Supporting Information

Copper-catalyzed enantioselective diyne cyclization via C(sp^2)–O bond cleavage

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General Information. Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1,2-dichloroethane (ACS grade) and benzotrifluoride (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 (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

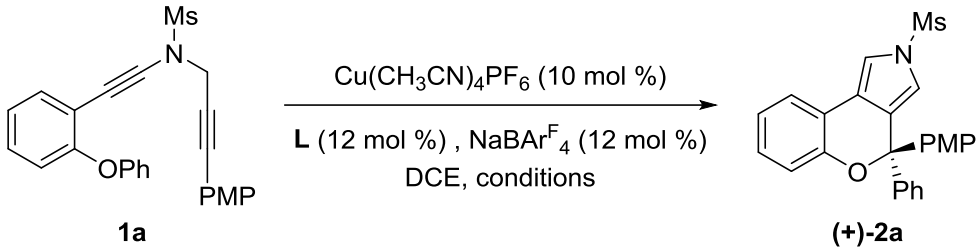
^{1}H NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved,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

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

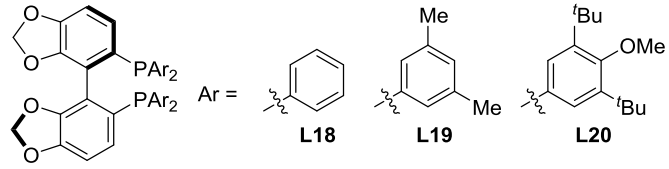
^{19}F NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d. Chemical shifts are reported in ppm.

More Reaction Condition Studies

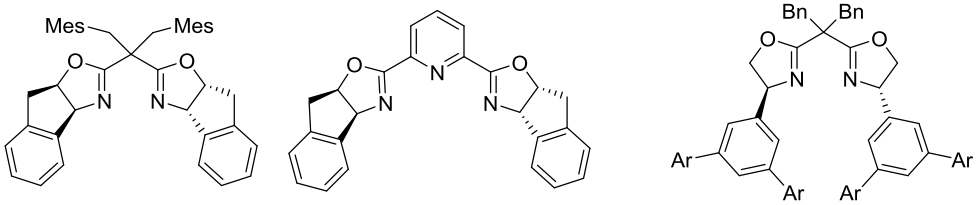
Supplementary Table 1. Other reaction condition studies for the formation of **(+)-2a**.



1a **(+)-2a**

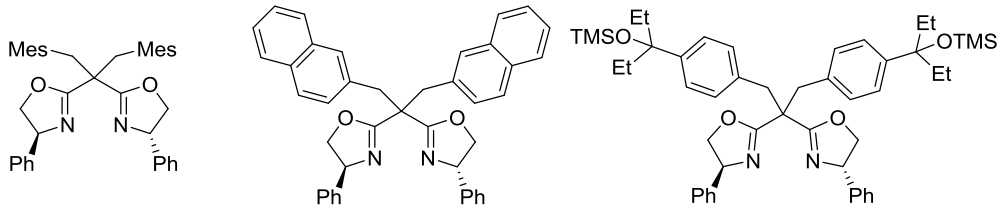


L18 **L19** **L20**



L21 **L22** **L23**

Ar = 2-naphthyl



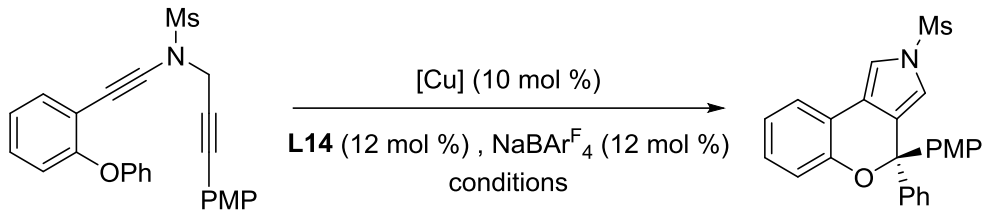
L24 **L25** **L26**

Entry	L	Conditions	Yield (%)[a]	ee (%)[b]
1	**L18**	40 °C, 10 h	72	12
2	**L19**	40 °C, 10 h	73	24
3	**L20**	40 °C, 72 h	<10	<10
4	**L21**	40 °C, 72 h	72	39
5	**L22**	40 °C, 72 h	65	<10
6	**L23**	40 °C, 96 h	52	18
7	**L24**	40 °C, 24 h	72	74
8	**L25**	40 °C, 20 h	72	59
9	**L26**	40 °C, 20 h	55	76

Reaction conditions: **1a** (0.05 mmol), $Cu(CH_3CN)_4PF_6$ (0.005 mmol), **L** (0.006 mmol), $NaBAr^F_4$ (0.006 mmol), DCE (1 mL), in vials. $NaBAr^F_4$ = sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate.

[a] Measured by ^1H NMR using 1,3,5-trimethoxybenzene as the internal standard. [b] Determined by HPLC analysis.

Supplementary Table 2. Other reaction condition studies for the formation of **(+)-2a**.

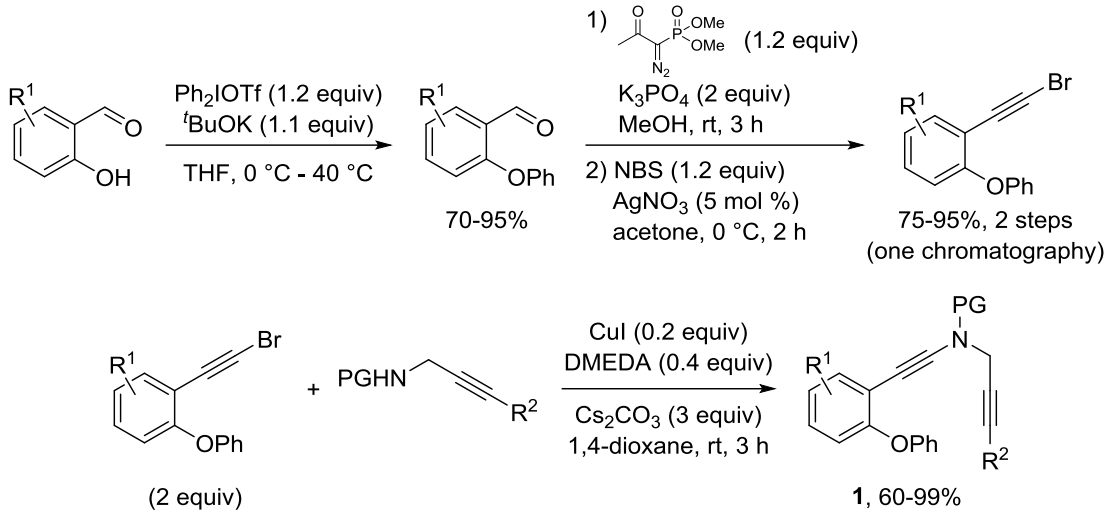


1a **(+)-2a**

Entry	Catalyst	Conditions	Yield (%)[a]	ee (%)[b]
1	$Cu(MeCN)_4PF_6$	DCE, 40 °C, 12 h	82	92
2[c]	$Cu(MeCN)_4PF_6$	DCE, 40 °C, 12 h	82	92
3[d]	$Cu(MeCN)_4PF_6$	DCE, 40 °C, 12 h	80	92
4[e]	$Cu(MeCN)_4PF_6$	DCE, 40 °C, 24 h	78	90
5	$Cu(MeCN)_4PF_6$	DCE, 30 °C, 50 h	72	93
6	$Cu(MeCN)_4PF_6$	DCM, 30 °C, 50 h	72	93
7	$Cu(MeCN)_4PF_6$	Et_2O, 30 °C, 50 h	<10	<10
8	$Cu(MeCN)_4PF_6$	PhMe, 30 °C, 50 h	74	94
9	$Cu(MeCN)_4PF_6$	PhMe, 40 °C, 12 h	82	93
10	$Cu(MeCN)_4PF_6$	*o*-xylene, 40 °C, 12 h	78	93
11	$Cu(MeCN)_4PF_6$	PhF, 40 °C, 12 h	85	92
12	$Cu(MeCN)_4PF_6$	PhCl, 40 °C, 12 h	84	92
13	$Cu(MeCN)_4PF_6$	$PhCF_3$, 40 °C, 12 h	92	94
14	$Cu(MeCN)_4BF_4$	$PhCF_3$, 40 °C, 12 h	90	93
15	CuCl	$PhCF_3$, 40 °C, 30 h	86	93
16	CuI	$PhCF_3$, 40 °C, 12 h	85	93
17	CuOTf	$PhCF_3$, 40 °C, 12 h	32	88
18	$Cu(OTf)_2$	$PhCF_3$, 40 °C, 12 h	<10	<10

Reaction conditions: **1a** (0.05 mmol), [Cu] (0.005 mmol), **L14** (0.006 mmol), NaBAr$^F_4$ (0.006 mmol), solvent (1 mL), in vials. NaBAr$^F_4$ = sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate. [a] Measured by ^1H NMR using 1,3,5-trimethoxybenzene as the internal standard. [b] Determined by HPLC analysis. [c] Using 3 Å MS (30 mg/0.1 mmol) as additive. [d] Using 4 Å MS (30 mg/0.1 mmol) as additive. [e] Using 5 Å MS (30 mg/0.1 mmol) as additive.

1. ***N*-propargyl ynamides 1a-1ab and 1ag-1ai were prepared according to the following procedures.**[1-4]



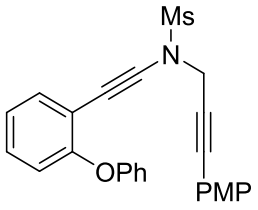
To a solution of salicylaldehyde derivative (3.0 mmol) in THF (10 mL) was added ^{t}BuOK (3.3 mmol, 370 mg) at 0 ℃ , the mixture solution was stirred at 0 ℃ for 0.5 h. Then, the Ph_2IOTf (3.6 mmol 1.55 g) was added to a stirred solution. The mixture solution was stirred at 40 ℃ for 6-10 h. The mixture was filtered, extracted by EtOAc and concentrated. The residue was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc) to afford the desired product (70-95%).[1]

To a solution of above product (2.7 mmol) in MeOH (15 mL) was added K_3PO_4 (5.4 mmol, 1.15 g) and dimethyl(1-diazo-2-oxopropyl)phosphonate (3.2 mmol, 622 mg) in sequence. The mixture solution was stirred at 25 ℃ for 3-8 h. The mixture was filtered, extracted by EtOAc and concentrated.[2] Then, NBS (3.2 mmol, 570 mg) and $AgNO_3$ (0.14 mmol, 23 mg) were added to a solution of the above crude product in acetone (15 mL) at 0 ℃ for about 1 h and the progress of the reaction was monitored by TLC. The solution was then concentrated under a reduced pressure, filtered and washed with hexanes, concentrated again under a reduced pressure to give the product without further purification (75-95%, 2 steps).[3]

To a dry flask was added CuI (0.2 mmol, 38 mg), DMEDA (0.4 mmol, 35 mg), Cs_2CO_3 (3.0 mmol, 977 mg), protected propargylamide derivative (1.0 mmol) and 1,4-dioxane (10 mL). To the mixture solution of the above product (2.0 mmol) was added. The reaction was stirred at rt for 2-6 h until the reaction was complete monitored by TLC.

Next, the mixture solution was filtered and concentrated to afford the crude product. The residue was purified by chromatography on silica gel (eluent: hexanes/EtOAc) to afford the desired product **1** (60-99%).[4]

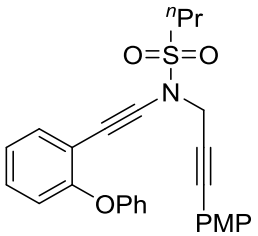
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)ethynyl)methane-sulfonamide) (1a)**



1a

The product **1a** was afforded as a pale yellow oil (90%, 388.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.32 (dd, *J* = 8.8, 1.6 Hz, 2H), 7.29 – 7.21 (m, 3H), 7.14 – 7.06 (m, 1H), 7.05 – 6.99 (m, 1H), 6.96 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.92 (dd, *J* = 8.4, 0.8 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 4.40 (s, 2H), 3.79 (s, 3H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.4, 156.9, 133.6, 133.3, 129.7, 129.6, 123.8, 122.7, 119.8, 117.6, 115.3, 114.0, 113.7, 86.9, 86.0, 80.1, 66.9, 55.2, 43.0, 38.3; IR (neat): 2961, 2932, 2838, 2239(s), 1606, 1509, 1363, 1167, 757, 518; HRESIMS Calcd for $[C_{25}H_{21}NNaO_4S]^+$ (M + Na^+) 454.1083, found 454.1072.

***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)ethynyl)propane-1-sulfonamide (1b)**

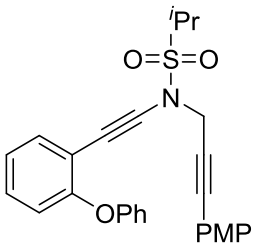


1b

The product **1b** was afforded as a pale yellow oil (99%, 459.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.28 – 7.20 (m, 3H), 7.10 – 7.05 (m, 1H), 7.05 – 6.99 (m, 1H), 6.93 (dd, *J* = 8.0, 2.8 Hz, 3H), 6.80 (d, *J* =

8.8 Hz, 2H), 4.40 (s, 2H), 3.77 (s, 3H), 3.23 – 3.13 (m, 2H), 1.93 – 1.81 (m, 2H), 0.92 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 157.3, 156.8, 133.3, 133.1, 129.5, 129.4, 123.6, 122.7, 119.5, 117.6, 115.4, 113.8(4), 113.7(5), 86.4, 86.3, 80.5, 66.6, 55.1, 53.8, 42.6, 16.7, 12.7; IR (neat): 2971, 2935, 2838, 2239(s), 1605, 1486, 1091, 753, 538; HRESIMS Calcd for $[C_{27}H_{25}NKO_4S]^+$ (M + K^+) 498.1136, found 498.1127.

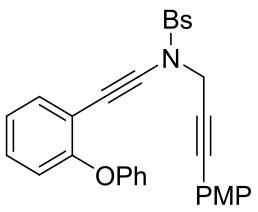
_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-_N_-((2-phenoxyphenyl)ethynyl)propane-2-sulfonamide (1c)



1c

The product **1c** was afforded as a pale yellow oil (98%, 449.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.28 – 7.20 (m, 3H), 7.11 – 7.04 (m, 1H), 7.04 – 6.98 (m, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 4.41 (s, 2H), 3.76 (s, 3H), 3.45 (hept, *J* = 6.8 Hz, 1H), 1.36 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 157.4, 156.5, 133.3, 133.1, 129.4, 129.3, 123.7, 122.5, 119.7, 117.4, 115.7, 113.9, 113.8, 86.6, 86.2, 80.6, 66.4, 55.1, 54.7, 42.6, 16.2; IR (neat): 2977, 2936, 2838, 2238(s), 1605, 1509, 1150, 757, 592; HRESIMS Calcd for $[C_{27}H_{25}NNaO_4S]^+$ (M + Na^+) 482.1397, found 482.1408.

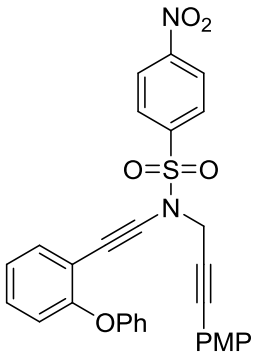
4-Bromo-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-_N_-((2-phenoxyphenyl)ethynyl)benzenesulfonamide (1d)



1d

The product **1d** was afforded as a pale yellow oil (85%, 485.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.6 Hz, 2H), 7.45 (d, *J* = 6.8 Hz, 1H), 7.41 – 7.18 (m, 5H), 7.17 – 6.84 (m, 7H), 6.75 (d, *J* = 7.6 Hz, 2H), 4.44 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 157.4, 157.2, 136.2, 133.5, 133.1, 132.0, 129.8, 129.7, 129.5, 128.9, 123.4, 123.3, 118.9, 118.5, 114.9, 113.9, 113.8, 86.9, 85.8, 79.4, 67.1, 55.3, 43.3; IR (neat): 2956, 2933, 2838, 2239(s), 1605, 1509, 1174, 750. 607; HRESIMS Calcd for $[C_{30}H_{22}BrNNaO_4S]^+$ (M + Na^+) 594.0345, found 594.0327.

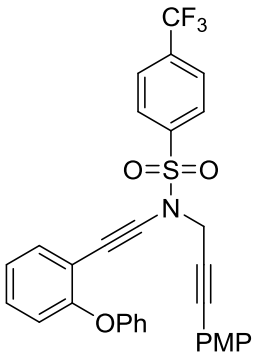
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-nitro-*N*-((2-phenoxyphenyl)ethynyl)-benzenesulfonamide (1e)**



1e

The product **1e** was afforded as a pale yellow oil (72%, 387.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.8 Hz, 2H), 7.93 (d, *J* = 8.8 Hz, 2H), 7.47 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.29 – 7.21 (m, 1H), 7.18 – 7.10 (m, 1H), 7.10 – 7.03 (m, 1H), 7.01 – 6.91 (m, 4H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 8.8 Hz, 2H), 4.50 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.6, 157.0, 150.1, 142.5, 133.5, 132.9, 129.9, 129.8, 129.4, 123.7, 123.5, 123.4, 118.7, 118.5, 114.4, 113.8, 113.2, 87.2, 85.0, 79.2, 67.3, 55.2, 43.6; IR (neat): 3104, 2925, 2839, 2240(s), 1606, 1509, 1177, 1032, 752, 612; HRESIMS Calcd for $[C_{30}H_{22}N_2NaO_6S]^+$ (M + Na^+) 561.1091, found 561.1077.

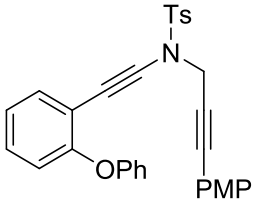
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)ethynyl)-4-(trifluoromethyl)benzenesulfonamide (1f)**



1f

The product **1f** was afforded as a pale yellow oil (93%, 522.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 2H), 7.46 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.35 – 7.26 (m, 2H), 7.26 – 7.18 (m, 1H), 7.14 – 7.07 (m, 1H), 7.07 – 7.00 (m, 1H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.69 (d, *J* = 8.8 Hz, 2H), 4.47 (s, 2H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 157.5, 157.1, 140.6, 134.6 (q, *J* = 33.0 Hz), 133.4, 132.9, 129.7, 129.6, 128.7, 125.7 (q, *J* = 3.0 Hz), 123.3, 123.0 (q, *J* = 271.0 Hz), 118.7, 118.5, 114.6, 113.7, 113.4, 87.0, 85.4, 79.1, 67.0, 55.1, 43.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3; IR (neat): 3059, 2936, 2839, 2240(s), 1607, 1487, 922, 753, 606; HRESIMS Calcd for $[C_{31}H_{22}F_3NNaO_4S]^+$ (M + Na^+) 584.1114, found 584.1101.

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

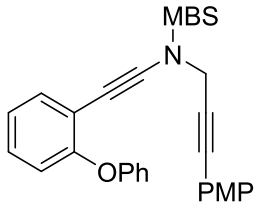


1g

The product **1g** was afforded as a pale yellow oil (85%, 431.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 6.0 Hz, 2H), 7.44 (d, *J* = 6.0 Hz, 1H), 7.38 – 7.15 (m, 3H), 7.15 – 6.99 (m, 6H), 6.99 – 6.81 (m, 3H), 6.72 (d, *J* = 6.0 Hz, 2H), 4.39 (s, 2H), 3.76 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 157.2, 144.5, 134.2, 133.3, 133.0, 129.6, 129.3, 129.1, 128.1, 123.2, 123.0, 118.8, 118.5, 115.2, 114.1, 113.6, 86.4, 86.3,

79.7, 66.8, 55.2, 42.9, 21.4; IR (neat): 3063, 2933, 2838, 2238(s), 1606, 1509, 1486, 1170, 754, 589; HRESIMS Calcd for $[C_{31}H_{25}NNaO_4S]^+$ (M + Na^+) 530.1397, found 530.1382.

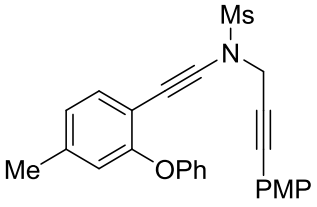
4-methoxy-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)-ethynyl)benzenesulfonamide (1h)



1h

The product **1h** was afforded as a pale yellow oil (75%, 392.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.8 Hz, 2H), 7.44 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.30 (dd, *J* = 8.4, 7.6 Hz, 2H), 7.23 – 7.15 (m, 1H), 7.12 – 7.00 (m, 4H), 6.97 (d, *J* = 7.6 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 1H), 6.71 (d, *J* = 8.8 Hz, 2H), 6.67 (d, *J* = 8.8 Hz, 2H), 4.39 (s, 2H), 3.76 (s, 3H), 3.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5, 159.6, 157.2(3), 157.1(9), 133.3, 133.1, 130.4, 129.6, 129.1, 128.7, 123.2, 123.1, 118.7, 118.6, 115.2, 114.1, 113.9, 113.6, 86.5, 86.3, 79.8, 66.8, 55.3, 55.2, 42.9; IR (neat): 2966, 2839, 2237(s), 1595, 1509, 1367, 1164, 833, 590, 558; HRESIMS Calcd for $[C_{31}H_{25}NNaO_5S]^+$ (M + Na^+) 546.1346, found 546.1334.

***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((4-methyl-2-phenoxyphenyl)-ethynyl)methanesulfonamide (1i)**

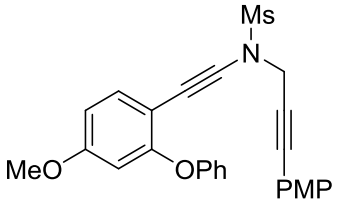


1i

The product **1i** was afforded as a pale yellow oil (99%, 441.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.26 – 7.19 (m, 2H), 7.03

– 6.96 (m, 1H), 6.94– 6.87 (m, 3H), 6.79 (d, *J* = 8.8 Hz, 3H), 4.37 (s, 2H), 3.77 (s, 3H), 2.96 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 157.4, 156.7, 140.5, 133.4, 133.2, 129.5, 124.7, 122.5, 120.4, 117.4, 113.8, 113.6, 112.1, 86.7, 85.2, 80.1, 66.8, 55.1, 42.9, 38.0, 21.3; IR (neat): 2958, 2931, 2839, 2241(s), 1606, 1360, 1166, 964, 738, 518; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1224.

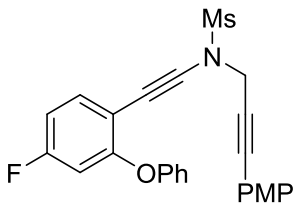
_N_-((4-methoxy-2-phenoxyphenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1j)



1j

The product **1j** was afforded as a pale yellow oil (60%, 276.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.28 – 7.18 (m, 2H), 7.06 – 6.97 (m, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 6.64 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.50 (d, *J* = 2.4 Hz, 1H), 4.39 (s, 2H), 3.77 (s, 3H), 3.71 (s, 3H), 2.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 159.9, 158.4, 157.0, 134.8, 133.1, 129.5, 122.7, 117.6, 113.8, 113.6, 109.5, 106.9, 105.7, 86.6, 84.5, 80.2, 66.5, 55.3, 55.1, 42.9, 37.8; IR (neat): 3010, 2934, 2839, 2242(s), 1608, 1509, 1362, 1031, 834, 525; HRESIMS Calcd for $[C_{26}H_{23}NNaO_5S]^+$ (M + Na^+) 484.1189, found 484.1179.

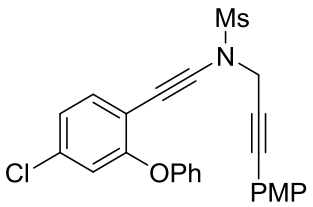
_N_-((4-fluoro-2-phenoxyphenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1k)



1k

The product **1k** was afforded as a pale yellow oil (83%, 373.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 8.8, 6.4 Hz, 1H), 7.35 – 7.24 (m, 4H), 7.12 – 7.05 (m, 1H), 6.96 (d, *J* = 7.6 Hz, 2H), 6.78 (d, *J* = 8.8 Hz, 3H), 6.61 (dd, *J* = 9.6, 2.4 Hz, 1H), 4.43 (s, 2H), 3.77 (s, 3H), 3.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 249.0 Hz), 159.9, 158.8 (d, *J* = 11.0 Hz), 156.2, 134.8 (d, *J* = 10.0 Hz), 133.1, 129.7, 123.7, 118.4, 113.9, 113.5, 110.5(1) (d, *J* = 3.0 Hz), 110.4(9) (d, *J* = 22.0 Hz), 106.4 (d, *J* = 25.0 Hz), 86.8, 85.5, 80.0, 65.9, 55.1, 42.8, 38.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.6; IR (neat): 3012, 2933, 2838, 2243(s), 1605, 1505, 1034, 834, 517; HRESIMS Calcd for $[C_{25}H_{20}FNNaO_4S]^+$ (M + Na^+) 472.0989, found 472.0976.

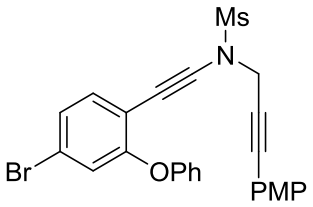
***N*-((4-chloro-2-phenoxyphenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1l)**



1l

The product **1l** was afforded as a pale yellow oil (91%, 424.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.0 Hz, 1H), 7.35 – 7.25 (m, 4H), 7.10 (d, *J* = 7.6 Hz, 1H), 7.06 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 1.6 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 2H), 4.43 (s, 2H), 3.80 (s, 3H), 3.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.9, 156.4, 134.9, 134.2, 133.3, 129.8, 123.8, 123.6, 119.3, 118.3, 114.0, 113.6, 113.4, 87.0, 86.7, 80.0, 66.2, 55.2, 43.0, 38.4; IR (neat): 3012, 2932, 2838, 2241(s), 1606, 1486, 1363, 1034, 929, 515; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0675.

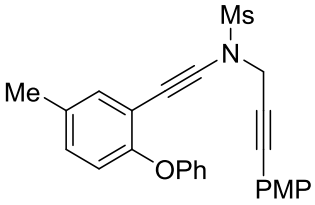
***N*-((4-bromo-2-phenoxyphenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1m)**



1m

The product **1m** was afforded as a pale yellow oil (76%, 387.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 5H), 7.21 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.12 – 7.07 (m, 1H), 7.06 (d, *J* = 2.0 Hz, 1H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 4.43 (s, 2H), 3.79 (s, 3H), 3.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.8, 156.5, 134.3, 133.3, 129.8, 126.7, 123.6, 122.6, 122.2, 118.3, 114.0, 113.6, 87.0, 86.9, 80.0, 66.3, 55.2, 42.9, 38.4; IR (neat): 2961, 2930, 2838, 2240(s), 1606, 1509, 1364, 1166, 923, 833; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_4S]^+$ (M + Na^+) 532.0189, found 532.0196.

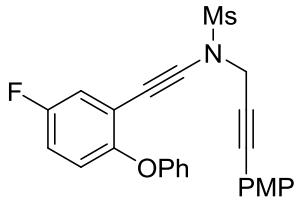
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((5-methyl-2-phenoxyphenyl)ethynyl)-methanesulfonamide (1n)**



1n

The product **1n** was afforded as a pale yellow oil (90%, 401.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.8 Hz, 2H), 7.30 (d, *J* = 1.6 Hz, 1H), 7.25 – 7.16 (m, 2H), 7.07 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.00 – 6.94 (m, 1H), 6.88 (d, *J* = 8.4 Hz, 3H), 6.80 (d, *J* = 8.8 Hz, 2H), 4.36 (s, 2H), 3.78 (s, 3H), 2.95 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 157.8, 154.2, 133.8, 133.6, 133.2, 130.4, 129.4, 122.2, 120.2, 117.0, 115.1, 113.9, 113.7, 86.8, 85.7, 80.1, 67.0, 55.1, 42.9, 38.1, 20.4; IR (neat): 2957, 2930, 2838, 2243(s), 1606, 1487, 1363, 1035, 833, 521; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1233.

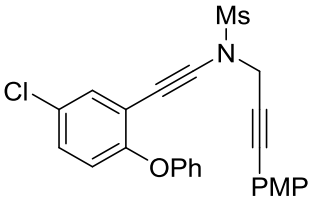
***N*-((5-fluoro-2-phenoxyphenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1o)**



1o

The product **1o** was afforded as a pale yellow oil (82%, 368.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.8 Hz, 2H), 7.28 – 7.21 (m, 2H), 7.18 (dd, *J* = 8.4, 2.8 Hz, 1H), 7.05 – 6.92 (m, 3H), 6.92 – 6.86 (m, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.37 (s, 2H), 3.79 (s, 3H), 2.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 158.4 (d, *J* = 243.0 Hz), 157.6, 152.5 (d, *J* = 2.0 Hz), 133.3, 129.6, 122.6, 121.6 (d, *J* = 8.0 Hz), 119.4 (d, *J* = 25.0 Hz), 117.1 (d, *J* = 11.0 Hz), 117.0, 116.4 (d, *J* = 23.0 Hz), 113.9, 113.6, 87.0, 86.9, 79.9, 66.2 (d, *J* = 3.0 Hz) , 55.2, 42.9, 38.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.5; IR (neat): 2931, 2839, 2245(s), 1606, 1510, 1486, 1250, 1167, 833, 522; HRESIMS Calcd for $[C_{25}H_{20}FNNaO_4S]^+$ (M + Na^+) 472.0989, found 472.0984.

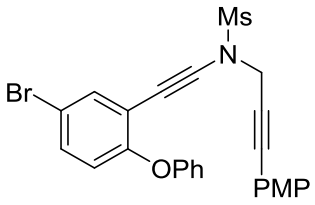
***N*-((5-chloro-2-phenoxyphenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1p)**



1p

The product **1p** was afforded as a pale yellow oil (87%, 405.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 2.4 Hz, 1H), 7.32 (d, *J* = 8.8 Hz, 2H), 7.30 – 7.26 (m, 2H), 7.22 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.08 – 7.02 (m, 1H), 6.92 (d, *J* = 7.6 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 1H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.41 (s, 2H), 3.81 (s, 3H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 157.1, 155.5, 133.3, 132.8, 129.7, 129.5, 128.7, 123.2, 120.8, 117.8, 116.9, 114.0, 113.7, 87.2, 87.0, 79.9, 66.2, 55.3, 43.0, 38.6; IR (neat): 3012, 2931, 2838, 2240(s), 1606, 1509, 1364, 1167, 834, 518; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0692.

