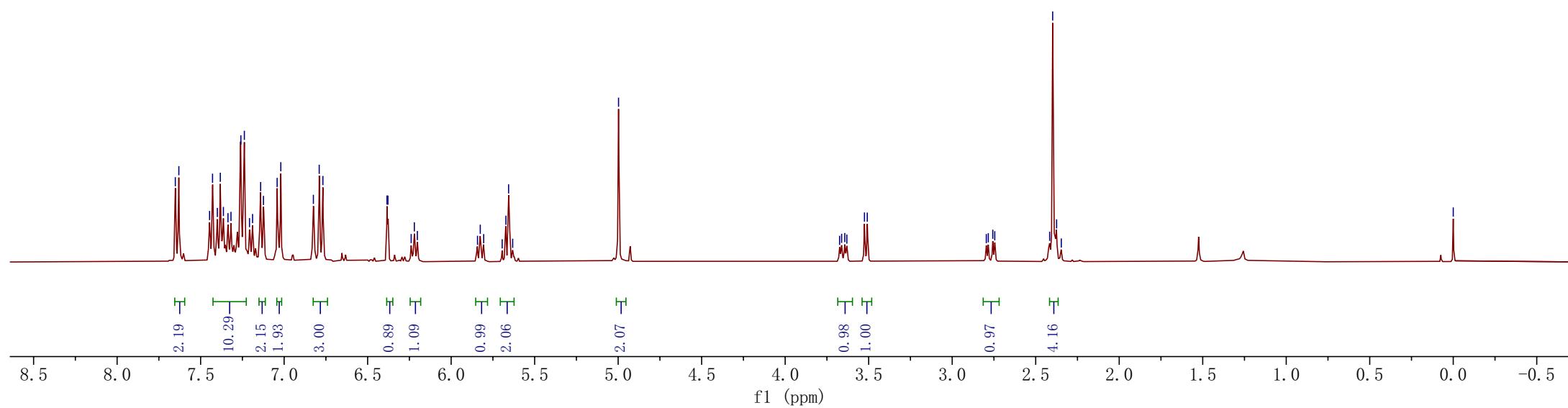
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



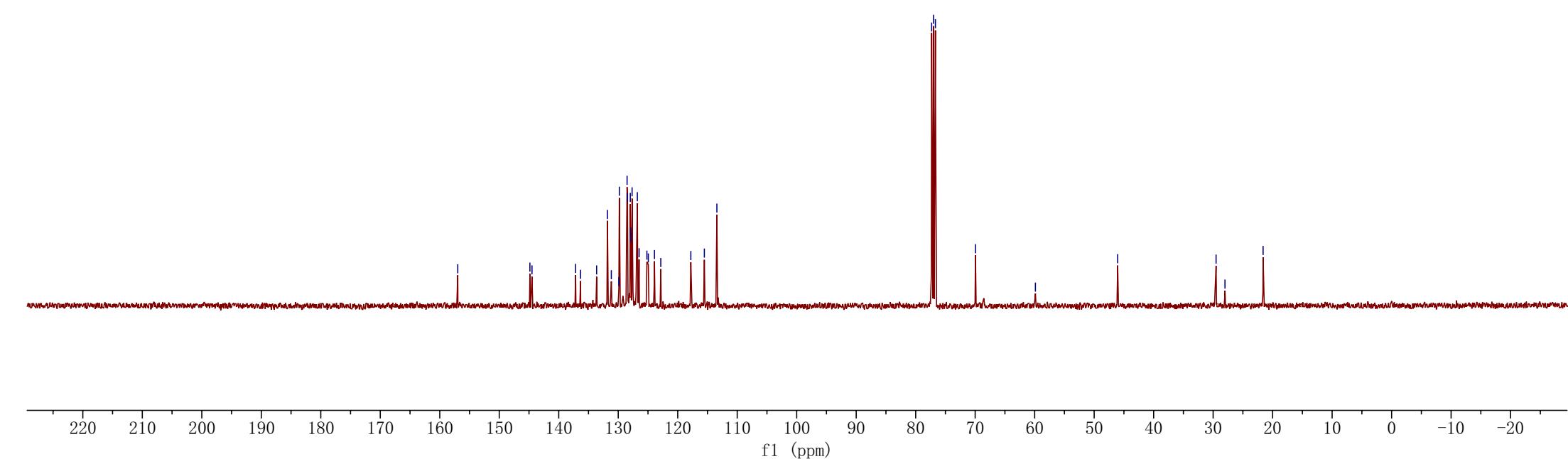
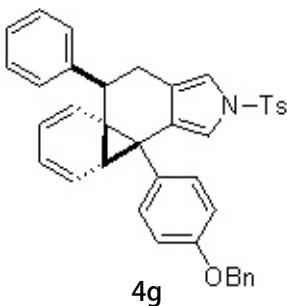
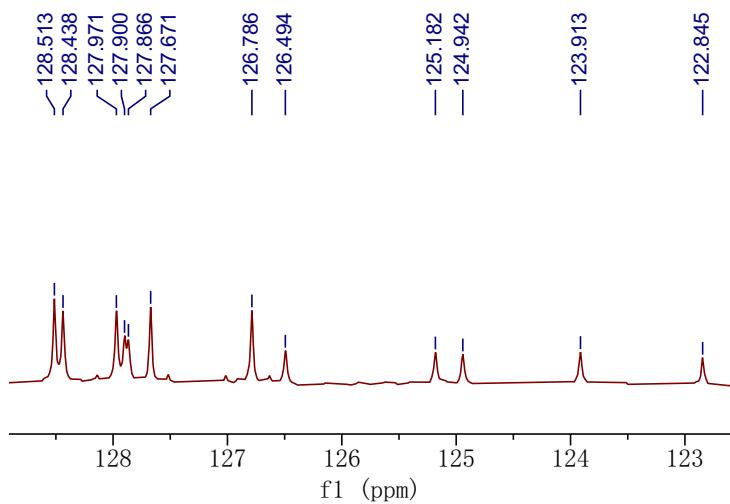
4g



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



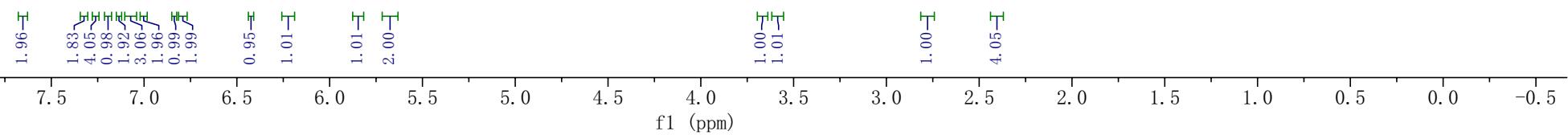
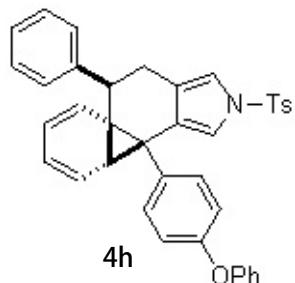
7.670  
7.653  
7.345  
7.340  
7.330  
7.317  
7.313  
7.277  
7.266  
7.260  
7.251  
7.247  
7.211  
7.197  
7.192  
7.182  
7.140  
7.127  
7.101  
7.086  
7.075  
7.071  
7.058  
7.008  
6.993  
6.842  
6.801  
6.784  
6.427  
6.423  
6.242  
6.226  
6.211  
5.865  
5.850  
5.834  
5.714  
5.697  
5.683  
5.664  
5.647  
3.687  
3.677  
3.662  
3.652  
3.581  
3.568  
2.809  
2.799  
2.778  
2.768  
2.431  
2.428  
2.408  
2.376  
2.372

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

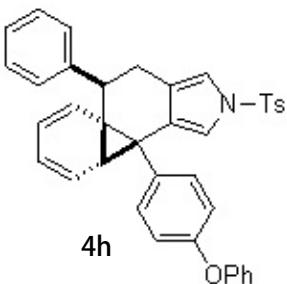
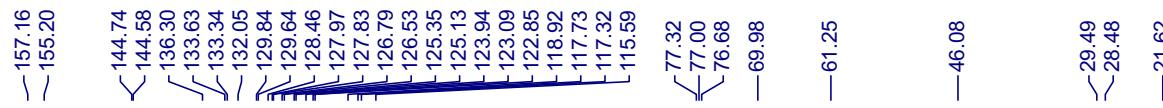
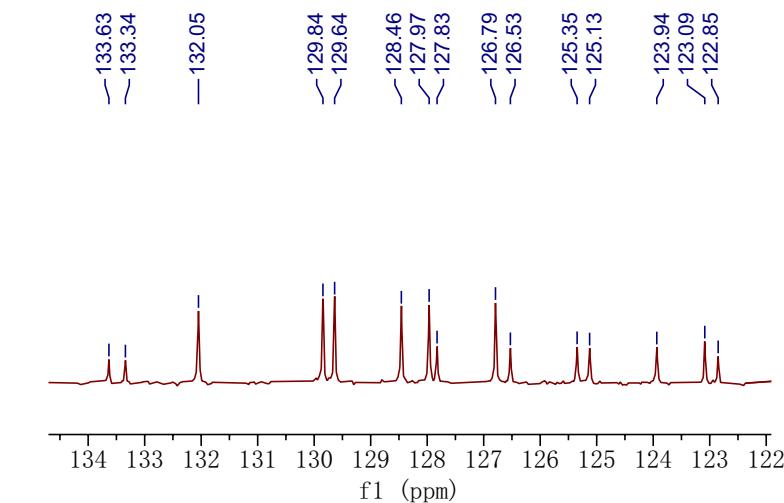
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz

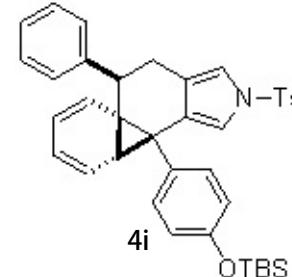


7.645  
7.624  
7.279  
7.262  
7.248  
7.243  
7.207  
7.189  
7.171  
7.139  
7.122  
6.959  
6.938  
6.825  
6.633  
6.611  
6.376  
6.370  
6.221  
6.201  
6.182  
5.815  
5.799  
5.779  
5.666  
5.644  
5.628  
5.608

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

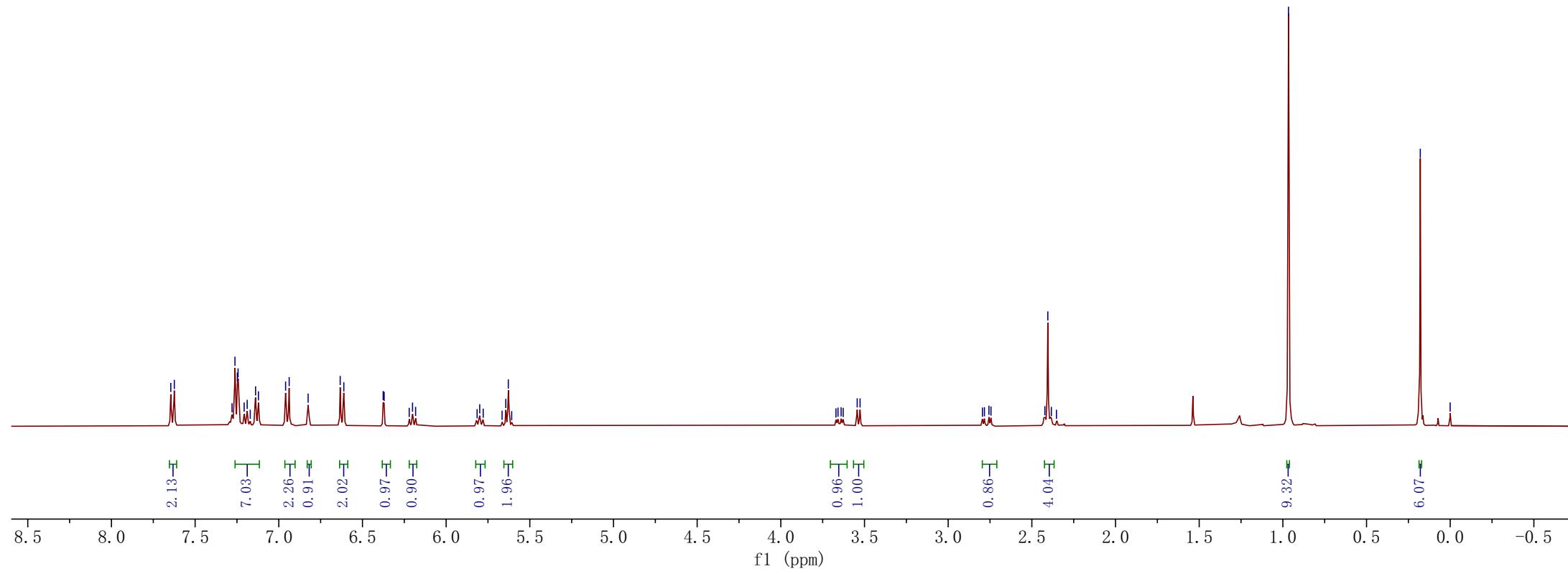
Field strength: 400 MHz



3.671  
3.658  
3.640  
3.627  
3.544  
3.527

2.795  
2.783  
2.756  
2.744  
2.422  
2.405  
2.383  
2.353

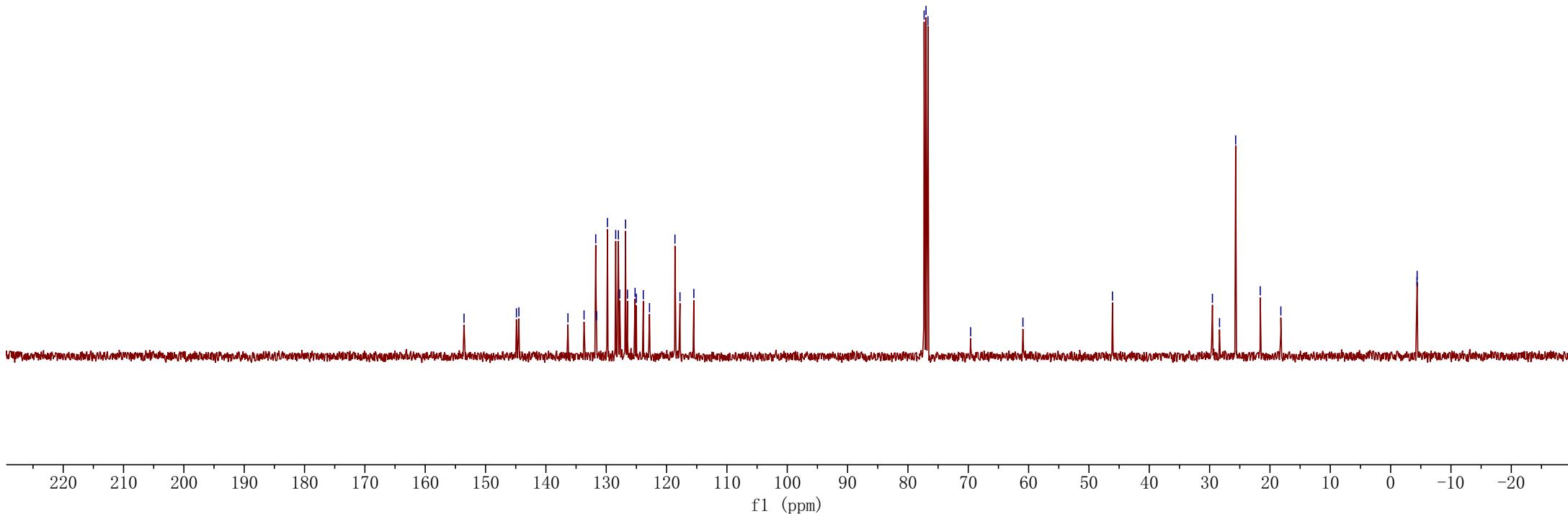
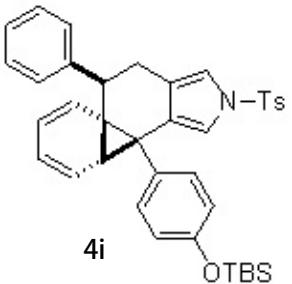
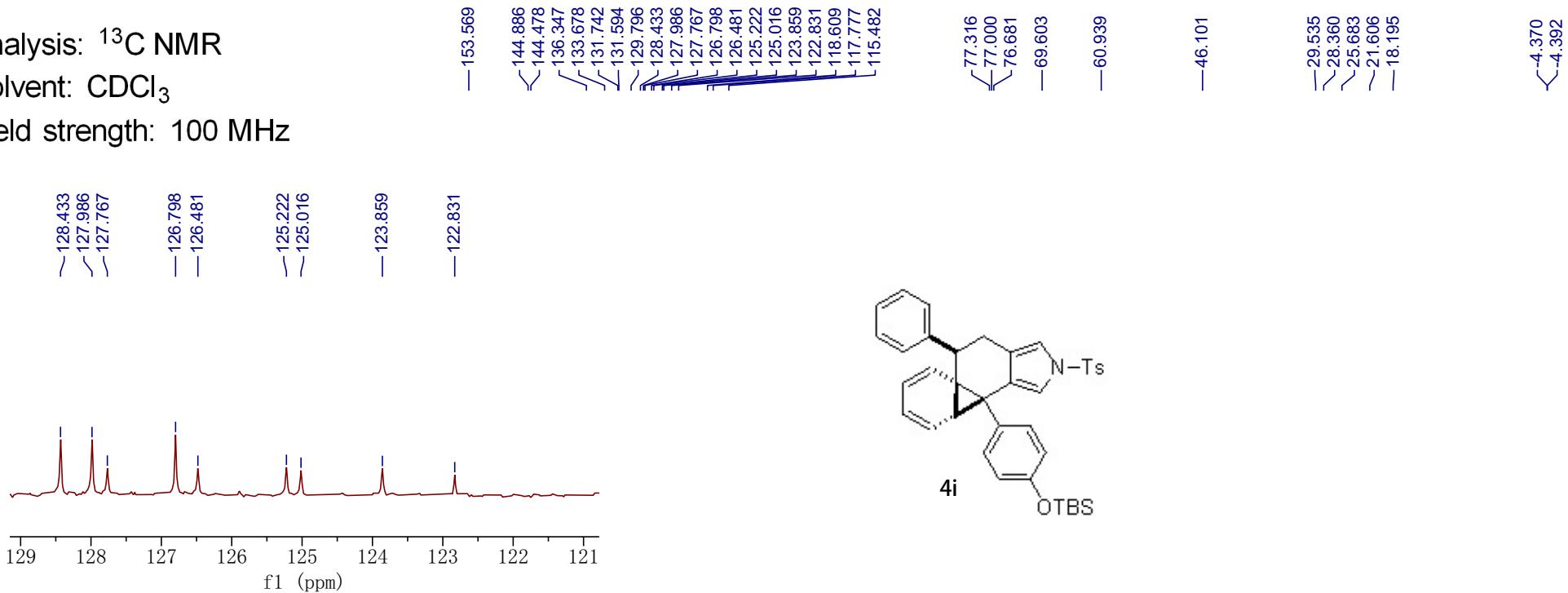
-0.966  
-0.179  
-0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

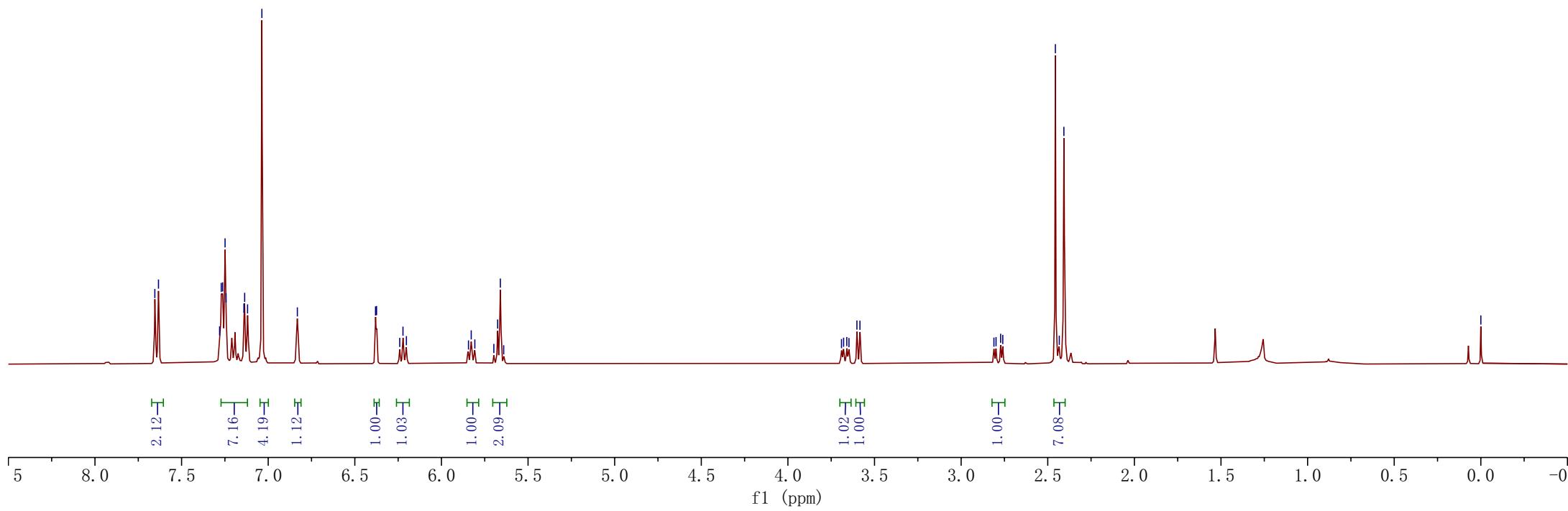
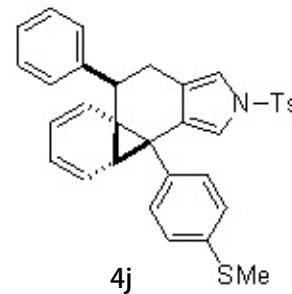