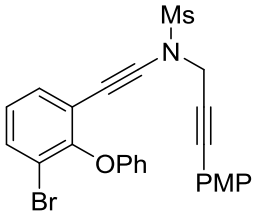
***N*-((4-methoxy-2-phenoxyphenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1q)**



1q

The product **1q** was afforded as a pale yellow oil (60%, 306.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 2.4 Hz, 1H), 7.35 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.32 (d, *J* = 8.8 Hz, 2H), 7.30 – 7.21 (m, 2H), 7.09 – 7.01 (m, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.81 (dd, *J* = 8.8, 2.4 Hz, 3H), 4.40 (s, 2H), 3.80 (s, 3H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 156.9, 156.0, 135.7, 133.3, 132.4, 129.7, 123.2, 121.0, 117.8, 117.2, 115.9, 114.0, 113.6, 87.3, 87.0, 79.9, 66.0, 55.2, 42.9, 38.5; IR (neat): 2931, 2838, 2239(s), 1606, 1509, 1480, 1364, 1167, 834, 518; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_4S]^+$ (M + Na^+) 532.0189, found 532.0177.

***N*-((3-bromo-2-phenoxyphenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1r)**

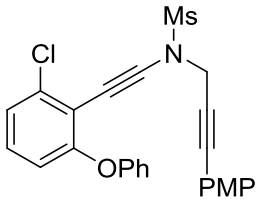


1r

The product **1r** was afforded as a pale yellow oil (62%, 316.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.44 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.35 (d, *J* = 8.8 Hz, 2H), 7.22 – 7.14 (m, 2H), 7.09 – 7.02 (m, 1H), 6.98 – 6.91 (m, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 4.28 (s, 2H), 3.79 (s, 3H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.1, 151.9, 133.4, 133.3, 132.3, 129.4, 126.1, 122.0, 119.2, 117.8, 115.1, 114.0, 113.5, 87.3, 86.8, 79.9, 66.2, 55.2, 42.8, 38.3; IR (neat):

3012, 2931, 2838, 2238(s), 1606, 1509, 1363, 1167, 1034, 752; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_4S]^+$ (M + Na^+) 532.0189, found 532.0181.

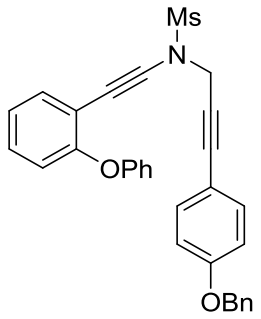
_N_-((2-chloro-6-phenoxyphenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1s)



1s

The product **1s** was afforded as a pale yellow oil (67%, 312.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.25 (m, 4H), 7.21 – 7.11 (m, 2H), 7.10 – 7.04 (m, 1H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.88 – 6.74 (m, 3H), 4.44 (s, 2H), 3.78 (s, 3H), 3.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 158.0, 156.6, 137.0, 133.3, 129.7, 129.0, 124.2, 123.4, 118.2, 117.1, 115.5, 113.9, 113.6, 91.0, 86.9, 79.9, 64.7, 55.2, 43.0, 38.5; IR (neat): 2931, 2838, 2239(s), 1606, 1509, 1480, 1364, 1167, 834, 518; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0692.

_N_-((5-bromo-2-phenoxyphenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1t)

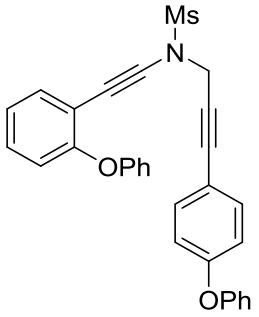


1t

The product **1t** was afforded as a pale yellow oil (77%, 390.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.2 Hz, 1H), 7.45 – 7.15 (m, 10H), 7.15 – 7.05 (m, 1H), 7.05 – 6.94 (m, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 8.0 Hz, 2H), 5.06 (s, 2H), 4.39 (s, 2H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 157.4, 156.9, 136.4, 133.6,

133.3, 129.7, 129.6, 128.6, 128.1, 127.4, 123.8, 122.8, 119.8, 117.7, 115.3, 114.9, 114.1, 86.8, 86.0, 80.2, 70.0, 67.0, 43.0, 38.3; IR (neat): 2927, 2239(s), 1604, 1508, 1485, 1363, 1232, 1167, 1037, 755; HRESIMS Calcd for $[C_{31}H_{25}NNaO_4S]^+$ (M + Na^+) 530.1397, found 530.1391.

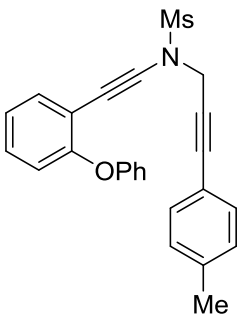
_N_-((2-phenoxyphenyl)ethynyl)-_N_-(3-(4-phenoxyphenyl)prop-2-yn-1-yl)methane-sulfonamide (1u)



1u

The product **1u** was afforded as a pale yellow oil (97%, 480.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.6 Hz, 1H), 7.39 – 7.28 (m, 4H), 7.27 – 7.17 (m, 3H), 7.15 – 7.08 (m, 1H), 7.08 – 7.02 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 3H), 6.91 (d, *J* = 8.0 Hz, 3H), 6.86 (d, *J* = 8.4 Hz, 2H), 4.38 (s, 2H), 2.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 157.1, 156.7, 155.8, 133.4, 133.3, 129.7, 129.6, 129.4, 123.9, 123.6, 122.6, 119.5, 119.3, 117.9, 117.5, 115.9, 115.0, 86.2, 85.9, 80.8, 66.9, 42.6, 38.0; IR (neat): 3064, 3040, 2929, 2239(s), 1588, 1488, 1364, 1167, 869, 757; HRESIMS Calcd for $[C_{30}H_{23}NNaO_4S]^+$ (M + Na^+) 516.1240, found 516.1224.

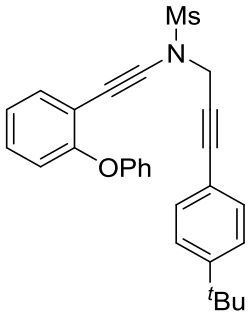
_N_-((2-phenoxyphenyl)ethynyl)-_N_-(3-(*p*-tolyl)prop-2-yn-1-yl)methanesulfonamide (1v)



1v

The product **1v** was afforded as a pale yellow oil (99%, 413.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.34 – 7.20 (m, 5H), 7.14 – 7.06 (m, 3H), 7.06 – 6.99 (m, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 2H), 4.40 (s, 2H), 3.00 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 156.9, 139.1, 133.6, 131.7, 129.7, 129.6, 129.1, 123.8, 122.7, 119.9, 118.7, 117.6, 115.3, 87.0, 86.0, 80.8, 67.0, 42.9, 38.3, 21.5; IR (neat): 3029, 2927, 2239(s), 1589, 1486, 11363, 1232, 1166, 757, 518; HRESIMS Calcd for $[C_{25}H_{21}NNaO_3S]^+$ (M + Na^+) 438.1134, found 438.1149.

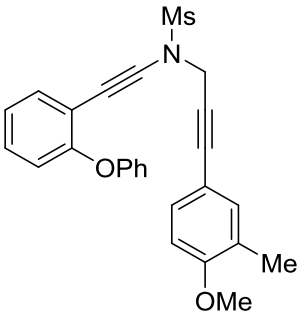
***N*-(3-(4-(*tert*-butyl)phenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)ethynyl)-methanesulfonamide (1w)**



1w

The product **1w** was afforded as a pale yellow oil (92%, 421.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.38 – 7.28 (m, 4H), 7.28 – 7.18 (m, 3H), 7.12 – 7.04 (m, 1H), 7.04 – 6.97 (m, 1H), 6.95 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.93 – 6.87 (m, 2H), 4.39 (s, 2H), 3.00 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 156.8, 152.2, 133.5, 131.5, 129.6, 129.5, 125.3, 123.7, 122.7, 119.7, 118.6, 117.6, 115.2, 86.9, 86.0, 80.8, 66.9, 42.8, 38.2, 34.7, 31.0; IR (neat): 2963, 2869, 2240(s), 1590, 1486, 1366, 1232, 1168, 756, 564; HRESIMS Calcd for $[C_{28}H_{27}NNaO_3S]^+$ (M + Na^+) 480.1604, found 480.1589.

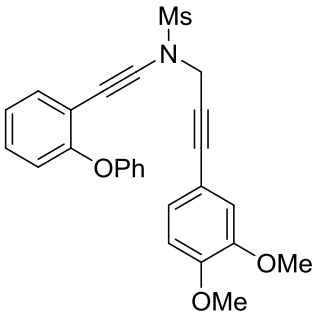
***N*-(3-(3,4-dimethoxyphenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)ethynyl)-methanesulfonamide (1x)**



1x

The product **1x** was afforded as a pale yellow oil (95%, 432.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.29 – 7.20 (m, 4H), 7.19 – 7.14 (m, 1H), 7.12 – 7.04 (m, 1H), 7.04 – 6.97 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 8.4 Hz, 1H), 4.38 (s, 2H), 3.79 (s, 3H), 2.99 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 157.3, 156.7, 133.8, 133.5, 130.9, 129.6, 129.5, 126.7, 123.7, 122.6, 119.7, 117.5, 115.3, 113.1, 109.6, 87.1, 86.1, 79.7, 66.8, 55.2, 42.9, 38.2, 15.9; IR (neat): 2929, 2837, 2238(s), 1604, 1502, 1363, 1241, 1167, 756, 517; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1222.

***N*-(3-(3,4-dimethoxyphenyl)prop-2-yn-1-yl)-*N*-((2-phenoxyphenyl)ethynyl)-methanesulfonamide (1y)**

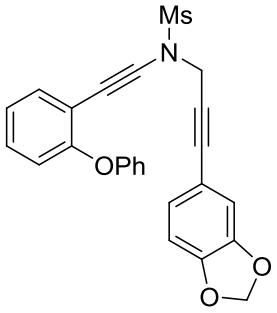


1y

The product **1y** was afforded as a pale yellow oil (96%, 443.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.32 – 7.19 (m, 3H), 7.14 – 7.05 (m, 1H), 7.05 – 6.98 (m, 2H), 6.96 (d, *J* = 8.4 Hz, 1H), 6.94 – 6.87 (m, 3H), 6.76 (d, *J* = 8.4 Hz, 1H), 4.40 (s, 2H), 3.86 (s, 3H), 3.81 (s, 3H), 2.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 156.6, 149.8, 148.4, 133.4, 129.6, 129.4, 125.1, 123.7, 122.6, 119.7, 117.4, 115.2, 114.2, 113.6, 110.8, 86.9, 86.0, 79.9, 66.8, 55.6, 42.7, 38.1; IR (neat): 2927, 2239(s),

1604, 1508, 1485, 1363, 1232, 1167, 1037, 755; IR (neat): 2933, 2837, 2238(s), 1598, 1514, 1486, 1363, 1167, 1025, 760; HRESIMS Calcd for $[C_{26}H_{23}NNaO_5S]^+$ (M + Na^+) 484.1189, found 484.1197.

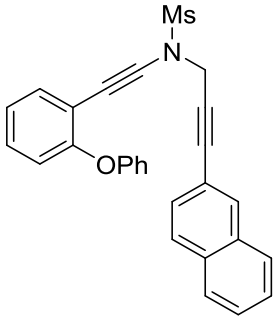
_N_-(3-(benzo[_d_][1,3]dioxol-5-yl)prop-2-yn-1-yl)-_N_-((2-phenoxyphenyl)ethynyl)-methanesulfonamide (1z)



1z

The product **1z** was afforded as a pale yellow oil (92%, 409.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.31 – 7.21 (m, 3H), 7.13 – 7.05 (m, 1H), 7.05 – 6.98 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.93 – 6.86 (m, 3H), 6.81 (d, *J* = 1.6 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 5.94 (s, 2H), 4.38 (s, 2H), 2.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 156.8, 148.3, 147.3, 133.5, 129.6, 129.5, 126.5, 123.7, 122.7, 119.7, 117.5, 115.2, 114.7, 111.5, 108.3, 101.3, 86.7, 85.9, 79.8, 66.9, 42.8, 38.1; IR (neat): 3014, 2902, 2239(s), 1589, 1487, 1360, 1038, 924, 757, 518; HRESIMS Calcd for $[C_{25}H_{19}NNaO_5S]^+$ (M + Na^+) 468.0876, found 468.0891.

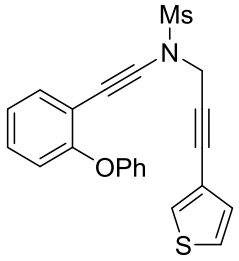
_N_-(3-(naphthalen-2-yl)prop-2-yn-1-yl)-_N_-((2-phenoxyphenyl)ethynyl)-methanesulfonamide (1aa)



1aa

The product **1aa** was afforded as a pale yellow oil (89%, 401.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.89 (m, 1H), 7.85 – 7.79 (m, 1H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.57 – 7.46 (m, 3H), 7.42 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.32 – 7.25 (m, 1H), 7.23 – 7.17 (m, 2H), 7.14 – 7.07 (m, 1H), 7.02 – 6.95 (m, 2H), 6.95 – 6.88 (m, 2H), 4.47 (s, 2H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 157.0, 133.7, 133.0, 132.8, 132.0, 129.8, 129.6, 128.2, 128.1, 127.8, 127.7, 127.0, 126.7, 123.8, 122.8, 119.8, 119.0, 117.6, 115.3, 87.2, 86.0, 81.8, 67.1, 43.0, 38.4; IR (neat): 3062, 3014, 2901, 2239(s), 1589, 1445, 1360, 1167, 757, 518; HRESIMS Calcd for $[C_{28}H_{21}NNaO_3S]^+$ (M + Na^+) 474.1134, found 474.1123.

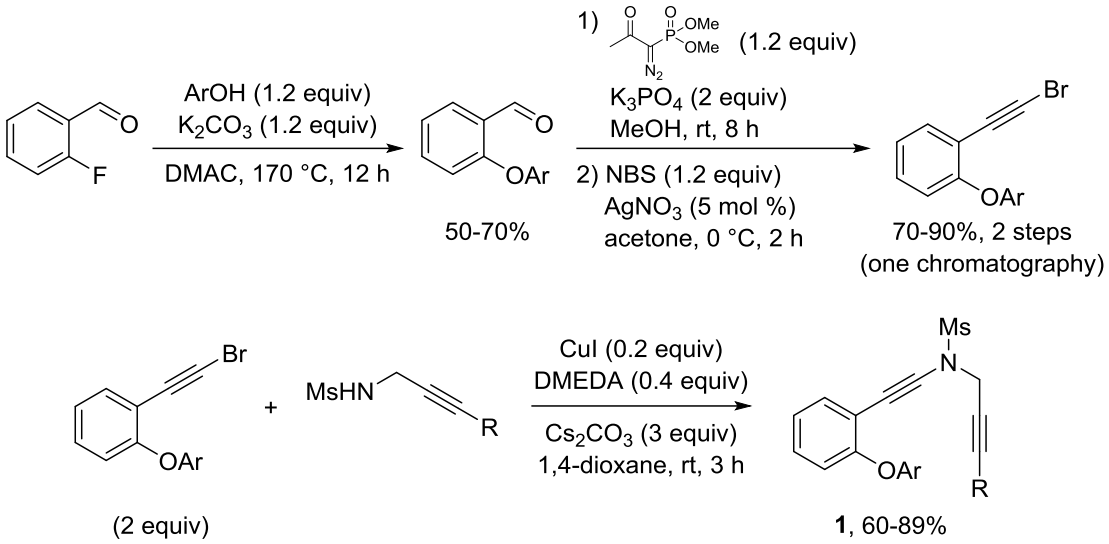
***N*-((2-phenoxyphenyl)ethynyl)-*N*-(3-(thiophen-3-yl)prop-2-yn-1-yl)-methanesulfonamide (1ab)**



1ab

The product **1ab** was afforded as a pale yellow oil (99%, 403.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.41 – 7.35 (m, 1H), 7.31 – 7.18 (m, 4H), 7.11 – 7.05 (m, 1H), 7.05 – 6.97 (m, 2H), 6.97 – 6.93 (m, 1H), 6.90 (d, *J* = 7.6 Hz, 2H), 4.37 (s, 2H), 2.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 156.6, 133.4, 129.8, 129.6(3), 129.5(7), 129.5, 125.5, 123.7, 122.6, 120.6, 119.7, 117.4, 115.1, 85.9, 81.9, 81.1, 66.9, 42.7, 38.1; IR (neat): 3109, 3021, 2929, 2240(s), 1589, 1486, 1362, 1166, 757, 515; HRESIMS Calcd for $[C_{22}H_{17}NNaO_3S_2]^+$ (M + Na^+) 430.0542, found 430.0527.

2. *N*-propargyl ynamides 1ac-1af were prepared according to the following procedures.[2-5]



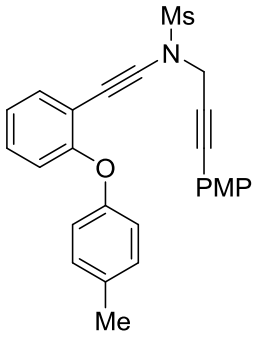
To a solution of 2-fluorobenzaldehyde (5.0 mmol, 621 mg) in DMAC (7.5 mL) was added K_2CO_3 (6 mmol, 830 mg) and ArOH (6.0 mmol) at rt , the mixture solution was stirred at 170 ℃ for 12 h. The mixture was filtered, extracted by EtOAc and concentrated. The residue was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc) to afford the desired product (50-70%).[5]

To a solution of above product (2.7 mmol) in MeOH (15 mL) was added K_3PO_4 (5.4 mmol, 1.15 g) and dimethyl(1-diazo-2-oxopropyl)phosphonate (3.2 mmol, 622 mg) in sequence. The mixture solution was stirred at 25 ℃ for 3-8 h. The mixture was filtered, extracted by EtOAc and concentrated.[2] Then, NBS (3.2 mmol, 577 mg) and $AgNO_3$ (0.14 mmol, 23 mg) were added to a solution of the above crude product in acetone (15 mL) at 0 ℃ for about 1 h and the progress of the reaction was monitored by TLC. The solution was then concentrated under a reduced pressure, filtered and washed with hexanes, concentrated again under a reduced pressure to give the product without further purification (70-90%, 2 steps).[3]

To a dry flask was added CuI (0.2 mmol, 38 mg), DMEDA (0.4 mmol, 35 mg), Cs_2CO_3 (3 mmol, 977 mg), protected propargylamide derivative (1.0 mmol) and 1,4-dioxane (8 mL). To the mixture solution of the above product (2.0 mmol) was added. The reaction was stirred at rt for 2-6 h until the reaction was complete monitored by TLC. Next, the mixture solution was filtered and concentrated to afford the crude solid. The residue

was purified by chromatography on silica gel (eluent: hexanes/EtOAc) to afford the desired product **1** (60-89%).[4]

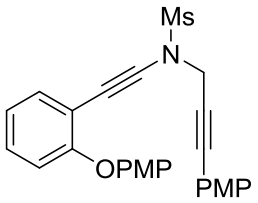
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-*N*-((2-(*p*-tolyloxy)phenyl)ethynyl)-methanesulfonamide (1ac)**



1ac

The product **1ac** was afforded as a pale yellow oil (89%, 396.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.27 – 7.19 (m, 1H), 7.09 – 7.00 (m, 3H), 6.89 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.84 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.8 Hz, 2H), 4.43 (s, 2H), 3.78 (s, 3H), 3.06 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.6, 154.9, 133.5, 133.2, 132.4, 130.0, 129.6, 123.2, 118.9, 118.0, 114.7, 113.9, 113.7, 86.8, 85.8, 80.1, 67.1, 55.2, 42.9, 38.2, 20.5; IR (neat): 2957, 2930, 2839, 2240(s), 1606, 1505, 1360, 1166, 1034, 775; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1253.

***N*-((2-(4-methoxyphenoxy)phenyl)ethynyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1ad)**

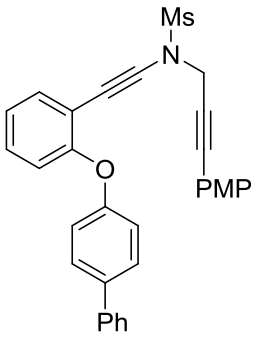


1ad

The product **1ad** was afforded as a pale yellow oil (60%, 276.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.24 – 7.17 (m,

1H), 7.06 – 6.97 (m, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.86 – 6.71 (m, 5H), 4.48 (s, 2H), 3.78 (s, 3H), 3.74 (s, 3H), 3.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 158.4, 155.6, 150.4, 133.5, 133.2, 129.5, 122.8, 119.8, 117.8, 114.7, 114.0, 113.9, 113.7, 86.9, 85.7, 80.1, 67.2, 55.5, 55.2, 43.0, 38.2; IR (neat): 2933, 2837, 2239(s), 1606, 1508, 1363, 1227, 1167, 1034, 834; HRESIMS Calcd for $[C_{26}H_{23}NNaO_5S]^+$ (M + Na^+) 484.1189, found 484.1174.

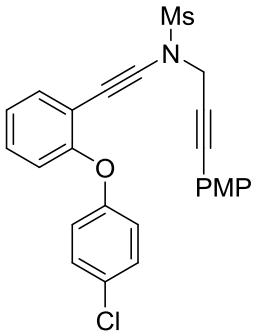
_N_-((4-chloro-2-phenoxyphenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1ae)



1ae

The product **1ae** was afforded as a pale yellow oil (76%, 385.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.42 – 7.34 (m, 2H), 7.34 – 7.24 (m, 4H), 7.15 – 7.07 (m, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 4.40 (s, 2H), 3.70 (s, 3H), 2.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 157.0, 156.7, 140.2, 135.6, 133.6, 133.2, 129.7, 128.7, 128.2, 126.9, 126.6, 123.9, 120.0, 117.8, 115.4, 113.9, 113.6, 86.8, 86.2, 80.1, 66.9, 55.1, 42.9, 38.2; IR (neat): 3032, 2931, 2838, 2240(s), 1606, 1509, 1363, 1249, 1167, 764; HRESIMS Calcd for $[C_{31}H_{25}NNaO_4S]^+$ (M + Na^+) 530.1397, found 530.1410.

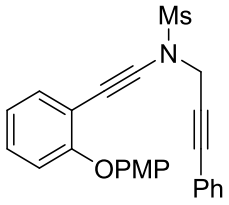
_N_-((2-(4-chlorophenoxy)phenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1af)



1af

The product **1af** was afforded as a pale yellow oil (81%, 377.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 6.8 Hz, 1H), 7.37 – 7.24 (m, 3H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.13 – 7.05 (m, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 4.42 (s, 2H), 3.78 (s, 3H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 156.2, 156.0, 133.5, 133.1, 129.7, 129.4, 127.5, 124.1, 119.8, 118.7, 115.3, 113.9, 113.5, 86.8, 86.2, 79.9, 66.7, 55.1, 42.8, 38.2; IR (neat): 2932, 2839, 2240(s), 1606, 1486, 1360, 1166, 1034, 964, 761; HRESIMS Calcd for $[C_{25}H_{19}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 487.0688.

***N*-((2-(4-methoxyphenoxy)phenyl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1ag)**

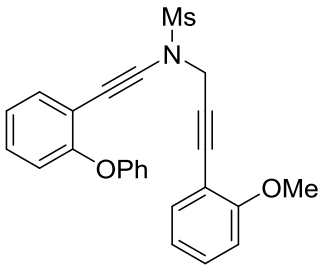


1ag

The product **1ag** was afforded as a pale yellow oil (80%, 345.2 mg). ^{1}H NMR (400 MHz, Acetone-d_6) δ 7.56 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.45 – 7.31 (m, 4H), 7.17 – 7.10 (m, 1H), 7.03 – 6.94 (m, 4H), 6.91 (dd, J = 8.0, 1.2 Hz, 1H), 4.64 (s, 2H), 3.80 (s, 3H), 3.31 (s, 3H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 159.2, 156.8, 151.1, 134.3, 132.5, 130.6, 129.8, 129.3, 123.8, 122.6, 120.6, 118.7, 115.7, 115.0, 87.1, 87.0, 82.9, 67.7, 55.9, 43.3, 38.6; IR (neat): 3009, 2932, 2836, 2239(s), 1505, 1444, 1166,

1035, 757, 517; HRESIMS Calcd for $[C_{25}H_{21}NNaO_4S]^+$ (M + Na^+) 454.1083, found 454.1077.

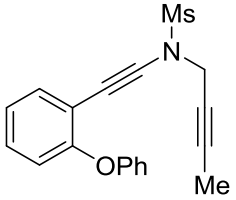
_N_-(3-(2-methoxyphenyl)prop-2-yn-1-yl)-_N_-((2-phenoxyphenyl)ethynyl)methane-sulfonamide (1ah)



1ah

The product **1ah** was afforded as a pale yellow oil (88%, 379.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.17 (m, 5H), 7.08 (t, *J* = 7.6 Hz, 1H), 7.03 – 6.93 (m, 2H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.88 – 6.81 (m, 2H), 4.43 (s, 2H), 3.77 (s, 3H), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 157.4, 156.8, 133.5(4), 133.4(8), 130.3, 129.6, 129.5, 123.7, 122.6, 120.4, 119.8, 117.6, 115.4, 111.0, 110.6, 86.2, 85.3, 83.4, 66.8, 55.4, 43.2, 38.1; IR (neat): 3016, 2931, 2838, 2239(s), 1595, 1447, 1163, 1024, 692, 518; HRESIMS Calcd for $[C_{25}H_{21}NNaO_4S]^+$ (M + Na^+) 454.1083, found 454.1074.

_N_-(but-2-yn-1-yl)-_N_-((2-phenoxyphenyl)ethynyl)methanesulfonamide (1ai)

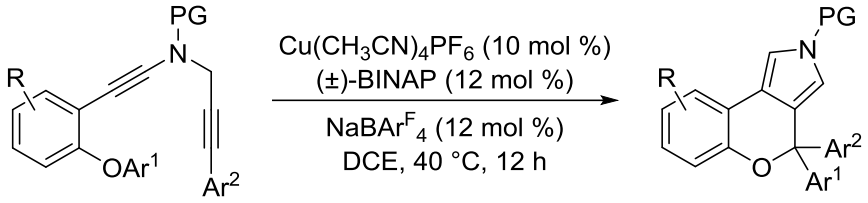


1ai

The product **1ai** was afforded as a pale yellow oil (94%, 319.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.34 – 7.23 (m, 3H), 7.14 – 7.07 (m, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 7.00 – 6.87 (m, 3H), 4.14 (q, *J* = 2.4 Hz, 2H), 2.96 (s, 3H), 1.78 (t, *J* = 2.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 156.6, 133.4, 129.6, 129.5, 123.8, 122.6, 119.9, 117.4, 115.4, 86.1, 83.1, 71.6, 66.7, 42.4, 38.2, 3.4; IR (neat): 3022,

2926, 2239(s), 1959, 1595, 1486, 1166, 1032, 754, 518; HRESIMS Calcd for $[C_{19}H_{17}NNaO_3S]^+$ (M + Na^+) 362.0821, found 362.0814.

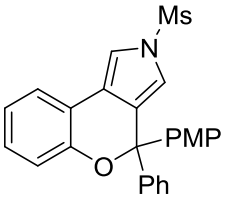
General procedure for the synthesis of racemic chromeno[3,4-*c*]pyrroles 2:



1 **2**

The powered $Cu(CH_3CN)_4PF_6$ (0.01 mmol, 3.7 mg), (±)-BINAP (0.012 mmol, 7.5 mg) and $NaBAr^F_4$ (0.012 mmol, 10.6 mg) were introduced into a vials. After DCE (2 mL) was injected into the vials, the solution was stirred at 40 ℃ for 2 h. Then the *N*-propargyl ynamide **1** (0.1 mmol) was introduced into the system subsequently. The resulting mixture was stirred at 40 ℃ and the progress of the reaction was monitored by TLC. After concentration in vacuo, the residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate) to give the desired chromeno[3,4-*c*]pyrrole **2**.

4-(4-Methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2a)

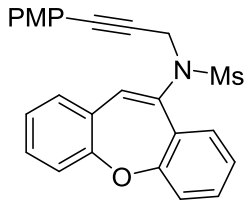


2a

Compound **2a** was prepared in 99% yield (42.7 mg) according to the general procedure. Pale yellow solid (mp 99-100 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.25 (m, 7H), 7.19 (d, *J* = 8.8 Hz, 2H), 7.14 – 7.08 (m, 1H), 7.03 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.94 – 6.86 (m, 1H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.70 (d, *J* = 2.0 Hz, 1H), 3.75 (s, 3H), 3.14 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.4, 143.4 135.3, 129.0, 128.8, 128.6, 128.0, 127.7, 127.5, 123.4, 122.0, 121.3, 118.9, 118.7, 117.6, 113.3(1), 113.2(7), 82.9, 55.2, 42.8; IR (neat): 3132, 3024, 2928, 1509, 1366, 1173, 1068, 769, 577; HRESIMS Calcd for $[C_{25}H_{21}NNaO_4S]^+$ (M + Na^+) 454.1083, found 454.1088.

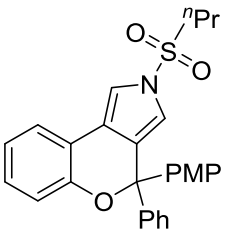
_N_-(dibenzo[_b_,_f_]oxepin-10-yl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (2a′)



2a′

Compound **2a′** was prepared in 15% yield (6.5 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.42 – 7.30 (m, 4H), 7.25 – 7.17 (m, 5H), 7.17 – 7.10 (m, 1H), 6.84 (d, *J* = 8.8 Hz, 2H), 4.62 (s, 2H), 3.80 (s, 3H), 3.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 158.0, 157.7, 138.1, 133.2, 131.4, 130.8, 129.8, 129.4, 129.3, 128.1, 127.8, 125.2, 125.0, 121.7, 121.2, 114.1(0), 114.0(6), 86.1, 82.2, 55.3, 41.5, 40.4; IR (neat): 2924, 2852, 1605, 1509, 1446, 1345, 1248, 1153, 1031, 787; HRESIMS Calcd for $[C_{25}H_{21}NNaO_4S]^+$ (M + Na^+) 454.1083, found 454.1074.