Analysis: <sup>1</sup>H NMR

Solvent: CDCl<sub>3</sub>

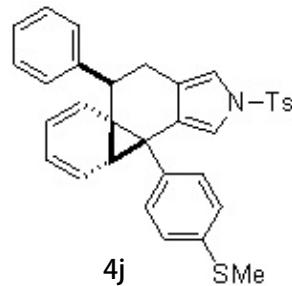
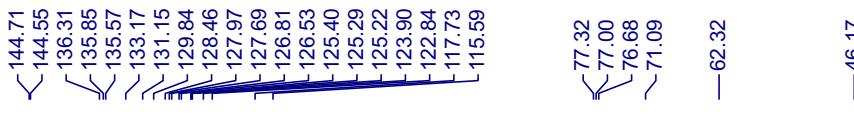
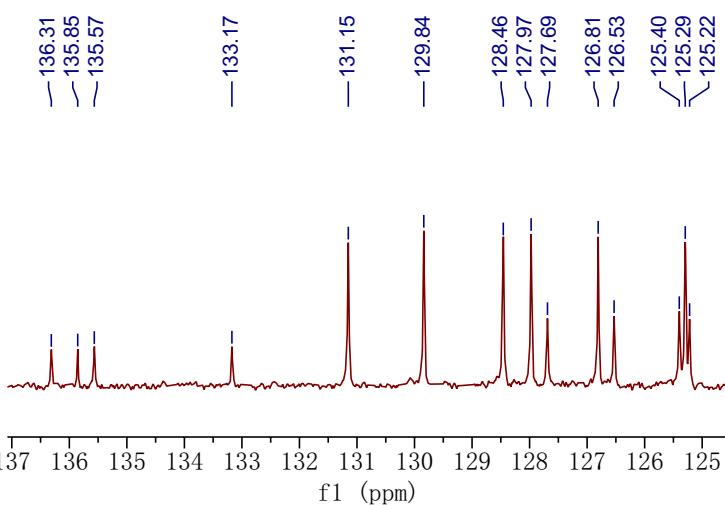
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

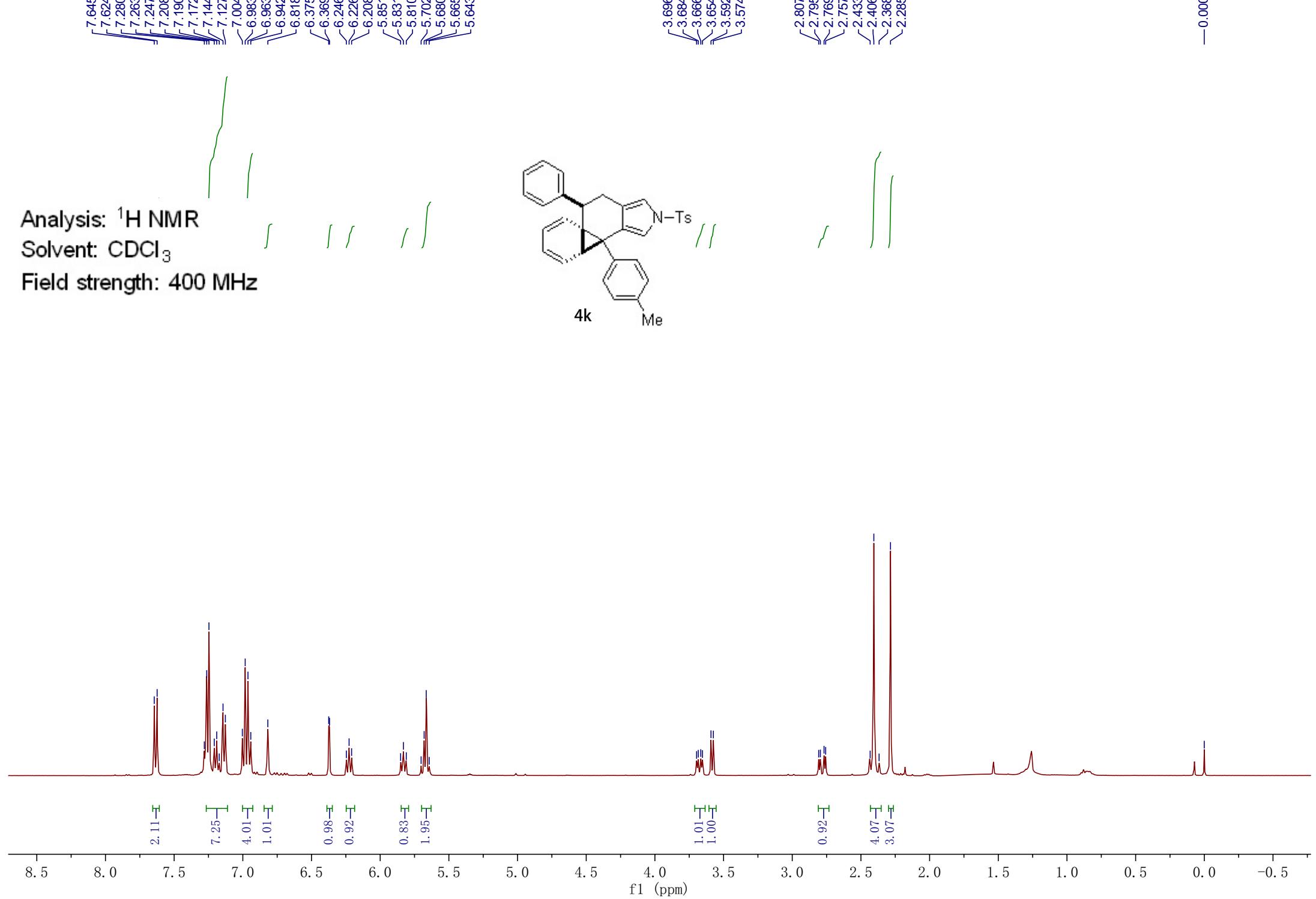




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

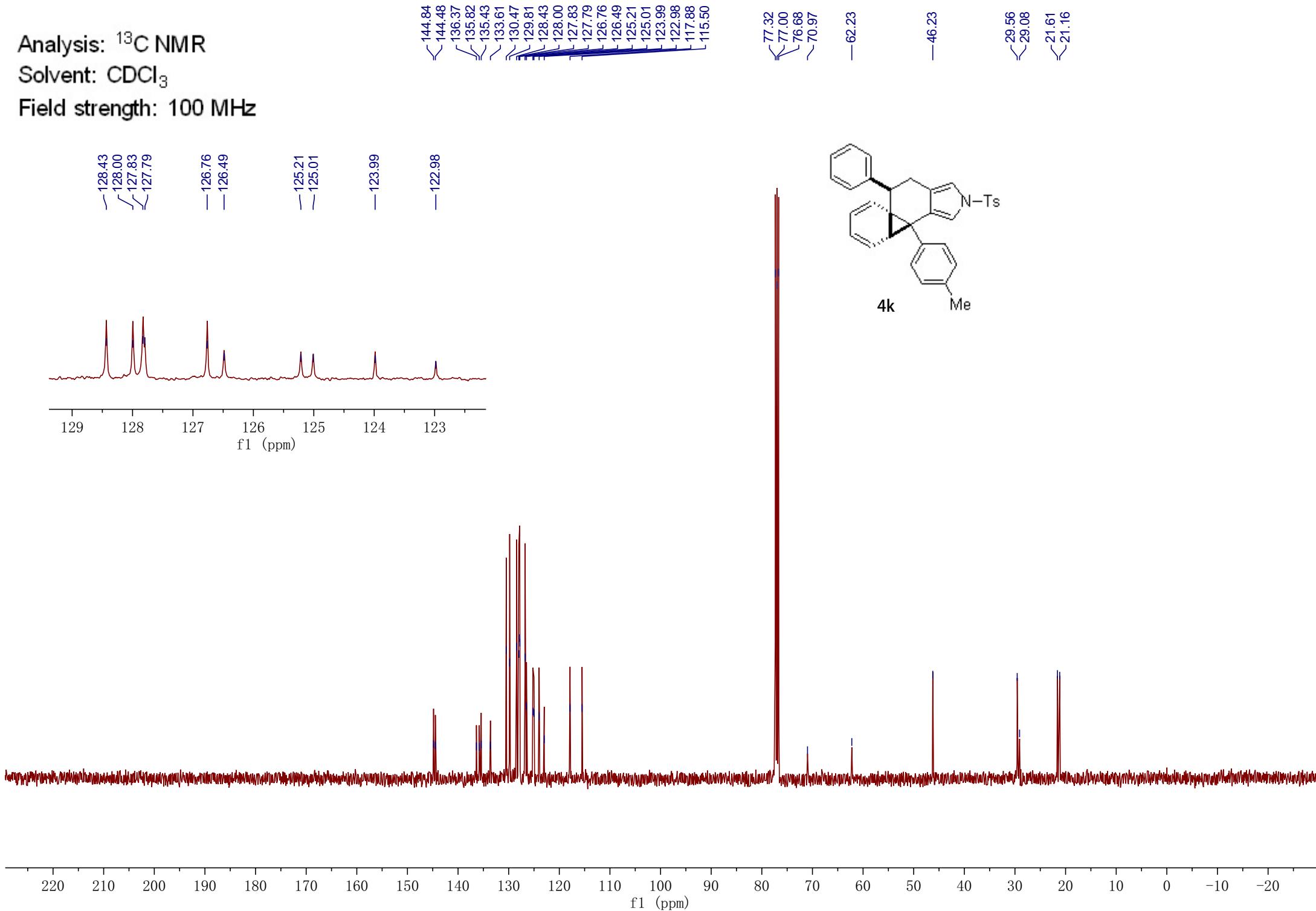
Field strength: 400 MHz



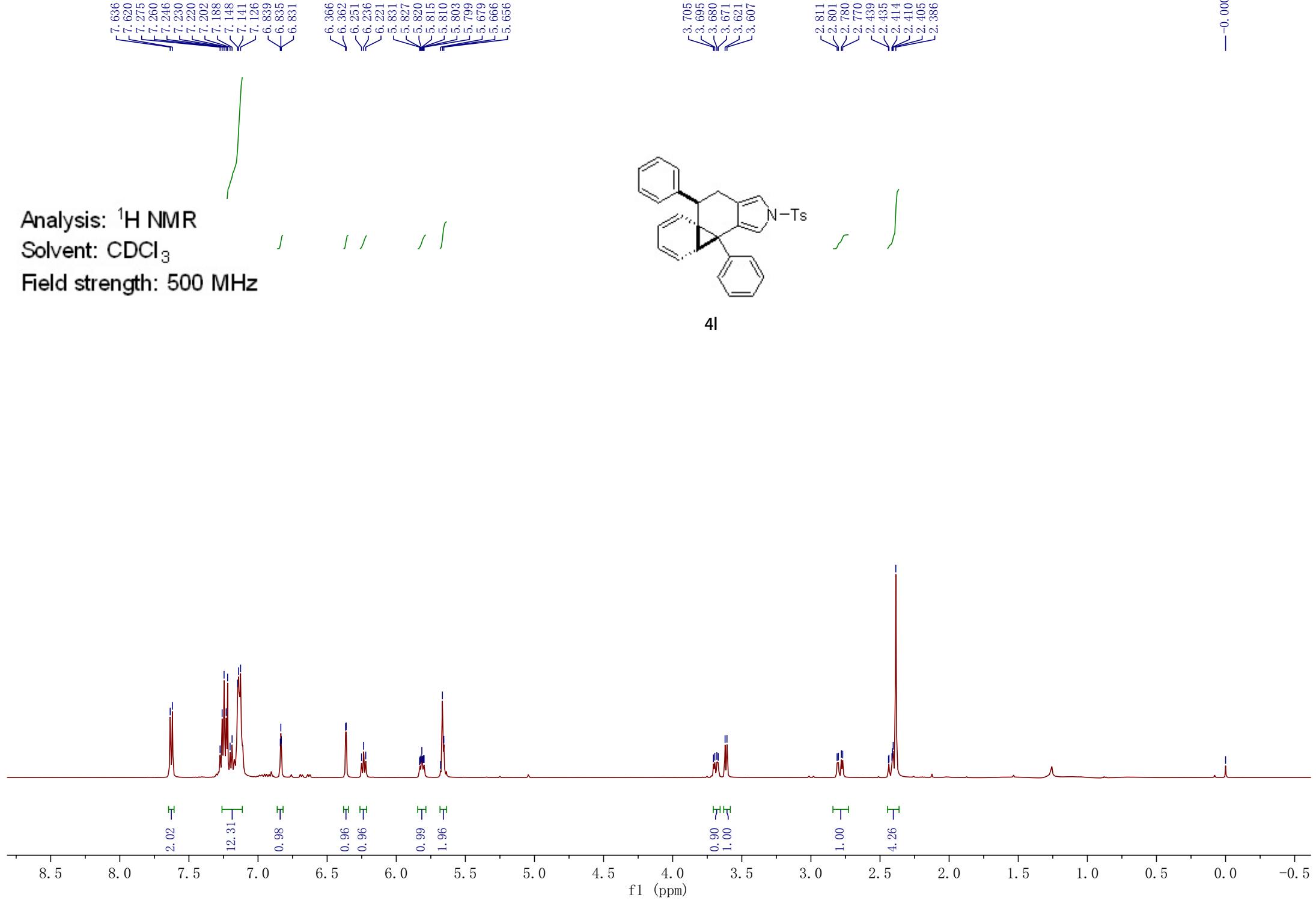
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



-0.000



Analysis:  $^{13}\text{C}$  NMR

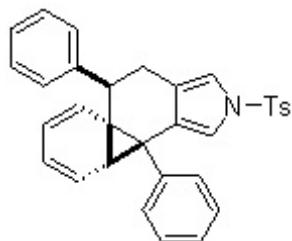
Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

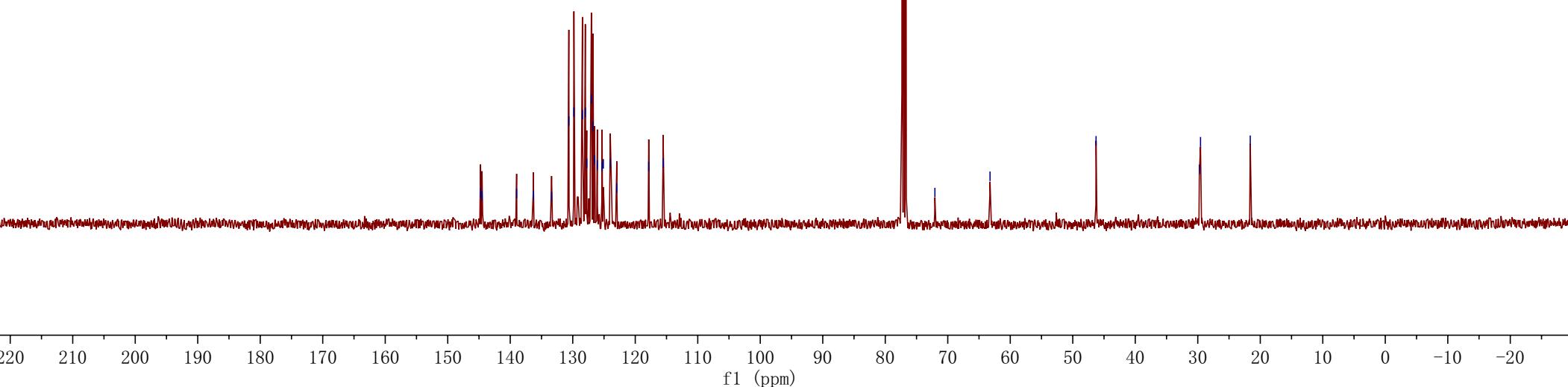
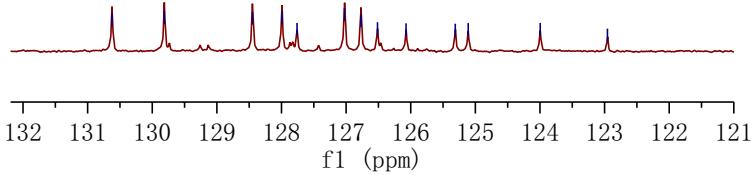
—130.62  
—129.81  
—128.45  
—127.99  
—127.76  
✓ 127.02  
✓ 126.77  
—126.51  
—126.07  
—125.31  
—125.11

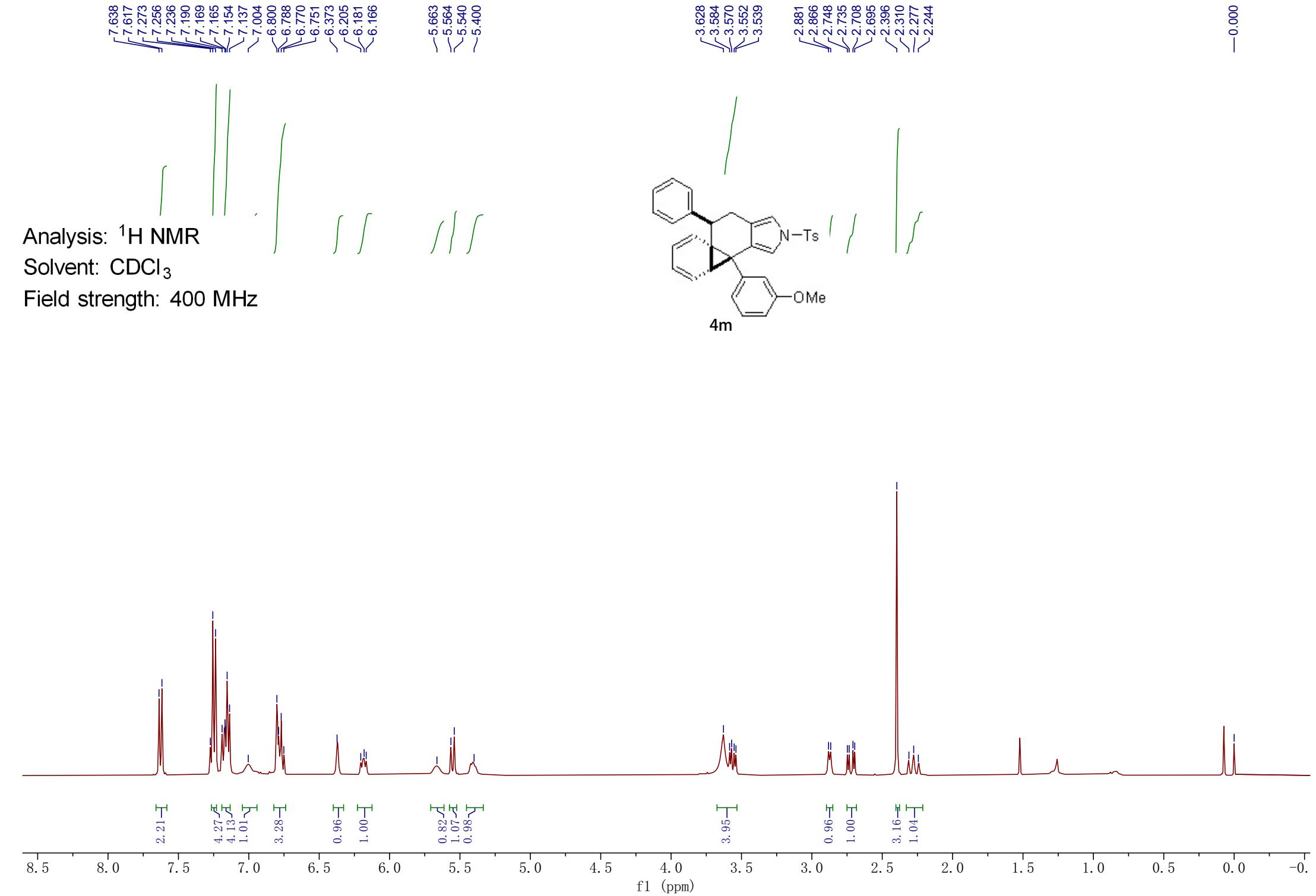
—124.00  
—122.96  
—144.75  
—144.52  
—138.98  
—136.31  
—133.39  
—130.62  
—129.81  
—128.45  
—127.99  
—127.76  
—127.02  
—126.77  
—126.51  
—126.07  
—125.31  
—125.11  
—117.84  
—115.54

—63.24  
—46.28  
—29.75  
✓ 29.56  
—21.60



4l

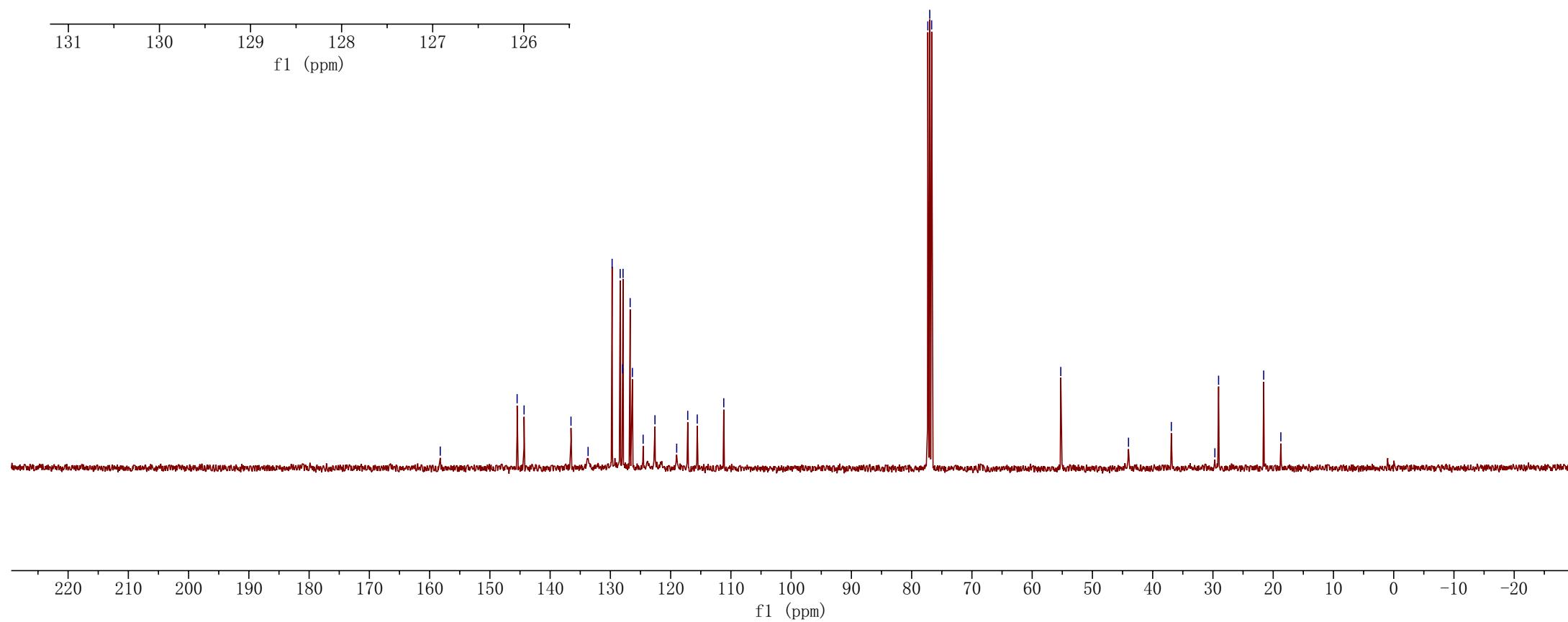
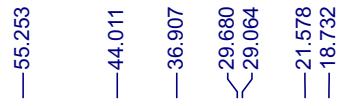
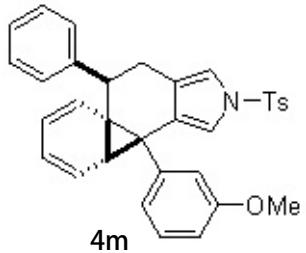
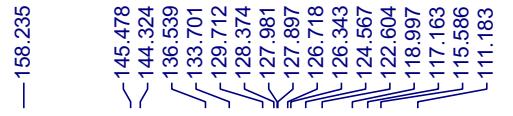
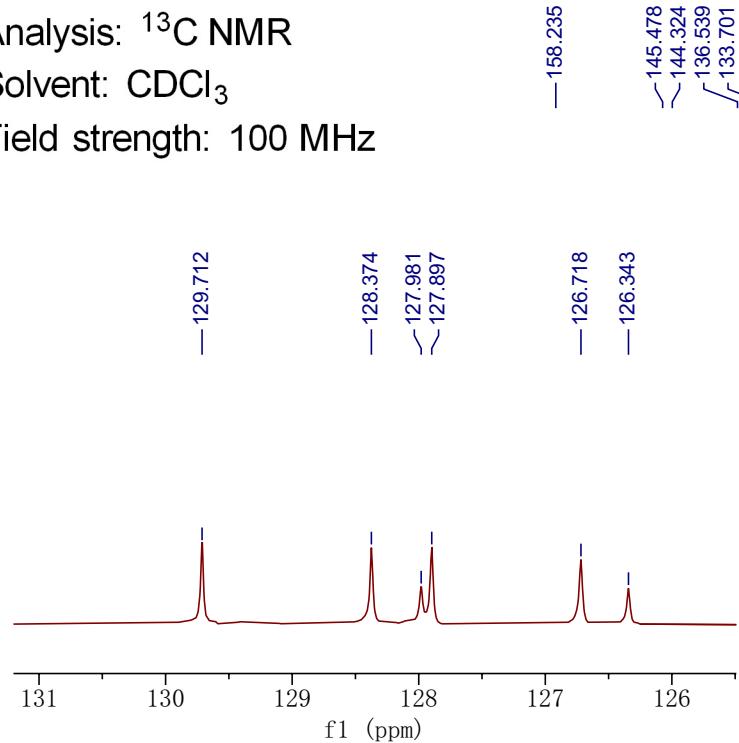


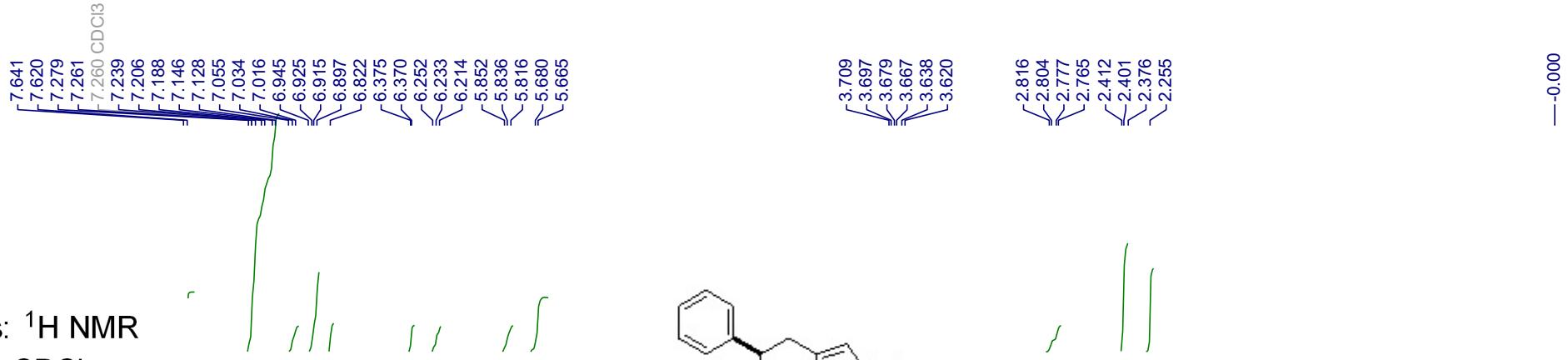


Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

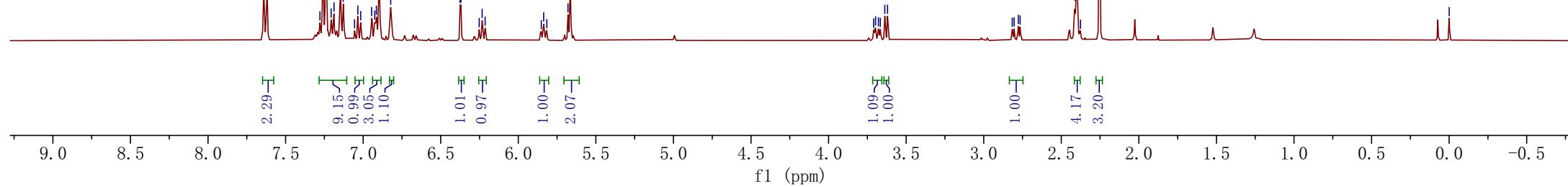
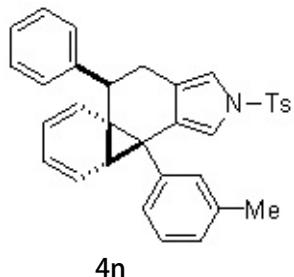




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

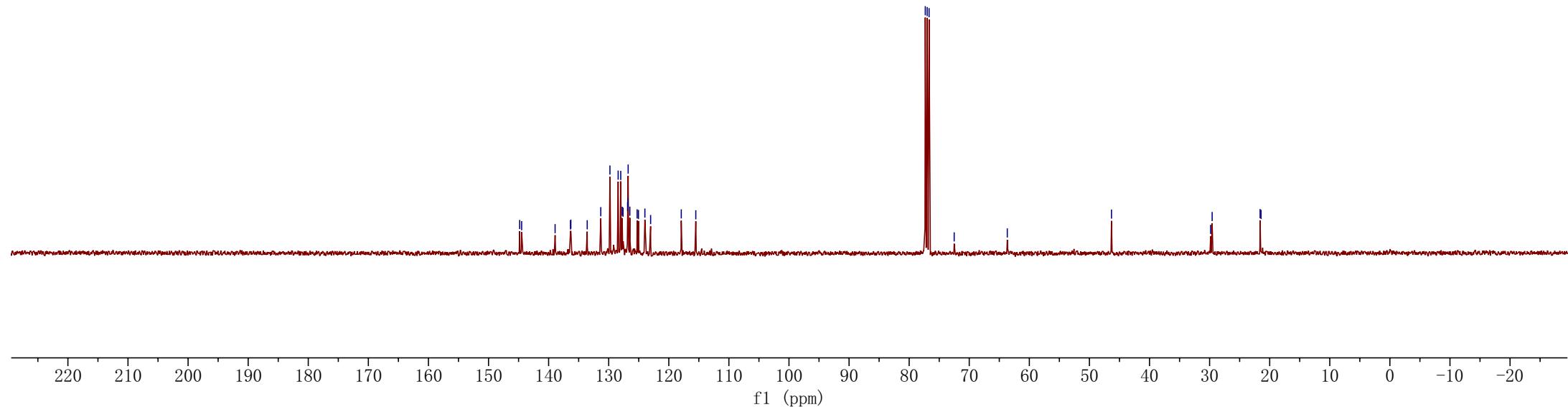
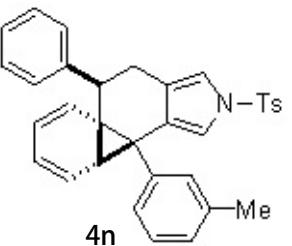
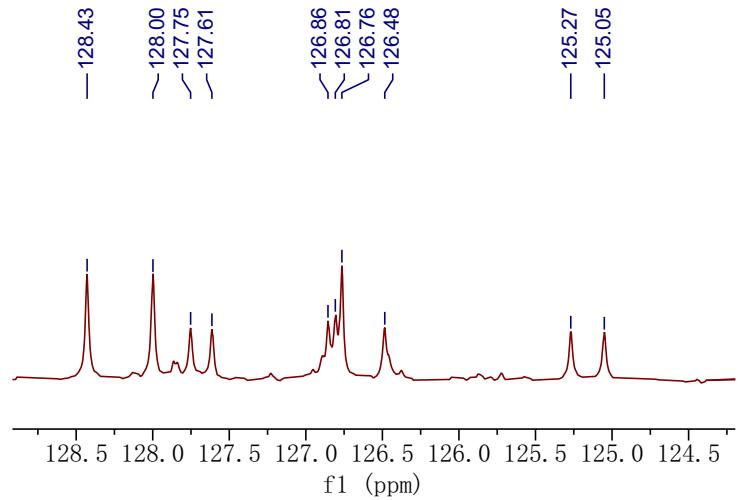
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

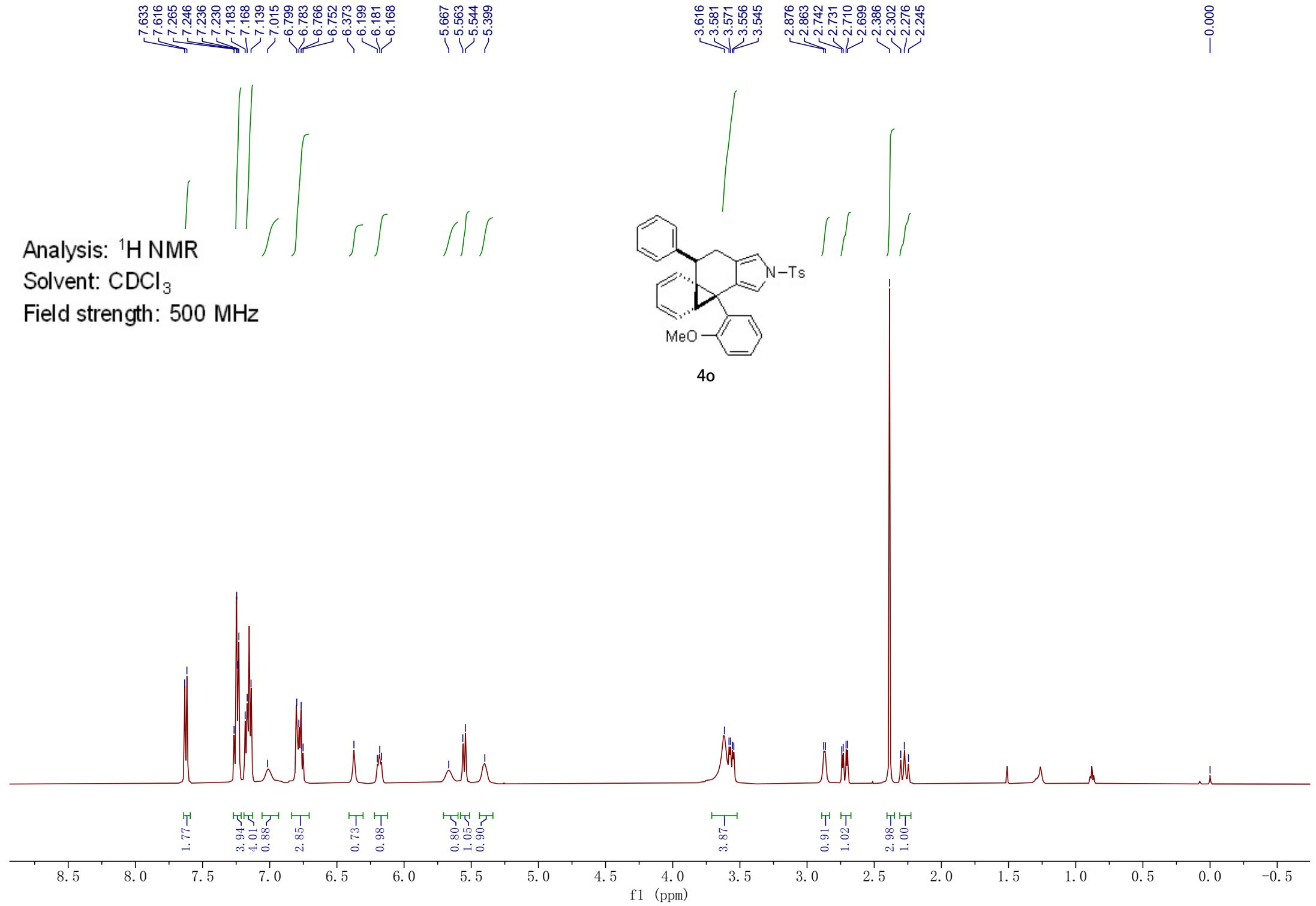
Field strength: 100 MHz



Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

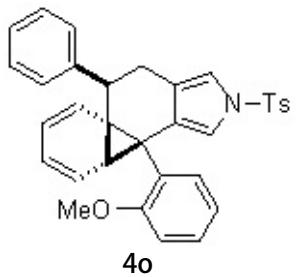
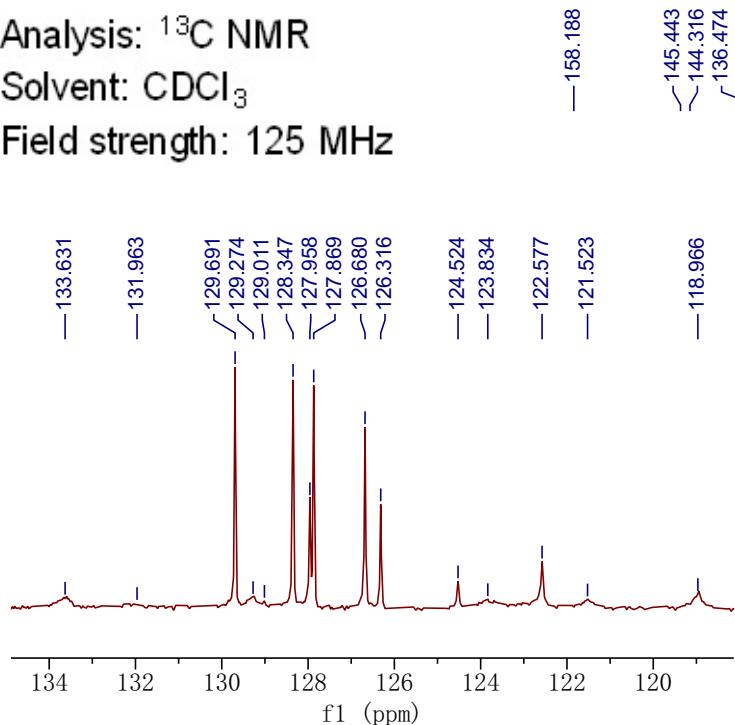
Field strength: 500 MHz



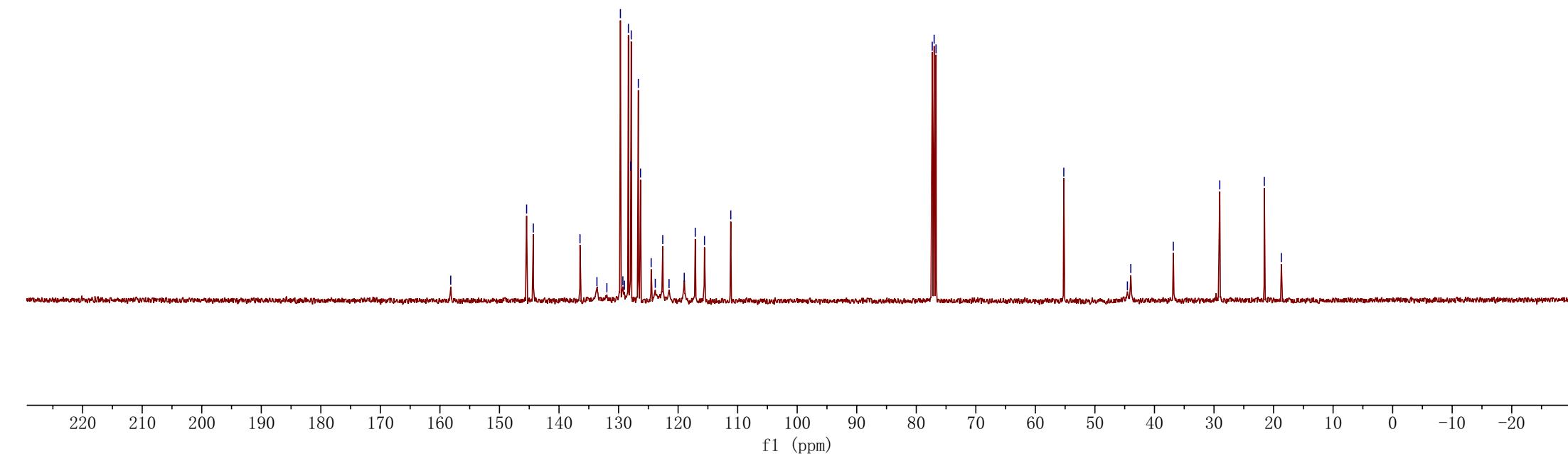
Analysis:  $^{13}\text{C}$  NMR

Solvent: CDCl<sub>3</sub>

Field strength: 125 MHz



40

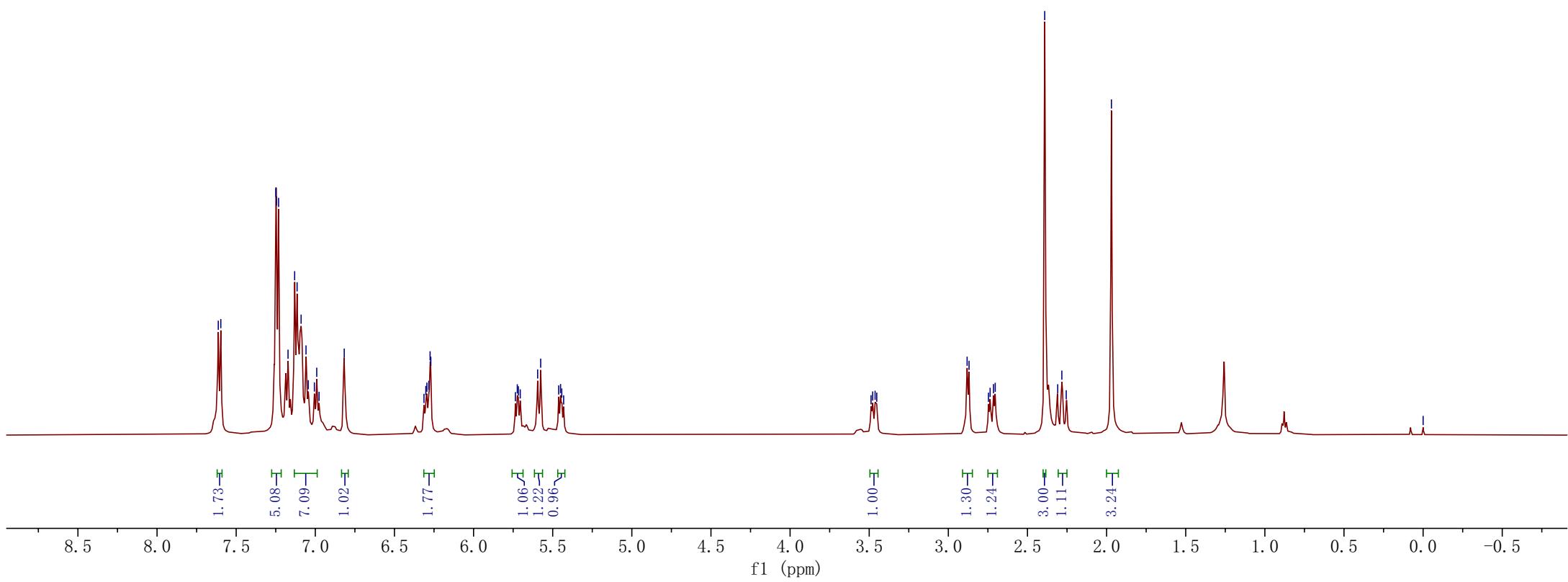
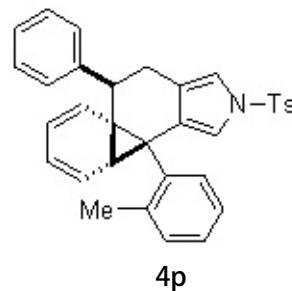




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

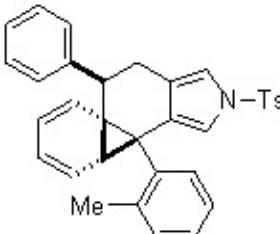
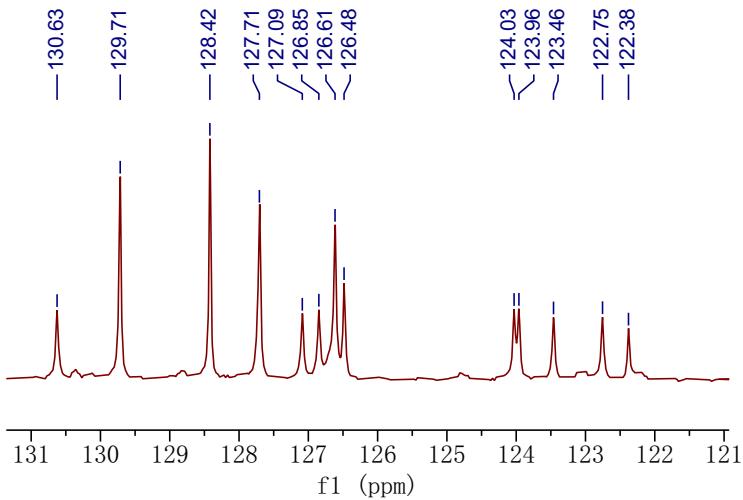
Field strength: 500 MHz