4-(4-Methoxyphenyl)-4-phenyl-2-(propylsulfonyl)-2,4-dihydrochromeno[3,4-_c_]pyrrole (2b)

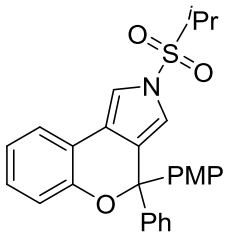


2b

Compound **2b** was prepared in 85% yield (39.1 mg) according to the general procedure. Pale yellow solid (mp 77-78 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.24 (m, 7H),

7.19 (d, *J* = 8.8 Hz, 2H), 7.15 – 7.07 (m, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.95 – 6.86 (m, 1H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.67 (d, *J* = 2.0 Hz, 1H), 3.76 (s, 3H), 3.21 (t, *J* = 7.6 Hz, 2H), 1.79 – 1.66 (m, 2H), 1.00 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.4, 143.4, 135.4, 129.0, 128.7, 128.2, 127.9, 127.7, 127.6, 123.4, 122.0, 121.0, 118.9, 118.8, 118.0, 113.6, 113.3, 83.0, 57.3, 55.2, 17.2, 12.6; IR (neat): 3133, 2963, 2927, 1608, 1510, 1469, 1163, 1063, 753, 700; HRESIMS Calcd for $[C_{27}H_{25}NNaO_4S]^+$ (M + Na^+) 482.1397, found 482.1388.

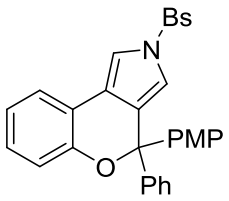
2-(Isopropylsulfonyl)-4-(4-methoxyphenyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2c)



2c

Compound **2c** was prepared in 82% yield (37.7 mg) according to the general procedure. Pale yellow solid (mp 66-67 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.33 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.24 (m, 5H), 7.19 (d, *J* = 8.8 Hz, 2H), 7.14 – 7.08 (m, 1H), 7.06 – 7.01 (m, 1H), 6.94 – 6.87 (m, 1H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.65 (d, *J* = 2.0 Hz, 1H), 3.76 (s, 3H), 3.48 – 3.34 (m, 1H), 1.32 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.4, 143.4, 135.4, 129.1, 128.7, 127.9(2), 127.9(1), 127.7, 127.6, 123.4, 122.0, 120.6, 118.8, 118.7, 114.2, 113.2, 83.0, 56.9, 55.2, 16.4; IR (neat): 3133, 2960, 2927, 1609, 1510, 1358, 1255, 1070, 708, 612; HRESIMS Calcd for $[C_{27}H_{25}NNaO_4S]^+$ (M + Na^+) 482.1397, found 482.1389.

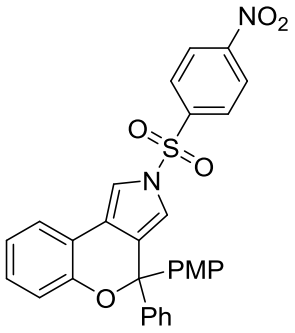
2-((4-Bromophenyl)sulfonyl)-4-(4-methoxyphenyl)-4-phenyl-2,4-dihydro-chromeno[3,4-*c*]pyrrole (2d)



2d

Compound **2d** was prepared in 84% yield (48.1 mg) according to the general procedure. Pale yellow solid (mp 70-71 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.8 Hz, 2H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.36 (d, *J* = 2.0 Hz, 1H), 7.33 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 – 7.19 (m, 5H), 7.08 (d, *J* = 8.8 Hz, 3H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.91 – 6.84 (m, 1H), 6.76 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 2.0 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.5, 143.1, 137.6, 135.1, 132.8, 129.4, 129.3, 129.0, 128.9, 128.2, 127.9, 127.8, 127.6, 123.5, 122.1, 122.0, 118.8, 118.4, 118.2, 113.6, 113.2, 82.9, 55.2; IR (neat): 2961, 2925, 1574, 1509, 1470, 1376, 1176, 1065, 745, 591; HRESIMS Calcd for $[C_{30}H_{22}BrNNaO_4S]^+$ (M + Na^+) 594.0345, found 594.0329.

4-(4-Methoxyphenyl)-2-((4-nitrophenyl)sulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2e)

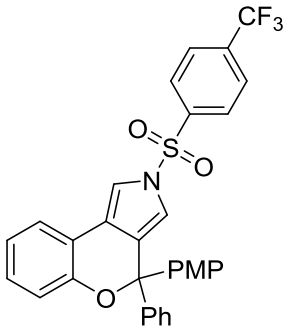


2e

Compound **2e** was prepared in 93% yield (50.1 mg) according to the general procedure. Pale yellow solid (mp 92-93 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.8 Hz, 2H), 7.98 (d, *J* = 8.8 Hz, 2H), 7.38 (d, *J* = 1.2 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.28 – 7.19 (m, 5H), 7.14 – 7.03 (m, 3H), 7.03 – 6.95 (m, 1H), 6.90 – 6.81 (m, 1H), 6.80 – 6.66 (m, 3H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.4, 150.6, 143.8, 142.9, 134.8, 130.1, 129.2, 128.9, 128.1, 127.9, 127.8, 127.5, 124.6, 123.5, 122.6, 122.0,

118.9, 118.1, 113.5, 113.2, 82.9, 55.1; IR (neat): 2960, 2926, 1609, 1533, 1181, 1067, 741, 633; HRESIMS Calcd for $[C_{30}H_{22}N_2NaO_6S]^+$ (M + Na^+) 561.1091, found 561.1076.

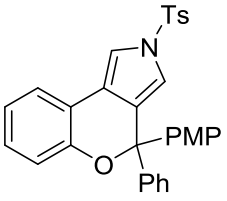
4-(4-Methoxyphenyl)-4-phenyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2f)



2f

Compound **2f** was prepared in 95% yield (53.8 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 2.0 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.19 (m, 5H), 7.08 (d, *J* = 8.8 Hz, 3H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.91 – 6.83 (m, 1H), 6.74 (d, *J* = 8.8 Hz, 3H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.5, 143.0, 142.0, 135.6 (q, *J* = 33.0 Hz), 134.9, 129.8, 129.1, 129.0, 127.9, 127.8, 127.5, 127.3, 126.6 (q, *J* = 4.0 Hz), 123.5, 122.9 (q, *J* = 272.0 Hz), 122.4, 122.0, 118.9, 118.3, 118.2, 113.6, 113.2, 82.9, 55.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3; IR (neat): 2959, 2926, 1609, 1509, 1381, 1323, 1179, 1063, 717, 633; HRESIMS Calcd for $[C_{31}H_{22}F_3NNaO_4S]^+$ (M + Na^+) 584.1114, found 584.1101.

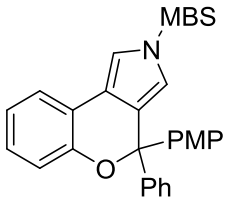
4-(4-Methoxyphenyl)-4-phenyl-2-tosyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2g)



2g

Compound **2g** was prepared in 73% yield (37.0 mg) according to the general procedure. Pale yellow solid (mp 154-155 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 2.0 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.20 (m, 5H), 7.10 (d, *J* = 8.8 Hz, 2H), 7.08 – 7.04 (m, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.90 – 6.82 (m, 1H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 2.0 Hz, 1H), 3.75 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 152.4, 145.2, 143.2, 135.8, 135.3, 130.0, 129.1, 128.7, 127.9, 127.7, 127.6, 126.8, 123.4, 121.9, 121.5, 118.8, 118.7, 118.2, 113.6, 113.2, 83.0, 55.2, 21.6; IR (neat): 2958, 2925, 2853, 1610, 1509, 1374, 1174, 1066, 753, 671; HRESIMS Calcd for $[C_{31}H_{25}NNaO_4S]^+$ (M + Na^+) 530.1397, found 530.1386.

4-(4-Methoxyphenyl)-2-((4-methoxyphenyl)sulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2h)

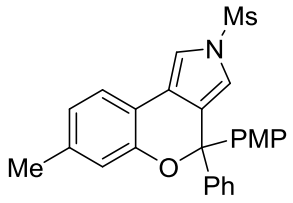


2h

Compound **2h** was prepared in 53% yield (26.2 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.8 Hz, 2H), 7.36 (d, *J* = 2.0 Hz, 1H), 7.33 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.25 – 7.20 (m, 5H), 7.10 (d, *J* = 8.8 Hz, 2H), 7.07 (dd, *J* = 7.6, 2.0 Hz, 1H), 6.99 (dd, *J* = 8.8, 1.2 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.90 – 6.84 (m, 1H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 2.0 Hz, 1H), 3.86 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 159.1, 152.4, 143.3, 135.3, 130.1, 129.2, 129.1, 128.6(4), 128.5(8), 127.9, 127.7, 127.6, 123.4, 121.9, 121.4, 118.8(0), 118.7(6), 118.1, 114.6, 113.6, 113.2, 83.0, 55.7, 55.2; IR (neat): 2960, 2928, 2840, 1594, 1469, 1166, 1065, 1034, 754, 603; HRESIMS Calcd for $[C_{31}H_{25}NNaO_5S]^+$ (M + Na^+) 546.1346, found 546.1346.

4-(4-Methoxyphenyl)-7-methyl-2-(methylsulfonyl)-4-phenyl-2,4-

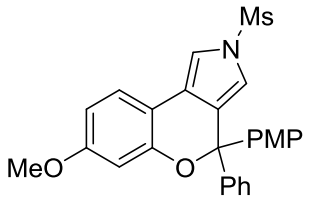
dihydrochromeno[3,4-*c*]pyrrole (2i)



2i

Compound **2i** was prepared in 91% yield (40.5 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.21 (m, 7H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.89 – 6.83 (m, 1H), 6.78 (d, *J* = 8.8 Hz, 2H), 6.71 (d, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 2.0 Hz, 1H), 3.74 (s, 3H), 3.11 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 152.3, 143.5, 139.1, 135.5, 128.9, 128.4, 127.9, 127.6, 127.5, 123.1, 122.9, 121.4, 119.2, 117.6, 115.7, 113.2, 112.8, 82.8, 55.1, 42.7, 21.4; IR (neat): 2958, 2927, 1735, 1610, 1509, 1252, 1171, 1067, 765, 561; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1226.

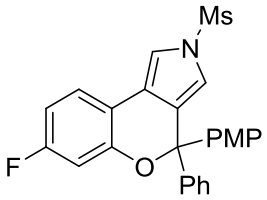
7-Methoxy-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2j)



2j

Compound **2j** was prepared in 90% yield (42.4 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.23 (m, 7H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.67 (d, *J* = 2.0 Hz, 1H), 6.60 (d, *J* = 2.0 Hz, 1H), 6.49 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 3.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 159.1, 153.6, 143.4, 135.3, 129.0, 128.1, 128.0, 127.7, 127.5, 124.1, 121.4, 117.6, 113.3, 112.1, 111.5, 108.6, 104.1, 83.2, 55.3, 55.2, 42.7; IR (neat): 2958, 2927, 2853, 1614, 1510, 1254, 1170, 1068, 765; HRESIMS Calcd for $[C_{26}H_{23}NNaO_5S]^+$ (M + Na^+) 484.1189, found 484.1175.

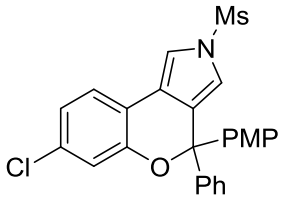
7-Fluoro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2k)



2k

Compound **2k** was prepared in 93% yield (42.2 mg) according to the general procedure. Pale yellow solid (mp 150-151 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 2.4 Hz, 1H), 7.32 – 7.26 (m, 6H), 7.17 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.76 (dd, *J* = 10.0, 2.4 Hz, 1H), 6.70 (d, *J* = 2.4 Hz, 1H), 6.67 – 6.59 (m, 1H), 3.76 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 245.0 Hz), 159.2, 153.6 (d, *J* = 12.0 Hz), 143.0, 134.9, 129.0, 128.0, 127.9(0), 127.8(7), 127.4, 124.3 (d, *J* = 10.0 Hz), 120.6, 117.7, 115.1 (d, *J* = 3.0 Hz), 113.3, 112.9, 109.4 (d, *J* = 22.0 Hz), 106.4 (d, *J* = 24.0 Hz), 83.6, 55.2, 42.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.6; IR (neat): 2959, 2929, 1609, 1510, 1367, 1172, 1068, 984, 769, 509; HRESIMS Calcd for $[C_{25}H_{20}FNNaO_4S]^+$ (M + Na^+) 472.0989, found 472.0975.

7-Chloro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2l)

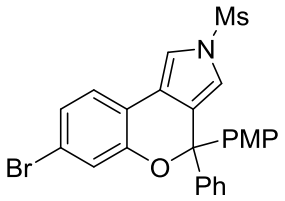


2l

Compound **2l** was prepared in 90% yield (42.0 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.27 (m, 5H), 7.26 (d, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.04 (d, *J* = 2.0 Hz, 1H), 6.89 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.70 (d, *J* = 2.0 Hz, 1H), 3.76 (s, 3H), 3.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 153.0, 143.0, 134.9, 133.7, 129.0, 128.1, 128.0, 127.9, 127.4, 124.1, 122.4, 120.4, 119.2, 117.8, 117.4, 113.4(2),

113.3(5), 83.5, 55.2, 42.9; IR (neat): 2959, 2929, 1609, 1510, 1255, 1172, 1033, 984, 768, 701; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0690.

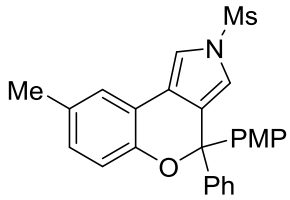
7-Bromo-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2m)



2m

Compound **2m** was prepared in 88% yield (45.0 mg) according to the general procedure. Pale yellow solid (mp 109-110 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.26 (m, 5H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.20 (d, *J* = 2.0 Hz, 1H), 7.15 (d, *J* = 8.8 Hz, 2H), 7.04 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 2.0 Hz, 1H), 3.77 (s, 3H), 3.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 153.1, 143.0, 134.9, 129.0, 128.1, 128.0, 127.9, 127.4, 125.2, 124.4, 122.0, 121.4, 120.5, 117.8(1), 117.7(7), 113.5, 113.4, 83.5, 55.2, 42.9; IR (neat): 2957, 2928, 1608, 1510, 1466, 1368, 1253, 1172, 1070, 770; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_4S]^+$ (M + Na^+) 532.0189, found 532.0180.

4-(4-Methoxyphenyl)-8-methyl-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2n)

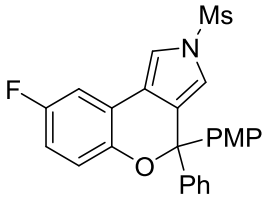


2n

Compound **2n** was prepared in 84% yield (35.6 mg) according to the general procedure. Pale yellow solid (mp 86-87 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.26 (m, 6H), 7.19 (d, *J* = 8.8 Hz, 3H), 6.95 – 6.90 (m, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 2.0

Hz, 1H), 3.76 (s, 3H), 3.16 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 150.3, 143.5, 135.4, 131.3, 129.6, 129.0, 128.8, 128.0, 127.7, 127.5, 123.7, 121.5, 118.6, 118.3, 117.6, 113.3, 113.2, 82.8, 55.2, 42.9, 20.7; IR (neat): 2960, 2927, 1609, 1509, 1366, 1255, 1171, 1069, 769, 507; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1225.

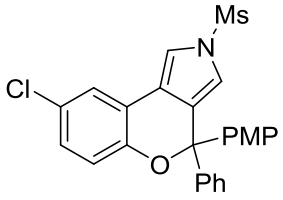
8-Fluoro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydro-chromeno[3,4-*c*]pyrrole (2o)



2o

Compound **2o** was prepared in 80% yield (39.6 mg) according to the general procedure. Pale yellow solid (mp 155-156 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 1H), 7.31 – 7.21 (m, 5H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.04 (dd, *J* = 8.4, 2.8 Hz, 1H), 6.97 (dd, *J* = 8.8, 4.8 Hz, 1H), 6.79 (d, *J* = 8.8 Hz, 3H), 6.73 – 6.66 (m, 1H), 3.75 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 157.8 (d, *J* = 238.0 Hz), 148.4, 143.1, 135.0, 129.0, 128.4, 128.0, 127.8, 127.5, 120.8 (d, *J* = 2.0 Hz), 120.0 (d, *J* = 8.0 Hz), 119.7 (d, *J* = 8.0 Hz), 117.7, 115.3 (d, *J* =24.0 Hz), 113.9, 113.3, 109.6 (d, *J* = 24.0 Hz), 83.1, 55.2, 42.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -121.2; IR (neat): 2958, 2930, 1609, 1510, 1478, 1369, 1176, 1068, 770, 508; HRESIMS Calcd for $[C_{25}H_{20}FNNaO_4S]^+$ (M + Na^+) 472.0989, found 472.0975.

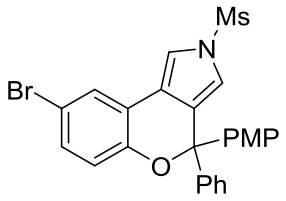
8-Chloro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydro-chromeno[3,4-*c*]pyrrole (2p)



2p

Compound **2p** was prepared in 92% yield (42.9 mg) according to the general procedure. Pale yellow solid (mp 94-95 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 2.0 Hz, 1H), 7.34 (d, *J* = 2.0 Hz, 1H), 7.32 – 7.25 (m, 5H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.05 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.70 (d, *J* = 2.0 Hz, 1H), 3.77 (s, 3H), 3.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 151.0, 143.0, 134.9, 129.0, 128.5, 128.2, 128.0, 127.9, 127.5, 126.9, 123.2, 120.4, 120.2(1), 120.1(9), 117.8, 113.8, 113.3, 83.3, 55.2, 43.0; IR (neat): 3135, 2930, 1609, 1510, 1369, 1172, 1067, 983, 770, 531; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0688.

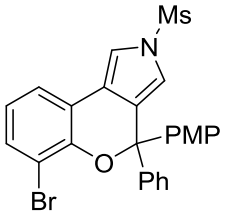
8-Bromo-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydro-chromeno[3,4-*c*]pyrrole (2q)



2q

Compound **2q** was prepared in 85% yield (43.4 mg) according to the general procedure. Pale yellow solid (mp 101-102 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 2.0 Hz, 1H), 7.38 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.26 (m, 5H), 7.19 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.16 (d, *J* = 8.8 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.70 (d, *J* = 2.0 Hz, 1H), 3.77 (s, 3H), 3.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 151.5, 143.0, 134.9, 131.4, 129.0, 128.2, 128.0, 127.9, 127.5, 126.1, 120.7(3), 120.6(5), 120.2, 117.8, 114.3, 113.8, 113.3, 83.3, 55.2, 43.0; IR (neat): 3134, 2930, 1609, 1510, 1368, 1252, 1172, 1067, 770, 701; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_4S]^+$ (M + Na^+) 532.0189, found 532.0176.

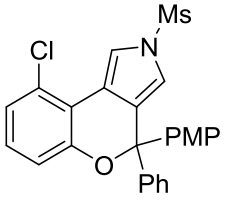
6-Bromo-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2r)



2r

Compound **2r** was prepared in 72% yield (36.7 mg) according to the general procedure. Pale yellow solid (mp 202-203 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 3H), 7.36 – 7.24 (m, 7H), 6.82 – 6.73 (m, 4H), 3.75 (s, 3H), 3.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 149.2, 143.0, 134.9, 132.1, 128.8, 128.1, 128.0, 127.8, 127.2, 122.9, 122.3, 120.8, 120.4, 117.6, 113.9, 113.3, 113.0, 84.1, 55.1, 42.9; IR (neat): 3133, 2929, 1608, 1510, 1437, 1368, 1174, 1064, 771; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_4S]^+$ (M + Na^+) 532.0189, found 532.0180.

9-Chloro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2s)

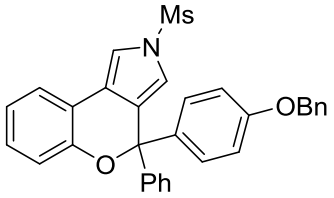


2s

Compound **2s** was prepared in 54% yield (25.2 mg) according to the general procedure. Pale yellow solid (mp 78-79 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.26 (m, 5H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.04 – 6.93 (m, 3H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 2.0 Hz, 1H), 3.76 (s, 3H), 3.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 153.7, 142.9, 134.8, 130.9, 129.0, 128.7, 128.2, 128.0, 127.9, 127.5, 123.6, 118.2(7), 118.2(5), 117.7, 117.6, 116.9, 113.3, 82.9, 55.2, 42.9; IR (neat): 3059, 2929, 1608, 1509, 1370, 1252, 1173, 1069, 983, 771; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0684.

4-(4-(Benzyloxy)phenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-

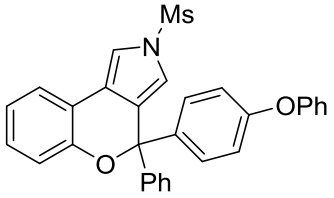
***c*]pyrrole (2t)**



2t

Compound **2t** was prepared in 92% yield (41.4 mg) according to the general procedure. Pale yellow solid (mp 93-94 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.29 (m, 8H), 7.29 – 7.21 (m, 3H), 7.19 (d, *J* = 8.8 Hz, 3H), 7.10 – 7.04 (m, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.93 – 6.77 (m, 3H), 6.70 (d, *J* = 2.0 Hz, 1H), 4.94 (s, 2H), 2.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 152.3, 143.3, 136.7, 135.5, 128.9, 128.7, 128.5, 128.3, 127.9(1), 127.8(9), 127.7, 127.4(3), 127.4(0), 123.3, 122.0, 121.1, 118.8, 118.6, 117.5, 114.1, 113.3, 82.9, 69.9, 42.6; IR (neat): 3032, 2927, 2855, 1738, 1606, 1508, 1367, 1069, 983, 769; HRESIMS Calcd for $[C_{31}H_{25}NNaO_4S]^+$ (M + Na^+) 530.1397, found 530.1391.

2-(Methylsulfonyl)-4-(4-phenoxyphenyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2u)

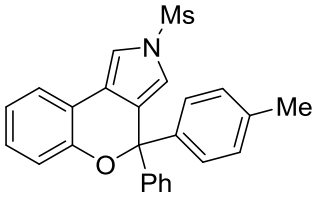


2u

Compound **2u** was prepared in 93% yield (45.9 mg) according to the general procedure. Pale yellow solid (mp 91-92 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.35 (m, 2H), 7.35 – 7.26 (m, 7H), 7.24 (d, *J* = 8.8 Hz, 2H), 7.15 – 7.07 (m, 2H), 7.04 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.02 – 6.97 (m, 2H), 6.93 (dd, *J* = 7.2, 1.2 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 2.4 Hz, 1H), 3.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 156.5, 152.3, 143.1, 137.8, 129.7, 129.2, 128.9, 128.3, 128.0, 127.8, 127.5, 123.6, 123.4, 122.1, 121.2, 119.4, 118.9, 118.6, 117.7, 117.6, 113.4, 82.9, 42.9; IR (neat): 2961, 2926, 2854,

1588, 1489, 1235, 1173, 1069, 753, 696; HRESIMS Calcd for $[C_{30}H_{23}NNaO_4S]^+$ (M + Na^+) 516.1240, found 516.1241.

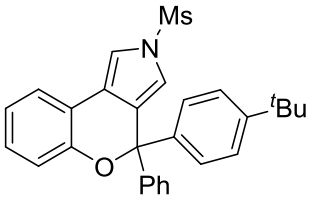
2-(Methylsulfonyl)-4-phenyl-4-(*p*-tolyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2v)



2v

Compound **2v** was prepared in 74% yield (30.8 mg) according to the general procedure. Pale yellow solid (mp 187-188 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.34 (m, 2H), 7.34 – 7.23 (m, 5H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.14 – 7.09 (m, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.04 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.94 – 6.86 (m, 1H), 6.71 (d, *J* = 2.0 Hz, 1H), 3.13 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 143.3, 140.2, 137.5, 128.8, 128.7, 128.4, 128.0, 127.7, 127.5, 123.4, 122.0, 121.3, 118.9, 118.7, 117.7, 113.3, 83.1, 42.8, 21.0; IR (neat): 3026, 2958, 2926, 1470, 1367, 1174, 1069, 769, 576; HRESIMS Calcd for $[C_{25}H_{21}NNaO_3S]^+$ (M + Na^+) 438.1134, found 438.1120.

4-(4-(*tert*-butyl)phenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2w)

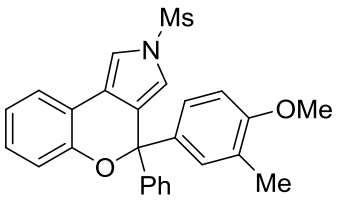


2w

Compound **2w** was prepared in 75% yield (34.3 mg) according to the general procedure. Pale yellow solid (mp 99-100 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 2H), 7.33 – 7.26 (m, 5H), 7.25 – 7.17 (m, 4H), 7.16 – 7.08 (m, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.94 – 6.86 (m, 1H), 6.73 (d, *J* = 2.0 Hz, 1H), 3.13 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 150.6, 143.2, 140.2, 128.8, 128.4, 127.9, 127.7, 127.6, 127.2, 124.9, 123.4, 122.0, 121.3, 118.9, 118.6, 117.7, 113.3, 83.1, 42.8, 34.5, 31.3; IR (neat):

2960, 2855, 1600, 1470, 1266, 1069, 983, 794; HRESIMS Calcd for $[C_{28}H_{27}NNaO_3S]^+$ (M + Na^+) 480.1604, found 480.1590.

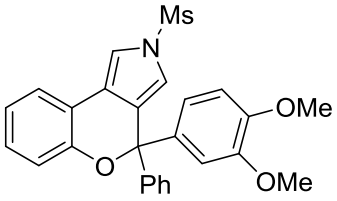
4-(3,4-Dimethoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2x)



2x

Compound **2x** was prepared in 83% yield (37.0 mg) according to the general procedure. Pale yellow solid (mp 184-185 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.20 (m, 7H), 7.15 – 7.07 (m, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.01 – 6.94 (m, 1H), 6.93 – 6.84 (m, 1H), 6.70 (d, *J* = 1.6 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 1H), 3.76 (s, 3H), 3.10 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 152.5, 143.5, 134.8, 129.9, 128.8, 128.6, 127.9, 127.6, 127.5, 126.3, 126.1, 123.3, 122.0, 121.3, 118.9, 118.7, 117.7, 113.3, 108.9, 83.0, 55.2, 42.8, 16.4; IR (neat): 2926, 2853, 1608, 1505, 1367, 1255, 1173, 1069, 982, 750; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1227.

4-(3,4-Dimethoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2y)

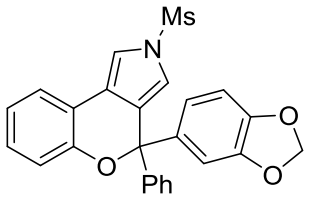


2y

Compound **2y** was prepared in 93% yield (42.9 mg) according to the general procedure. Pale yellow solid (mp 90-91 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.25 (m, 7H), 7.15 – 7.09 (m, 1H), 7.05 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.99 (d, *J* = 2.0 Hz, 1H), 6.94 – 6.87 (m, 1H), 6.74 – 6.67 (m, 2H), 6.64 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 3.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 148.6(4), 148.5(8), 143.2, 135.6,

128.8, 128.5, 127.9, 127.8, 127.5, 123.4, 122.1, 121.2, 120.5, 118.8, 118.7, 117.6, 113.3, 111.0, 110.0, 83.1, 55.8, 55.7, 42.8; IR (neat): 3022, 2929, 2837, 1738, 1600, 1514, 1367, 1173, 1070, 753; HRESIMS Calcd for $[C_{26}H_{23}NNaO_5S]^+$ (M + Na^+) 484.1189, found 484.1178.

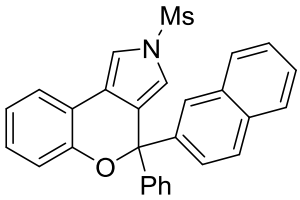
4-(Benzo[*d*][1,3]dioxol-5-yl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno-[3,4-*c*]pyrrole (2z)



2z

Compound **2z** was prepared in 95% yield (42.7 mg) according to the general procedure. Pale yellow solid (mp 74-75 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.25 (m, 7H), 7.15 – 7.08 (m, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.94 – 6.89 (m, 1H), 6.87 – 6.82 (m, 1H), 6.71 (d, *J* = 2.0 Hz, 1H), 6.68 – 6.62 (m, 2H), 5.90 (s, 2H), 3.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 147.6, 147.2, 143.2, 137.2, 128.8, 128.3, 128.0, 127.8, 127.4, 123.4, 122.1, 121.5, 121.2, 118.9, 118.7, 117.7, 113.4, 108.4, 107.3, 101.1, 83.0, 42.8; IR (neat): 2955, 2925, 1738, 1601, 1487, 1367, 1173, 1068, 1038, 756; HRESIMS Calcd for $[C_{25}H_{19}NNaO_5S]^+$ (M + Na^+) 468.0876, found 468.0867.

2-(Methylsulfonyl)-4-(naphthalen-2-yl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (2aa)

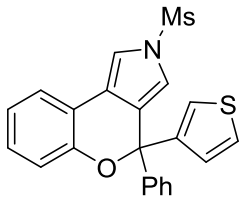


2aa

Compound **2aa** was prepared in 87% yield (39.3 mg) according to the general procedure. Pale yellow solid (mp 117-118 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.69 (m, 3H), 7.65 – 7.58 (m, 1H), 7.53 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.48 – 7.42 (m, 2H),

7.41 (d, *J* = 2.0 Hz, 1H), 7.39 – 7.34 (m, 3H), 7.33 – 7.25 (m, 3H), 7.15 – 7.05 (m, 2H), 6.94 – 6.86 (m, 1H), 6.75 (d, *J* = 2.0 Hz, 1H), 3.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 143.1, 140.6, 132.8, 132.6, 128.9, 128.4, 128.1, 128.0, 127.9, 127.5(3), 127.4(7), 126.7, 126.4, 126.2, 125.6, 123.4, 122.2, 121.3, 118.9, 118.7, 117.8, 113.5, 83.2, 42.9; IR (neat): 3058, 2928, 1600, 1368, 1174, 1069, 770, 574; HRESIMS Calcd for $[C_{28}H_{21}NNaO_3S]^+$ (M + Na^+) 474.1134, found 474.1119.

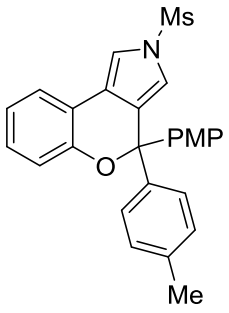
2-(Methylsulfonyl)-4-phenyl-4-(thiophen-3-yl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2ab)



2ab

Compound **2ab** was prepared in 71% yield (29.0 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 4H), 7.33 – 7.25 (m, 3H), 7.24 – 7.20 (m, 1H), 7.16 – 7.09 (m, 1H), 7.07 – 7.00 (m, 2H), 6.96 – 6.88 (m, 2H), 6.76 (d, *J* = 2.0 Hz, 1H), 3.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 144.9, 142.7, 128.9, 128.3, 128.1, 127.9, 127.3, 127.1, 125.9, 124.3, 123.4, 122.2, 121.1, 118.7, 118.5, 117.1, 113.3, 80.8, 42.8; IR (neat): 2960, 2926, 2854, 1599, 1470, 1367, 1172, 1069, 765; HRESIMS Calcd for $[C_{22}H_{17}NNaO_3S_2]^+$ (M + Na^+) 430.0542, found 430.0524.

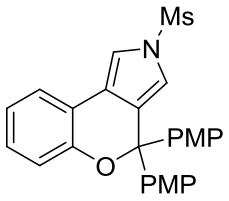
4-(4-Methoxyphenyl)-2-(methylsulfonyl)-4-(*p*-tolyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2ac)



2ac

Compound **2ac** was prepared in 87% yield (35.2 mg) according to the general procedure. Pale yellow solid (mp 156-157 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.32 (m, 2H), 7.23 – 7.15 (m, 4H), 7.13 – 7.05 (m, 3H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.92 – 6.86 (m, 1H), 6.78 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 1.6 Hz, 1H), 3.74 (s, 3H), 3.11 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 152.5, 140.4, 137.4, 135.5, 128.9, 128.7(7), 128.7(5), 128.7, 127.5, 123.3, 122.0, 121.3, 118.9, 118.7, 117.6, 113.3, 113.2, 82.9, 55.1, 42.8, 21.0; IR (neat): 3025, 2927, 2854, 1608, 1510, 1367, 1254, 1174, 1070, 765; HRESIMS Calcd for $[C_{26}H_{23}NNaO_4S]^+$ (M + Na^+) 468.1240, found 468.1226.

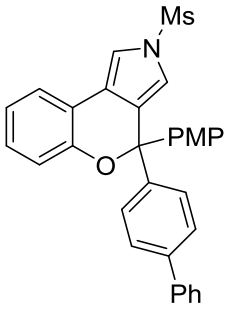
4,4-Bis(4-methoxyphenyl)-2-(methylsulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2ad)



2ad

Compound **2ad** was prepared in 90% yield (41.5 mg) according to the general procedure. Pale yellow solid (mp 117-118 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.33 (m, 2H), 7.21 (d, *J* = 8.8 Hz, 4H), 7.15 – 7.07 (m, 1H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.93 – 6.87 (m, 1H), 6.80 (d, *J* = 8.8 Hz, 4H), 6.68 (d, *J* = 2.4 Hz, 1H), 3.76 (s, 6H), 3.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 152.5, 135.5, 128.9, 128.8, 123.3, 122.0, 121.4, 118.9, 118.7, 117.5, 113.2, 82.8, 55.2, 42.8; IR (neat): 2956, 2930, 2837, 1608, 1509, 1367, 1252, 1174, 1069, 769; HRESIMS Calcd for $[C_{26}H_{23}NNaO_5S]^+$ (M + Na^+) 484.1189, found 484.1178.

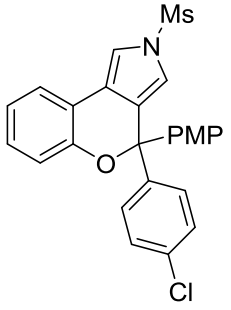
4-([1,1'-Biphenyl]-4-yl)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2ae)



2ae

Compound **2ae** was prepared in 52% yield (26.4 mg) according to the general procedure. Pale yellow solid (mp 200-201 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.44 – 7.34 (m, 6H), 7.34 – 7.28 (m, 1H), 7.24 (d, *J* = 8.8 Hz, 2H), 7.15 – 7.09 (m, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.95 – 6.87 (m, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.77 – 6.71 (m, 1H), 3.74 (s, 3H), 3.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.4, 142.4, 140.5, 135.2, 129.0, 128.8, 128.7, 128.5, 127.9, 127.3, 127.0, 126.7, 123.4, 122.1, 121.3, 118.9, 118.6, 117.6, 113.3(4), 113.3(1), 82.8, 55.1, 42.8; IR (neat): 3029, 2926, 2854, 1607, 1506, 1471, 1259, 1069, 1034, 764; HRESIMS Calcd for $[C_{31}H_{25}NNaO_4S]^+$ (M + Na^+) 530.1397, found 530.1386.

4-(4-Chlorophenyl)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole (2af)

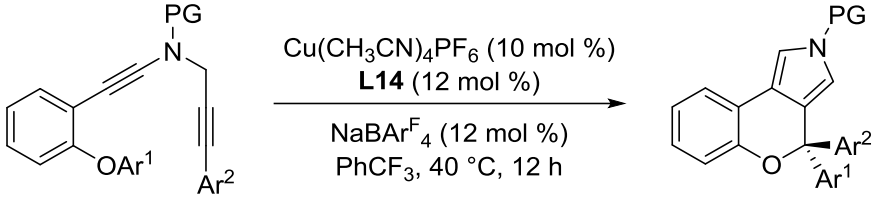


2af

Compound **2af** was prepared in 85% yield (39.6 mg) according to the general procedure. Pale yellow solid (mp 88-89 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.0 Hz, 2H), 7.28 – 7.22 (m, 4H), 7.18 (d, *J* = 8.8 Hz, 2H), 7.15 – 7.08 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.95 – 6.88 (m, 1H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.70 – 6.66 (m, 1H), 3.76 (s, 3H), 3.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 152.2, 142.0, 134.9, 133.7,

129.0, 128.9(1), 128.8(6), 128.2, 123.4, 122.3, 121.2, 118.8, 118.6, 117.5, 113.5, 113.4, 82.5, 55.2, 42.9; IR (neat): 3010, 2929, 2854, 1608, 1510, 1367, 1174, 1070, 765; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_4S]^+$ (M + Na^+) 488.0694, found 488.0681.

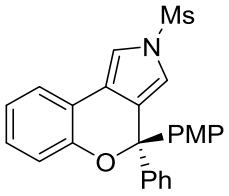
General procedure for the synthesis of chiral chromeno[3,4-*c*]pyrroles (+)-2:



1 **(+)-2**

The powered $Cu(CH_3CN)_4PF_6$ (0.01 mmol, 3.7 mg), **L14** (0.012 mmol, 8.0 mg) and $NaBAr^F_4$ (0.012 mmol, 10.6 mg) were introduced into a vial. After $PhCF_3$ (2 mL) was injected into the vial, the solution was stirred at 40 ℃ for 2 h. Then, the *N*-propargyl ynamide **1** (0.1 mmol) was introduced into the system subsequently. The resulting mixture was stirred at 40 ℃ and the progress of the reaction was monitored by TLC. After concentration in vacuo, the residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate) to give the desired chiral chromeno[3,4-*c*]pyrrole **(+)-2**.

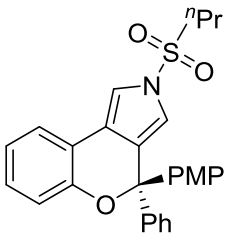
(*R*)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2a)



(+)-2a

Compound **(+)-2a** was prepared in 96% yield (41.4 mg) according to the general procedure. $[\alpha]_D^{20}$ = +63.1 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 16.67 min (major), 18.96 min (minor)).

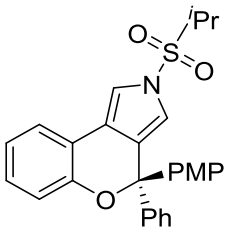
(*R*)-4-(4-methoxyphenyl)-4-phenyl-2-(propylsulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2b)



(+)-2b

Compound **(+)-2b** was prepared in 84% yield (38.6 mg) according to the general procedure. $[\alpha]_D^{20}$ = +48.5 °(c = 1.0, $CHCl_3$). 85% ee (determined by HPLC: Chiralpak IA Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 10.79 min (minor), 13.57 min (major)).

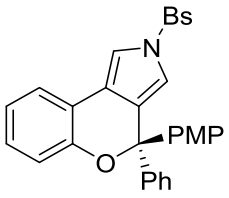
(*R*)-2-(isopropylsulfonyl)-4-(4-methoxyphenyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2c)



(+)-2c

Compound **(+)-2c** was prepared in 77% yield (35.4 mg) according to the general procedure. $[\alpha]_D^{20}$ = +35.4 °(c = 1.0, $CHCl_3$). 86% ee (determined by HPLC: Chiralpak IE Column, 98/2 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 32.86 min (minor), 34.66 min (major)).

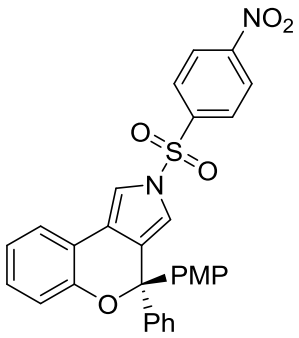
(*R*)-2-((4-bromophenyl)sulfonyl)-4-(4-methoxyphenyl)-4-phenyl-2,4-dihydro-chromeno[3,4-*c*]pyrrole ((+)-2d)



(+)-2d

Compound **(+)-2d** was prepared in 85% yield (48.7 mg) according to the general procedure. $[\alpha]_D^{20}$ = +33.8 °(c = 1.0, $CHCl_3$). 88% ee (determined by HPLC: Chiralpak IE Column, 95/5 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 15.41 min (minor), 16.18 min (major)).

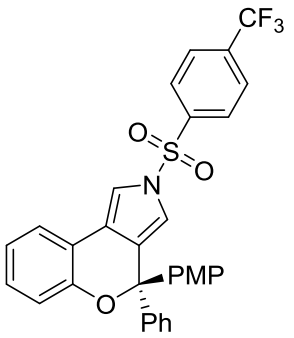
(*R*)-4-(4-methoxyphenyl)-2-((4-nitrophenyl)sulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2e)



(+)-2e

Compound **(+)-2e** was prepared in 96% yield (51.7 mg) according to the general procedure. $[\alpha]_D^{20}$ = +26.9 °(c = 1.0, $CHCl_3$). 85% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 32.73 min (major), 40.80 min (minor)).

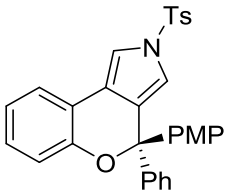
(*R*)-4-(4-methoxyphenyl)-4-phenyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2f)



(+)-2f

Compound **(+)-2f** was prepared in 99% yield (56.1 mg) according to the general procedure. $[\alpha]_D^{20}$ = +36.1 °(c = 1.0, $CHCl_3$). 86% ee (determined by HPLC: Chiralpak IE Column, 98/2 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 14.51 min (minor), 15.37 min (major)).

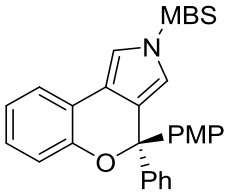
(*R*)-4-(4-methoxyphenyl)-4-phenyl-2-tosyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2g)



(+)-2g

Compound **(+)-2g** was prepared in 69% yield (35.0 mg) according to the general procedure. $[\alpha]_D^{20}$ = +30.2 °(c = 1.0, $CHCl_3$). 78% ee (determined by HPLC: Chiralpak IG Column, 80/20 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 14.46 min (minor), 17.37 min (major)).

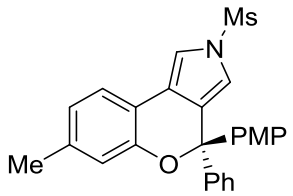
(*R*)-4-(4-methoxyphenyl)-2-((4-methoxyphenyl)sulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2h)



(+)-2h

Compound **(+)-2h** was prepared in 60% yield (29.7 mg) according to the general procedure. $[\alpha]_D^{20}$ = +40.8 °(c = 1.0, $CHCl_3$). 79% ee (determined by HPLC: Chiralpak IE Column, 95/5 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 33.87 min (minor), 37.48 min (major)).

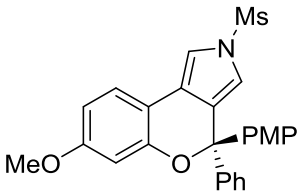
(*R*)-4-(4-methoxyphenyl)-7-methyl-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2i)



(+)-2i

Compound **(+)-2i** was prepared in 91% yield (40.5 mg) according to the general procedure. $[\alpha]_D^{20}$ = +29.5 °(c = 1.0, $CHCl_3$). 91% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 13.07 min (major), 14.11 min (minor)).

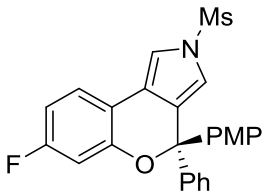
(*R*)-7-methoxy-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2j)



(+)-2j

Compound **(+)-2j** was prepared in 91% yield (42.0 mg) according to the general procedure. $[\alpha]_D^{20}$ = +23.8 °(c = 1.0, $CHCl_3$). 91% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 16.01 min (major), 17.57 min (minor)).

(*R*)-7-fluoro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2k)

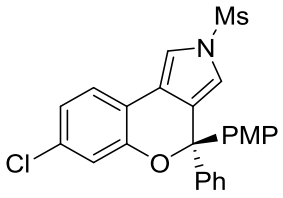


(+)-2k

Compound **(+)-2k** was prepared in 99% yield (44.9 mg) according to the general procedure. $[\alpha]_D^{20}$ = +38.2 °(c = 1.0, $CHCl_3$). 91% ee (determined by HPLC: Chiralpak

IA Column, 80/20 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 10.38 min (minor), 11.85 min (major)).

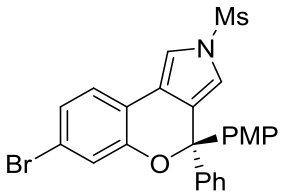
(*R*)-7-chloro-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2l)



(+)-2l

Compound **(+)-2l** was prepared in 92% yield (42.9 mg) according to the general procedure. $[\alpha]_D^{20}$ = +36.3 °(c = 1.0, $CHCl_3$). 90% ee (determined by HPLC: Chiralpak IA Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 20.29 min (minor), 26.31 min (major)).

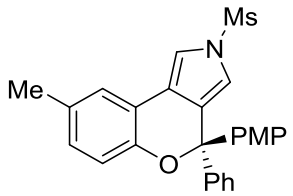
(*R*)-7-bromo-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2m)



(+)-2m

Compound **(+)-2m** was prepared in 92% yield (47.0 mg) according to the general procedure. $[\alpha]_D^{20}$ = +33.1 °(c = 1.0, $CHCl_3$). 85% ee (determined by HPLC: Chiralpak IG Column, 50/50 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 8.54 min (minor), 12.58 min (major)).

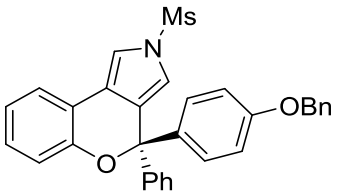
(*R*)-4-(4-methoxyphenyl)-8-methyl-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2n)



(+)-2n

Compound **(+)-2n** was prepared in 80% yield (35.6 mg) according to the general procedure. $[\alpha]_D^{20}$ = +38.9 °(c = 1.0, $CHCl_3$). 80% ee (determined by HPLC: Chiralpak IG Column, 50/50 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 7.68 min (minor), 8.99 min (major)).

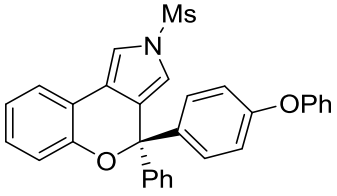
(*R*)-4-(4-(benzyloxy)phenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2t)



(+)-2t

Compound **(+)-2t** was prepared in 94% yield (42.3 mg) according to the general procedure. $[\alpha]_D^{20}$ = +43.0 °(c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IA Column, 70/30 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 12.12 min (major), 16.63 min (minor)).

(*R*)-2-(methylsulfonyl)-4-(4-phenoxyphenyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2u)

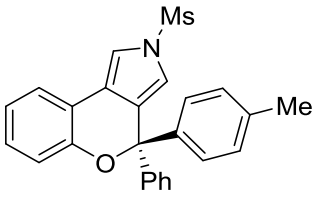


(+)-2u

Compound **(+)-2u** was prepared in 94% yield (46.4 mg) according to the general procedure. $[\alpha]_D^{20}$ = +25.5 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak

IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 19.01 min (minor), 28.11 min (major)).

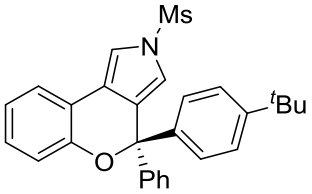
(*R*)-2-(methylsulfonyl)-4-phenyl-4-(*p*-tolyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2v)



(+)-2v

Compound **(+)-2v** was prepared in 83% yield (34.5 mg) according to the general procedure. $[\alpha]_D^{20}$ = +28.8 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 10.05 min (major), 10.98 min (minor)).

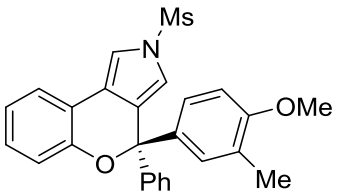
(*R*)-4-(4-(*tert*-butyl)phenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2w)



(+)-2w

Compound **(+)-2w** was prepared in 92% yield (42.1 mg) according to the general procedure. $[\alpha]_D^{20}$ = +38.9 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IA Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 7.69 min (major), 9.09 min (minor)).

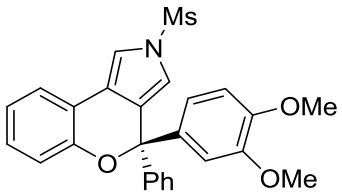
(*R*)-4-(3,4-dimethoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2x)



(+)-2x

Compound **(+)-2x** was prepared in 96% yield (42.8 mg) according to the general procedure. $[\alpha]_D^{20}$ = +43.1 °(c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IB Column, 80/20 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 8.29 min (major), 9.82 min (minor)).

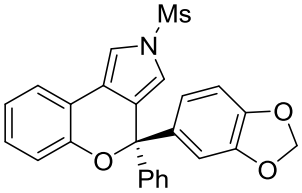
(*R*)-4-(3,4-dimethoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2y)



(+)-2y

Compound **(+)-2y** was prepared in 95% yield (43.8 mg) according to the general procedure. $[\alpha]_D^{20}$ = +74.1 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IA Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 21.20 min (minor), 31.28 min (major)).

(*R*)-4-(benzo[*d*][1,3]dioxol-5-yl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno-[3,4-*c*]pyrrole ((+)-2z)

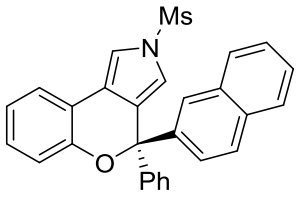


(+)-2z

Compound **(+)-2z** was prepared in 99% yield (44.5 mg) according to the general procedure. $[\alpha]_D^{20}$ = +41.8 °(c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak

IA Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 19.21 min (major), 22.56 min (minor)).

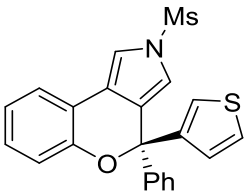
(*R*)-2-(methylsulfonyl)-4-(naphthalen-2-yl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2aa)



(+)-2aa

Compound **(+)-2aa** was prepared in 86% yield (38.8 mg) according to the general procedure. $[\alpha]_D^{20}$ = +25.6 °(c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 11.77 min (major), 12.77 min (minor)).

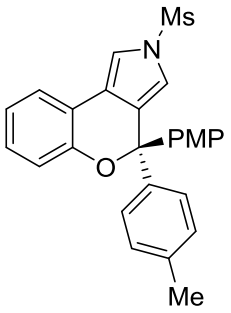
(*S*)-2-(methylsulfonyl)-4-phenyl-4-(thiophen-3-yl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2ab)



(+)-2ab

Compound **(+)-2ab** was prepared in 93% yield (38.0 mg) according to the general procedure. $[\alpha]_D^{20}$ = +39.8 °(c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IG Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 12.59 min (minor), 13.32 min (major)).

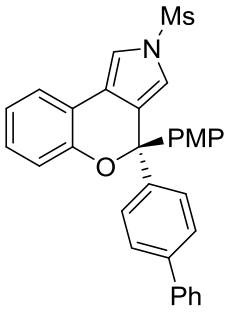
(*R*)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-(*p*-tolyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2ac)



(+)-2ac

Compound **(+)-2ac** was prepared in 96% yield (38.8 mg) according to the general procedure. $[\alpha]_D^{20}$ = +26.8 °(c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IB Column, 95/5 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 21.76 min (major), 23.59 min (minor)).

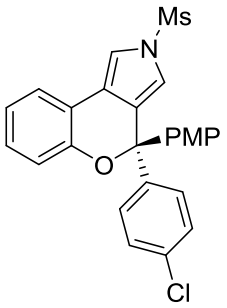
(*R*)-4-([1,1'-biphenyl]-4-yl)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2ae)



(+)-2ae

Compound **(+)-2ae** was prepared in 95% yield (48.2 mg) according to the general procedure. $[\alpha]_D^{20}$ = +24.0 °(c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 23.23 min (minor), 26.67 min (major)).

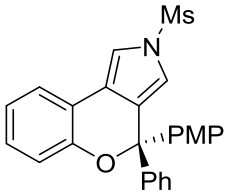
(*S*)-4-(4-chlorophenyl)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-2,4-dihydrochromeno[3,4-*c*]pyrrole ((+)-2af)



(+)-2af

Compound **(+)-2af** was prepared in 99% yield (46.1 mg) according to the general procedure. $[\alpha]_D^{20}$ = +28.0 °(c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IB Column, 95/5 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 25.07 min (major), 28.32 min (minor)).

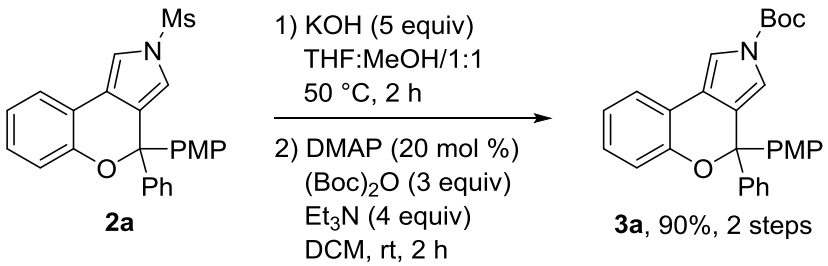
(*S*)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole ((-)-2a)



(-)-2a

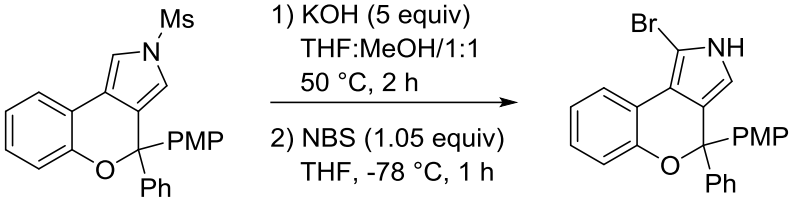
Compound **(-)-2a** was prepared in 96% yield (41.4 mg) according to the general procedure. $[\alpha]_D^{20}$ = -57.2 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IB Column, 90/10 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 17.70 min (minor), 19.31 min (major)).

***Tert*-butyl 4-(4-methoxyphenyl)-4-phenylchromeno[3,4-*c*]pyrrole-2(4*H*)-carboxylate (3a)**



Compound **3a** was prepared in 90% yield (40.8 mg, two steps) according to the known procedure (0.10 mmol scale).[4] Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 1.2 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.32 – 7.22 (m, 5H), 7.11 – 7.04 (m, 1H), 7.04 – 6.98 (m, 1H), 6.92 – 6.84 (m, 1H), 6.83 – 6.75 (m, 3H), 3.75 (s, 3H), 1.59 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 152.4, 148.9, 143.9, 135.9, 129.1, 128.1, 127.8, 127.7, 127.5, 126.9, 123.2, 121.8, 119.6, 119.5, 118.7, 117.1, 113.2, 112.7, 84.2, 83.1, 55.2, 28.0; IR (neat): 2980, 2933, 1743, 1510, 1397, 1254, 1153, 979, 753; HRESIMS Calcd for $[C_{29}H_{27}NNaO_4]^+$ (M + Na^+) 476.1832, found 476.1821.

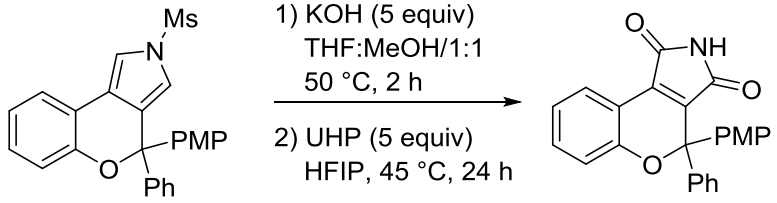
1-Bromo-4-(4-methoxyphenyl)-4-phenyl-2,4-dihydrochromeno[3,4-*c*]pyrrole (4a)



2a **4a**, 65%, 2 steps

Compound **4a** was prepared in 65% yield (56.2 mg, two steps) according to the known procedure (0.20 mmol scale).[4] White solid (mp 82-83 ℃). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.89 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.29 – 7.22 (m, 3H), 7.21 (d, *J* = 8.8 Hz, 2H), 7.09 – 6.98 (m, 2H), 6.95 – 6.88 (m, 1H), 6.77 (d, *J* = 8.8 Hz, 2H), 6.23 (d, *J* = 2.4 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 152.0, 144.1, 136.2, 129.2, 127.8, 127.7, 127.4, 125.1, 122.3, 121.4, 120.1, 118.5, 116.0, 114.0, 113.1, 94.1, 83.2, 55.2; IR (neat): 3399, 2932, 1608, 1508, 1466, 1242, 1176, 1032, 754, 700; HRESIMS Calcd for $[C_{24}H_{18}BrNNaO_2]^+$ (M + Na^+) 454.0413, found 454.0410.

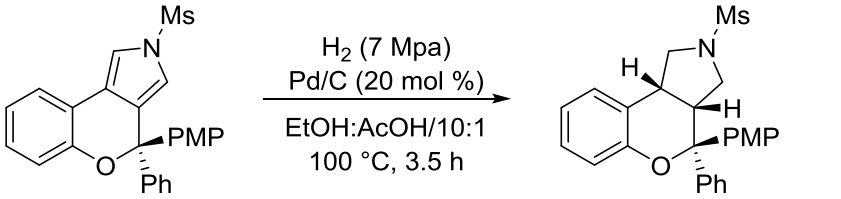
4-(4-methoxyphenyl)-4-phenylchromeno[3,4-*c*]pyrrole-1,3(2*H*,4*H*)-dione (5a)



2a **5a**, 60%, 2 steps

Compound **5a** was prepared in 60% yield (46.0 mg, two steps) according to the known procedure (0.20 mmol scale).[6] Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.49 – 7.39 (m, 3H), 7.39 – 7.32 (m, 4H), 7.30 (d, *J* = 8.8 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 167.7, 159.7, 154.5, 141.4, 133.8, 133.4, 133.3, 133.0, 129.1, 128.6, 128.2, 127.6, 126.3, 122.2, 117.1, 114.6, 113.6, 83.6, 55.3; IR (neat): 2924, 1766, 1729, 1712, 1604, 1511, 1337, 1255, 1176, 758; HRESIMS Calcd for $[C_{24}H_{17}NNaO_4]^+$ (M + Na^+) 406.1050, found 406.1042.

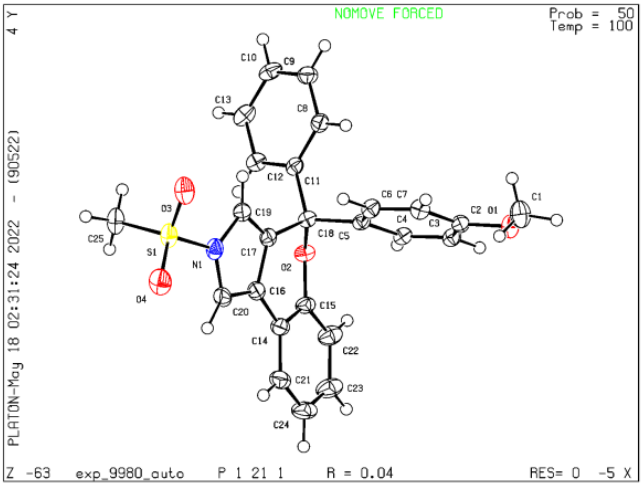
(3a*R*,4*R*,9b*R*)-4-(4-methoxyphenyl)-2-(methylsulfonyl)-4-phenyl-1,2,3,3a,4,9b-hexahydrochromeno[3,4-*c*]pyrrole ((-)-6a)

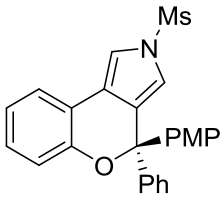


(+)-2a, 94% ee **(-)-6a**, 63%, 94% ee, 3:1 d.r

Compound **(-)-6a** was prepared in 63% yield (51.5 mg) according to the known procedure (0.20 mmol scale).[4] Pale yellow oil. $[\alpha]_D^{20}$ = -39.0 °(c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IA Column, 95/5 hexane/*i*-PrOH, 1.0 mL/min, 254 nm; TR = 43.53 min (major), 50.95 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.8 Hz, 4H), 7.25 – 7.10 (m, 5H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.94 – 6.88 (m, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 3.97 – 3.86 (m, 2H), 3.81 – 3.68 (m, 4H), 3.45 (t, *J* = 6.0 Hz, 1H), 3.36 – 3.22 (m, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 153.0, 143.7, 135.9, 128.8, 128.6(9), 128.6(5), 127.4, 125.7(4), 125.7(2), 122.0, 118.1, 114.0, 80.0, 55.9, 55.3, 47.6, 45.2, 36.7, 33.9; IR (neat): 3059, 2930, 2853, 1610, 1512, 1454, 1334, 1251, 1152, 737; HRESIMS Calcd for $[C_{25}H_{25}NNaO_4S]$+ (M + Na+) 458.1397, found 458.1393.

Crystal data and structure refinement for (+)-2a. CCDC Number = 2192857





Bond precision: C-C = 0.0050 A Wavelength=1.54184

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alpha=90 beta=94.829(1) gamma=90
Temperature: 100 K

	Calculated	Reported
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Hall group	P 2yb	P 2yb
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Sum formula	C25 H21 N O4 S	C25 H21 N O4 S
Mr	431.49	431.49
Dx,g cm-3	1.311	1.311
Z	2	2
Mu (mm-1)	1.578	1.578
F000	452.0	452.0
F000'	453.97	
h,k,lmax	11,10,18	11,9,18
Nref	4496[2417]	4228
Tmin,Tmax	0.963,0.969	0.042,1.000
Tmin'	0.924	

Correction method= # Reported T Limits: Tmin=0.042 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.94 Theta(max)= 75.086

R(reflections)= 0.0419(4077) wR2(reflections)= 0.1248(4228)

S = 1.167 Npar= 282

Computational Methods.