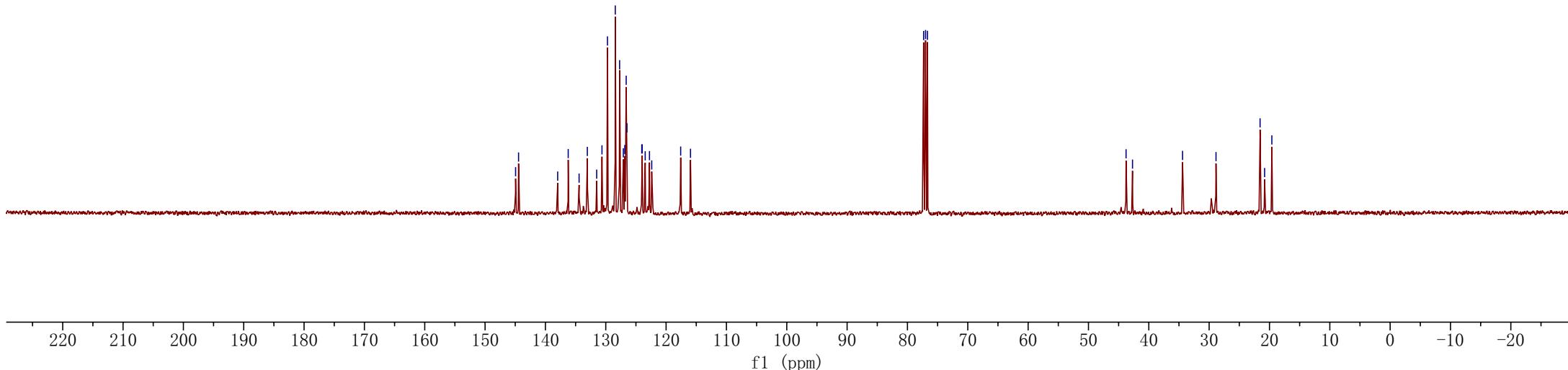
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



4p



7.648  
7.644  
7.631  
7.272  
7.257  
7.241  
7.236  
7.198  
7.184  
7.145  
7.142  
7.129  
6.902  
6.897  
6.885  
6.881  
6.833  
6.828  
6.820  
6.816  
6.611  
6.594  
6.383  
6.379  
6.231  
6.215  
6.200  
5.838  
5.824  
5.808  
5.686  
5.669  
5.655  
5.649  
5.631

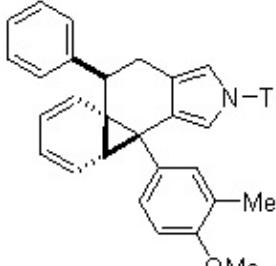
3.775  
3.678  
3.668  
3.653  
3.644  
3.509  
3.495  
2.789  
2.779  
2.758  
2.748  
2.422  
2.408  
2.397  
2.383  
2.121

-0.000

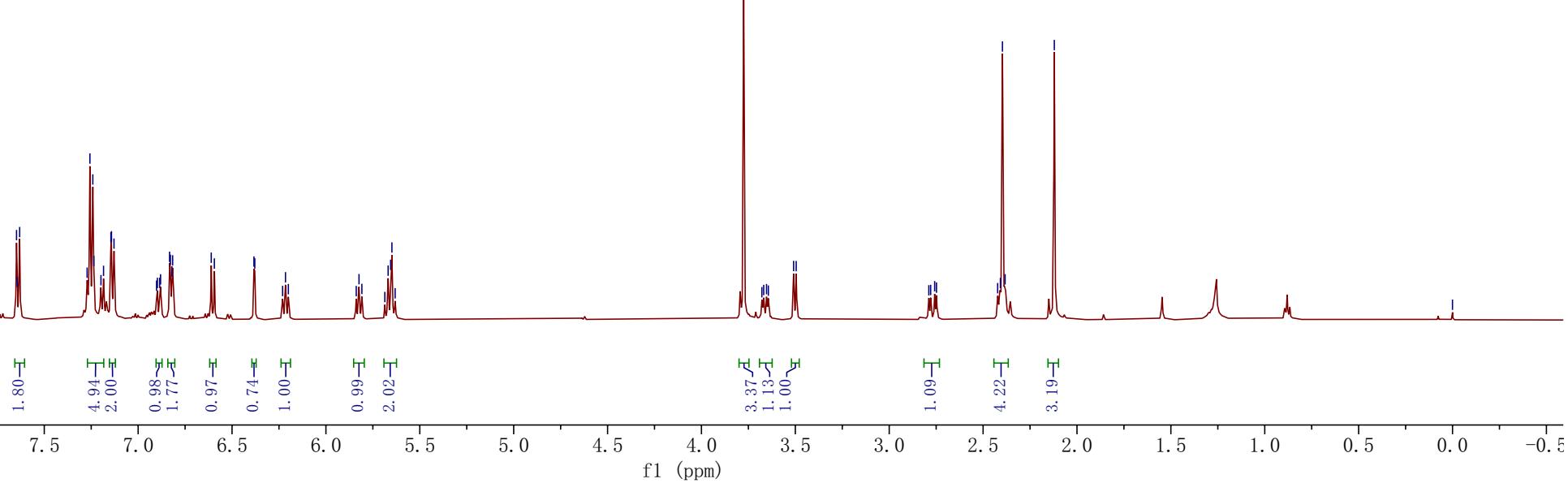
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz



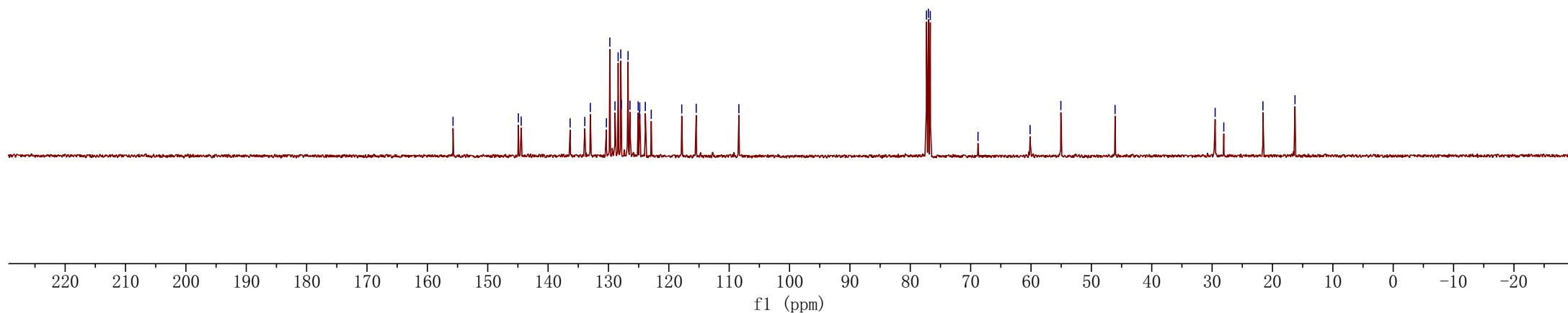
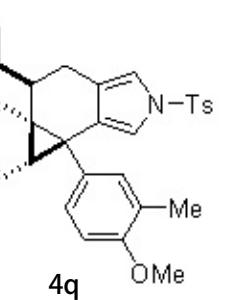
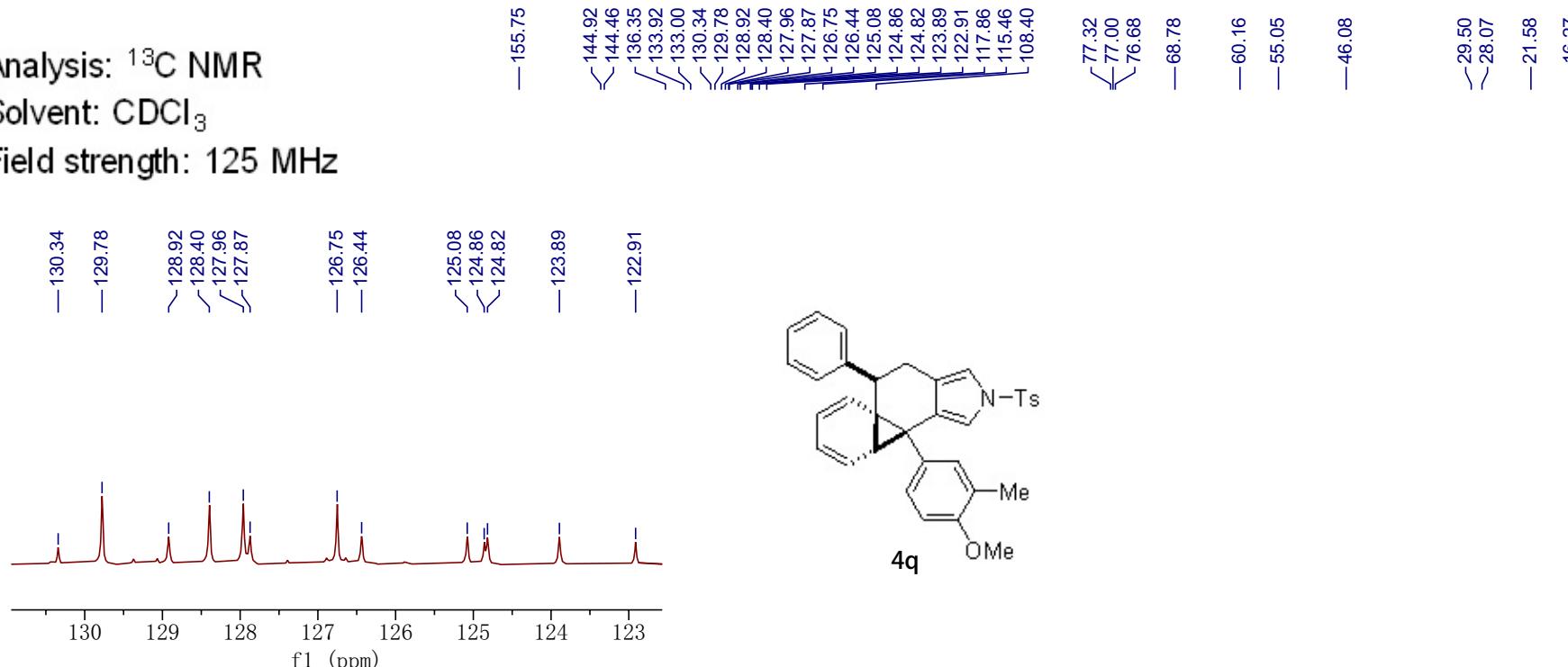
4q



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



7.656  
7.639  
7.271  
7.257  
7.241  
7.199  
7.184  
7.170  
7.140  
7.126  
6.842  
6.668  
6.663  
6.626  
6.408  
6.403  
6.228  
6.213  
6.197  
5.851  
5.836  
5.820  
5.693  
5.675  
5.662  
5.645  
5.627

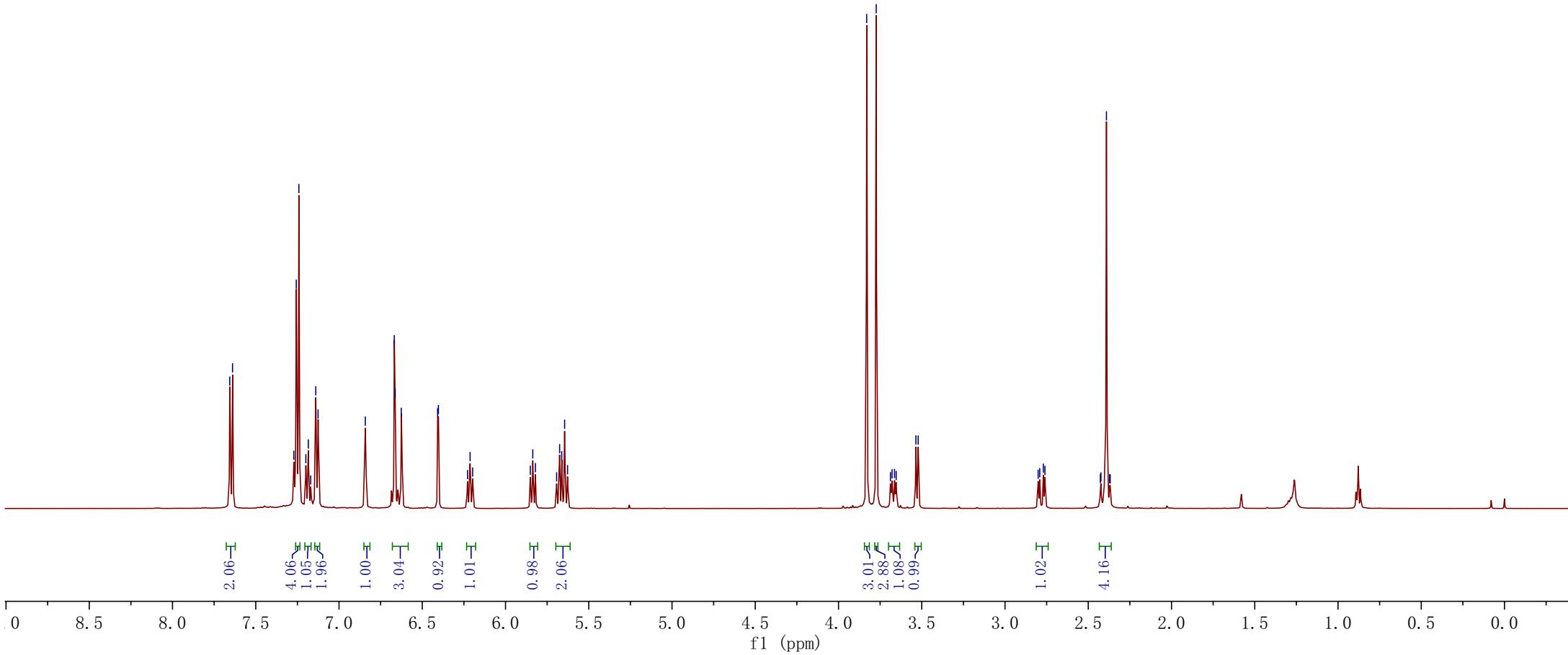
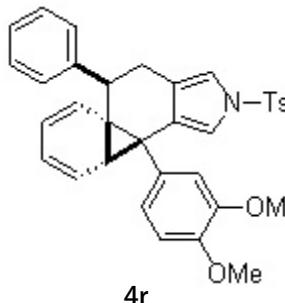
3.831  
3.774  
3.688  
3.678  
3.663  
3.654  
3.535  
3.521

2.801  
2.791  
2.770  
2.760  
2.427  
2.424  
2.391  
2.372  
2.368

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

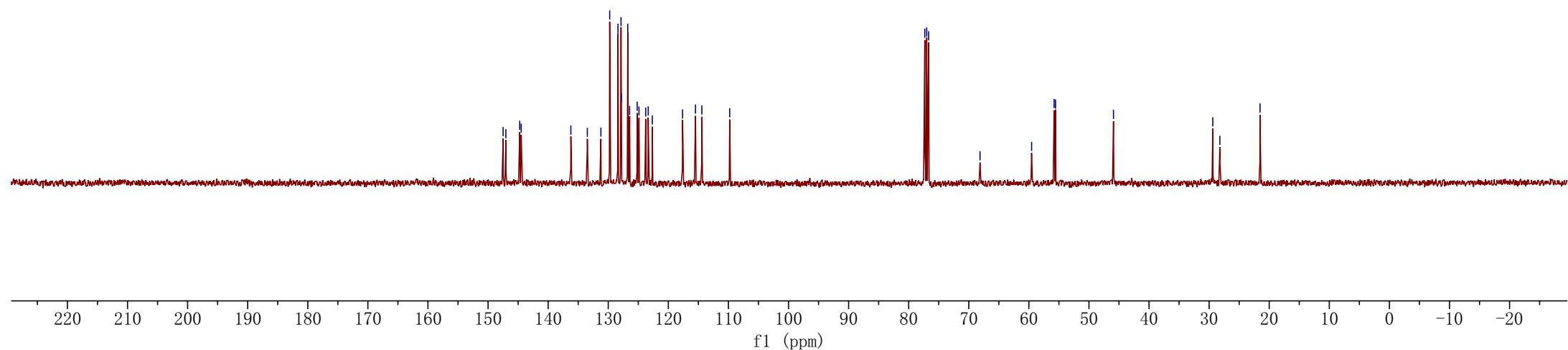
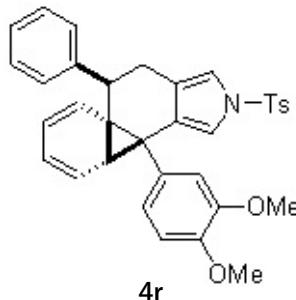
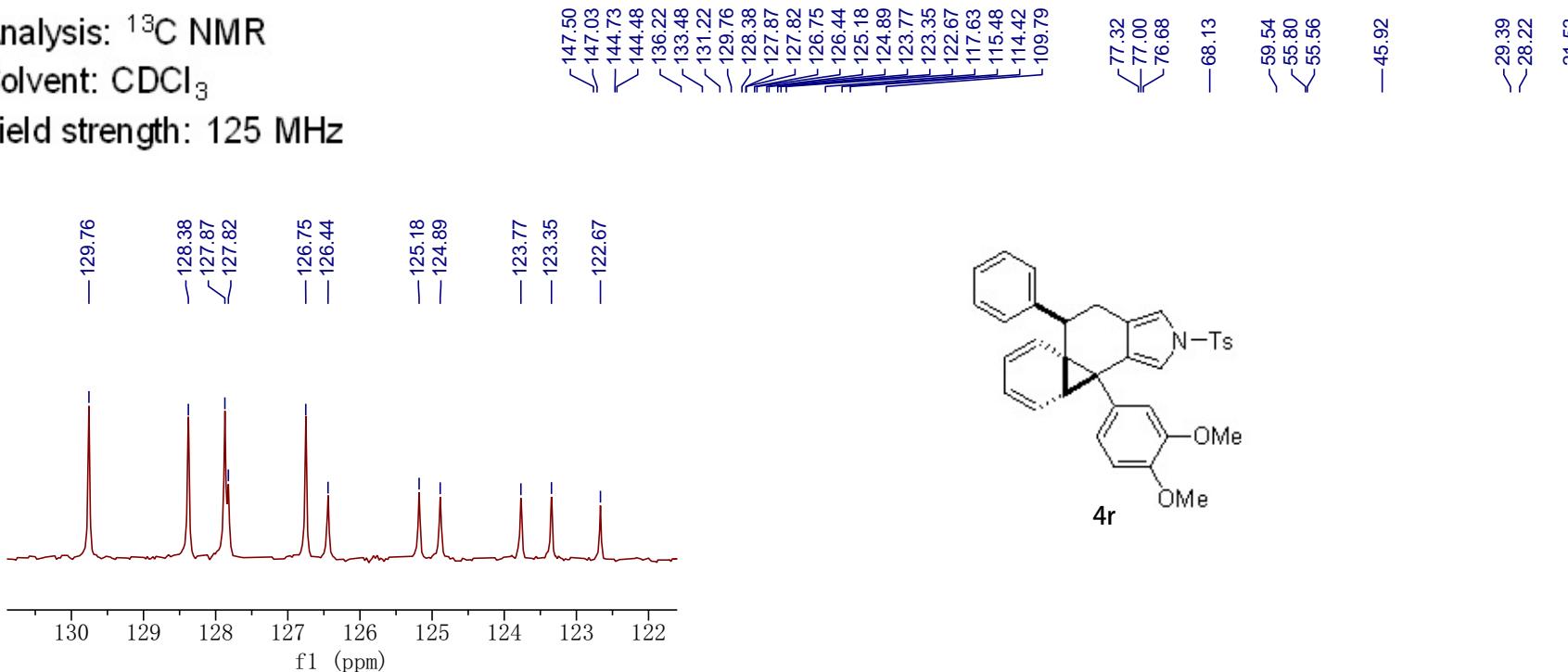
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



7.667  
7.646  
7.270  
7.250  
7.236  
7.202  
7.184  
7.166  
7.128  
7.110  
6.829  
6.619  
6.600  
6.587  
6.578  
6.553  
6.441  
6.436  
6.223  
6.203  
6.184  
5.888  
5.869  
5.849  
5.738  
5.716  
5.698  
5.651  
5.629