All calculations were performed using Gaussian 16 package.[7] Geometry optimizations and vibration frequencies were calculated by using M06[8] level of density function theory with the LANL2DZ[9,10] basis set and pseudopotential for the Cu atom, and the 6-31G(d,p) basis set[11,12] for C, H, O, N, P and S atom. All local minimums were confirmed with no imaginary frequency and all transition states had only one imaginary frequency. And every transition state was checked by intrinsic reaction coordinate (IRC). Single-point energies of all the transition states and intermediates were further recomputed at the M06-D3/def2TZVPP level of theory. The SMD solvation model[13] with $PhCF_3$ was used for all calculations. The ball stick models of molecules were drawn by CYLview 2.0.[14]

Reference

1. N. Jalalian, E. E. Ishikawa, L. F. Silva and B. Olofsson, *Org. Lett.,* 2011, **13**, 1552.

2. J. D. Priest, L. Male, P. W. Davies, *Tetrahedron,* 2021, **78**, 131757.

3. F.-L. Hong, Z.-S. Wang, D.-D. Wei, T.-Y. Zhai, G.-C. Deng, X. Lu, R.-S. Liu and L.-W. Ye, *J. Am. Chem. Soc.*, 2019, **141**, 16961.

4. F.-L. Hong, C.-Y. Shi, P. Hong, T.-Y. Zhai, X.-Q. Zhu, X. Lu and L.-W. Ye, *Angew. Chem. Int. Ed.,* 2022, **61**, e202115554.

5. S. Wertz, D. Leifert and A. Studer, *Org. Lett.,* 2013, **15**, 928.

6. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M.

Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16, Revision B.01, Gaussian, Inc., Wallingford CT,* 2016.

8. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.,* 2008, **120**, 215.

9. W. R. Wadt and P. J. Hay, *J. Chem. Phys.,* 1985, **82**, 284.

10. P. J. Hay and W. R. Wadt, *J. Chem. Phys.,* 1985, **82**, 270.

11. R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.,* 1971, **54**, 724.

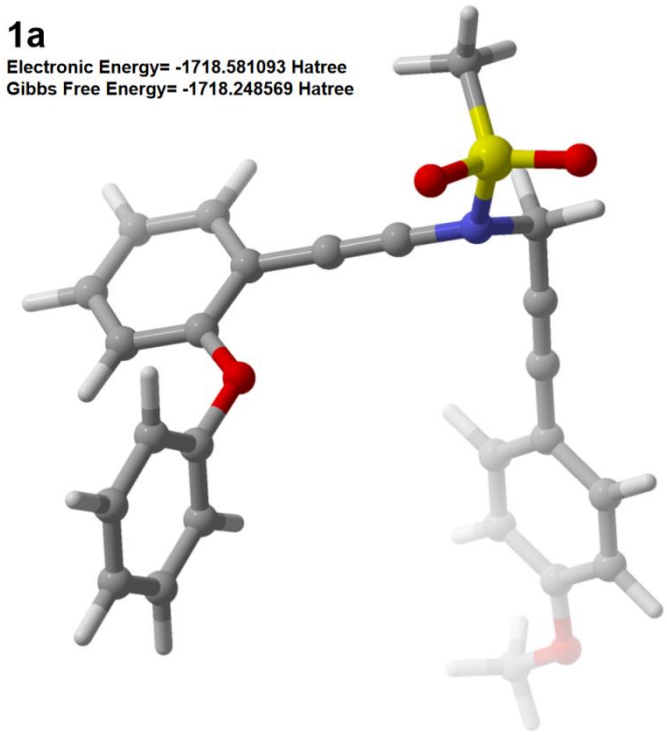
12. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.,* 1972, **56**, 2257.

13. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.,* 2009, **113**, 6378.

14. CYLview20; Legault, C. Y. Université de Sherbrooke, 2020, *(http://www.cylview.org)*..

XYZ Coordinates

1a



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H	-6.20713500	0.33755400	-2.03204500
O	-6.91793800	-1.36921500	-0.31447800
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C	2.11129200	-0.33488800	1.69080300
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C	2.29891500	-1.57249900	1.04237500
C	2.77051100	-1.36576600	3.78808900
H	2.21105600	0.70430500	3.56206800
C	2.72053700	-2.68808200	1.75877100
C	2.95187500	-2.57741000	3.12644800
H	2.95447300	-1.28823700	4.85598600
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C	1.11482200	-3.65536600	-1.07294700
C	3.40279500	-3.05755600	-1.61879500
C	1.25131000	-4.82608700	-1.81290900
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C	3.52623200	-4.23088100	-2.35733500
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H	2.55462600	-6.02928900	-3.03317300
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O	3.09490000	2.98583300	-1.56762700
O	1.45005000	4.89004800	-1.76357600
C	2.83266100	4.63355700	0.47700400
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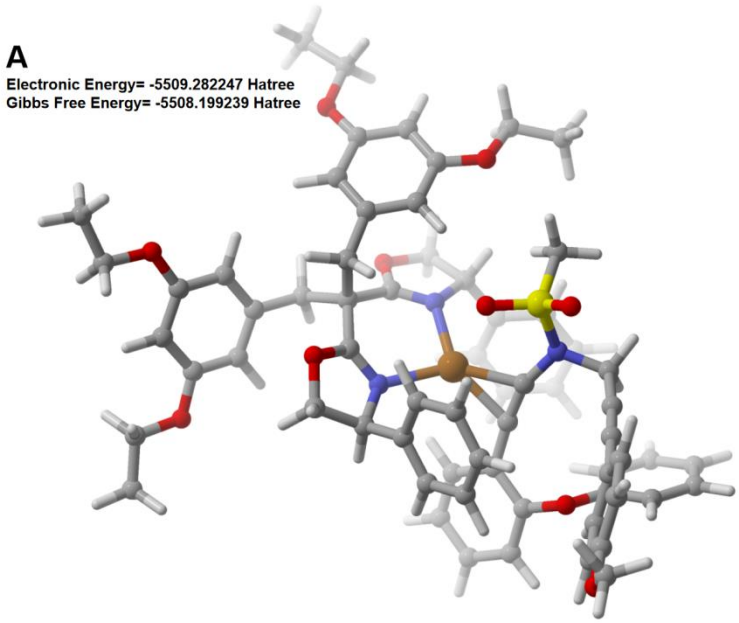

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C	7.03058900	2.03017500	-4.10595400
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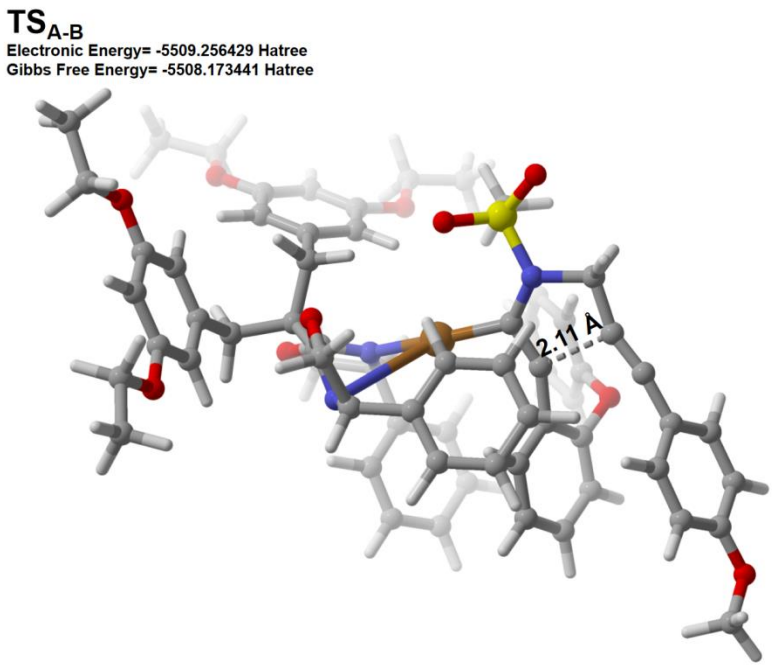
TS_{A-B}



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O	-8.11570800	-1.52520800	1.04795500
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H	-8.03536000	5.76294700	-0.44326000
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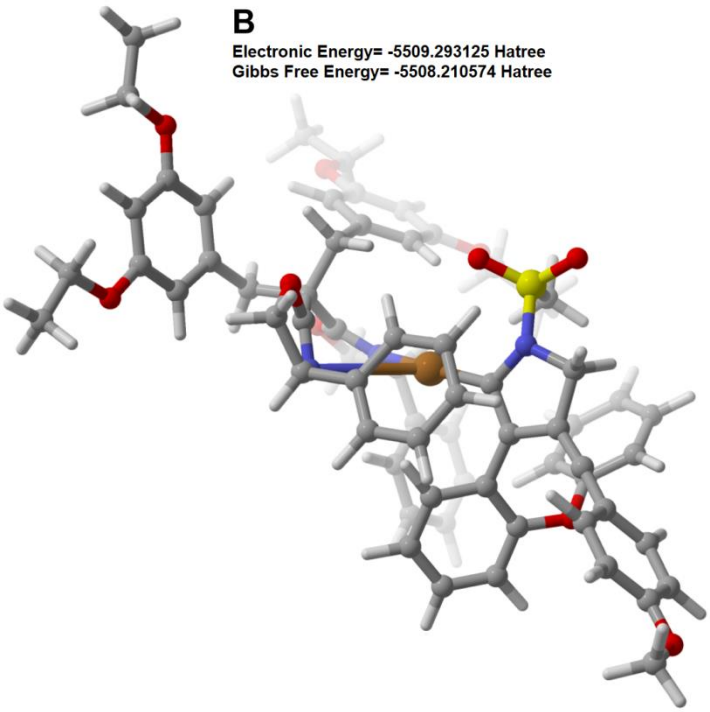

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C	-3.27295600	-0.27526000	-0.29250600
C	-3.58328000	-0.47178900	1.12742800

C	-2.79891700	-1.29301500	1.94639500
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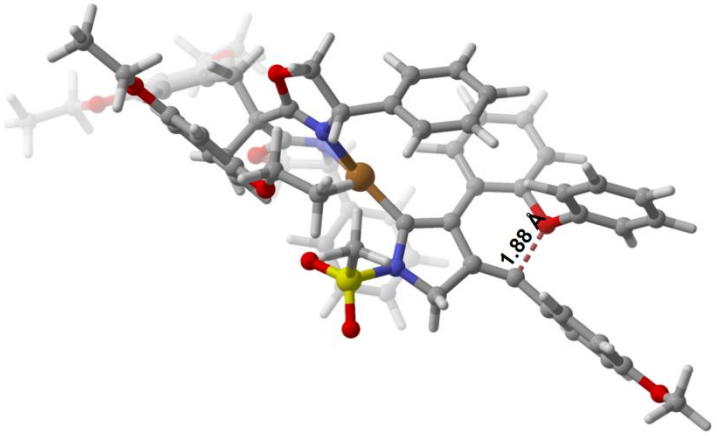

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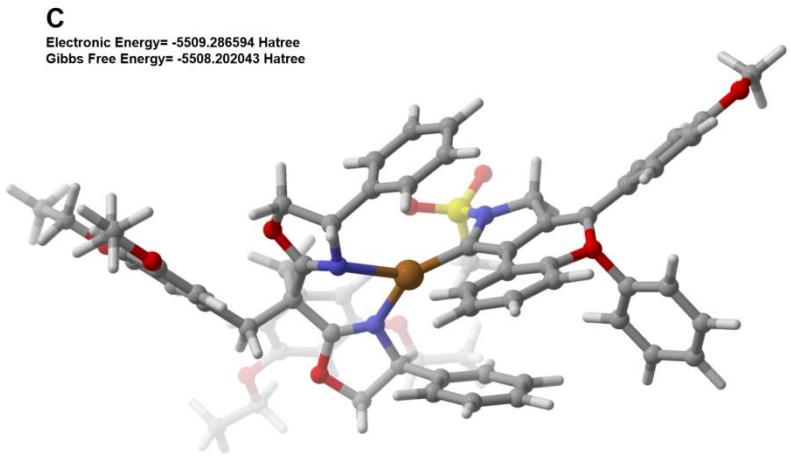
C



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C	-4.49192900	-1.78991300	1.70797400
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C	-3.73936500	-3.24374800	3.42014100
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H	-0.71426400	2.71277400	-0.67724500
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H	-2.18199600	3.33134500	-1.52365800
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H	-1.05153300	-4.12803300	0.48129600
C	-0.94878600	-2.50623300	-3.03228000
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C	6.30939700	-7.25030300	1.56245900
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H	6.35669800	-7.13645300	2.65071900
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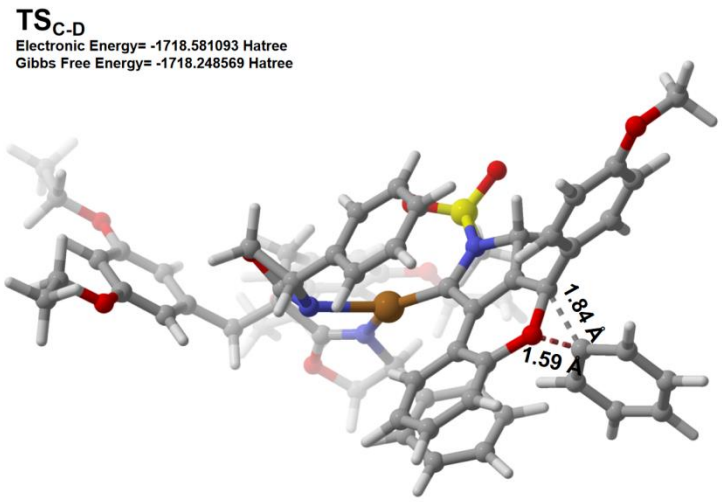
TS_{C-D}



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C	-5.49656000	-0.38501000	-0.03940900
C	-6.44205300	-0.97063600	-0.99934700
C	-6.73321700	-2.34150200	-1.00171700
C	-7.05502300	-0.14433700	-1.94050700
C	-7.60485100	-2.86686400	-1.93843100
H	-6.27230000	-2.99473300	-0.26270800
C	-7.92034000	-0.66724800	-2.89828100
H	-6.85460600	0.92632300	-1.92478400
C	-8.19860600	-2.03398200	-2.89499900
H	-7.83993400	-3.92841200	-1.95421100
H	-8.37839000	-0.00246600	-3.62415400
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C	-9.66295700	-1.83940300	-4.75471900
H	-10.28197100	-2.50944900	-5.35429900
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C	-1.91735200	0.30406300	-0.19465500
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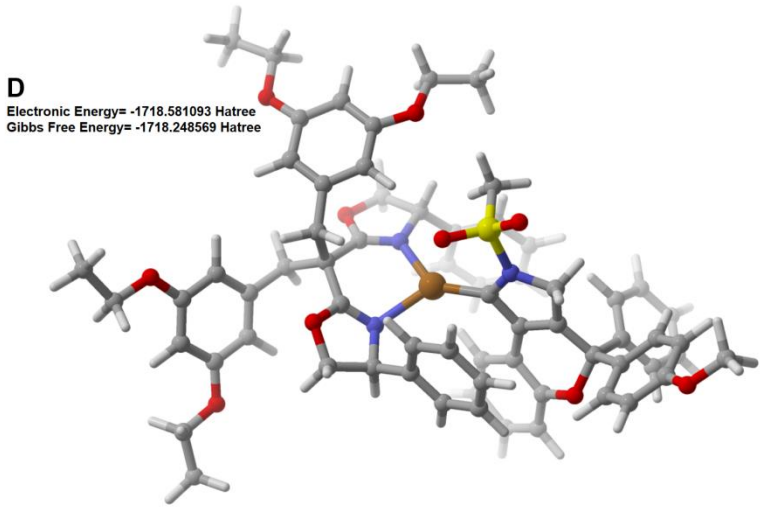

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H	-3.54043700	-2.89569000	-2.83056600
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H	0.91477600	1.21018600	3.99063800
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H	4.49715000	-7.51569600	1.60866500
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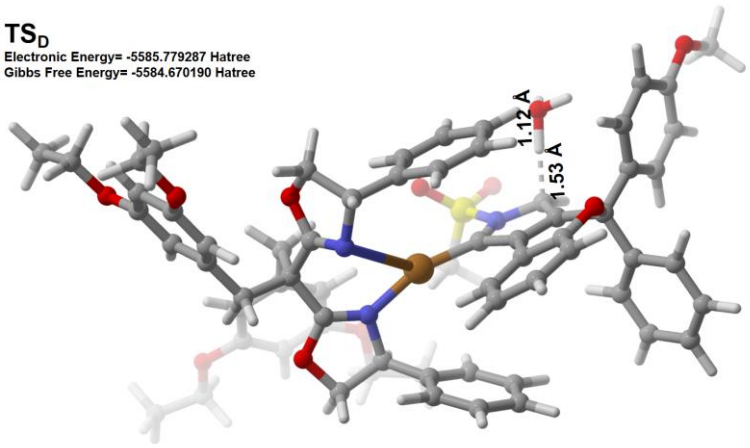

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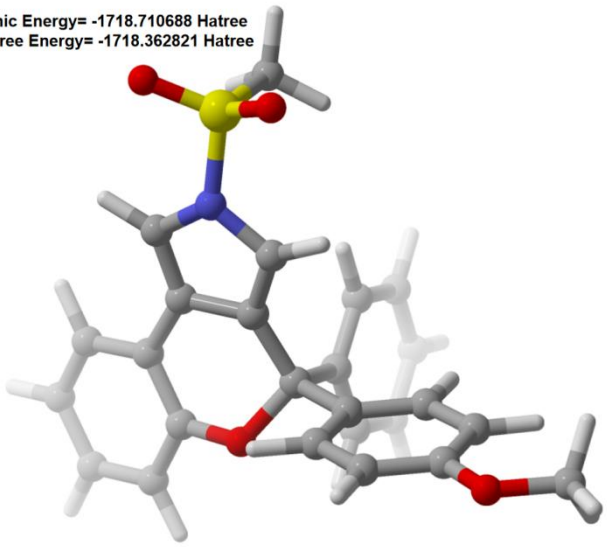

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C	3.63713900	-3.28594400	-1.68287400
H	4.32494300	-1.31788500	-1.13397800

C	1.24127300	-3.60489000	-1.68023400
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H	3.06262900	4.10591400	2.39647400
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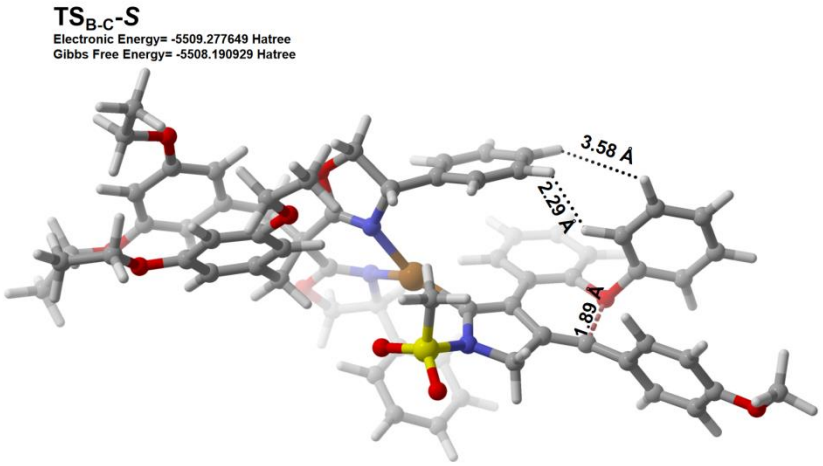

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C	-8.50796900	2.31173000	-1.63614600
H	-6.52023300	2.37791000	-0.83228000
C	-9.50617100	1.48317100	-2.16851500
H	-10.07484700	-0.50120900	-2.76279900
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O	-10.72042000	1.91708800	-2.54130700
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C	-3.91035800	-1.53358900	0.98180100
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C	-4.75105200	-3.14655900	3.16334000
H	-2.66986500	-3.68685500	3.32901400
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C	-6.91470900	0.08302700	1.44888100
C	-6.18842300	1.10208600	2.04565800
C	-8.29679700	0.01729200	1.49473500
C	-6.88390300	2.09562700	2.72461400
H	-5.10261800	1.11366300	1.96616900
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H	-10.06563000	1.00087100	2.21517600
H	-8.81633800	2.84578500	3.30507000
S	-1.13974200	1.04328900	-2.55086600
O	0.08236000	0.23905500	-2.52558700
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C	-0.92456200	2.42855700	-1.46828800
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H	-1.85830300	2.99769400	-1.44138700
Cu	-0.50368700	-0.84636500	0.14595000
C	2.89403500	-1.45998600	0.71802900
C	4.04390200	-2.00427500	1.63021800
H	3.74552300	-1.85028600	2.67263400
H	4.09117200	-3.08537400	1.48108500
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C	1.93818600	-2.60821700	0.44926800
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C	0.19983600	-3.93847600	0.02911300
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C	-2.19837100	-3.33791300	-3.49186000
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H	-0.39170000	-2.59006200	-4.40068300
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C	-0.71066800	0.04723400	3.50363700
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C	3.49270800	1.51449300	-0.58195100
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H	2.45080800	1.58145000	-0.28033400
C	6.11357000	1.47383300	-1.49064300
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H	8.33214600	3.78403500	2.96440400
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C	4.21577800	5.08206200	-0.43350600
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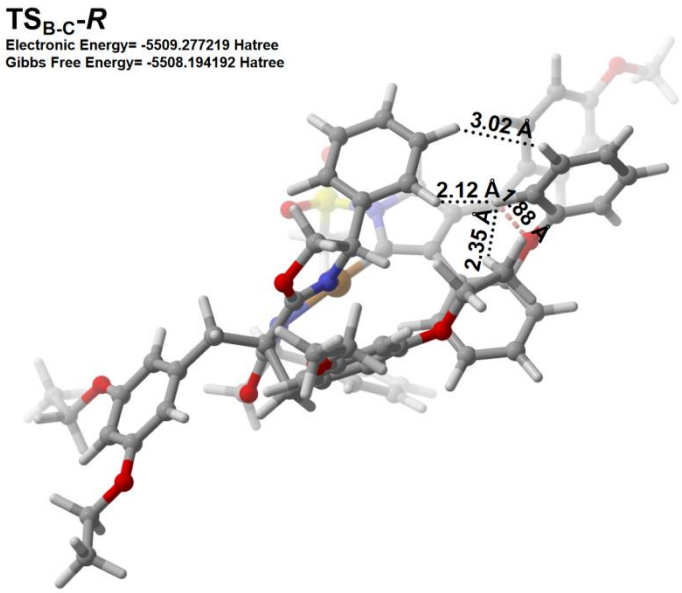

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C	3.93598900	-1.52313400	0.13892100
C	5.16528700	-1.19785800	0.50580700
C	6.53191900	-1.22773900	0.15282700
C	6.95158200	-0.68309800	-1.08424600
C	7.50346700	-1.72003400	1.04303800
C	8.28610000	-0.65431800	-1.41614800
H	6.20067700	-0.29180300	-1.77040300
C	8.84811900	-1.68184800	0.72478900
H	7.18280400	-2.12296200	2.00129800

C	9.24224100	-1.14657000	-0.51069800
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H	9.58171200	-2.06516500	1.42649700
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C	1.62388800	-1.66323300	-0.11244700
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C	1.31976400	0.51784800	2.04349200
C	3.68627200	0.67180400	2.07480300
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H	0.40214600	0.07256200	1.66110200
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C	5.19843800	2.09824700	0.00248000
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C	5.97986500	3.08739800	-0.58283800
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O	-2.44704100	1.92359100	-1.92352000
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O	0.21875900	4.08510500	1.18418800
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C	-4.26085900	8.14872800	-1.51236400
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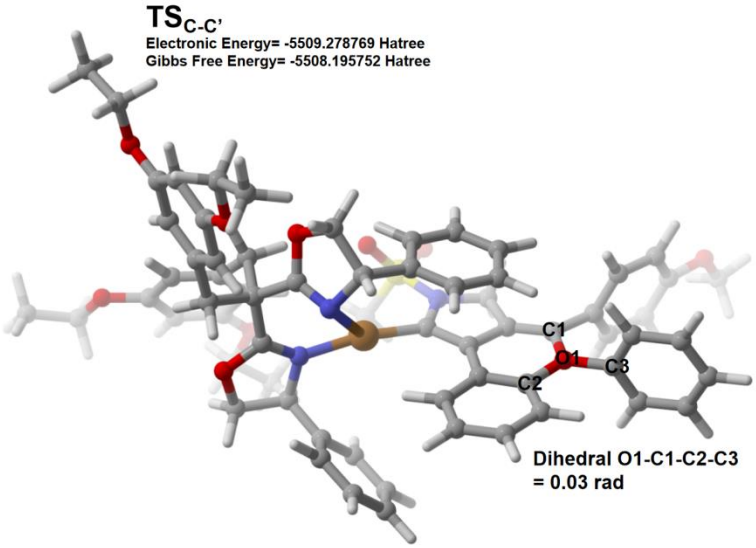

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H	9.05604500	-2.32209000	-1.91953900
O	9.83846100	-0.44353200	-3.73226800
C	10.66825200	-1.59525300	-3.70024800
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C	6.73177700	1.61091300	0.96819100
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C	-3.39537200	0.30767900	0.38434600
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H	-2.63596100	-0.33922400	-1.54311300
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C	1.77334700	1.85930800	-2.00999800
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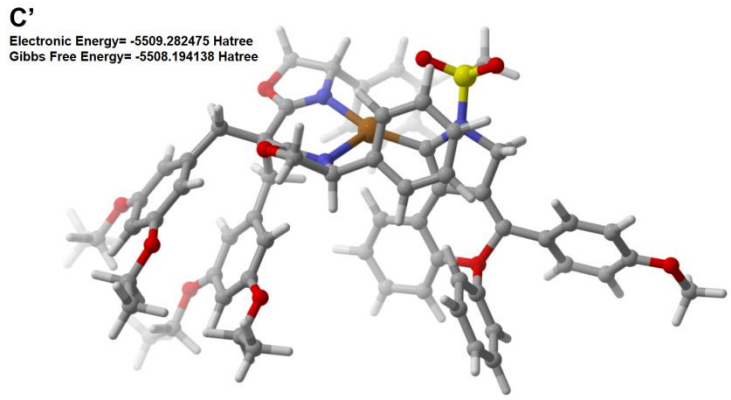
C’



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C	-7.06606600	1.39276600	0.31774400
C	-6.78434900	2.20085700	-1.93436400
C	-8.38788900	1.79882700	0.29842700
H	-6.65547900	0.94744400	1.22228800
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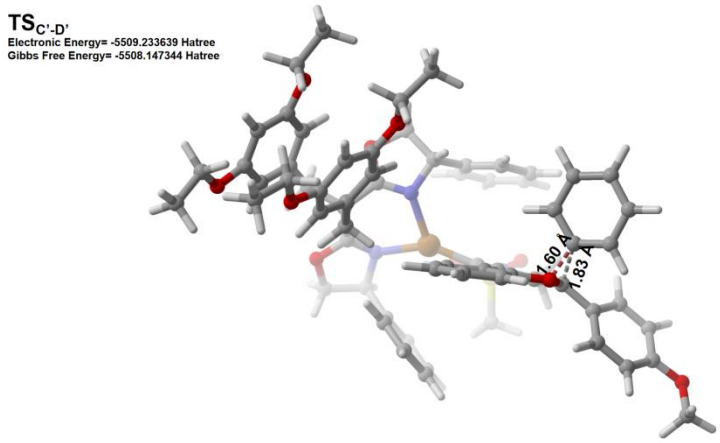

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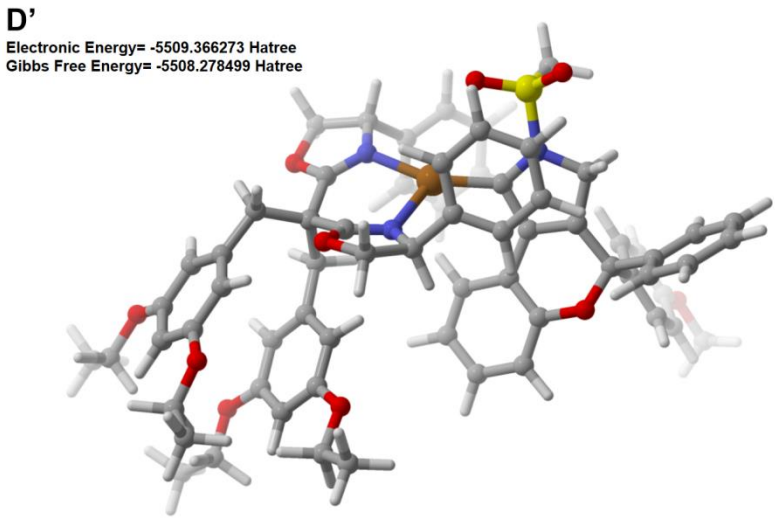

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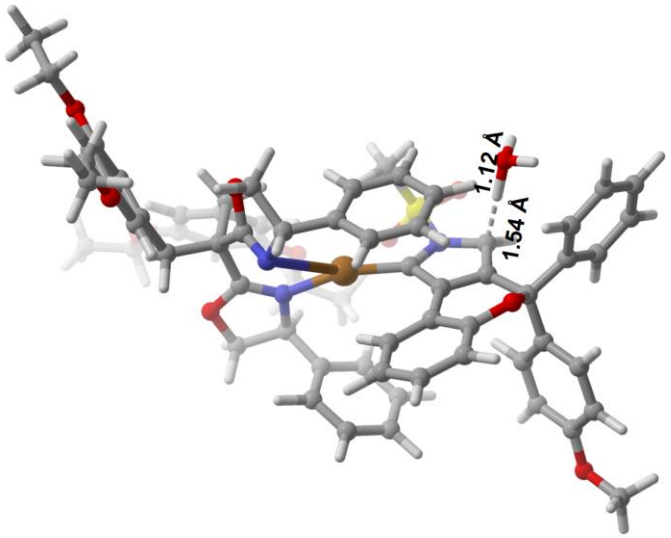