3.662  
3.650  
3.631  
3.619  
3.566  
3.549

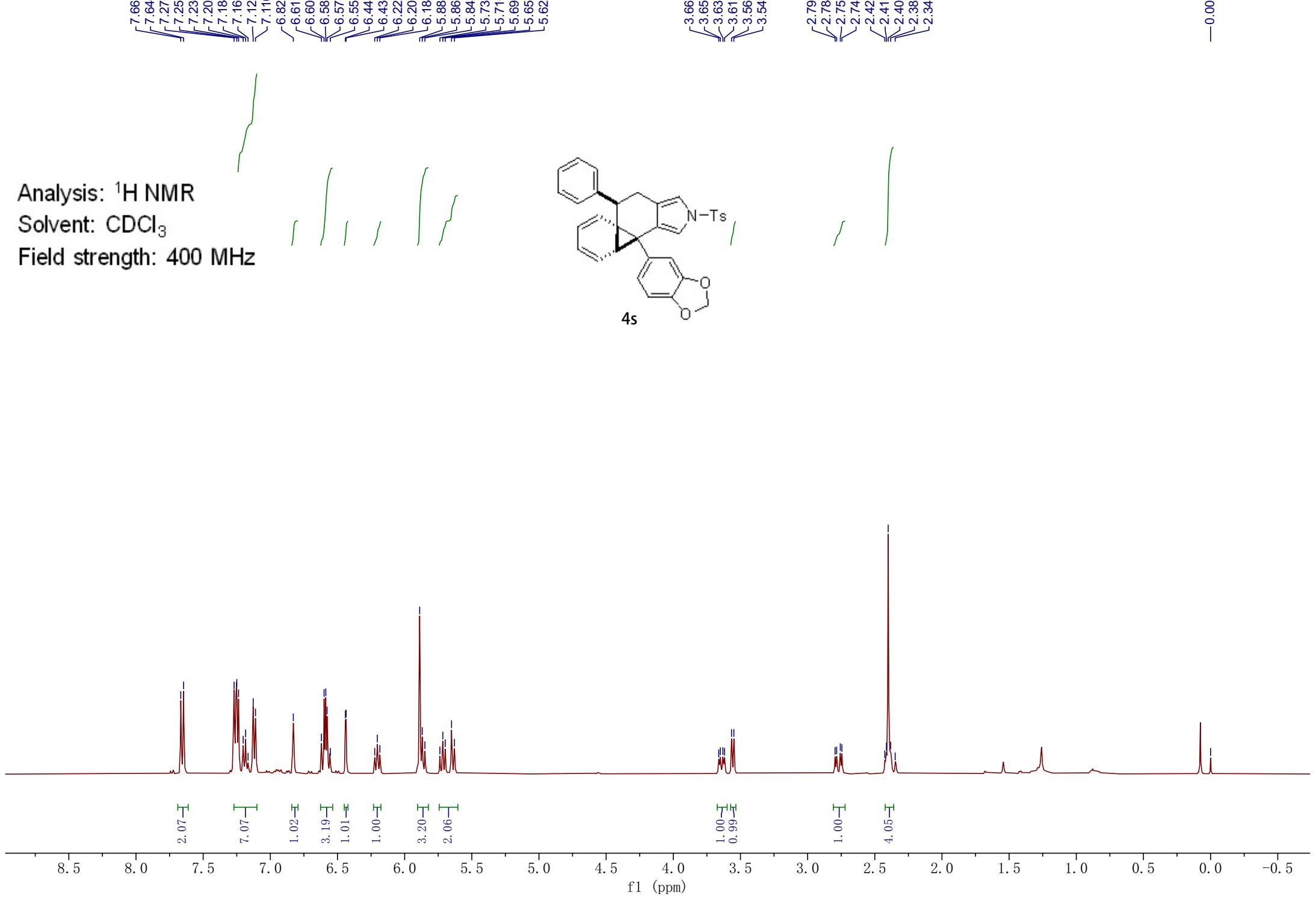
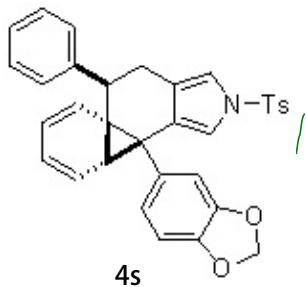
2.796  
2.784  
2.757  
2.745  
2.425  
2.413  
2.400  
2.382  
2.348

-0.000

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

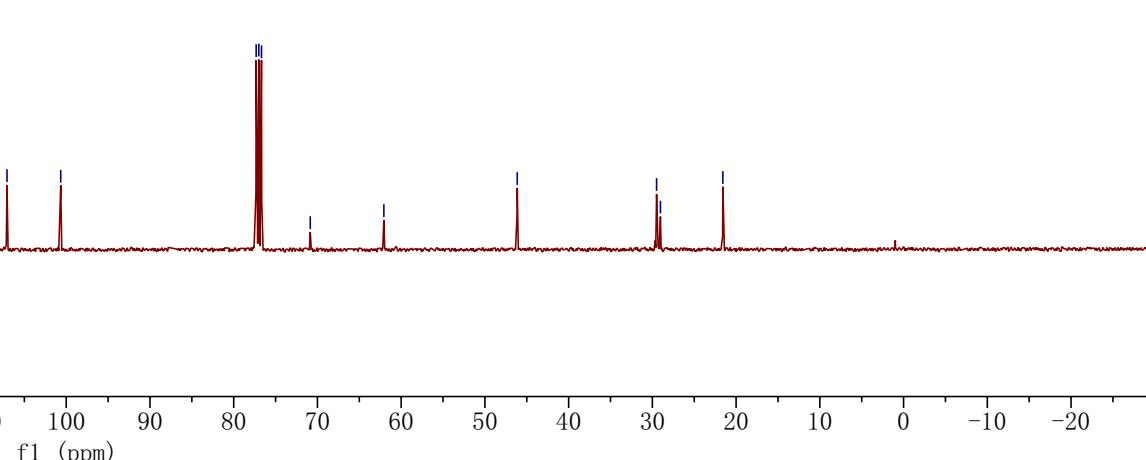
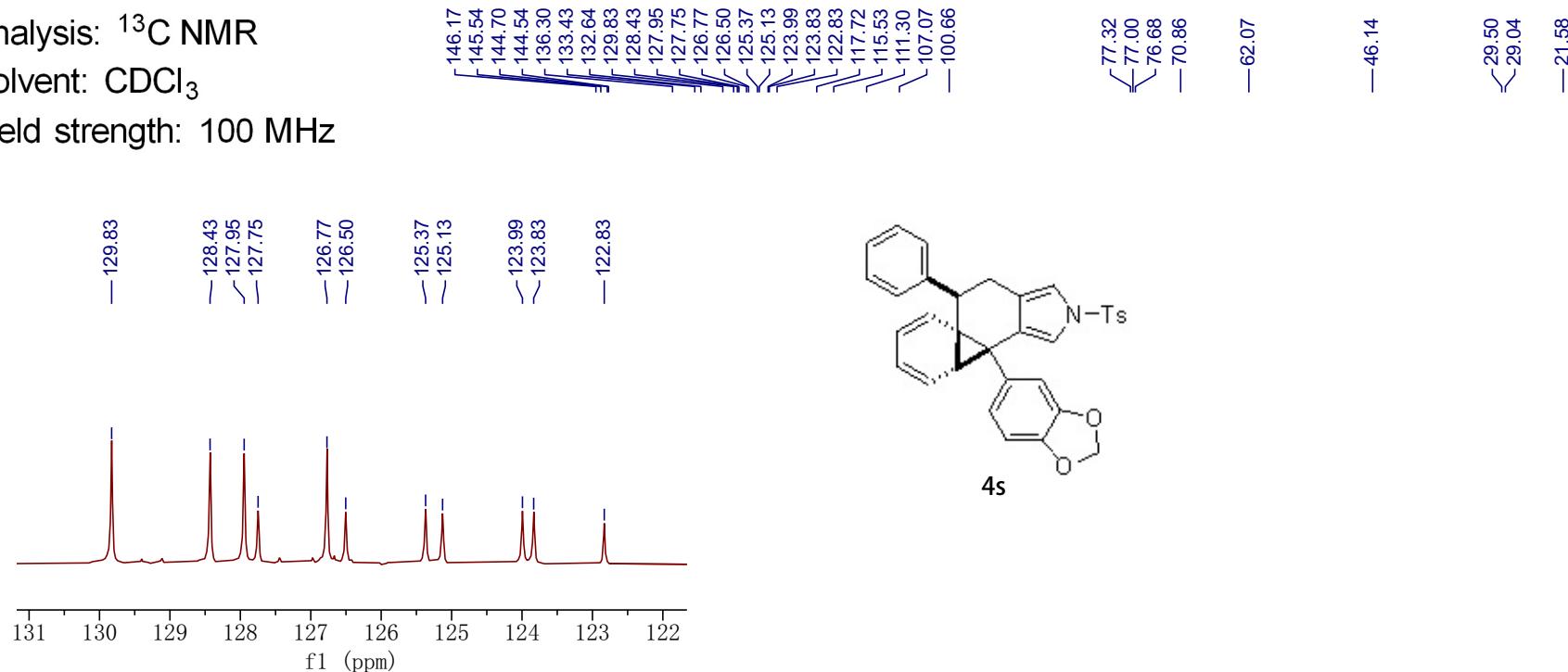
Field strength: 400 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

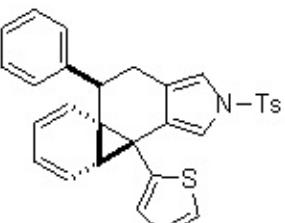




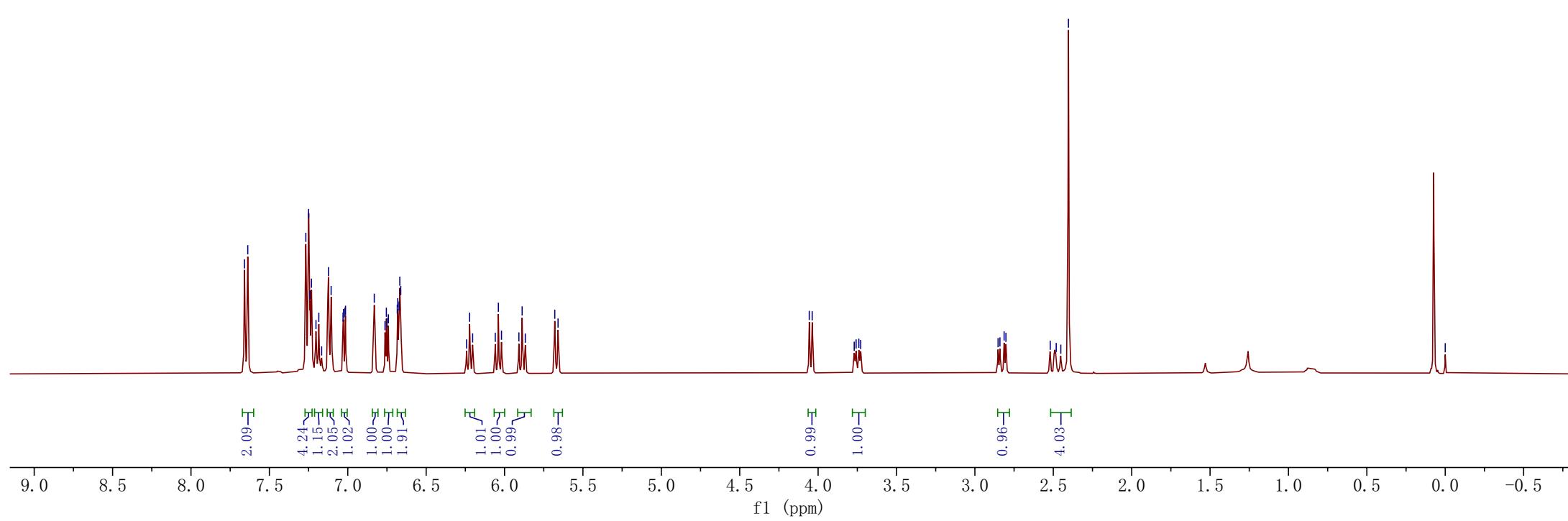
Analysis: <sup>1</sup>H NMR

Solvent: CDCl<sub>3</sub>

Field strength: 400 MHz



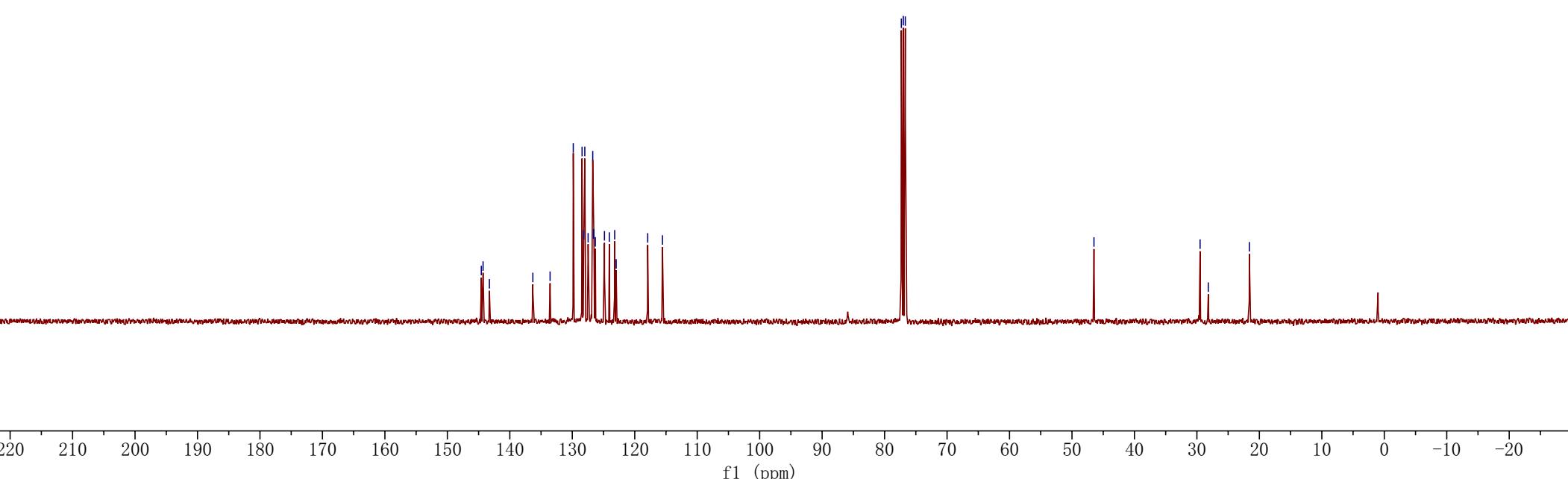
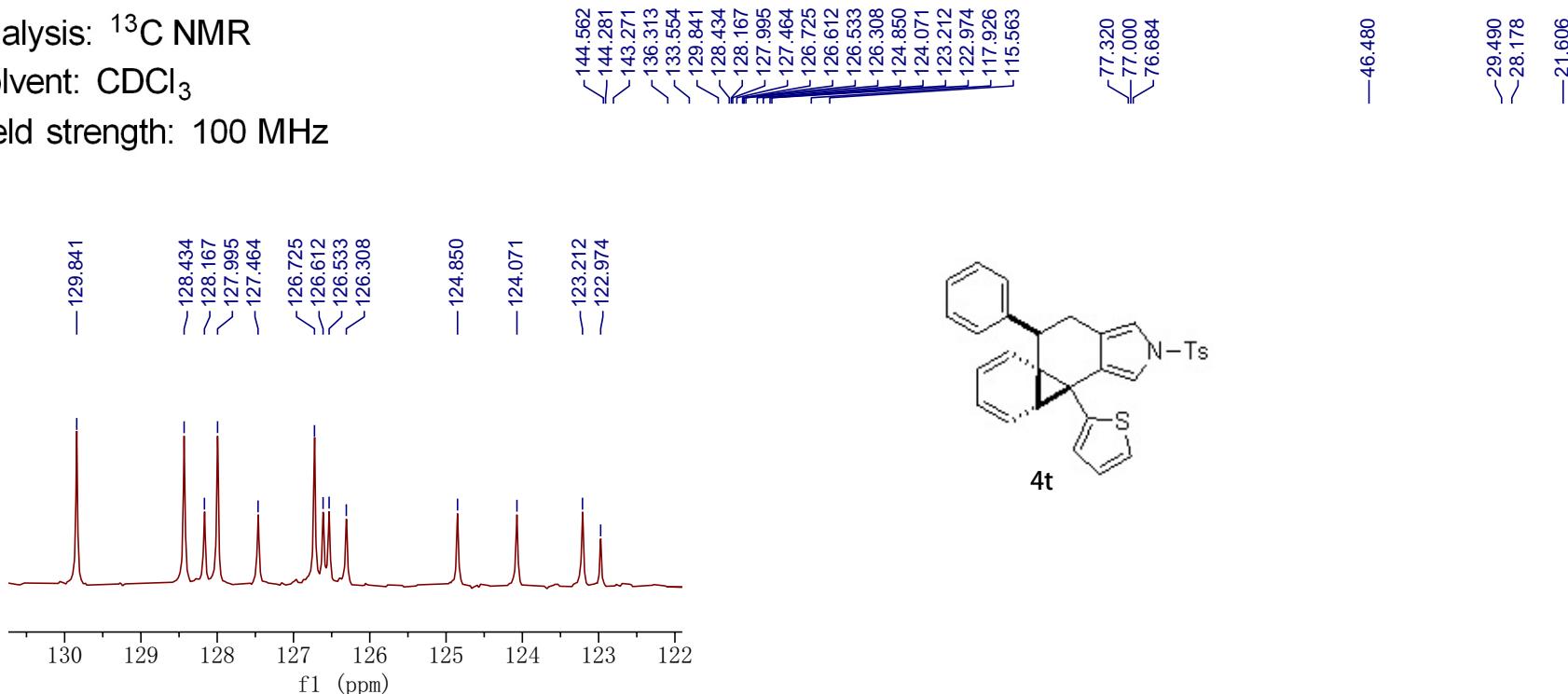
**4t**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



7.646  
7.625  
7.261  
7.240  
7.082  
7.061  
7.038  
7.014  
6.992  
6.800  
6.697  
6.675  
6.340  
6.334

5.911  
5.895  
5.574  
5.551  
5.444  
5.421

3.772  
3.577  
3.565  
3.547  
3.534  
3.279  
3.263

2.751  
2.739  
2.712  
2.699  
2.429  
2.399  
2.373  
2.338  
2.319  
2.298

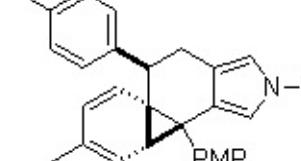
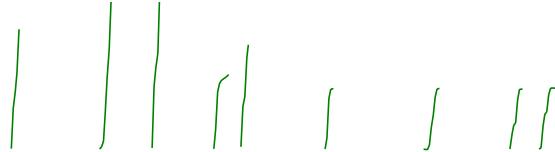
-1.563

-0.000

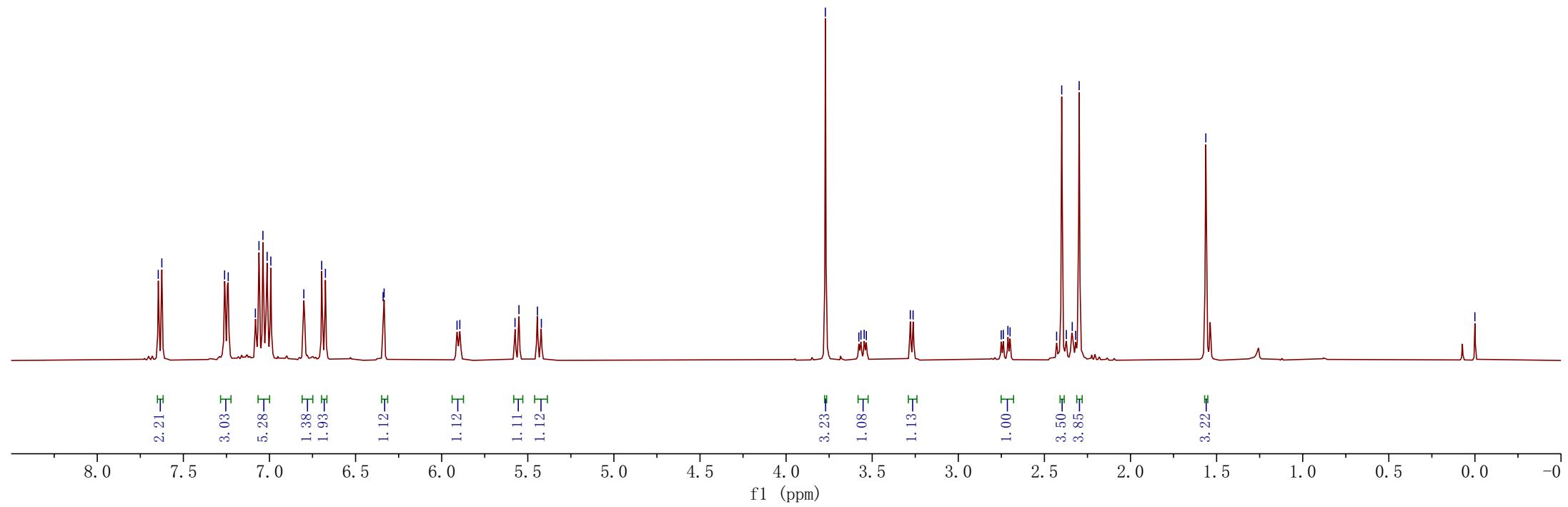
Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz



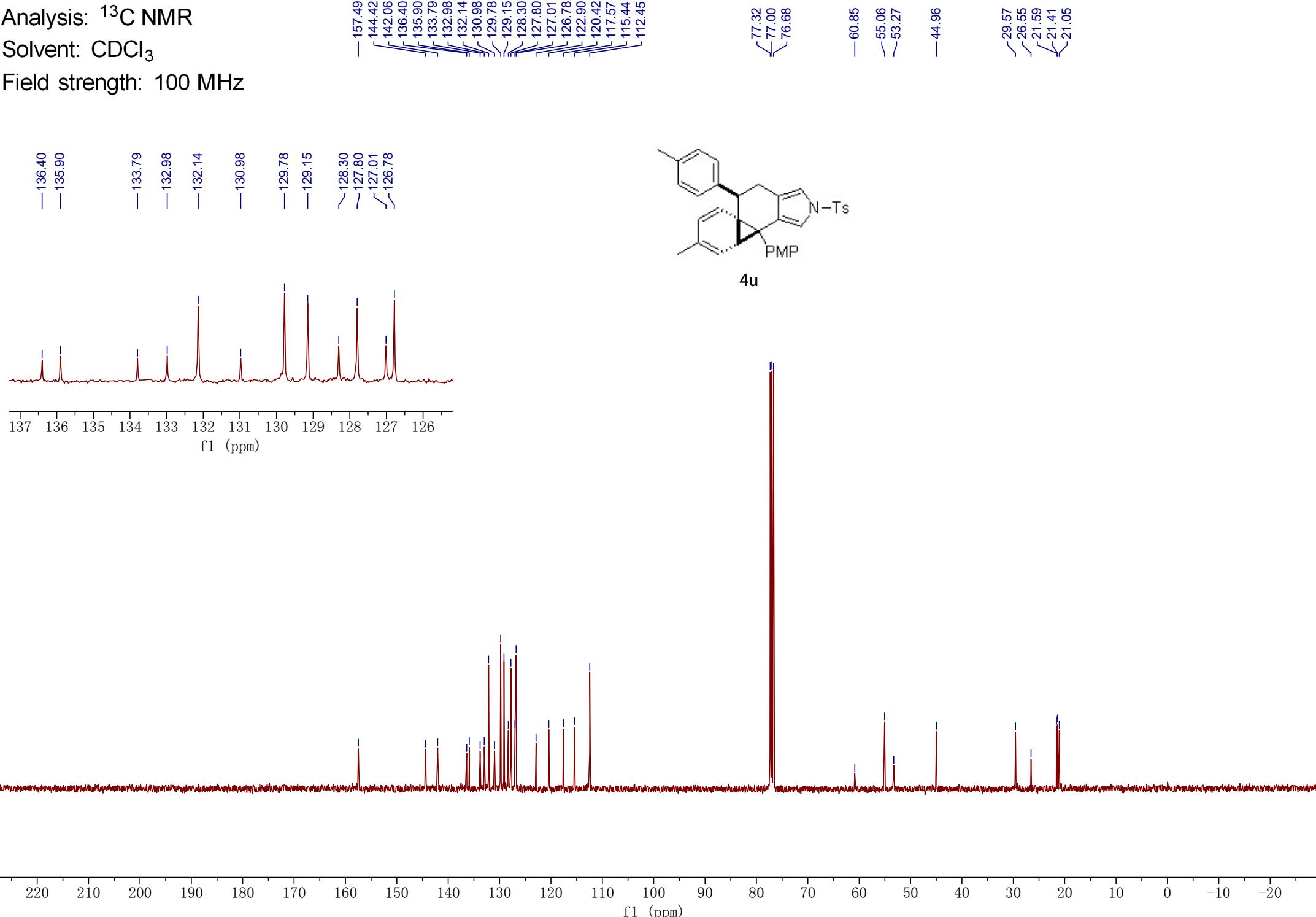
4u

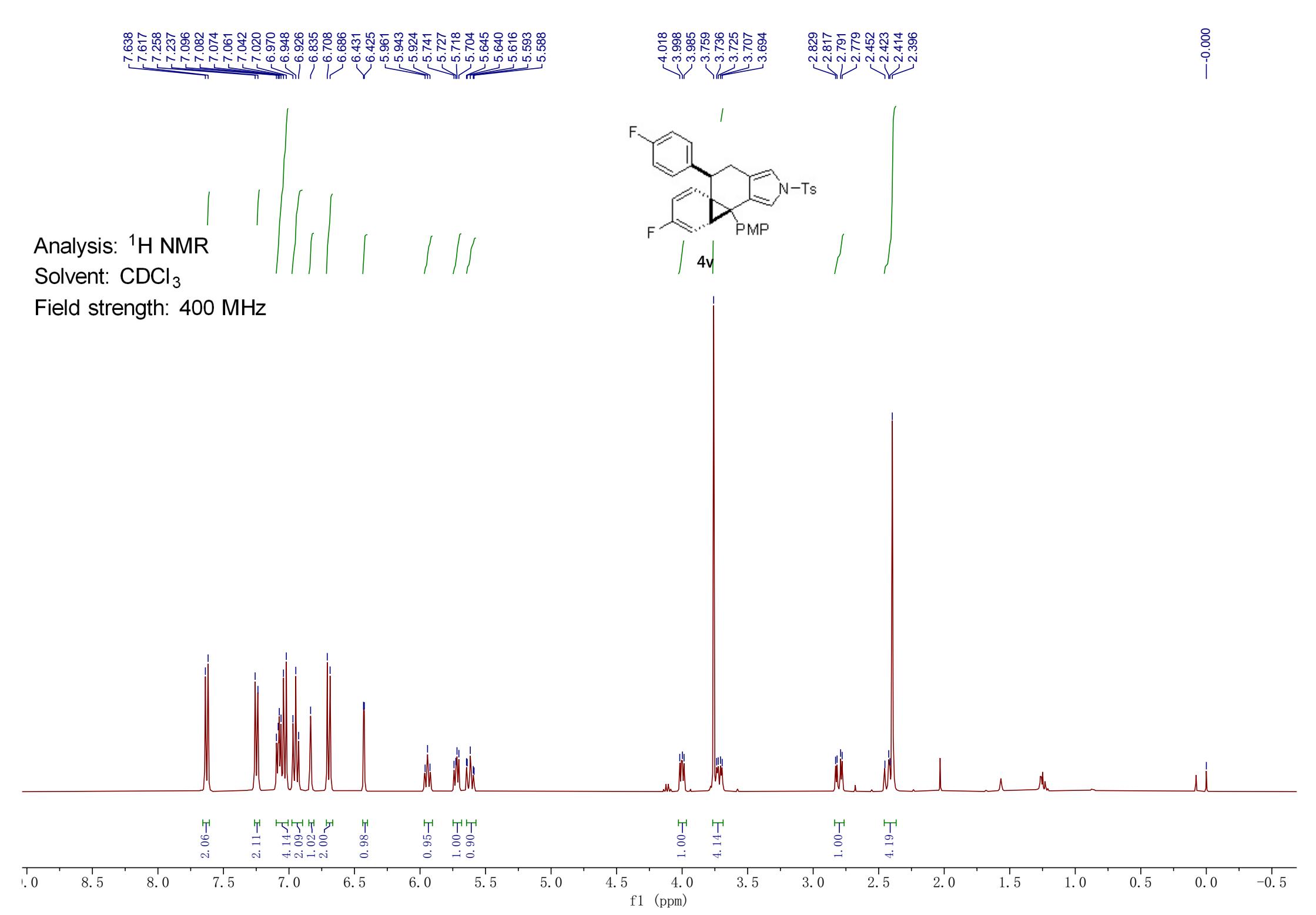


Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



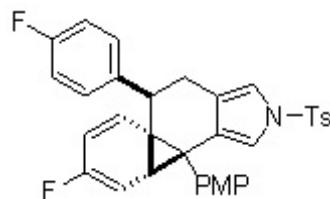


Analysis:  $^{19}\text{F}$  NMR

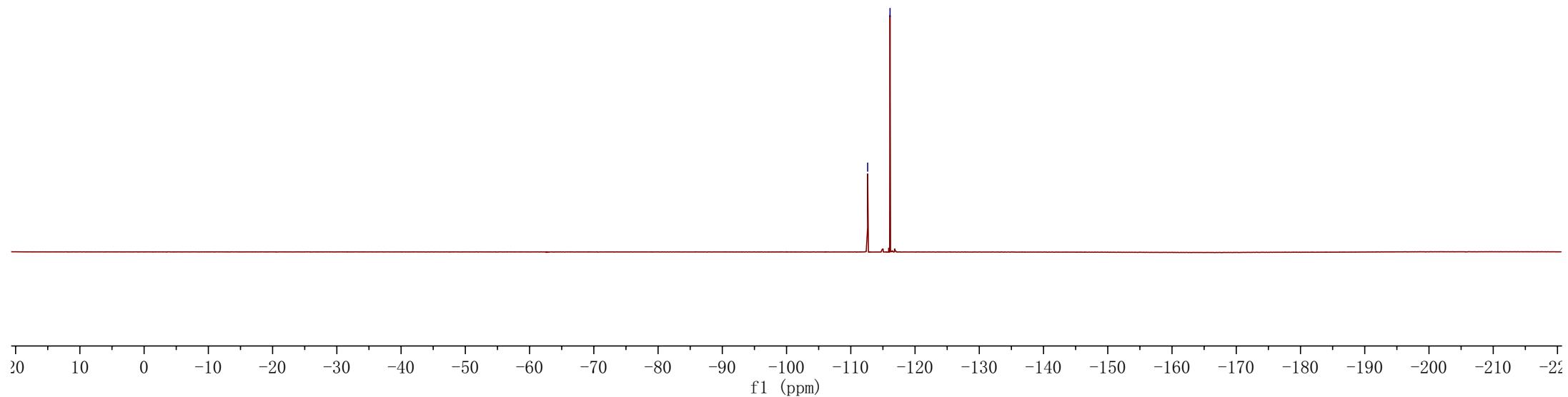
Solvent:  $\text{CDCl}_3$

Field strength: 471 MHz

-112.63  
-116.11



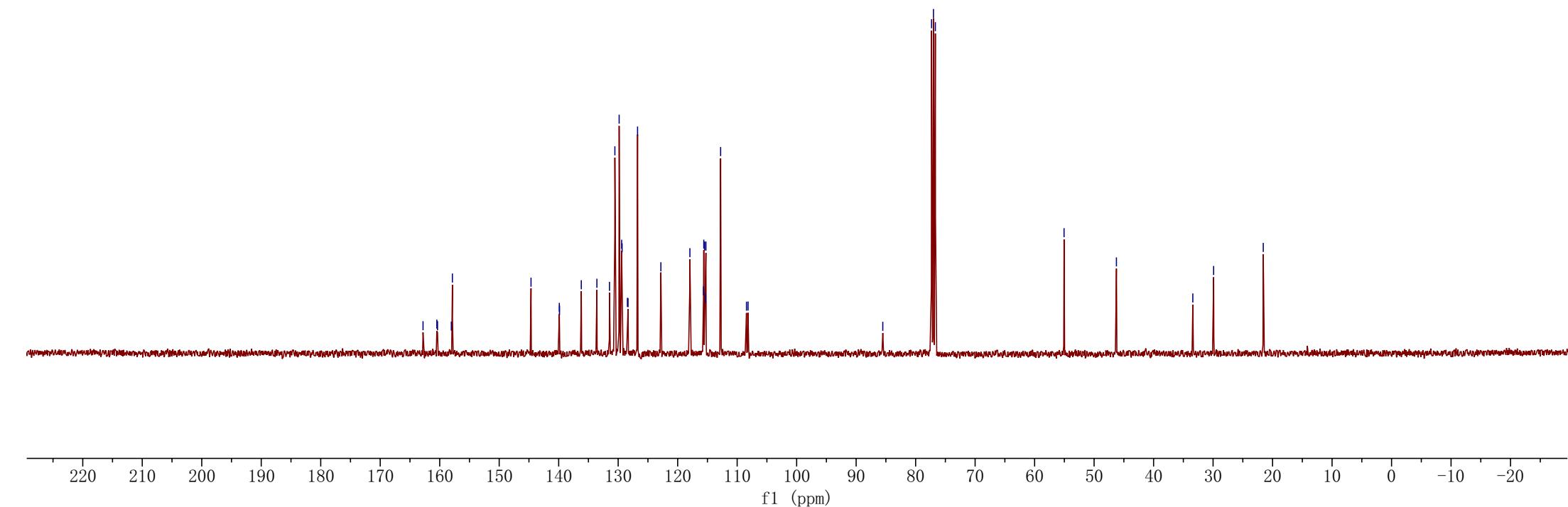
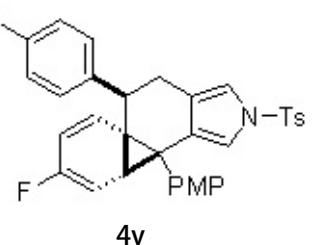
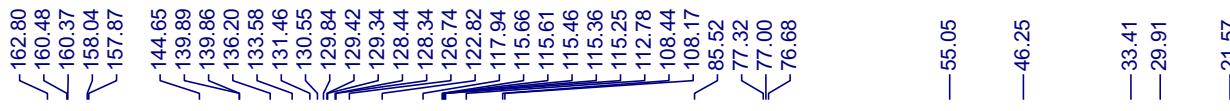
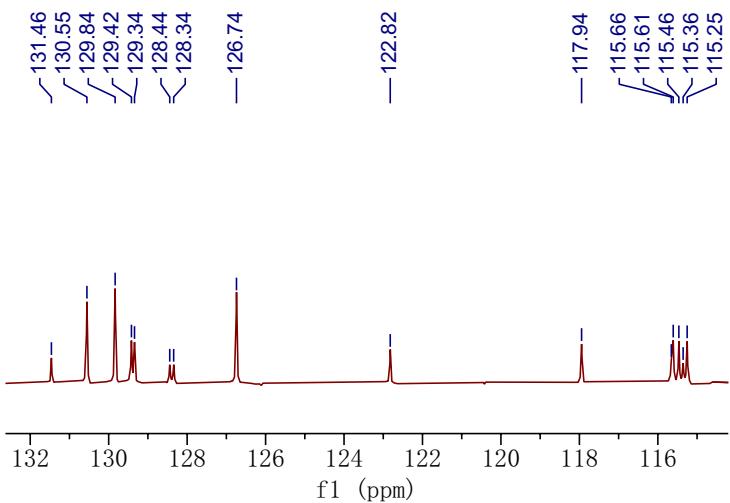
4v



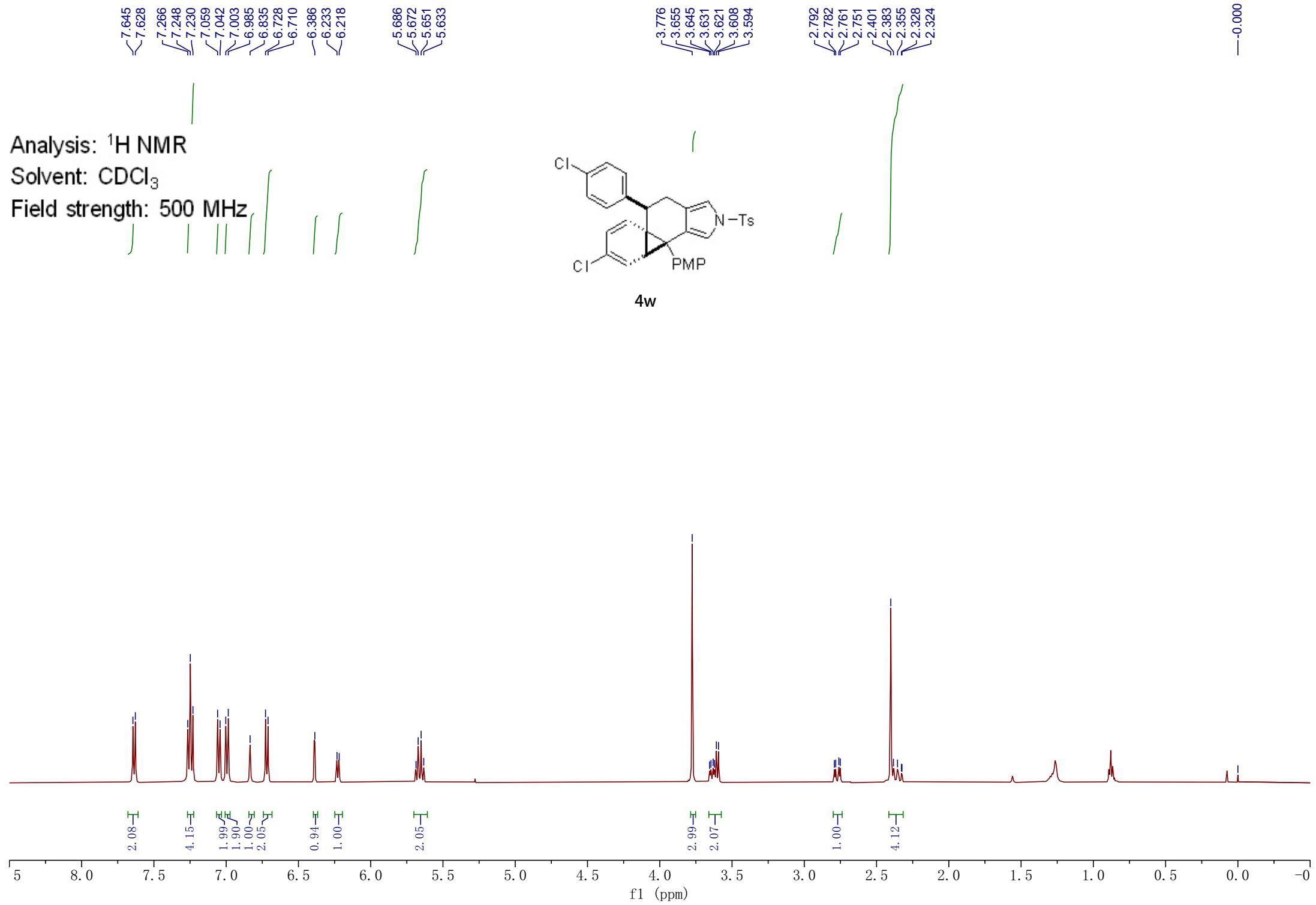
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz



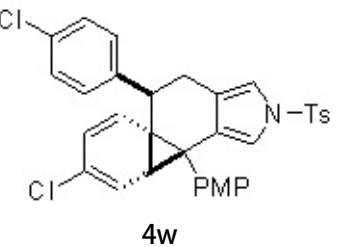
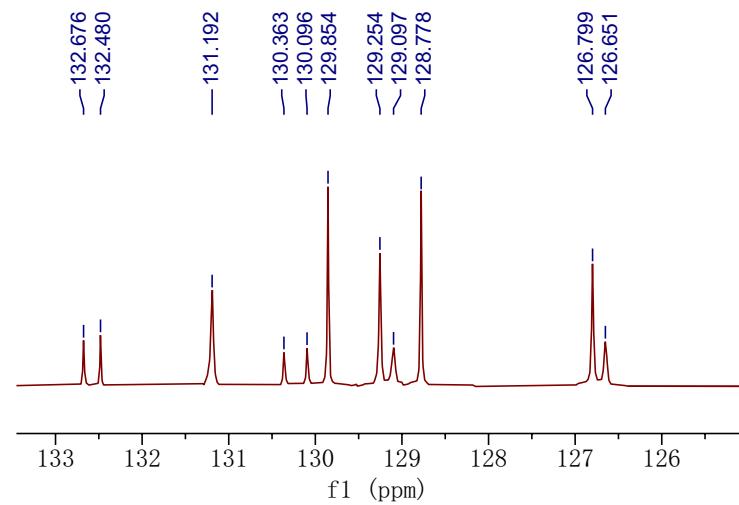
-0.000



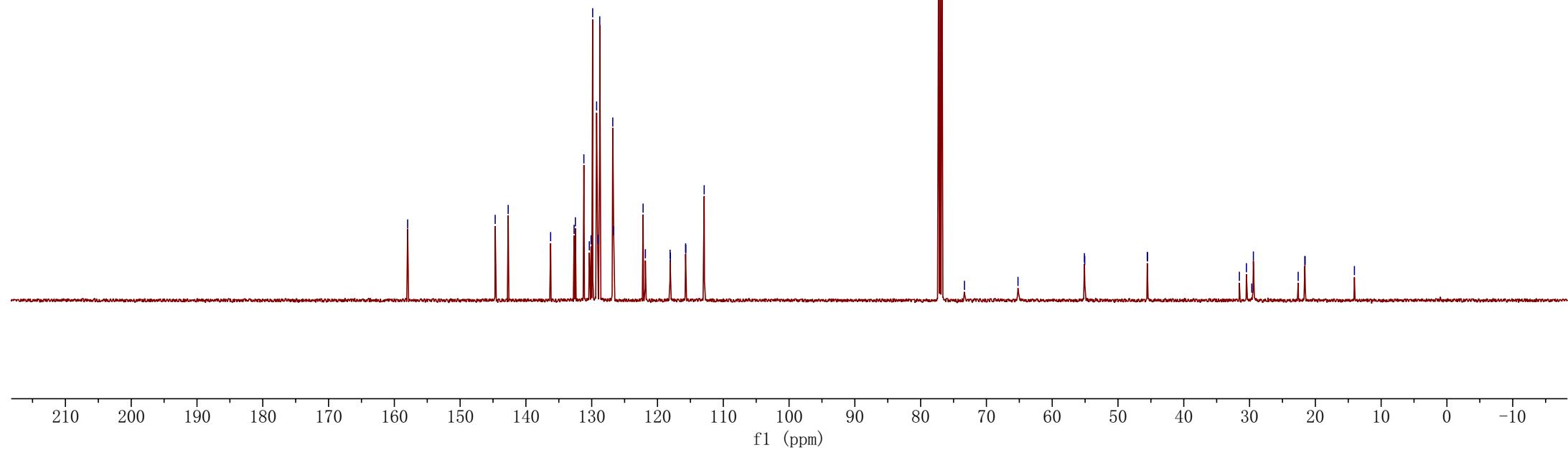
Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



**4w**

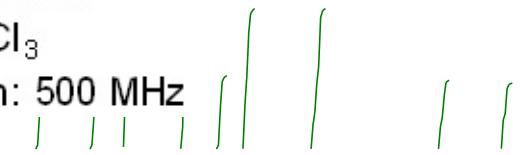


7.641  
7.625  
7.399  
7.382  
7.264  
7.249  
6.997  
6.983  
6.980  
6.834  
6.725  
6.708  
6.423  
6.394  
6.389