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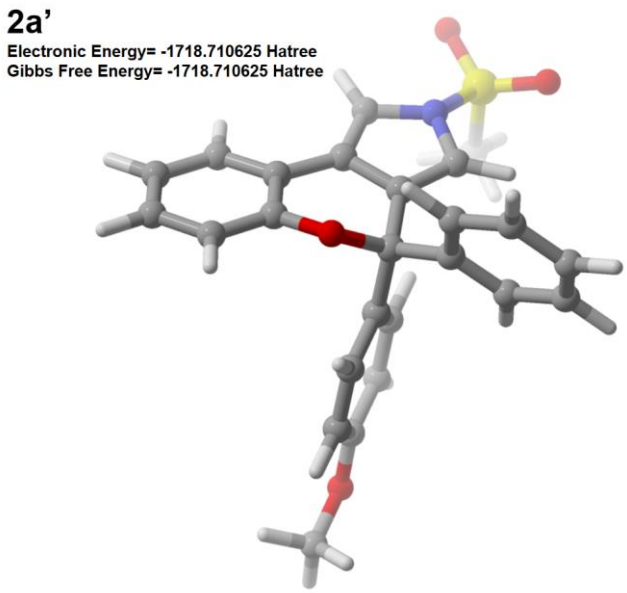
H	0.59772300	6.34011500	1.86320000
C	-6.25558000	6.08343700	0.15011200
H	-5.57794800	6.43669100	-0.64104800
H	-5.93895900	6.54609900	1.09654700
C	-7.68680300	6.41974100	-0.16828000
H	-8.35509800	6.06720300	0.62454400
H	-7.80493400	7.50364100	-0.26095600
H	-7.99436100	5.95798500	-1.11256500
O	3.59767000	-1.45541000	4.02572600
H	3.59021400	-0.94548100	4.85626500
H	4.38956700	-2.03235700	4.04626300
H	7.71997500	-2.64919800	5.20572300
O	8.63106100	1.96799200	-2.96647800
C	9.82184500	1.43107600	-3.51812800
H	9.61611800	0.54049000	-4.12556400
H	10.24333700	2.21006900	-4.15627200
H	10.54683400	1.17591800	-2.73477200

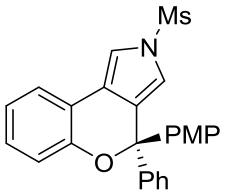
2a’

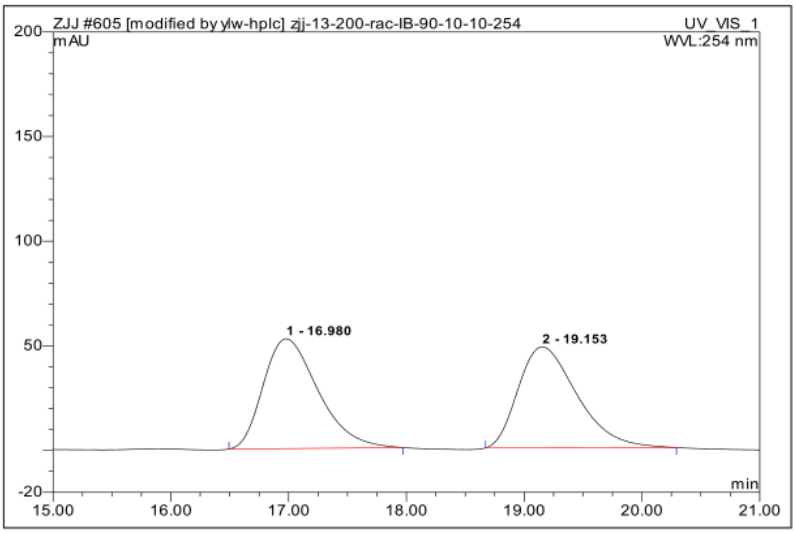


N	-2.94591800	0.32038200	0.22177700
C	-1.96471900	-0.66539800	0.10106000
H	-2.14530800	-1.67590300	0.44604600
C	-0.88927800	-0.07863900	-0.48891000
C	0.47642400	-0.59812900	-0.82304400
C	0.42369300	-2.07680900	-1.16694500
C	0.18678400	-2.49961000	-2.47568800
C	0.52490600	-3.02956700	-0.15143500
C	0.07683900	-3.85622200	-2.76575100
H	0.09220400	-1.76510500	-3.27088900
C	0.40073000	-4.38485600	-0.44128200
H	0.70228900	-2.70923200	0.87410700
C	0.18290100	-4.80289700	-1.75078700
H	-0.09637500	-4.17331800	-3.79165400
H	0.48232300	-5.11568900	0.35996900
C	-2.44720000	1.54120200	-0.23215800
C	-1.18503800	1.30592100	-0.70398000
C	-0.20542100	2.13682200	-1.37979500
C	-0.25107800	3.53080000	-1.45868000
C	0.85219400	1.45896700	-2.01085500
C	0.72525500	4.23419500	-2.15252500
H	-1.06563600	4.05879600	-0.96526500
C	1.83493500	2.15866000	-2.70178800
C	1.76614800	3.54573900	-2.77544600
H	0.67835900	5.31881900	-2.20584000
H	2.64039900	1.60186600	-3.17537800

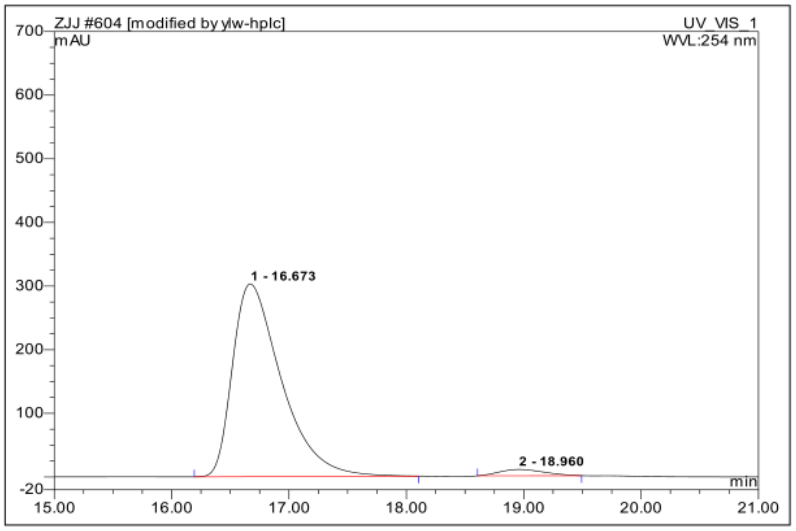
H	2.53630100	4.09223100	-3.31439600
O	0.92377600	0.08884800	-2.01991800
C	1.48210800	-0.30182400	0.28637400
C	1.10308600	0.06374400	1.57927100
C	2.84276900	-0.42377400	0.00273100
C	2.05725400	0.29997100	2.55847300
H	0.04797900	0.16853100	1.83035400
C	3.81201100	-0.18581200	0.97031200
H	3.15504500	-0.70930100	-1.00093700
C	3.41570800	0.17890800	2.25937300
H	1.76800000	0.58611200	3.56702300
H	4.86215300	-0.28651400	0.71291800
S	-4.19511400	0.21147400	1.36448600
O	-5.12337600	1.28894800	1.05180600
O	-4.64498300	-1.17353000	1.34239500
C	-3.36298300	0.55026800	2.88621700
H	-2.90100100	1.53864000	2.81075700
H	-4.11081900	0.53263100	3.68432700
H	-2.61043300	-0.22712000	3.04564300
H	-3.06567000	2.42933300	-0.22140000
H	0.09473700	-5.86241800	-1.97939200
O	4.27630700	0.43509300	3.28117900
C	5.66409100	0.32419700	3.01421900
H	5.98075000	1.02935600	2.23509200
H	6.17725600	0.56736000	3.94664400
H	5.93420100	-0.69533500	2.71059000

(+)-2a: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



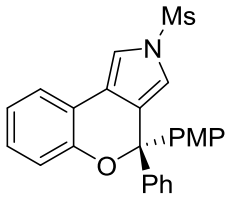


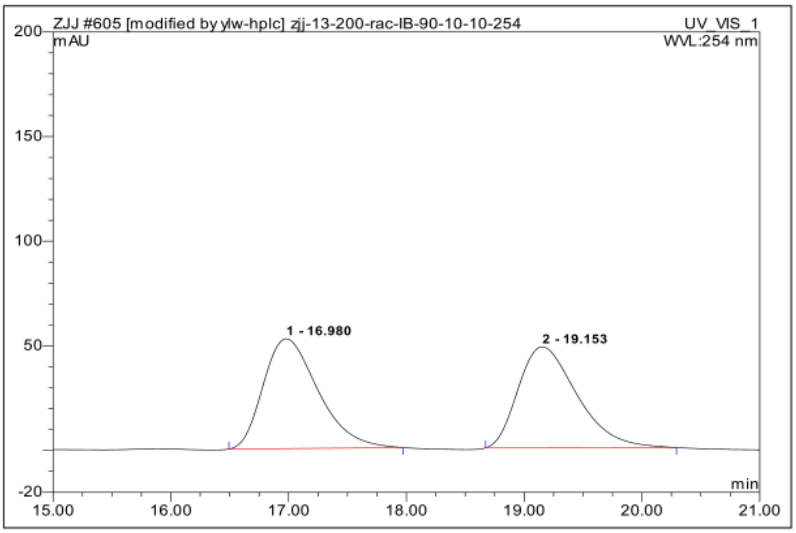
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.98	n.a.	52.440	28.336	50.39	n.a.	BMB*
2	19.15	n.a.	48.211	27.897	49.61	n.a.	BMB*
Total:			100.652	56.233	100.00	0.000	



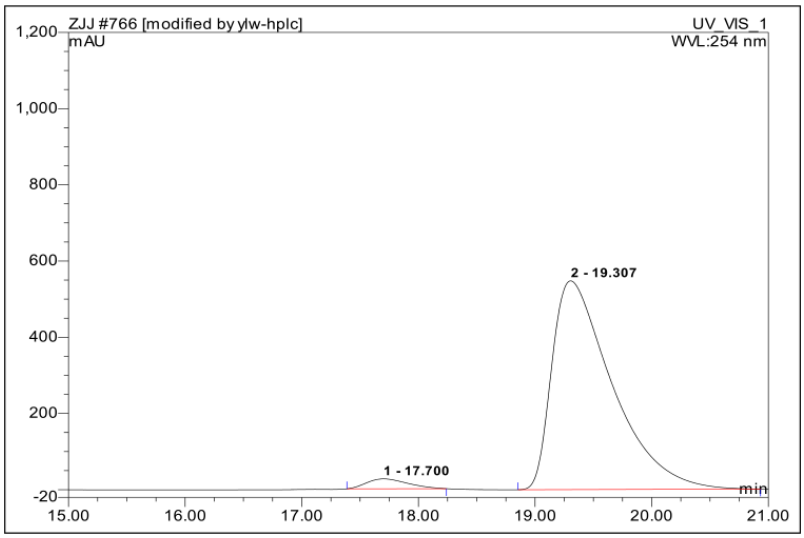
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.67	n.a.	302.792	145.986	97.10	n.a.	BMB*
2	18.96	n.a.	9.877	4.359	2.90	n.a.	BMB*
Total:			312.669	150.345	100.00	0.000	

(-)-2a: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



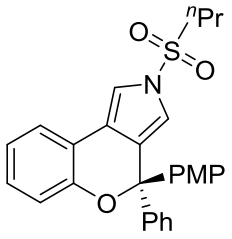


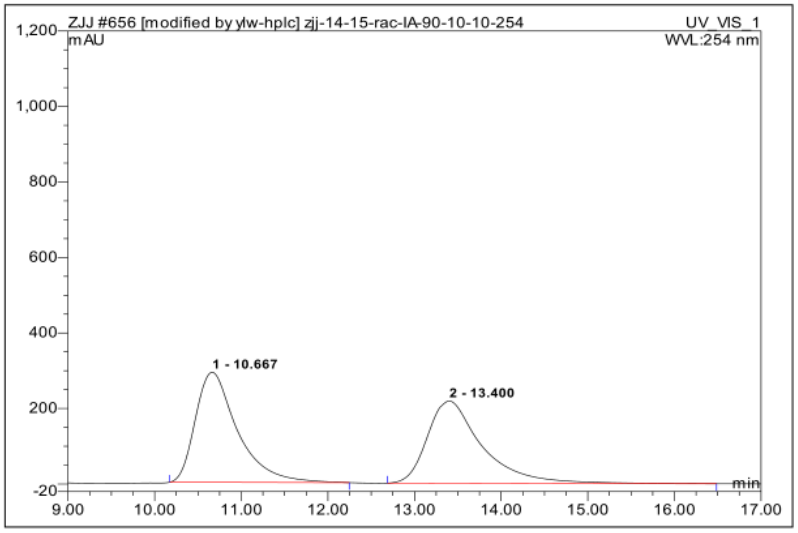
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.98	n.a.	52.440	28.336	50.39	n.a.	BMB*
2	19.15	n.a.	48.211	27.897	49.61	n.a.	BMB*
Total:			100.652	56.233	100.00	0.000	



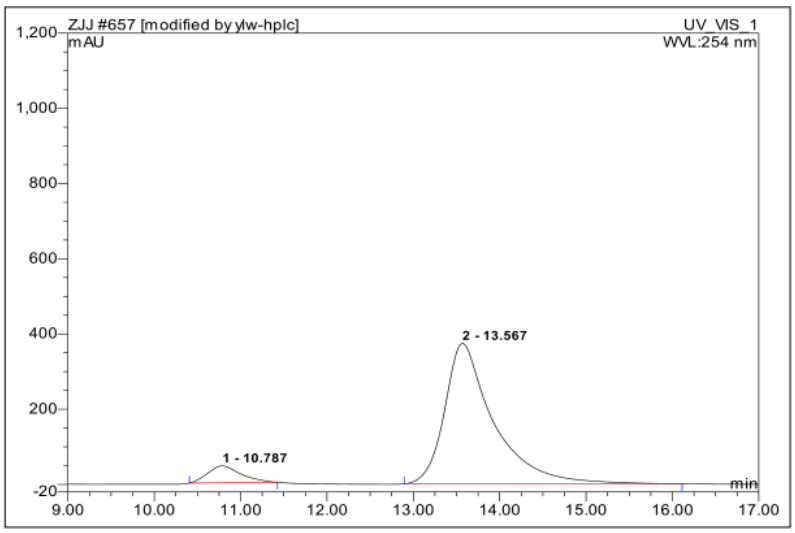
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	17.70	n.a.	25.991	10.602	3.13	n.a.	BMB*
2	19.31	n.a.	547.788	328.245	96.87	n.a.	BMB*
Total:			573.779	338.847	100.00	0.000	

(+)-2b: IA, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



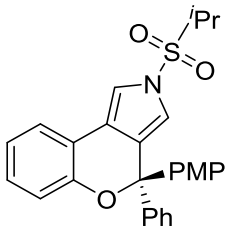


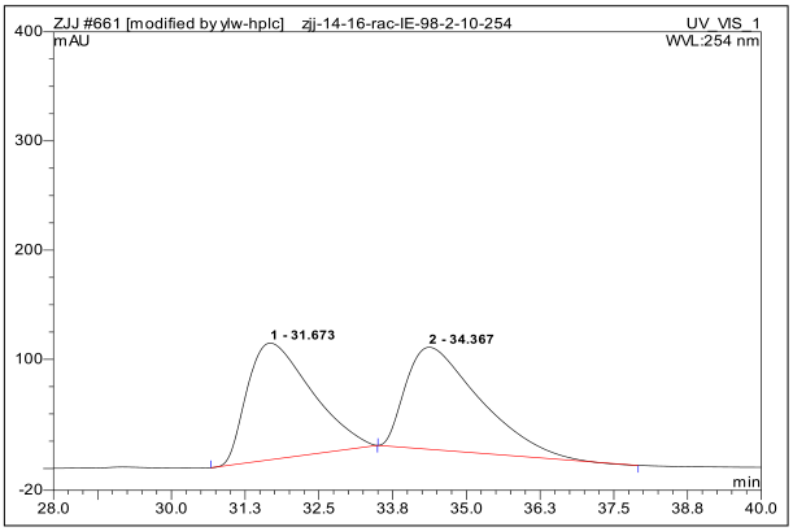
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.67	n.a.	291.577	164.271	50.68	n.a.	BMB*
2	13.40	n.a.	218.055	159.846	49.32	n.a.	BMB*
Total:			509.631	324.117	100.00	0.000	



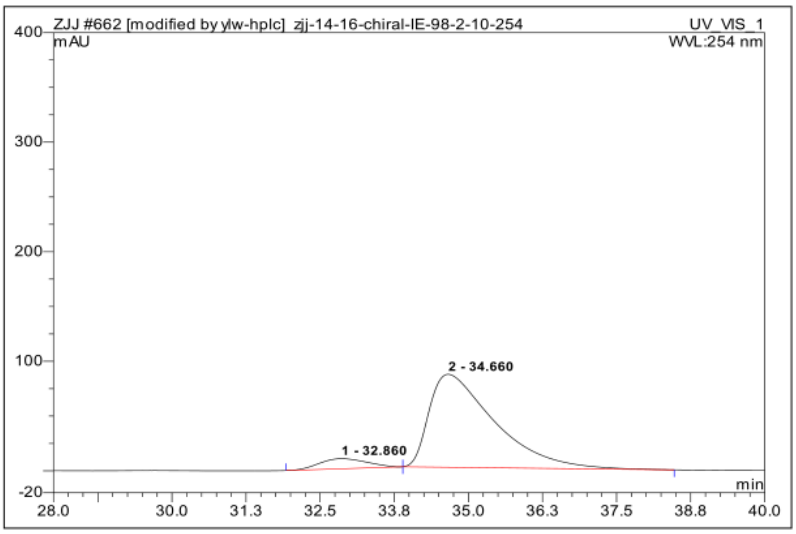
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.79	n.a.	44.860	19.995	7.54	n.a.	BMB*
2	13.57	n.a.	373.569	245.349	92.46	n.a.	BMB*
Total:			418.429	265.344	100.00	0.000	

(+)-2c: IE, *n*-hexane/2-propanol = 98/2, v = 1.0 mL·min^{-1}, λ = 254 nm



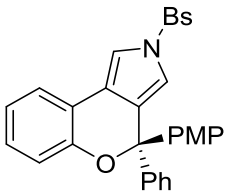


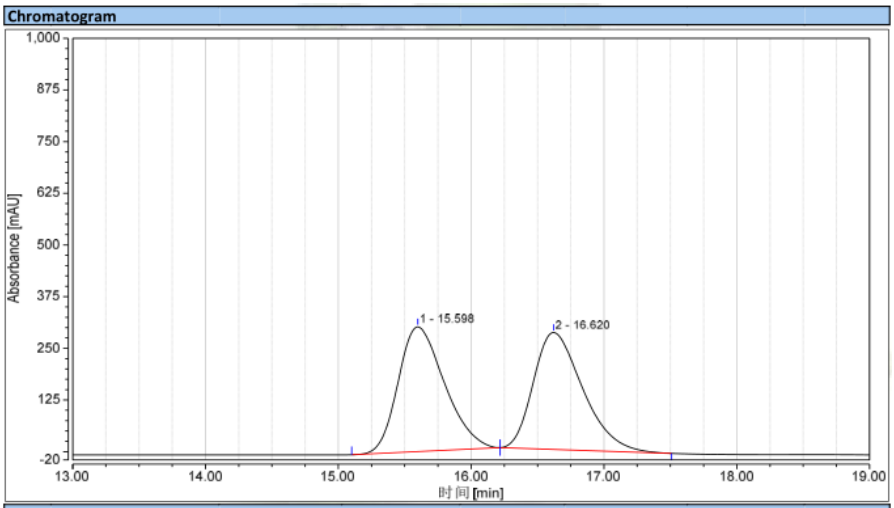
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	31.67	n.a.	106.941	134.765	49.65	n.a.	BMB*
2	34.37	n.a.	93.464	136.656	50.35	n.a.	BMB*
Total:			200.405	271.421	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	32.86	n.a.	9.201	8.472	7.25	n.a.	BMb*
2	34.66	n.a.	84.869	108.326	92.75	n.a.	bMB*
Total:			94.070	116.798	100.00	0.000	

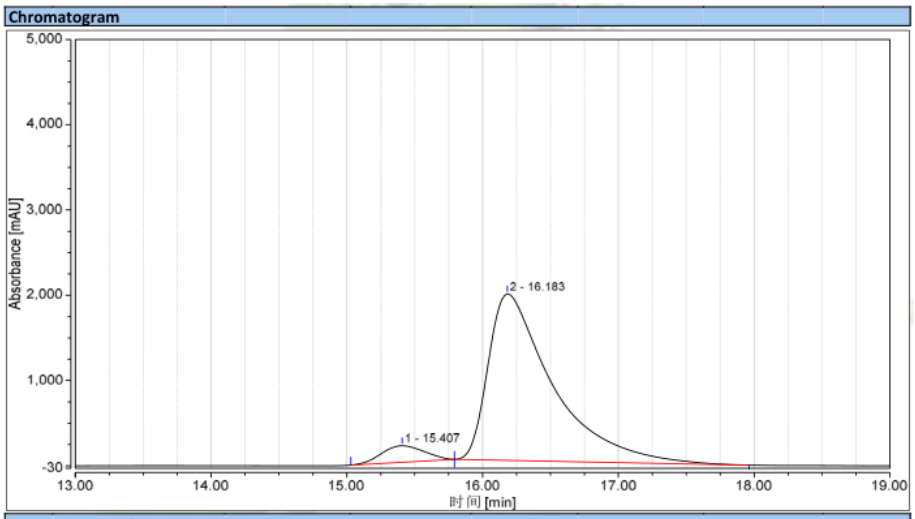
(+)-2d: IE, *n*-hexane/2-propanol = 95/5, v = 1.0 mL min^{-1}, λ = 254 nm





Integration Results

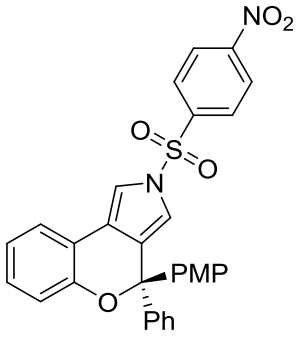
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.598	121.798	301.871	50.00	51.63	n.a.
2		16.620	121.787	282.759	50.00	48.37	n.a.
Total:			**243.585**	**584.630**	**100.00**	**100.00**	

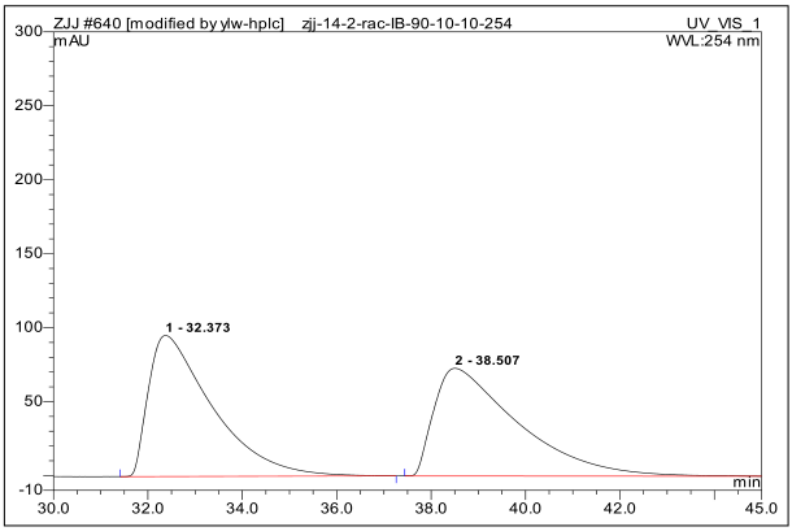


Integration Results

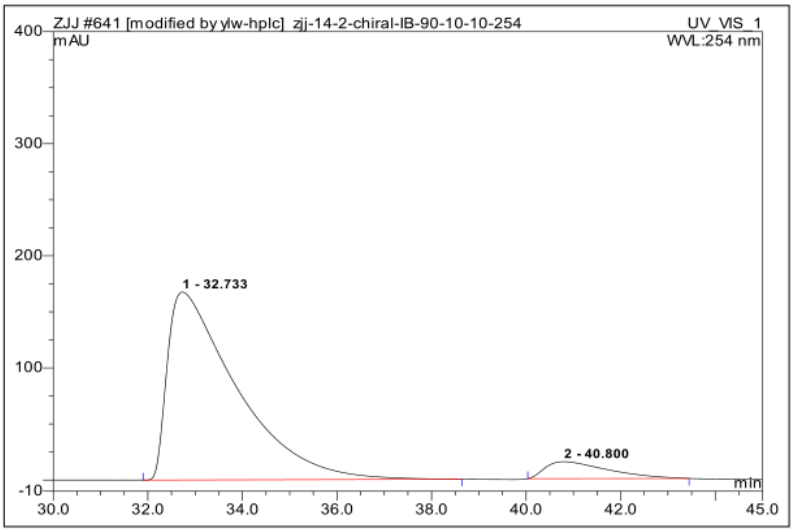
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.407	70.838	194.071	6.18	9.04	n.a.
2		16.183	1075.155	1952.437	93.82	90.96	n.a.
Total:			**1145.993**	**2146.508**	**100.00**	**100.00**	

(+)-2e: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



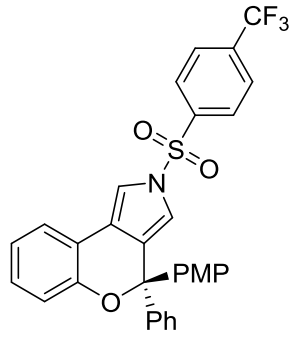


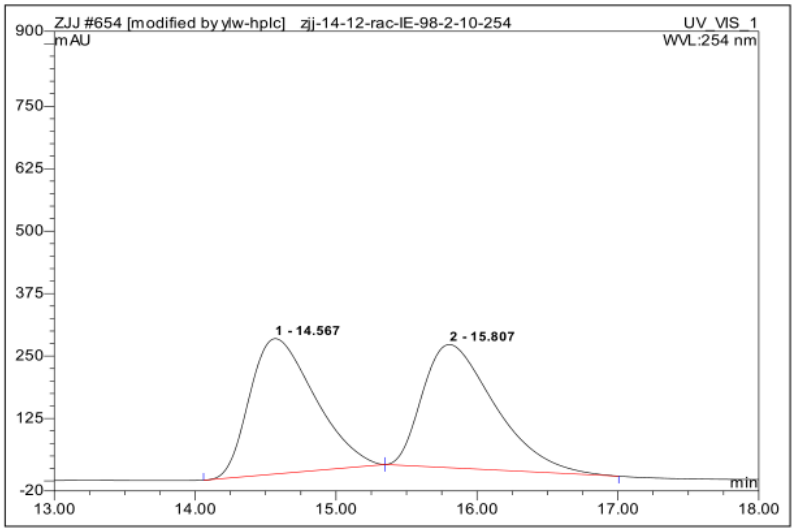
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	32.37	n.a.	95.394	149.351	49.98	n.a.	BMB*
2	38.51	n.a.	72.834	149.498	50.02	n.a.	BMB*
Total:			168.228	298.849	100.00	0.000	



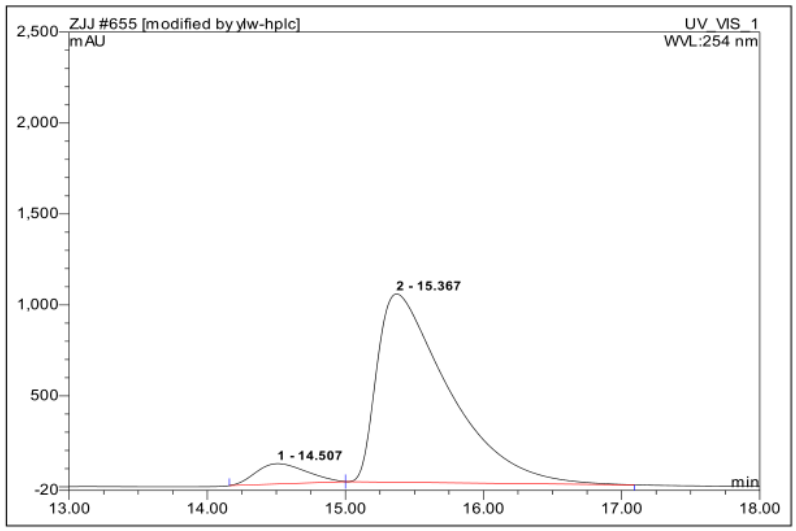
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	32.73	n.a.	167.535	284.562	92.55	n.a.	BMB*
2	40.80	n.a.	15.096	22.914	7.45	n.a.	BMB*
Total:			182.631	307.476	100.00	0.000	

(+)-2f: IE, *n*-hexane/2-propanol = 98/2, v = 1.0 mL min^{-1}, λ = 254 nm



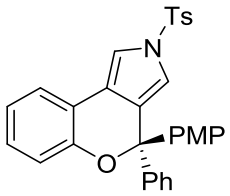


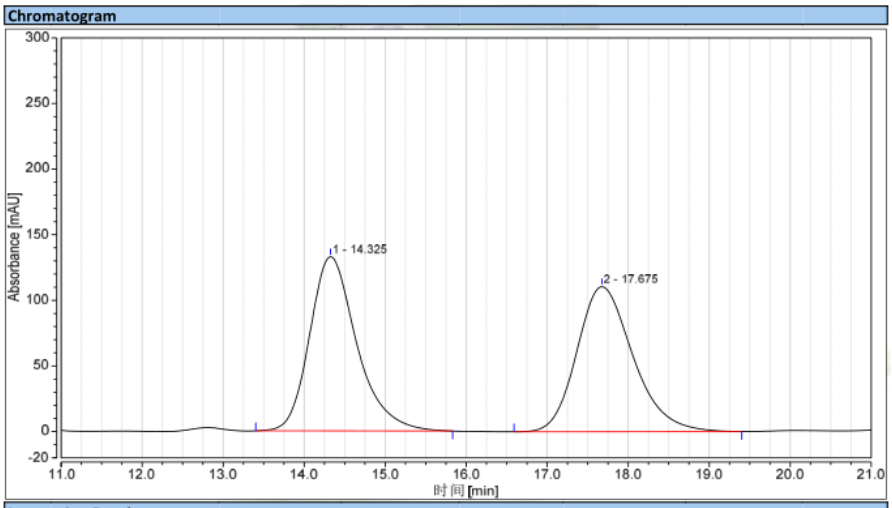
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.57	n.a.	271.003	144.871	49.64	n.a.	BMb*
2	15.81	n.a.	246.636	146.982	50.36	n.a.	bMB*
Total:			517.639	291.852	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.51	n.a.	111.696	47.054	7.03	n.a.	BMb*
2	15.37	n.a.	1035.430	622.363	92.97	n.a.	bMB*
Total:			1147.125	669.417	100.00	0.000	