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

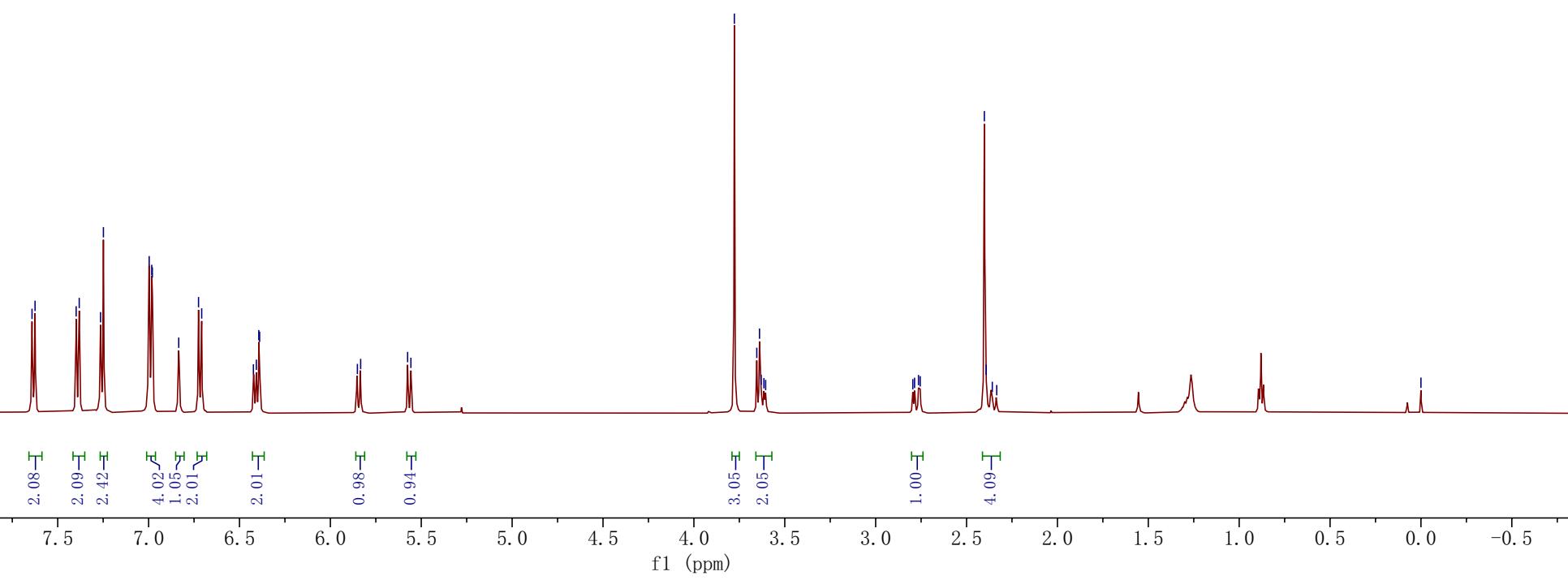
Field strength: 500 MHz



3.777  
3.654  
3.639  
3.630  
3.615  
3.605

2.796  
2.786  
2.764  
2.755  
2.402  
2.393  
2.358  
2.334

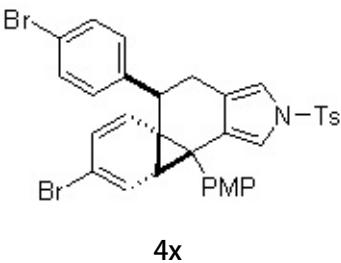
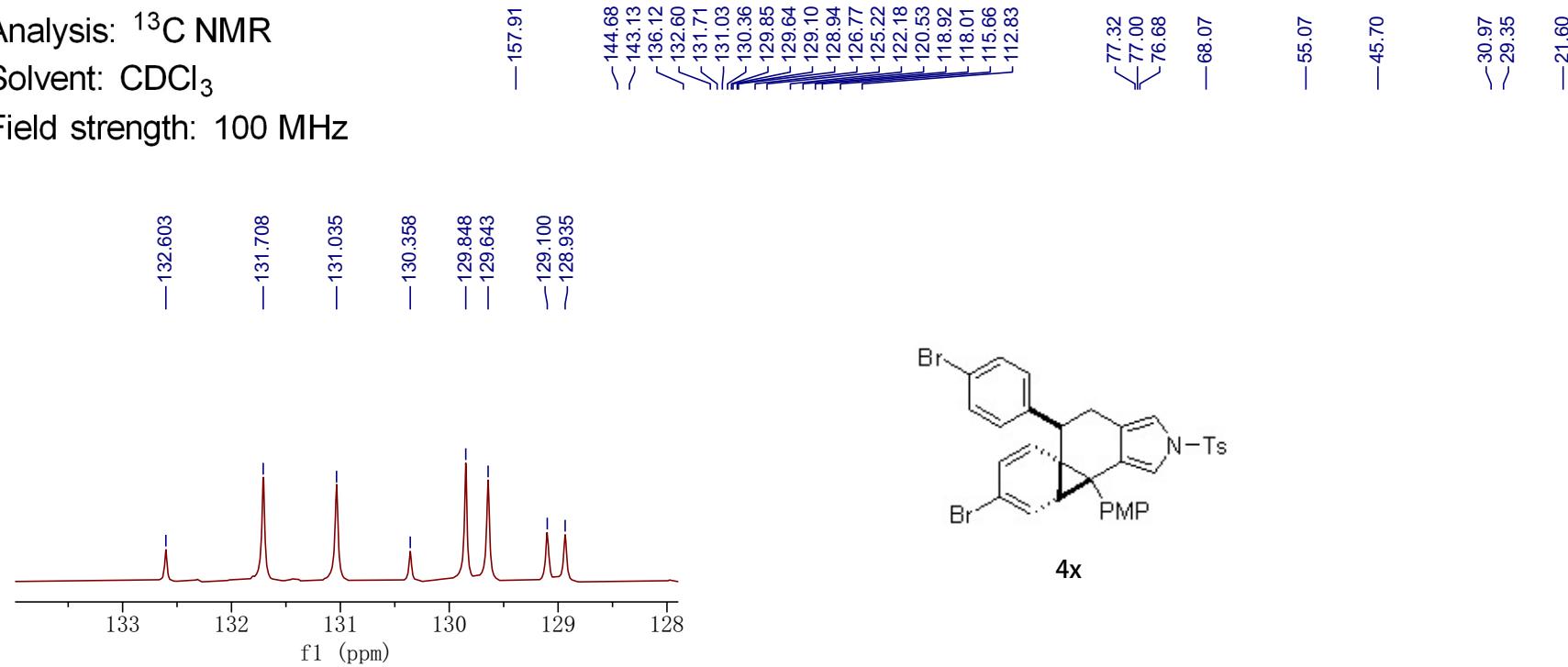
-0.000



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

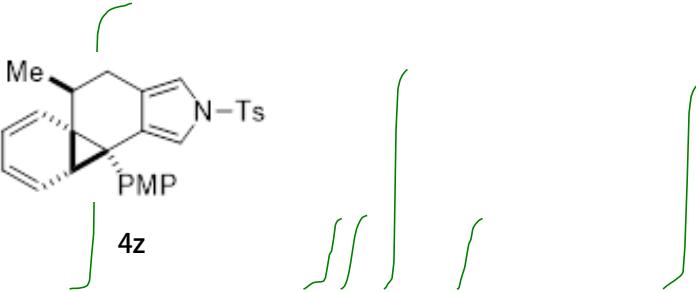
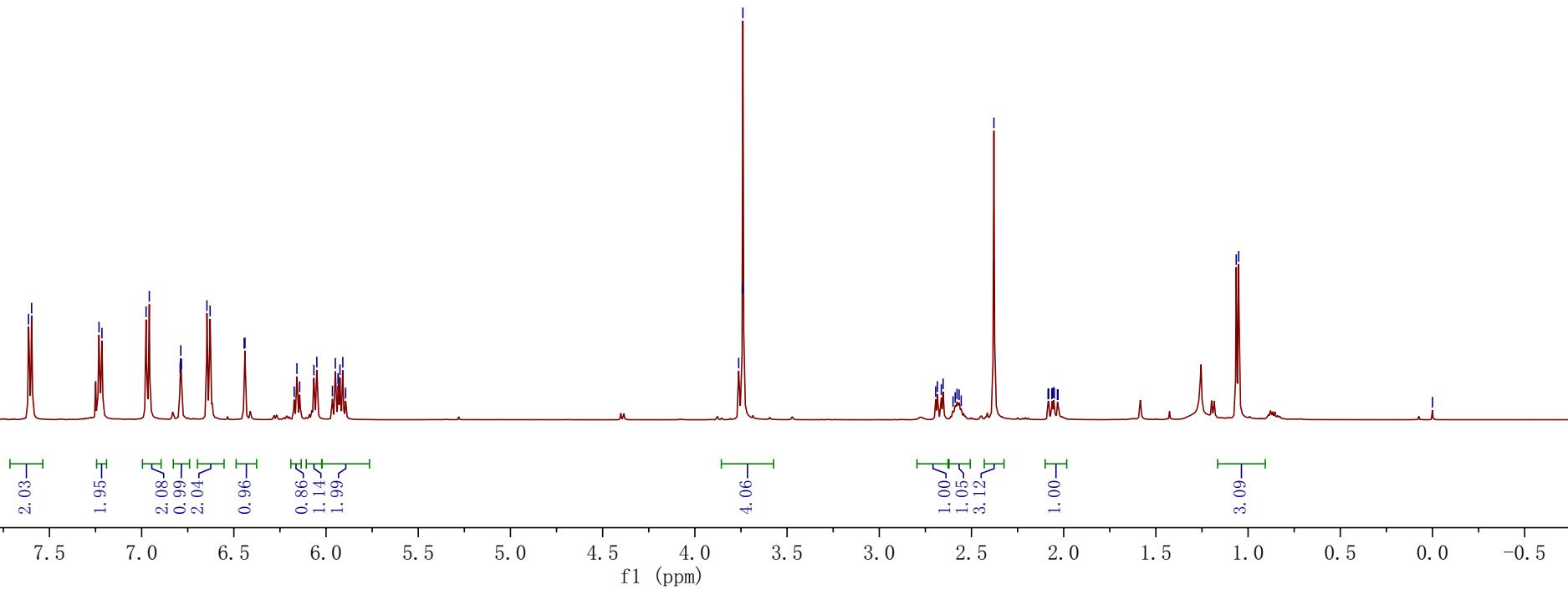




Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz



-0.000

Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

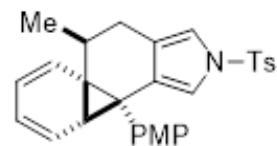
-157.40

144.38  
136.38  
134.46  
132.80  
130.68  
129.73  
126.63  
126.40  
125.56  
125.25  
124.74  
123.20  
117.64  
115.45  
112.31

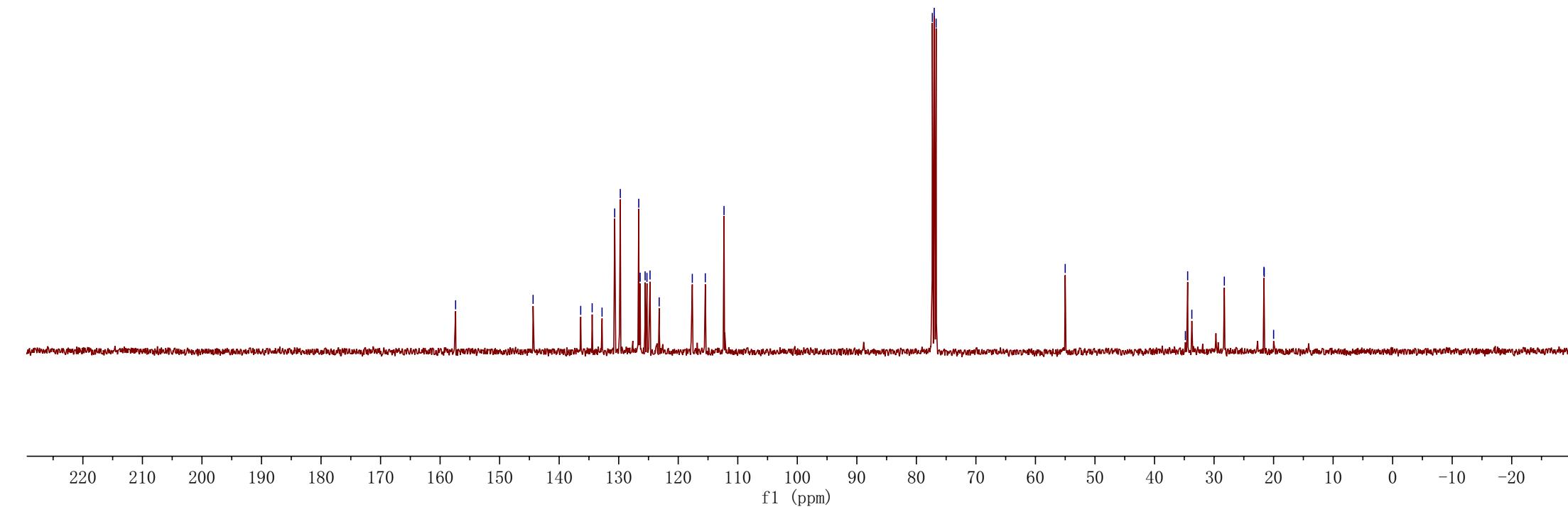
77.32  
77.00  
76.68

-55.00

34.82  
34.43  
33.73  
-28.27  
21.61  
21.57  
20.00



**4z**



<7.084

6.606  
6.585  
6.327  
6.313  
6.280  
6.255  
6.185  
6.173  
6.162  
6.007  
6.002

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

<5.081

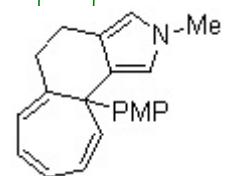
<5.059

<3.698

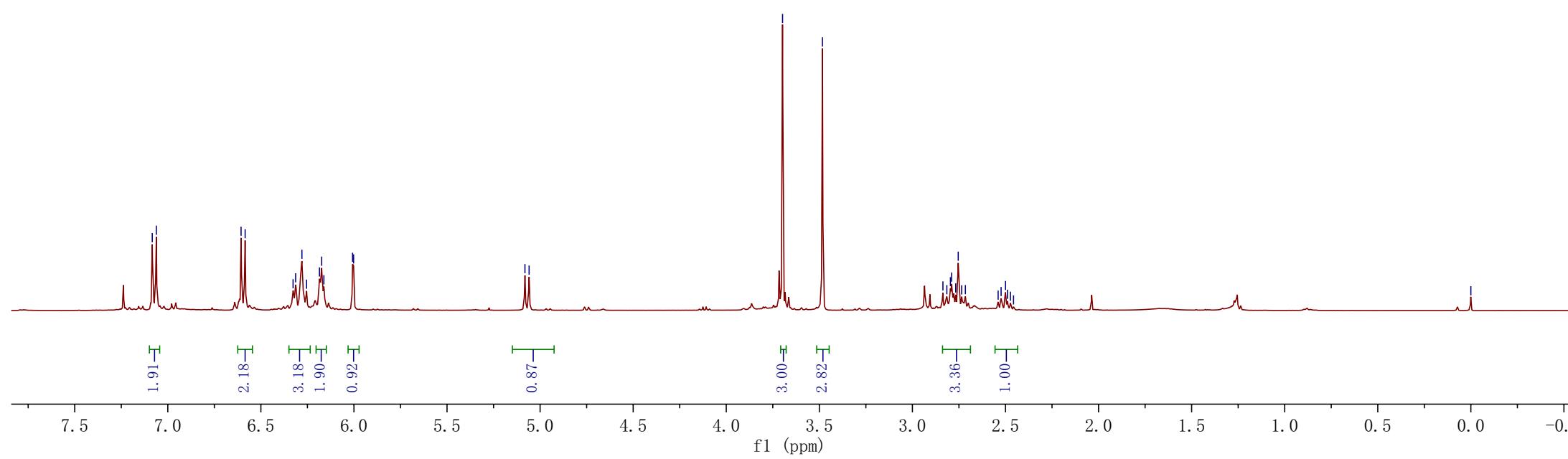
<3.483

2.836  
2.815  
2.796  
2.789  
2.767  
2.754  
2.735  
2.715  
2.539  
2.524  
2.500  
2.489  
2.473  
2.457

-0.000



5a



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

—130.40

—156.96

—137.25  
—130.40  
—128.46  
—128.41  
—127.49  
—125.57  
—124.68  
—123.40  
—118.87  
—118.46  
—116.82  
—116.26  
—111.91

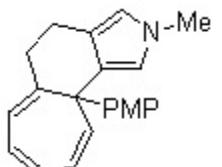
—77.32  
—77.00  
—76.68

—54.93

—43.81  
—36.01  
—35.08

—21.84

—128.46  
—128.41



5a

130.0 129.5 129.0 128.5 128.0

f1 (ppm)

f1 (ppm)

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

-0.000

7.735  
7.719  
7.332  
7.315  
7.189  
7.179  
7.174  
7.167  
7.160  
7.155  
7.146  
7.049  
7.033  
6.920  
6.903  
6.721  
6.703

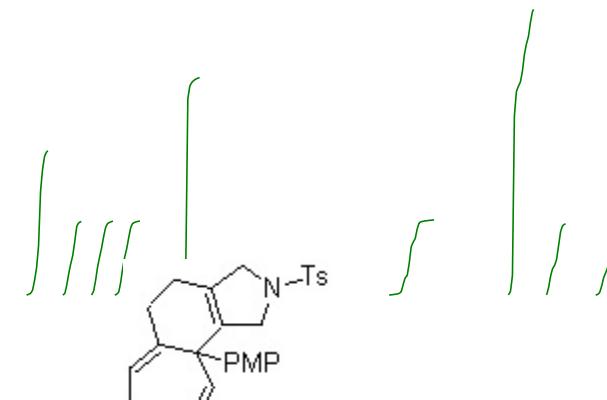
4.334  
4.216  
4.190  
4.110  
4.077  
4.004  
3.978  
-3.747

Analysis:  $^1\text{H}$  NMR

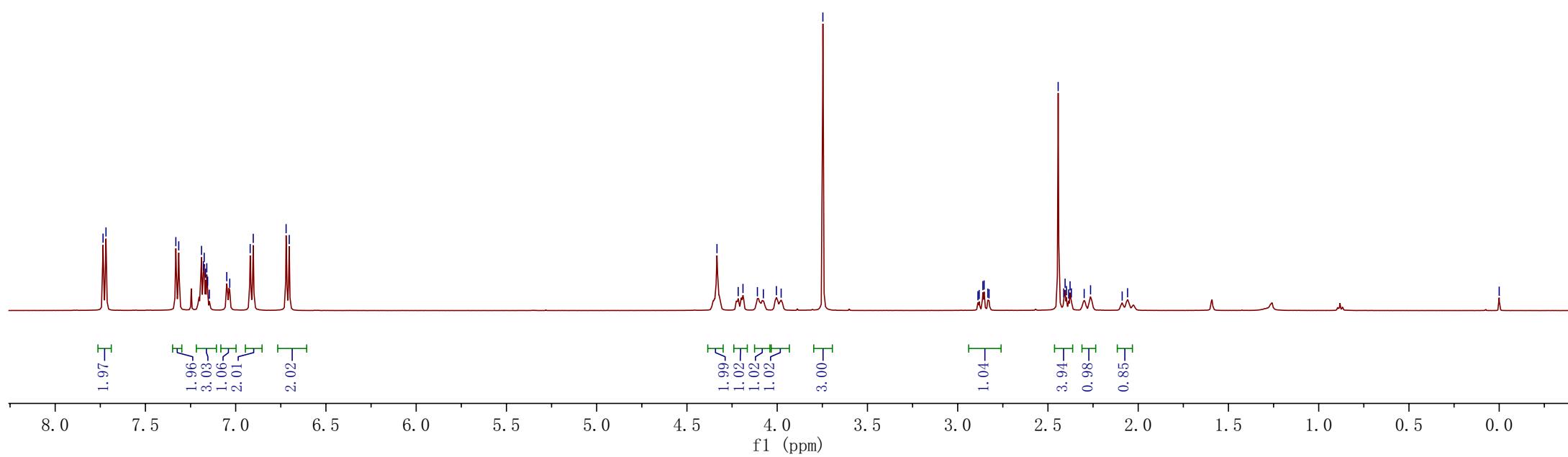
Solvent:  $\text{CDCl}_3$

Field strength: 500 MHz

J J J J J



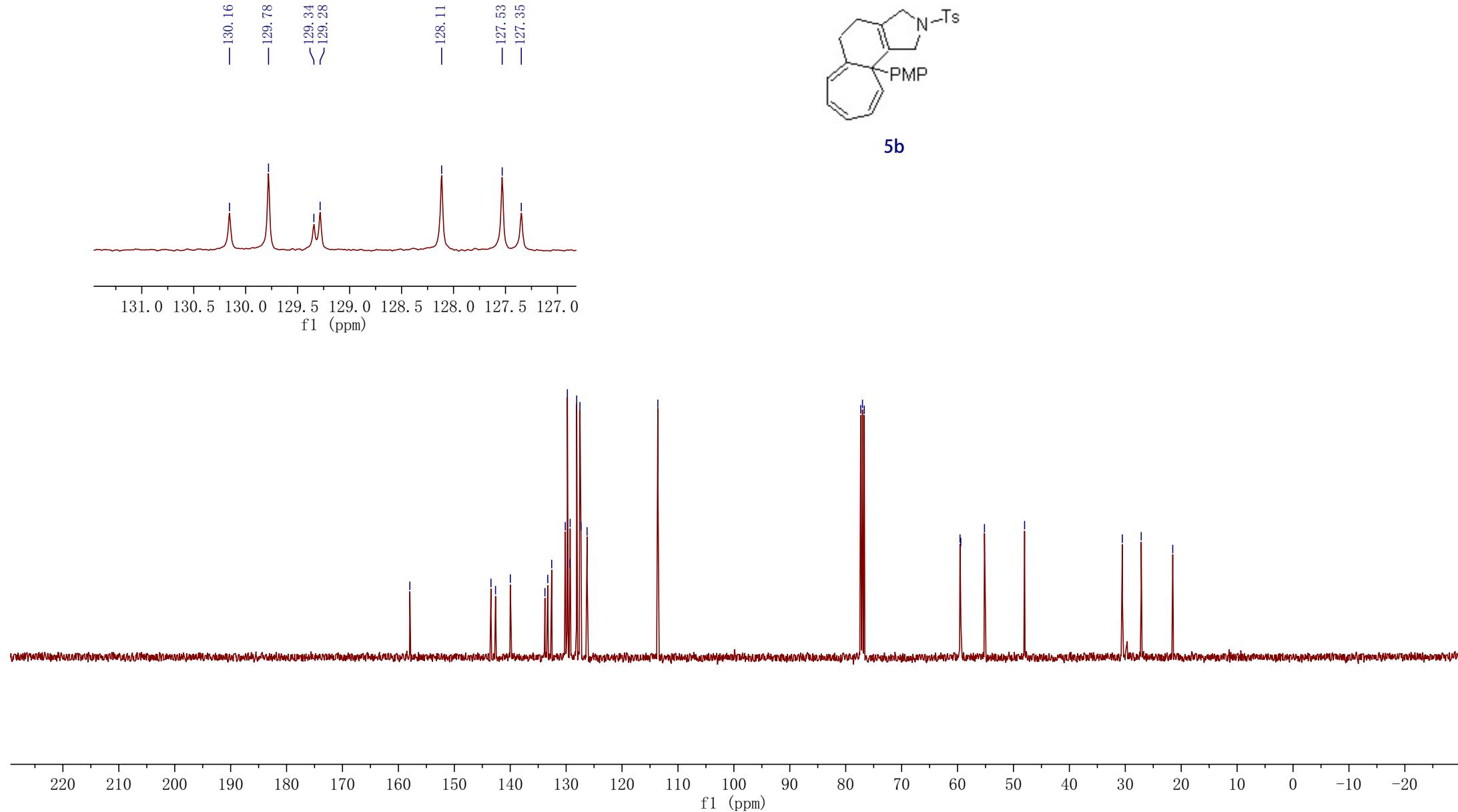
**5b**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