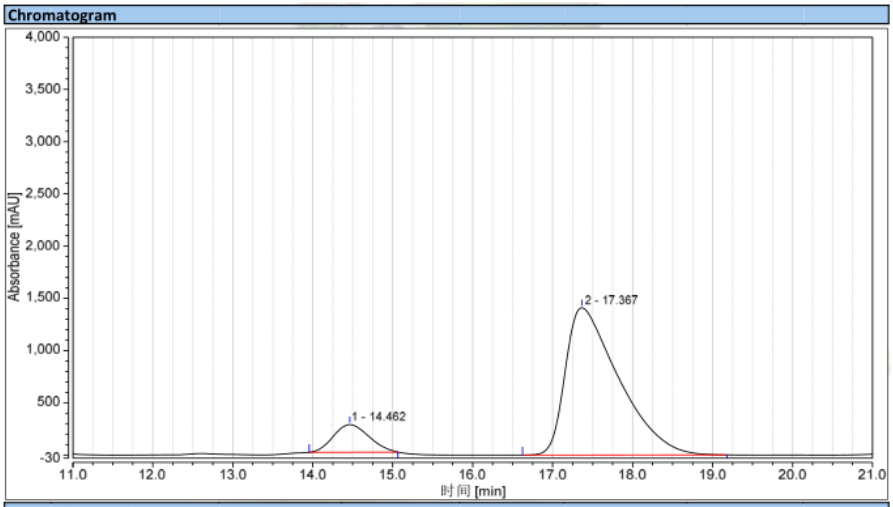
(+)-2g: IG, *n*-hexane/2-propanol = 80/20, v = 1.0 mL min^{-1}, λ = 254 nm





Integration Results

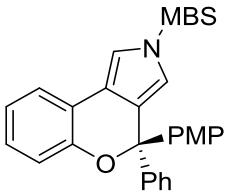
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.325	89.379	132.634	50.20	54.56	n.a.
2		17.675	88.670	110.469	49.80	45.44	n.a.
Total:			**178.049**	**243.103**	**100.00**	**100.00**	

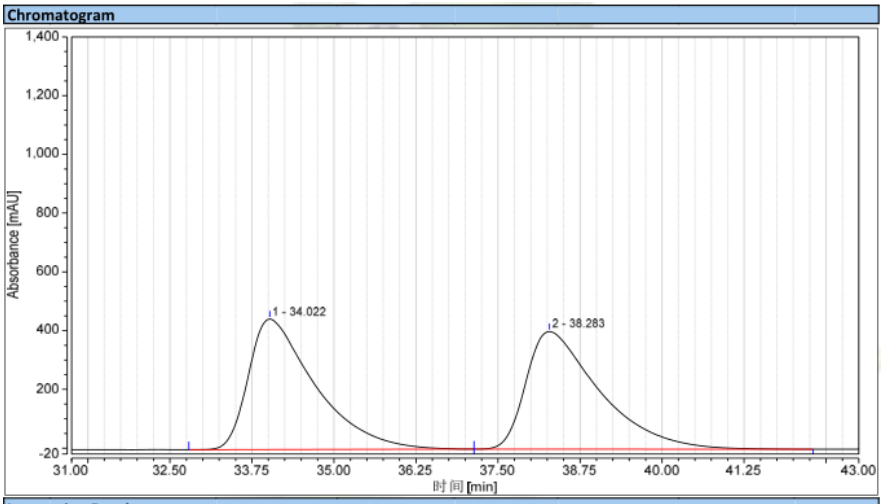


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.462	135.913	263.585	11.10	15.76	n.a.
2		17.367	1088.841	1409.083	88.90	84.24	n.a.
Total:			**1224.753**	**1672.669**	**100.00**	**100.00**	

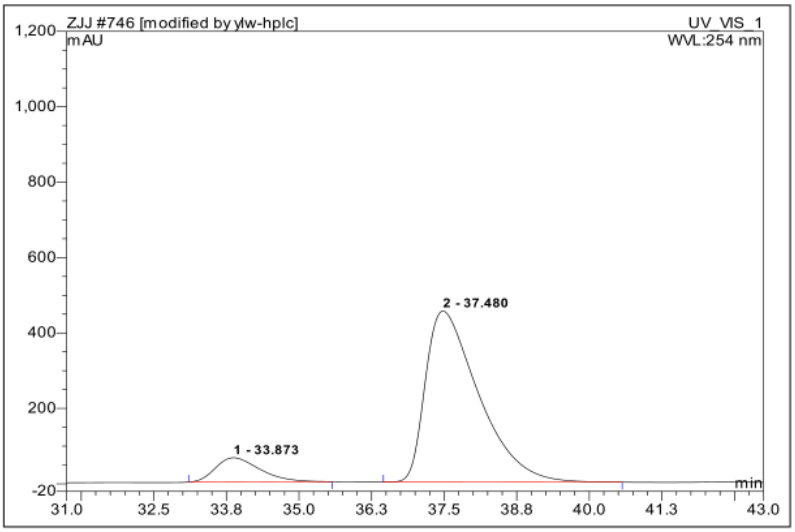
(+)-2h: IE, *n*-hexane/2-propanol = 95/5, v = 1.0 mL min^{-1}, λ = 254 nm





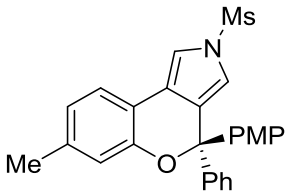
Integration Results

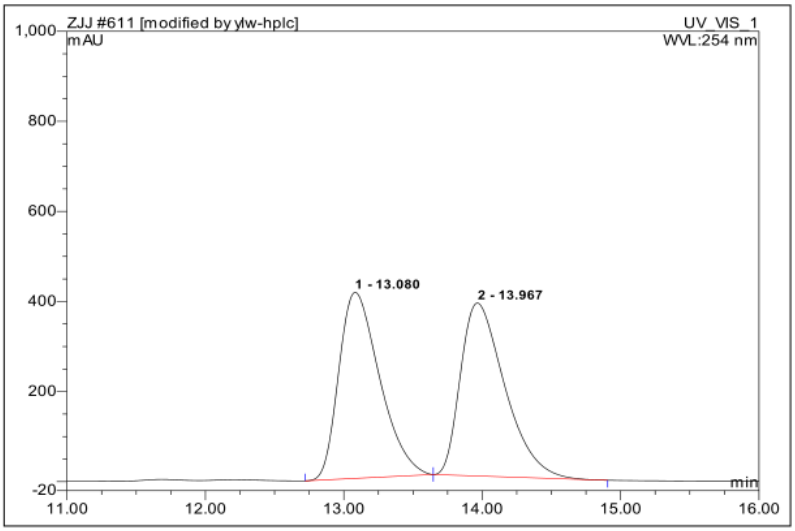
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		34.022	522.197	443.955	50.12	52.59	n.a.
2		38.283	519.680	400.288	49.88	47.41	n.a.
Total:			**1041.877**	**844.243**	**100.00**	**100.00**	



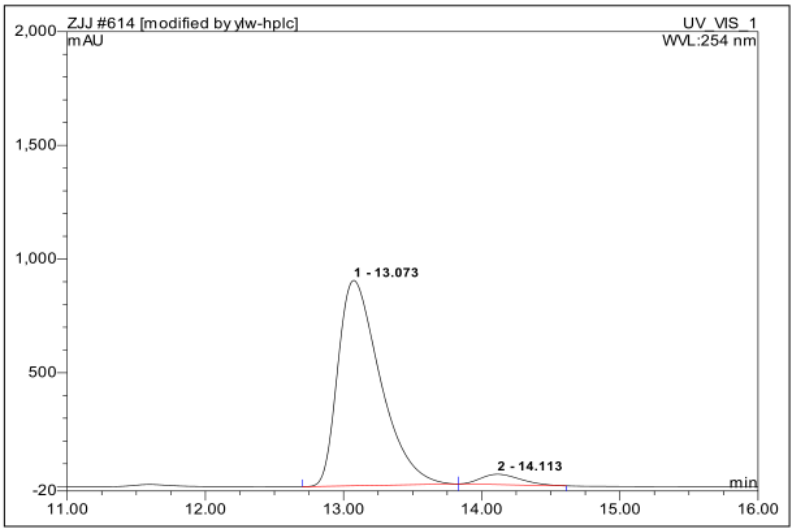
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	33.87	n.a.	64.255	56.908	10.55	n.a.	BMB*
2	37.48	n.a.	453.692	482.752	89.45	n.a.	BMB*
Total:			517.947	539.660	100.00	0.000	

(+)-2i: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



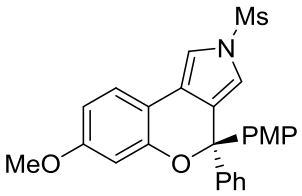


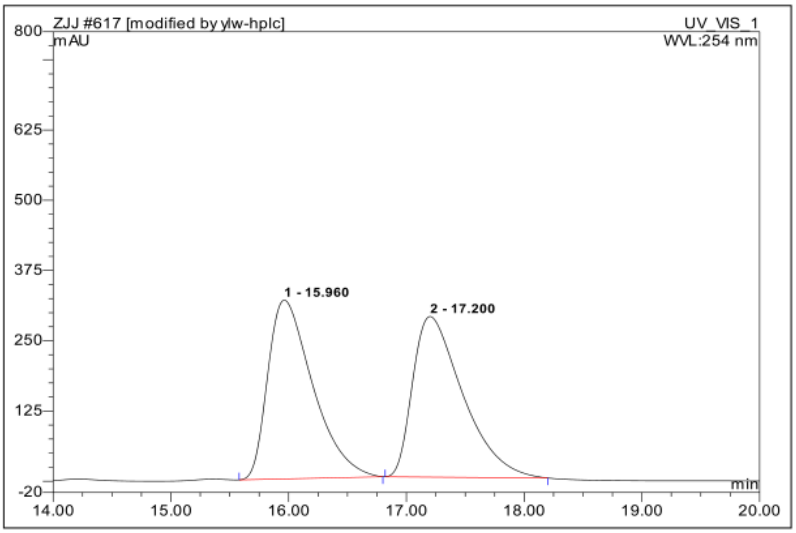
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.08	n.a.	413.183	141.223	49.75	n.a.	BMb*
2	13.97	n.a.	384.021	142.626	50.25	n.a.	bMB*
Total:			797.205	283.849	100.00	0.000	



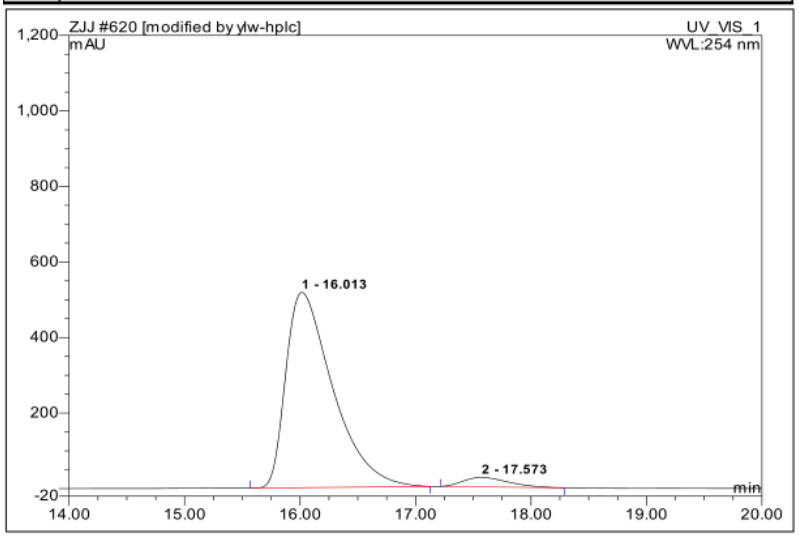
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.07	n.a.	902.784	320.449	95.47	n.a.	BMb*
2	14.11	n.a.	45.644	15.221	4.53	n.a.	bMB*
Total:			948.429	335.670	100.00	0.000	

(+)-2j: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



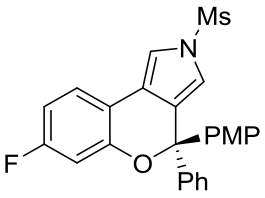


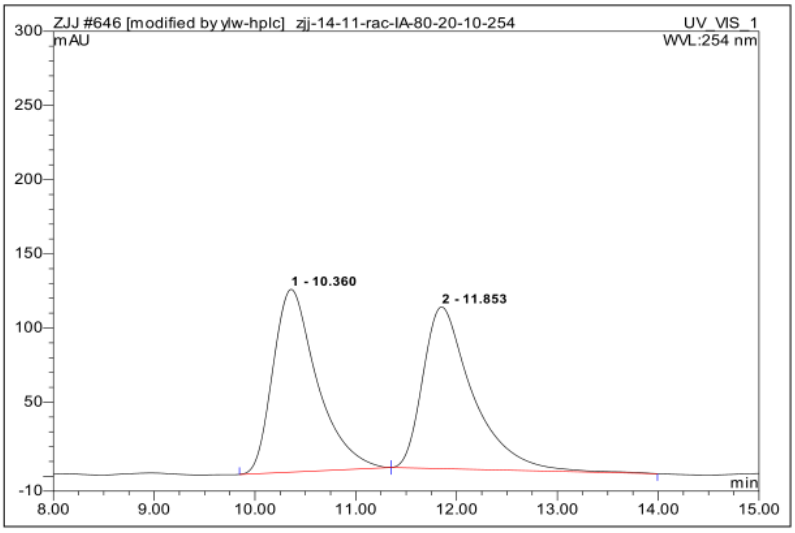
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.96	n.a.	318.077	140.783	49.95	n.a.	BMB*
2	17.20	n.a.	285.703	141.063	50.05	n.a.	BMB*
Total:			603.780	281.846	100.00	0.000	



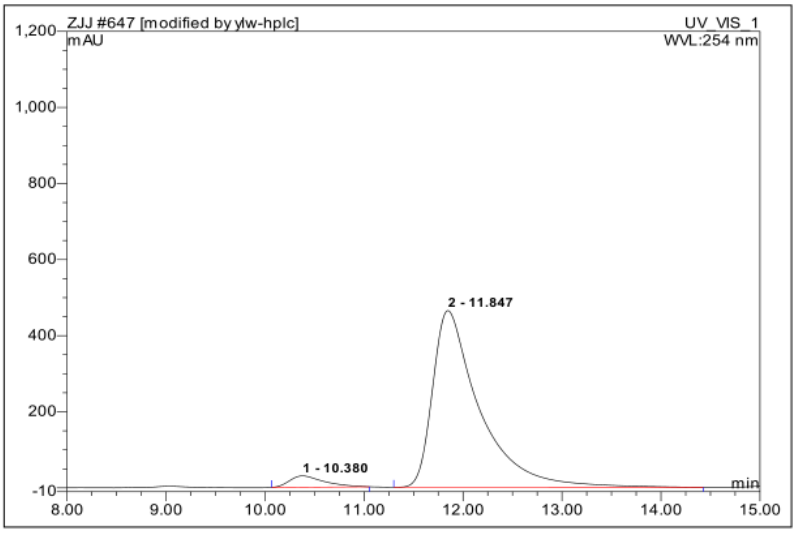
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.01	n.a.	516.886	243.700	95.57	n.a.	BMB*
2	17.57	n.a.	24.941	11.283	4.43	n.a.	BMB*
Total:			541.827	254.983	100.00	0.000	

(+)-2k: IA, *n*-hexane/2-propanol = 80/20, v = 1.0 mL min^{-1}, λ = 254 nm



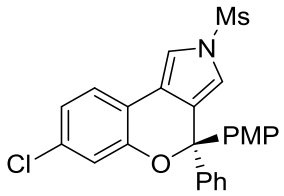


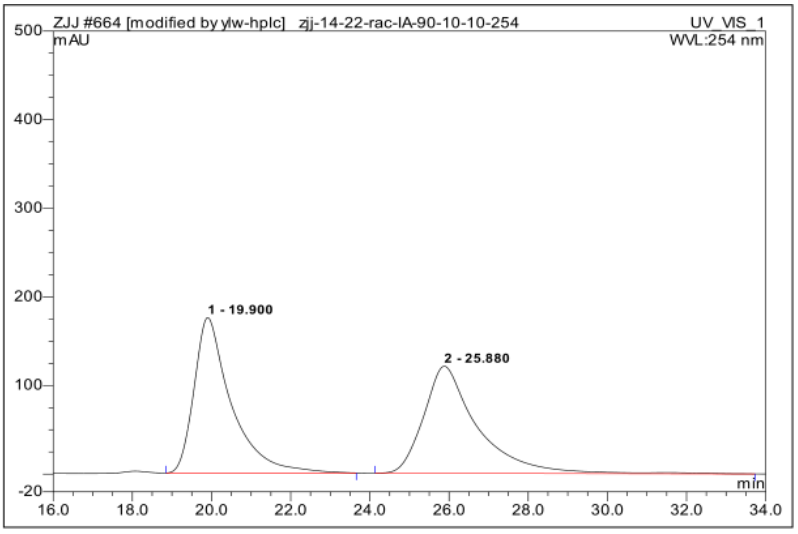
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.36	n.a.	123.172	62.411	50.01	n.a.	BMb*
2	11.85	n.a.	109.022	62.398	49.99	n.a.	bMB*
Total:			232.194	124.809	100.00	0.000	



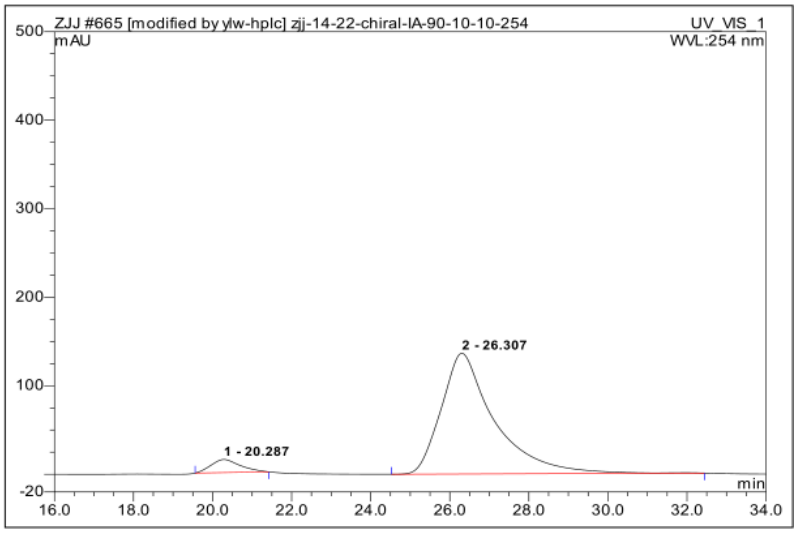
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.38	n.a.	29.786	11.972	4.47	n.a.	BMB*
2	11.85	n.a.	464.360	255.595	95.53	n.a.	BMB*
Total:			494.146	267.567	100.00	0.000	

(+)-2l: IA, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



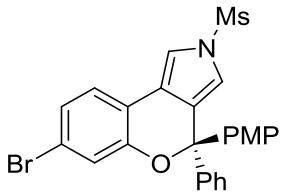


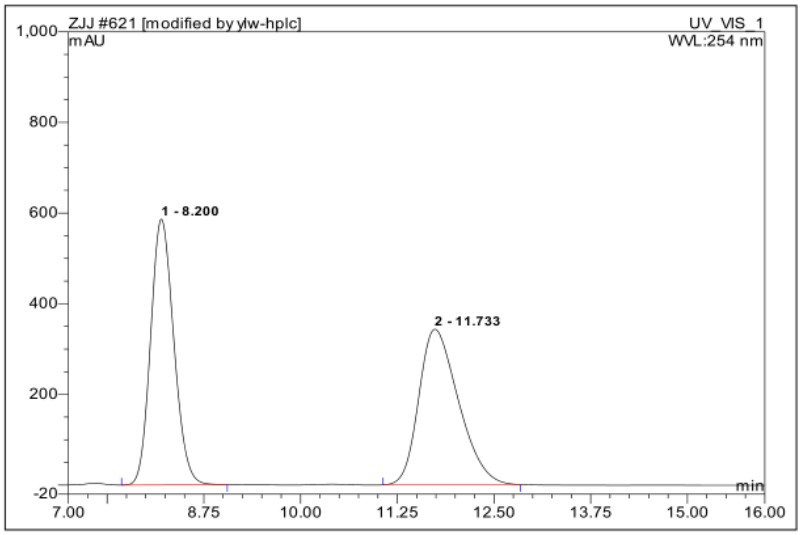
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.90	n.a.	175.326	190.812	50.00	n.a.	BMB*
2	25.88	n.a.	120.859	190.836	50.00	n.a.	BMB*
Total:			296.185	381.648	100.00	0.000	



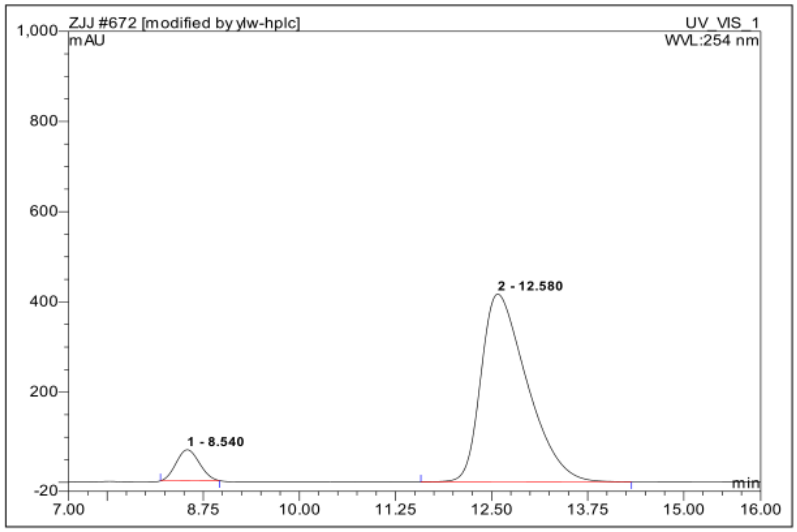
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	20.29	n.a.	14.787	12.680	5.64	n.a.	BMB*
2	26.31	n.a.	136.382	212.253	94.36	n.a.	BMB*
Total:			151.168	224.933	100.00	0.000	

(+)-2m: IG, *n*-hexane/2-propanol = 50/50, v = 1.0 mL·min^{-1}, λ = 254 nm



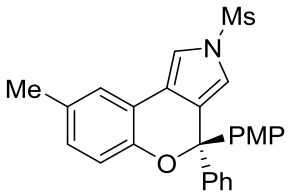


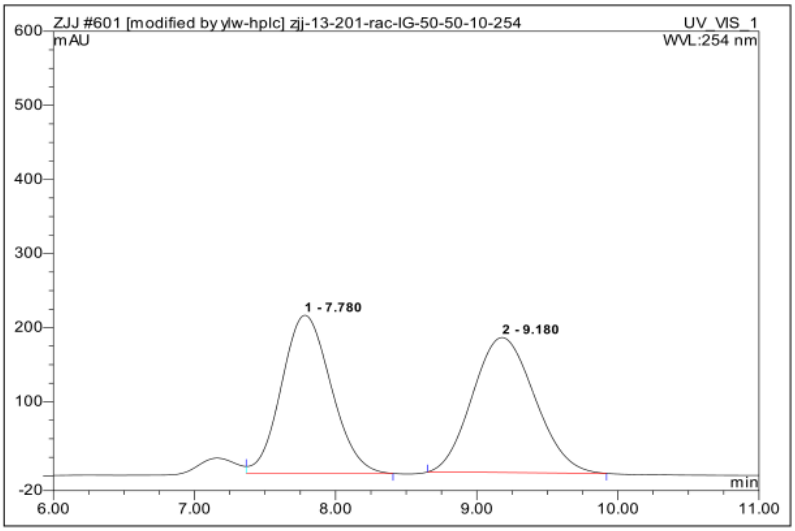
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.20	n.a.	586.328	203.664	49.92	n.a.	BMB*
2	11.73	n.a.	343.080	204.304	50.08	n.a.	BMB*
Total:			929.408	407.968	100.00	0.000	



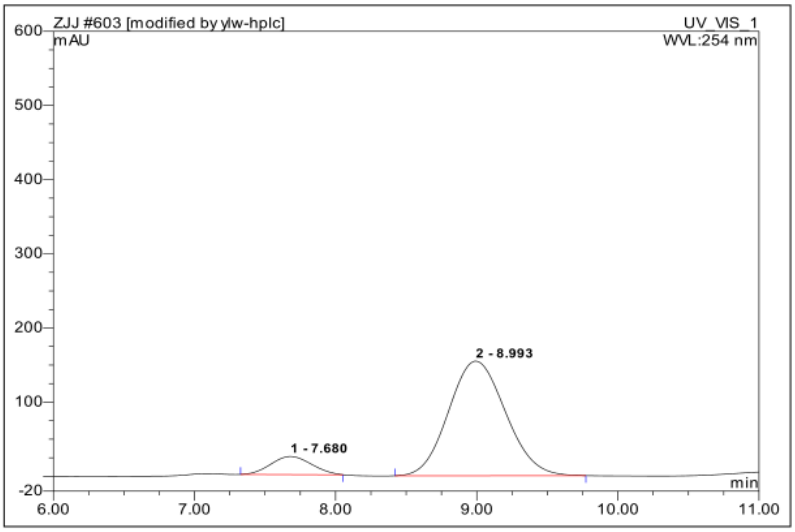
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.54	n.a.	68.638	24.071	7.68	n.a.	BMB*
2	12.58	n.a.	416.534	289.462	92.32	n.a.	BMB*
Total:			485.172	313.533	100.00	0.000	

(+)-2n: IG, *n*-hexane/2-propanol = 50/50, v = 1.0 mL·min^{-1}, λ = 254 nm



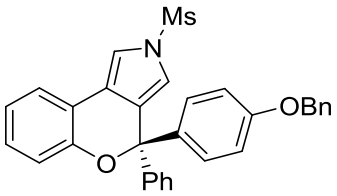


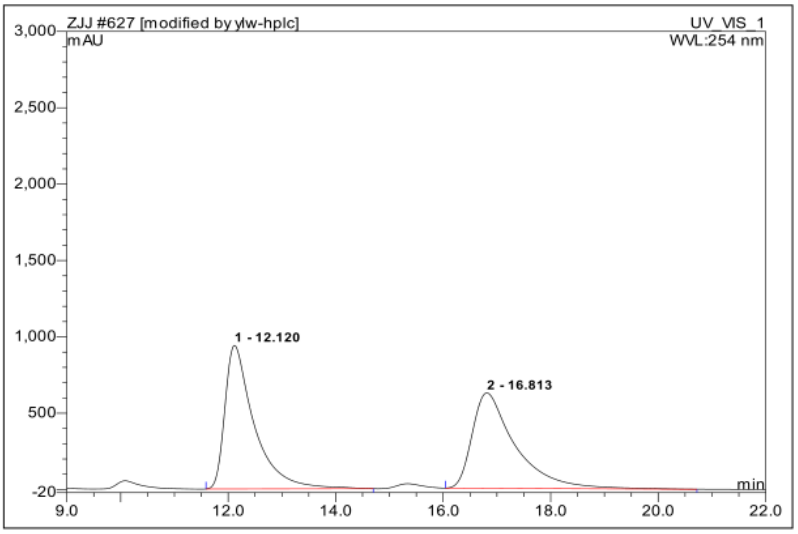
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.78	n.a.	213.476	87.018	48.30	n.a.	MB*
2	9.18	n.a.	182.174	93.134	51.70	n.a.	BMB*
Total:			395.650	180.152	100.00	0.000	



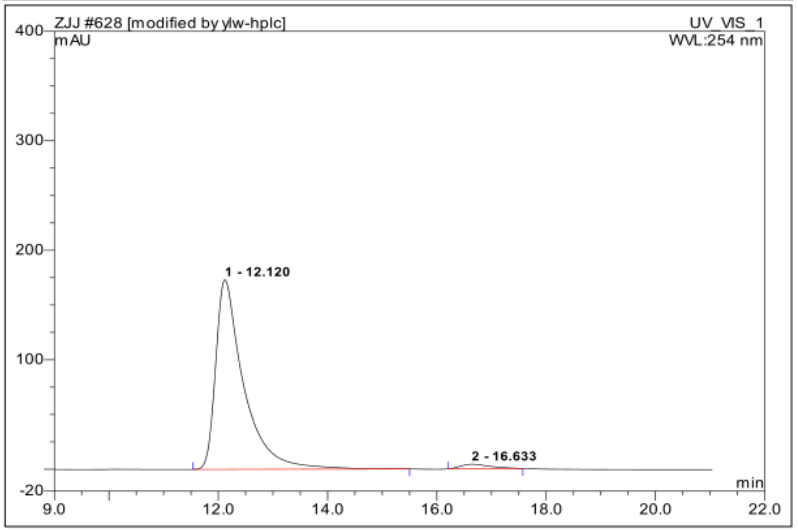
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.68	n.a.	24.388	8.146	10.13	n.a.	BMB*
2	8.99	n.a.	154.492	72.286	89.87	n.a.	BMB*
Total:			178.880	80.432	100.00	0.000	

(+)-2t: IA, *n*-hexane/2-propanol = 70/30, v = 1.0 mL·min^{-1}, λ = 254 nm



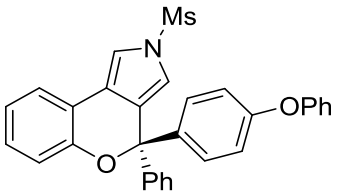


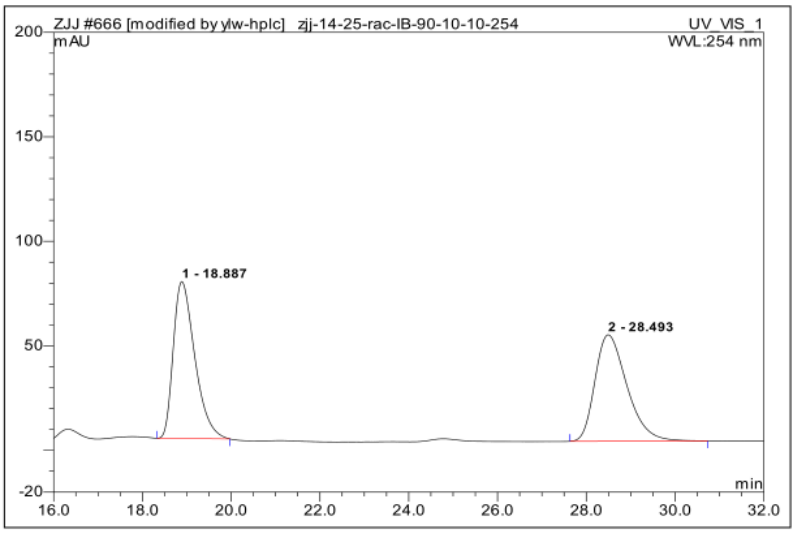
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.12	n.a.	939.596	595.337	50.66	n.a.	BMB*
2	16.81	n.a.	624.379	579.748	49.34	n.a.	BMB*
Total:			1563.975	1175.085	100.00	0.000	