$\sim$ 7.591

$\sim$ 7.245

$\sim$ 7.225

$\sim$ 6.893

$\sim$ 6.873

$\sim$ 6.813

$\sim$ 6.792

$\sim$ 6.741

$\sim$ 6.697

$\sim$ 6.676

—6.023

Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 400 MHz

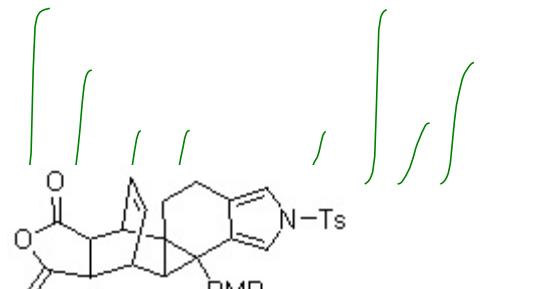
5.386  
5.368  
5.351  
5.292  
5.276  
5.258

—3.814  
—3.611  
—3.394  
 $\sim$ 3.204  
 $\sim$ 3.191

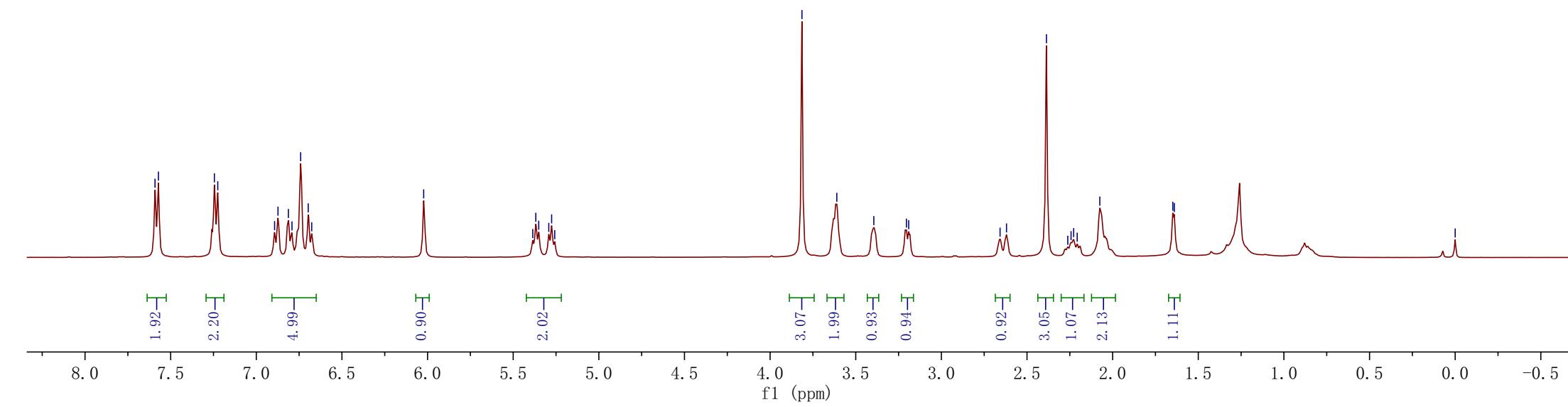
$\sim$ 2.657  
 $\sim$ 2.620  
2.387  
2.262  
2.243  
2.228  
2.207  
 $\sim$ 2.075

$\sim$ 1.649  
 $\sim$ 1.640

—0.000



**5c**



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 100 MHz

>172.30  
<171.67

-157.83

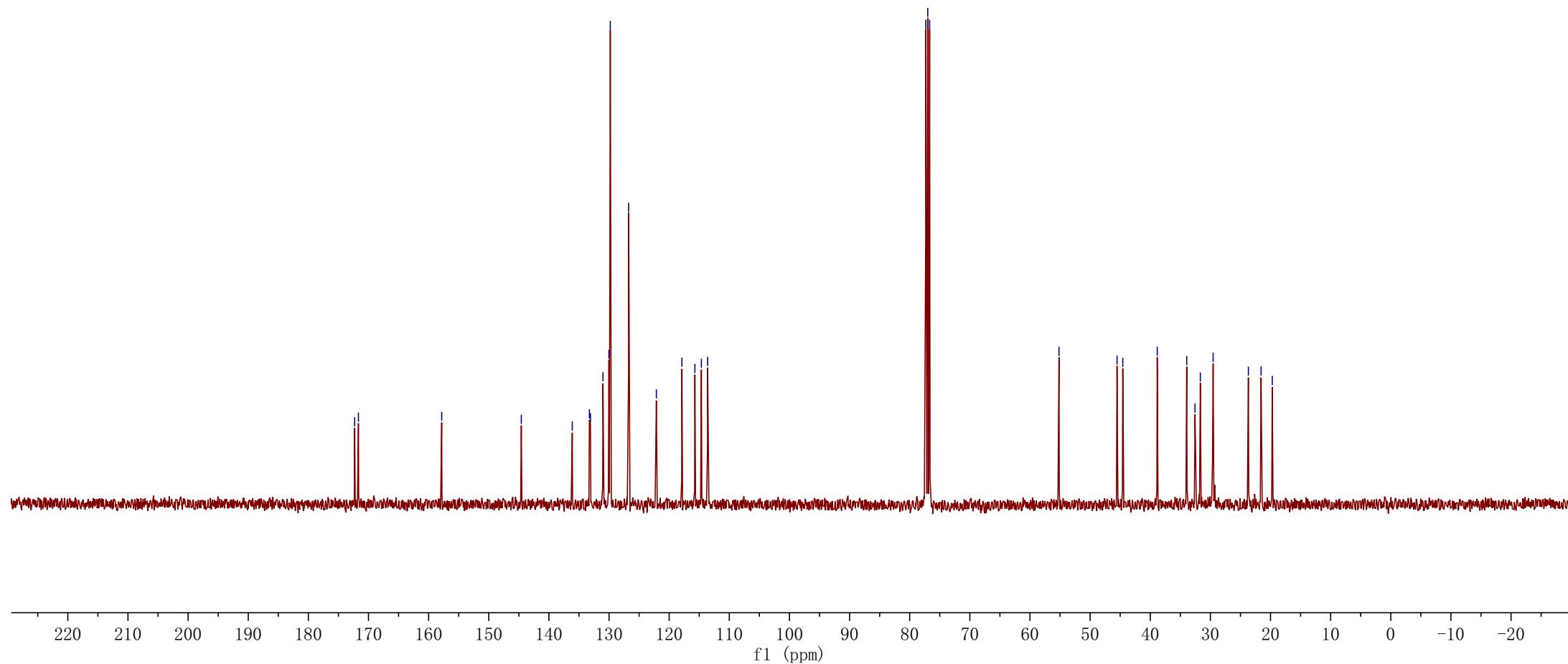
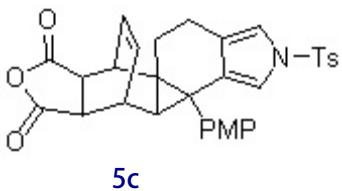
-144.59

136.12  
133.27  
133.09  
131.01  
130.02  
129.79  
126.74  
122.13  
117.88  
115.72  
114.64  
113.61

77.32  
77.00  
76.68

-55.17

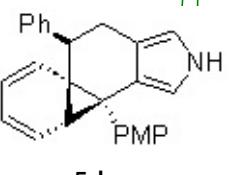
>45.52  
>44.57  
-38.84  
-33.93  
-32.55  
-31.67  
-29.54  
-23.68  
-21.57  
-19.71



-0.000

2.908  
2.898  
2.878  
2.868  
2.550  
2.525  
2.495

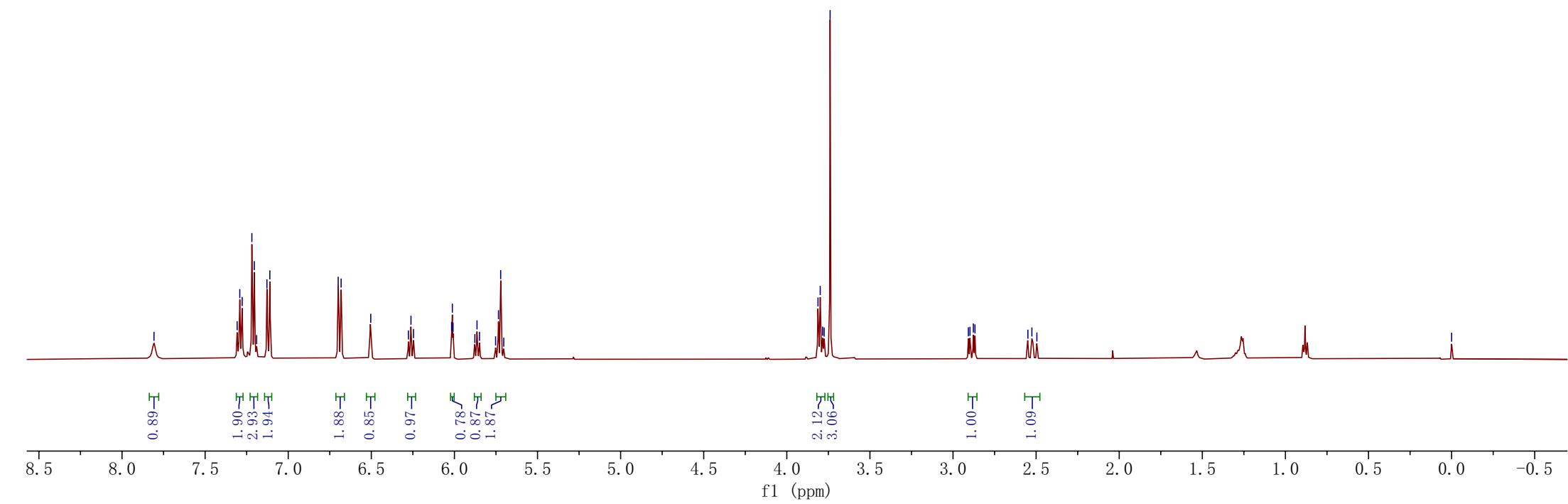
3.812  
3.799  
3.785  
3.775  
3.740



Analysis:  $^1\text{H}$  NMR

Solvent:  $\text{CDCl}_3$

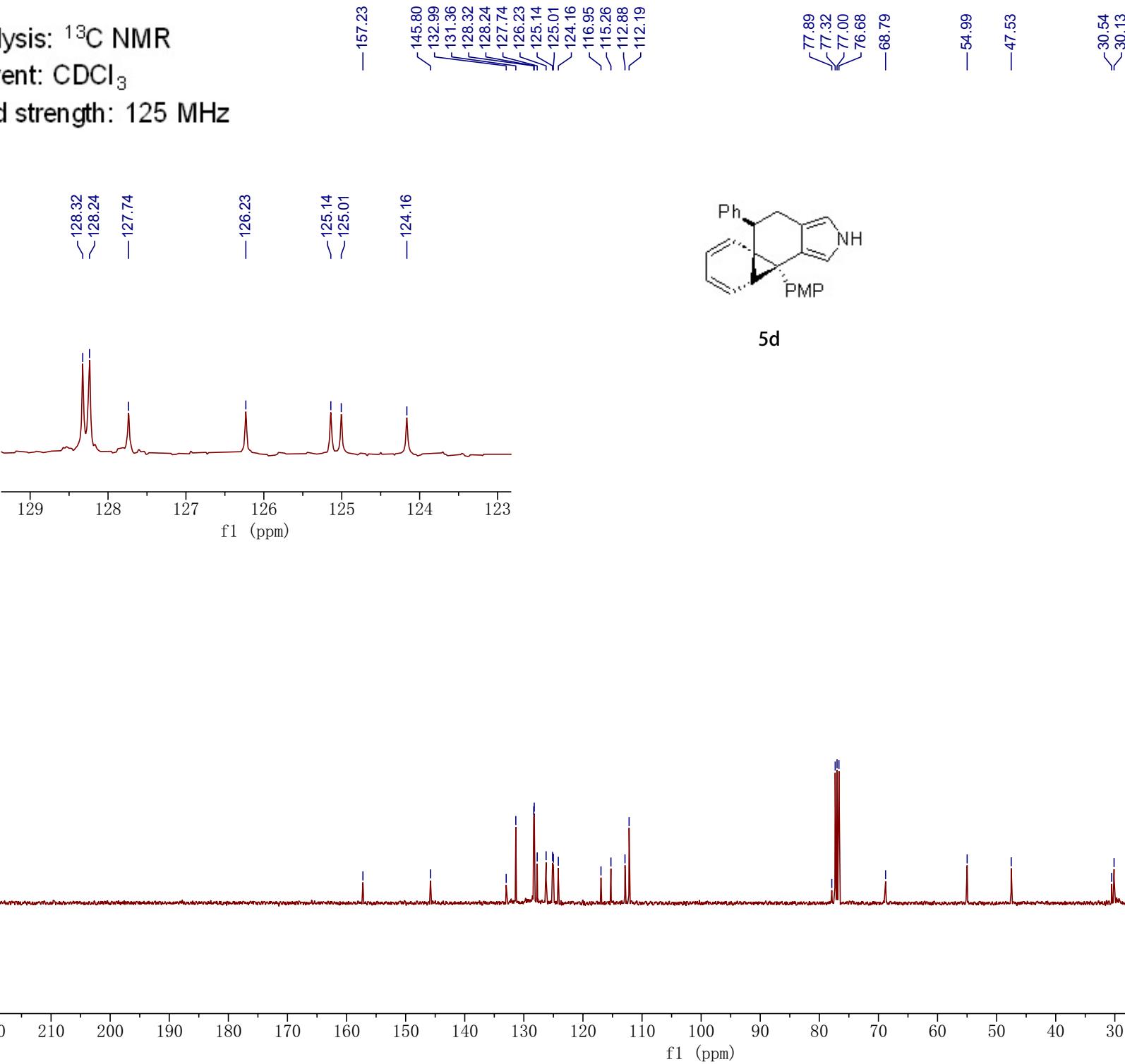
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent: CDCl<sub>3</sub>

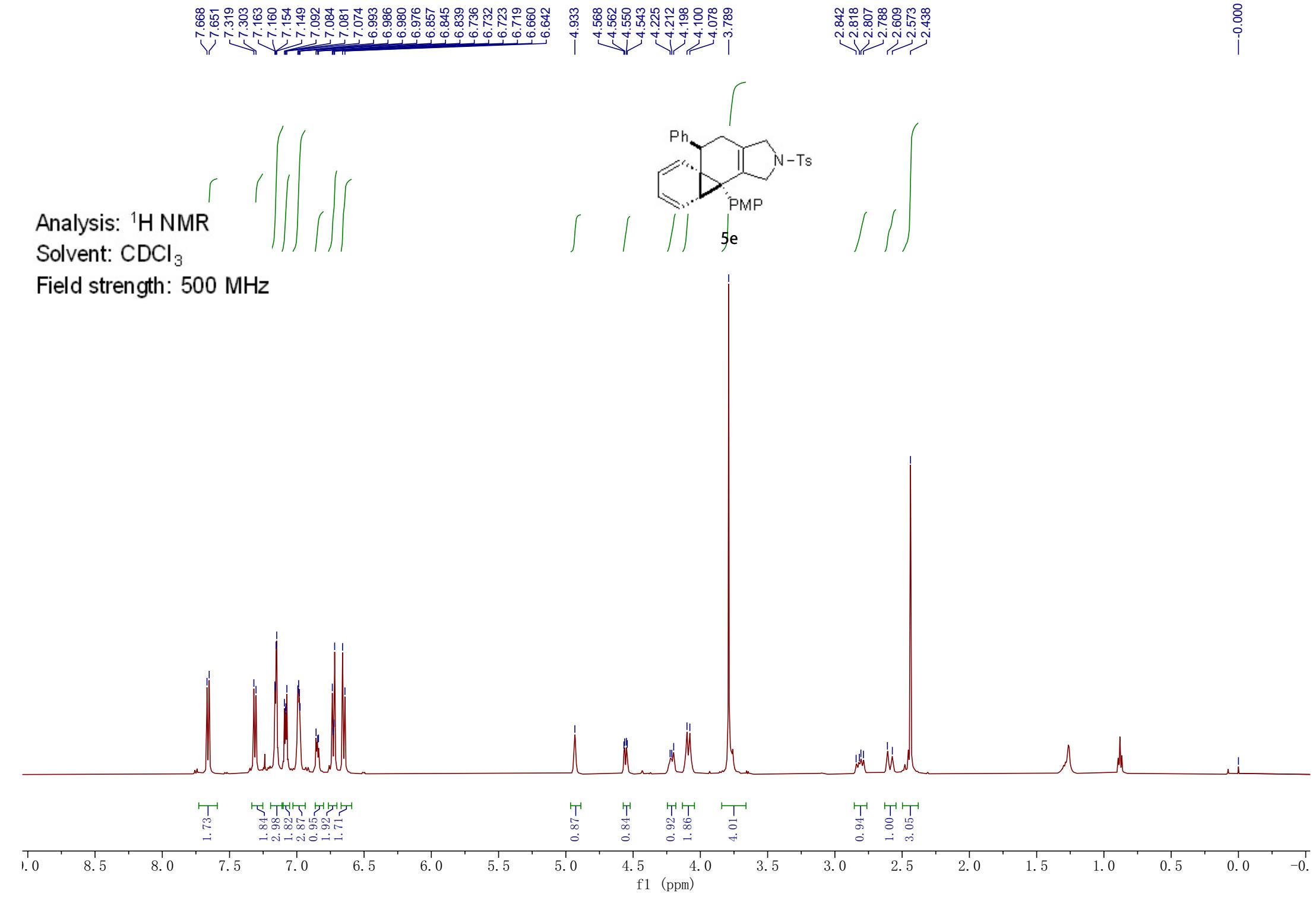
Field strength: 125 MHz



## Analysis: $^1\text{H}$ NMR

Solvent: CDCl<sub>3</sub>

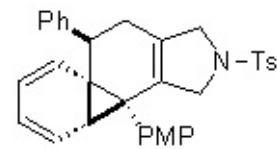
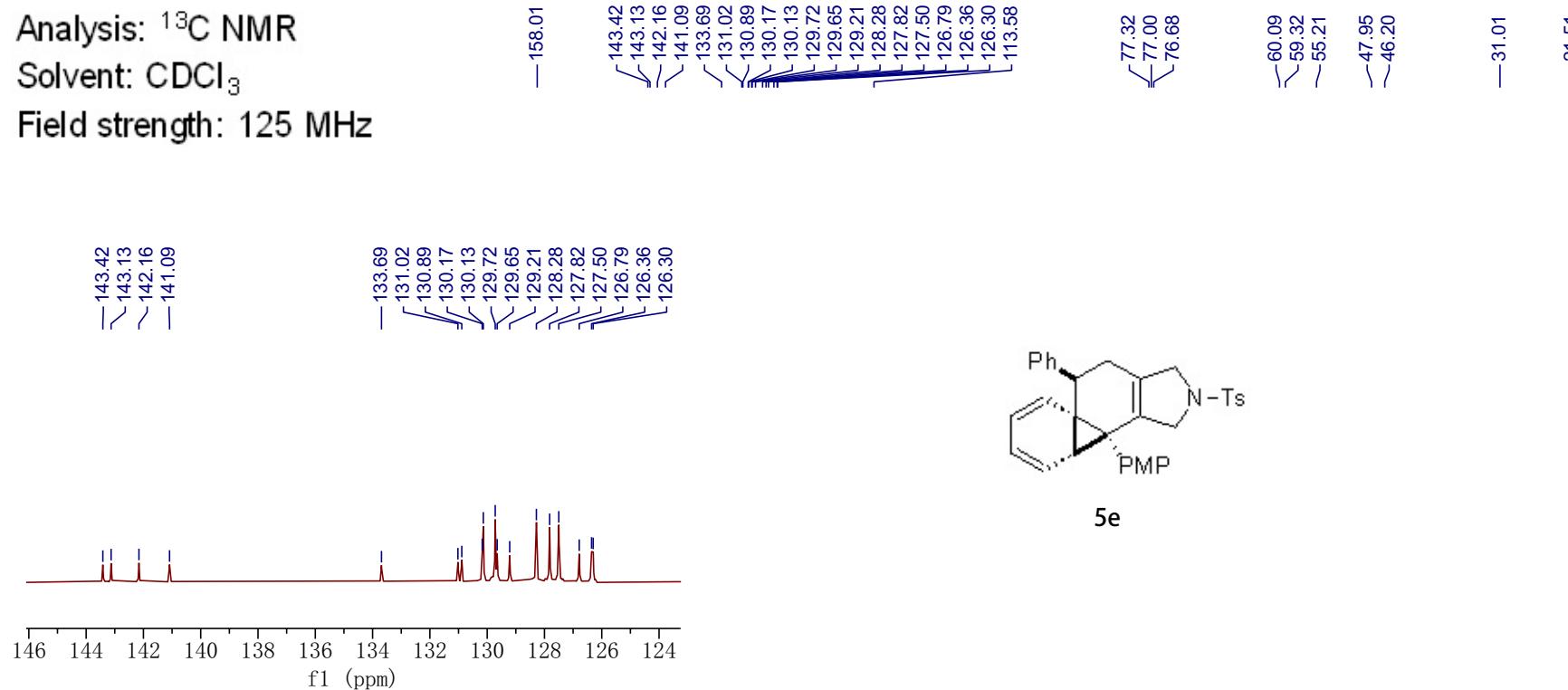
Field strength: 500 MHz



Analysis:  $^{13}\text{C}$  NMR

Solvent:  $\text{CDCl}_3$

Field strength: 125 MHz



**5e**