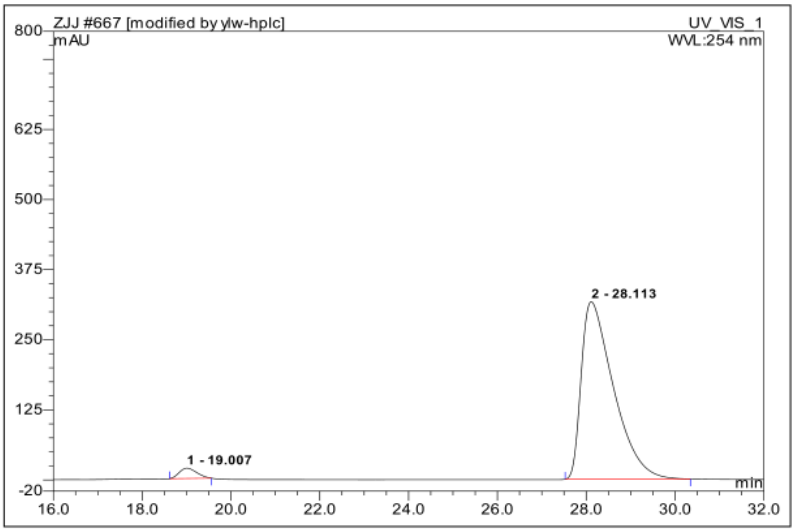
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.12	n.a.	173.132	102.904	97.54	n.a.	BMB*
2	16.63	n.a.	4.107	2.591	2.46	n.a.	BMB*
Total:			177.240	105.496	100.00	0.000	

(+)-2u: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



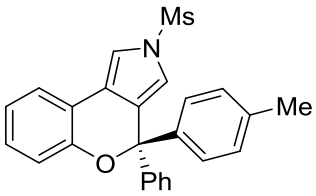


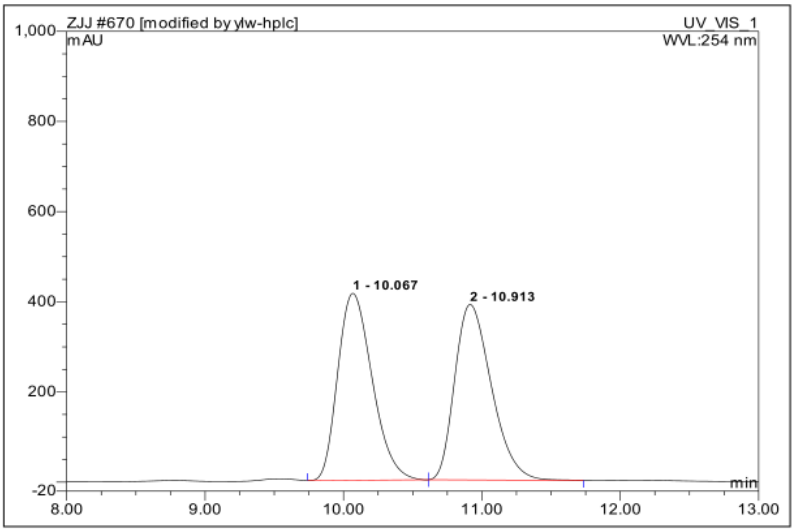
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.89	n.a.	75.054	42.161	49.79	n.a.	BMB*
2	28.49	n.a.	50.906	42.508	50.21	n.a.	BMB*
Total:			125.960	84.669	100.00	0.000	



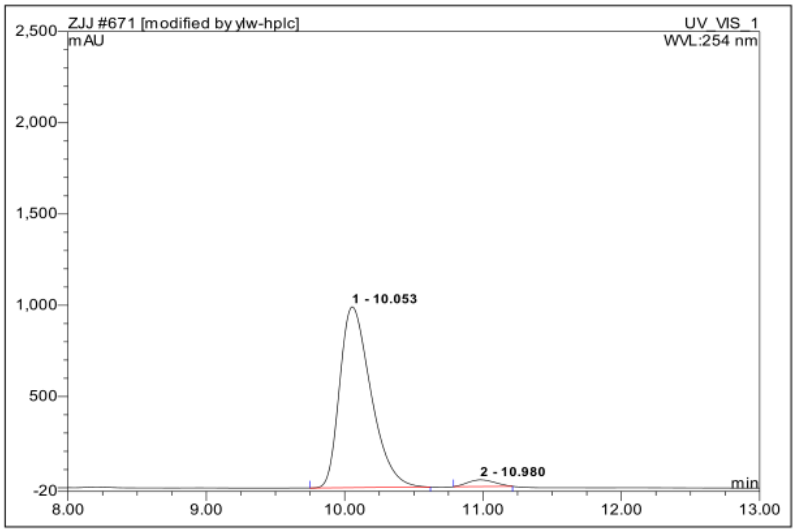
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.01	n.a.	18.363	8.386	3.06	n.a.	BMB*
2	28.11	n.a.	316.440	266.018	96.94	n.a.	BMB*
Total:			334.802	274.404	100.00	0.000	

(+)-2v: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



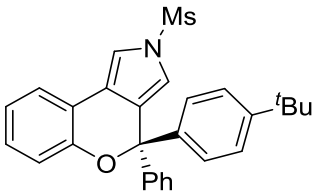


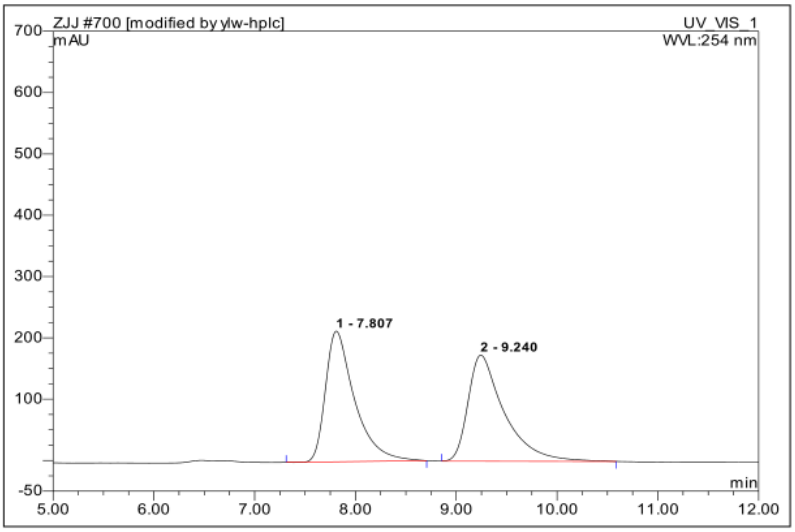
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.07	n.a.	414.639	119.565	50.00	n.a.	BMb*
2	10.91	n.a.	389.216	119.574	50.00	n.a.	bMB*
Total:			803.855	239.139	100.00	0.000	



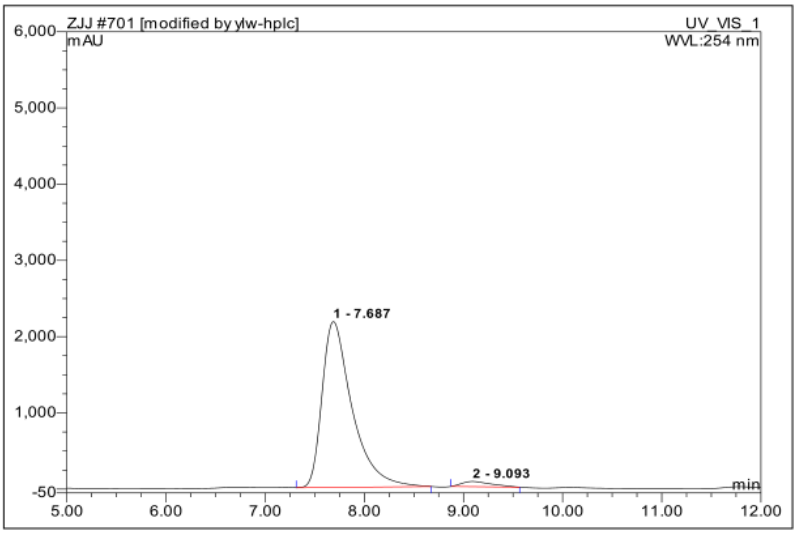
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.05	n.a.	991.206	259.722	96.91	n.a.	BMB*
2	10.98	n.a.	36.331	8.272	3.09	n.a.	BMB*
Total:			1027.537	267.994	100.00	0.000	

(+)-2w: IA, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



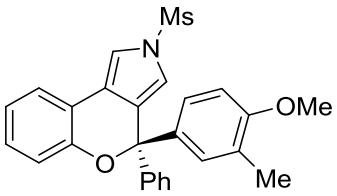


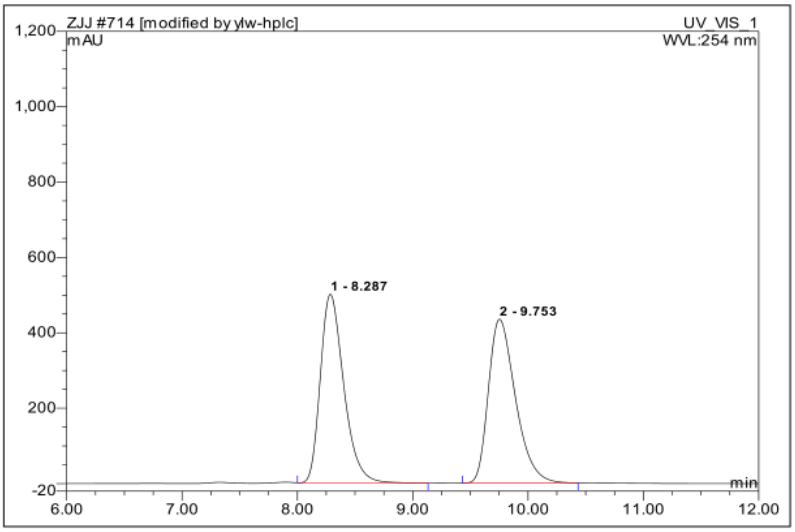
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.81	n.a.	212.988	71.186	49.76	n.a.	BMB*
2	9.24	n.a.	173.065	71.864	50.24	n.a.	BMB*
Total:			386.053	143.051	100.00	0.000	



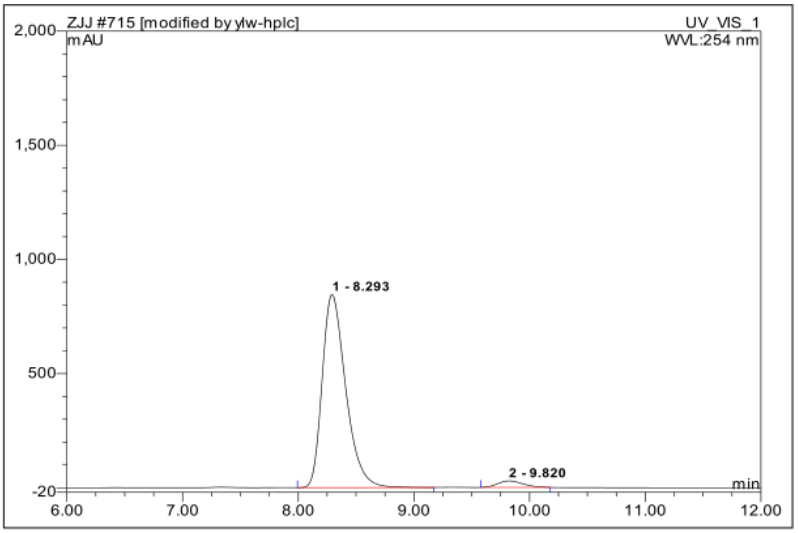
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.69	n.a.	2174.886	762.994	97.00	n.a.	BMB*
2	9.09	n.a.	67.971	23.637	3.00	n.a.	BMB*
Total:			2242.858	786.631	100.00	0.000	

(+)-2x: IB, *n*-hexane/2-propanol = 80/20, v = 1.0 mL min^{-1}, λ = 254 nm



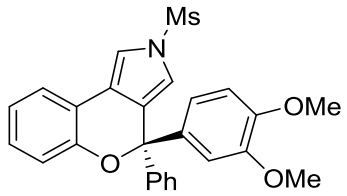


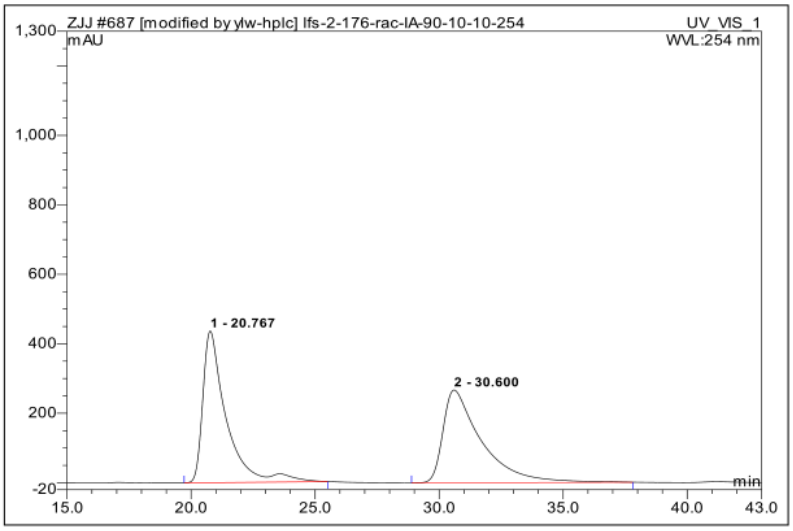
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.29	n.a.	500.525	117.863	49.95	n.a.	BMB*
2	9.75	n.a.	434.689	118.092	50.05	n.a.	BMB*
Total:			935.214	235.955	100.00	0.000	



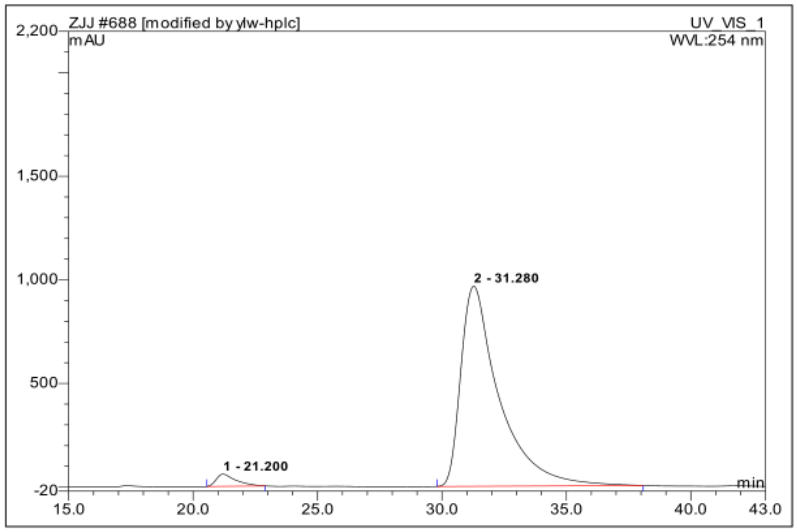
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.29	n.a.	845.601	199.127	96.50	n.a.	BMB*
2	9.82	n.a.	28.492	7.232	3.50	n.a.	BMB*
Total:			874.093	206.359	100.00	0.000	

(+)-2y: IA, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



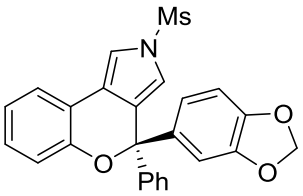


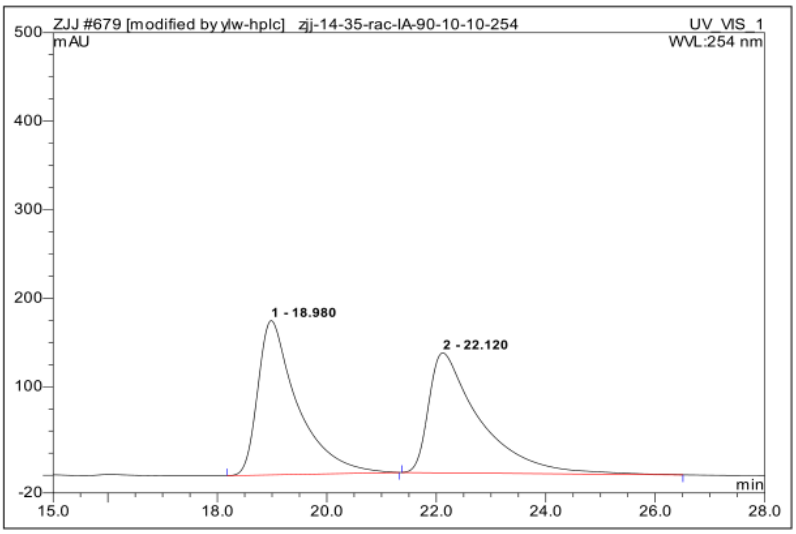
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	20.77	n.a.	436.336	477.144	50.00	n.a.	BMB*
2	30.60	n.a.	266.746	477.174	50.00	n.a.	BMB*
Total:			703.082	954.318	100.00	0.000	



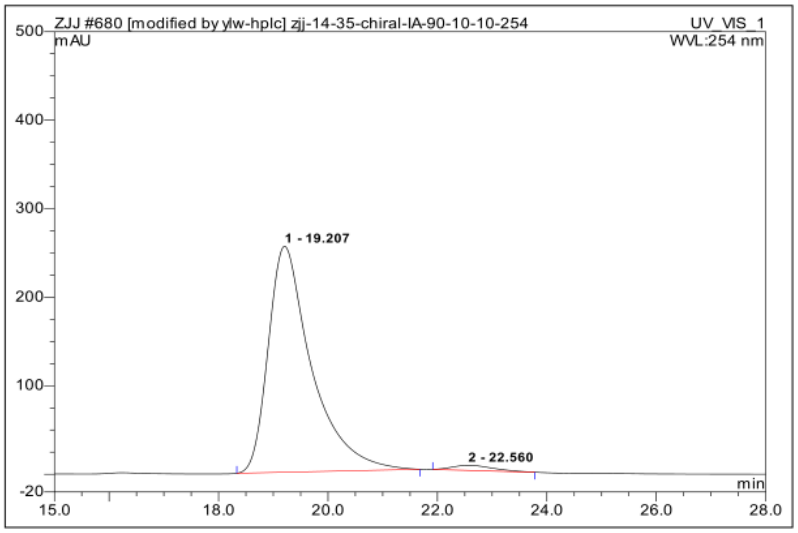
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	21.20	n.a.	58.941	54.211	3.04	n.a.	BMB*
2	31.28	n.a.	966.180	1729.808	96.96	n.a.	BMB*
Total:			1025.121	1784.019	100.00	0.000	

(+)-2z: IA, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



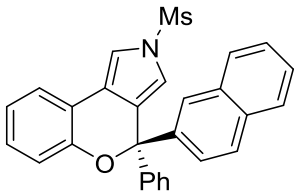


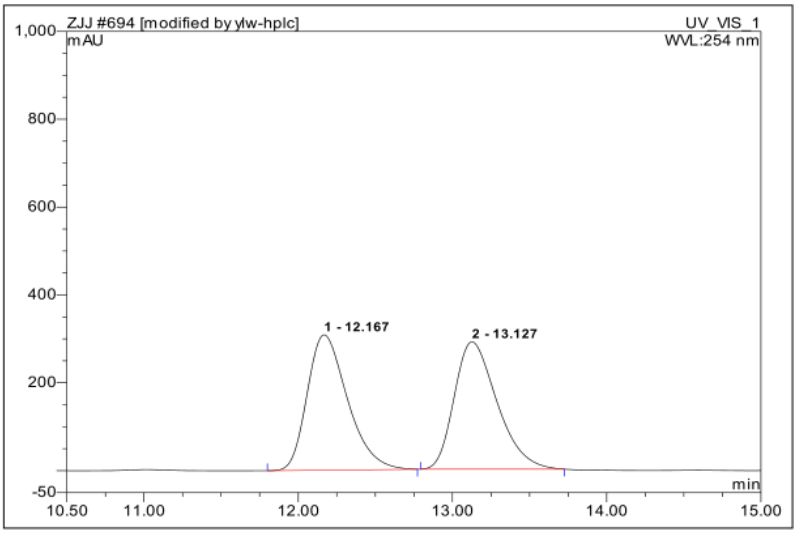
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.98	n.a.	174.239	146.203	50.00	n.a.	BMB*
2	22.12	n.a.	135.467	146.183	50.00	n.a.	BMB*
Total:			309.706	292.386	100.00	0.000	



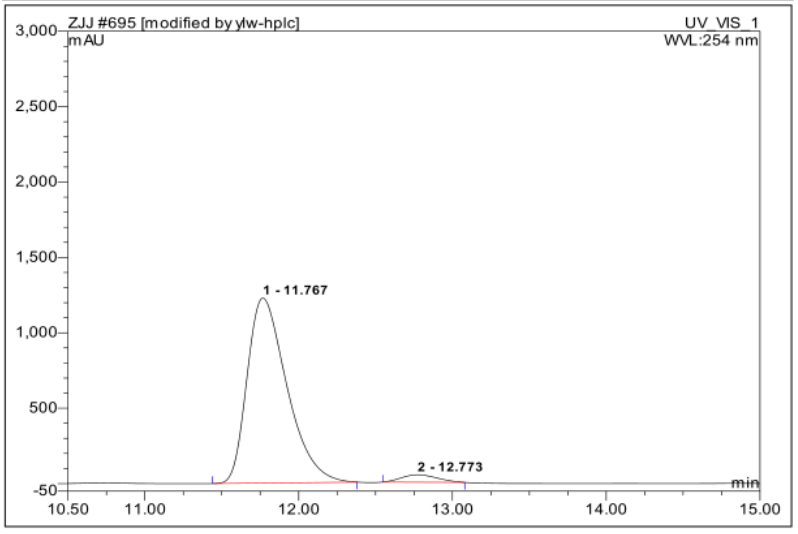
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.21	n.a.	255.271	234.103	97.93	n.a.	BMB*
2	22.56	n.a.	5.732	4.956	2.07	n.a.	BMB*
Total:			261.004	239.058	100.00	0.000	

(+)-2aa: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



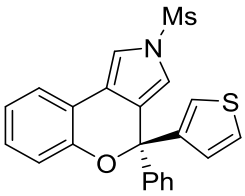


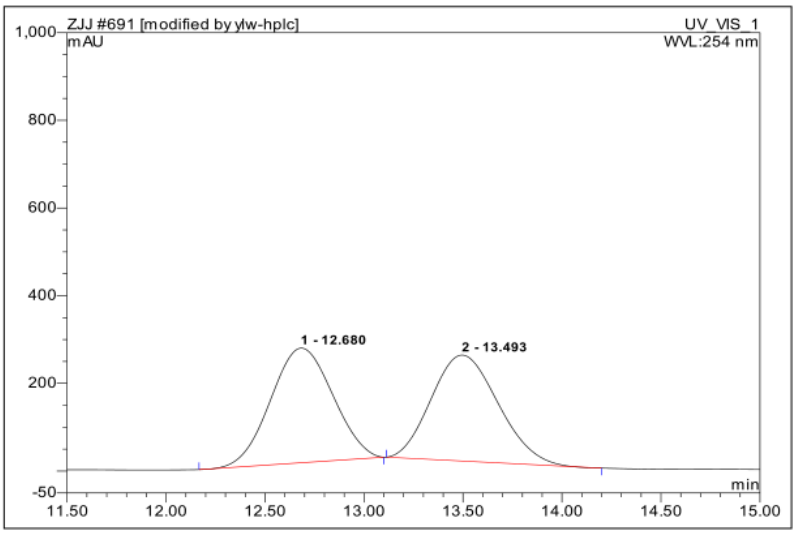
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.17	n.a.	308.238	93.237	50.00	n.a.	BMB*
2	13.13	n.a.	290.041	93.227	50.00	n.a.	BMB*
Total:			598.279	186.463	100.00	0.000	



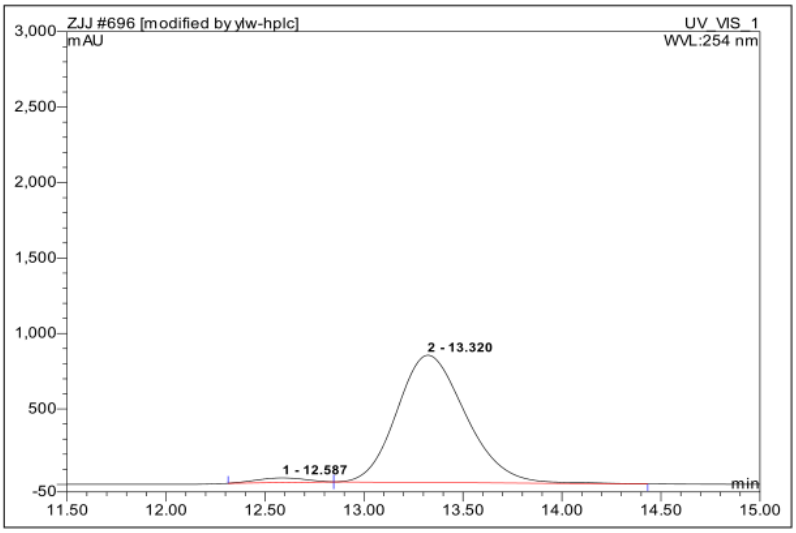
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.77	n.a.	1227.707	367.958	96.52	n.a.	BMB*
2	12.77	n.a.	49.193	13.271	3.48	n.a.	BMB*
Total:			1276.899	381.229	100.00	0.000	

(+)-2ab: IG, *n*-hexane/2-propanol = 90/10, v = 1.0 mL min^{-1}, λ = 254 nm



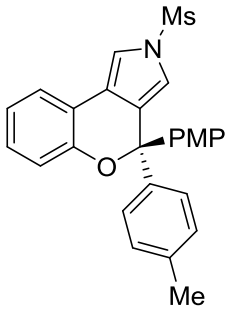


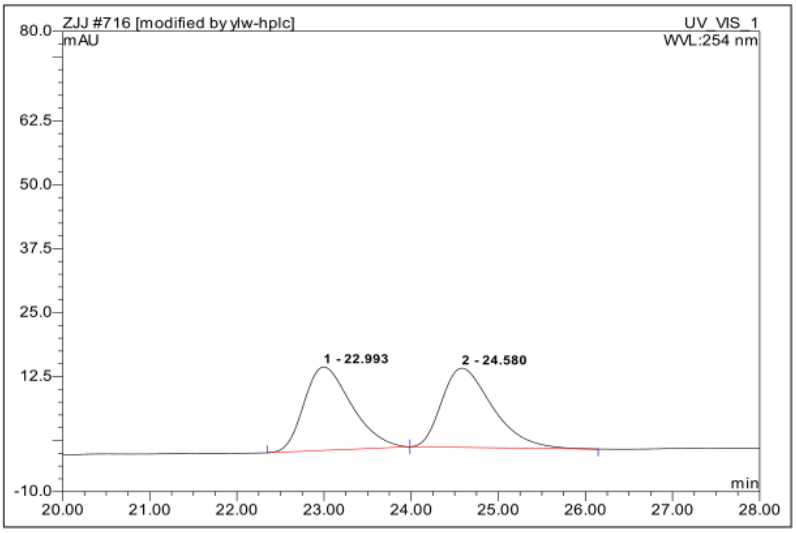
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.68	n.a.	261.518	95.147	50.14	n.a.	BMB*
2	13.49	n.a.	241.530	94.628	49.86	n.a.	BMB*
Total:			503.047	189.775	100.00	0.000	



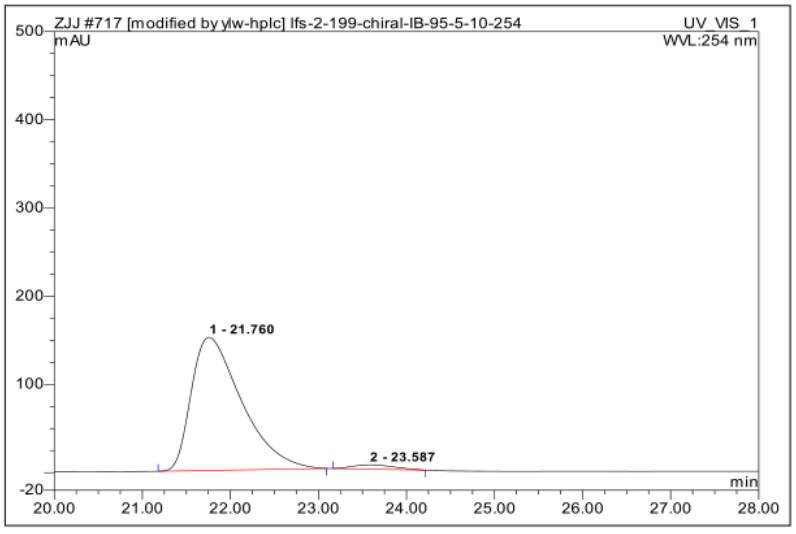
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.59	n.a.	30.731	8.742	2.51	n.a.	BMb*
2	13.32	n.a.	843.077	340.068	97.49	n.a.	bMB*
Total:			873.808	348.811	100.00	0.000	

(+)-2ac: IB, *n*-hexane/2-propanol = 95/5, v = 1.0 mL·min^{-1}, λ = 254 nm



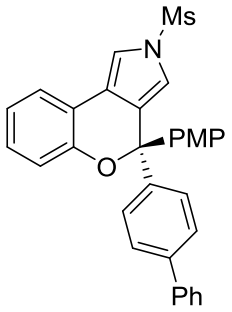


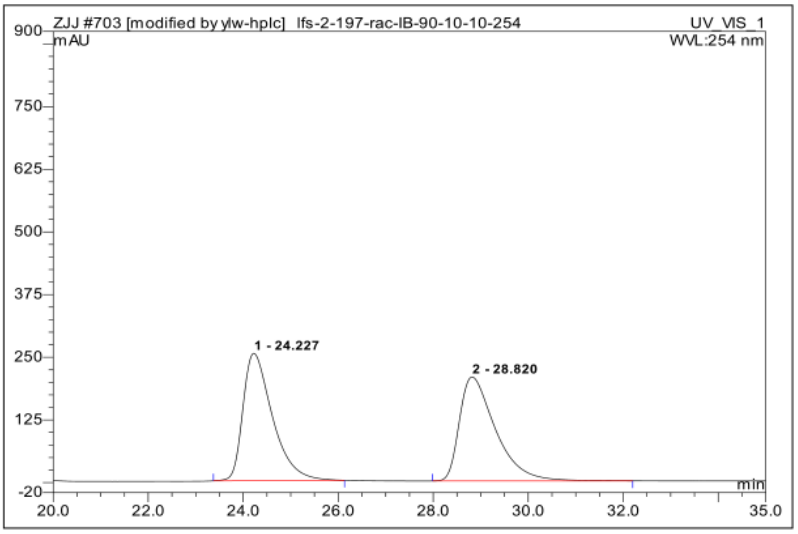
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	22.99	n.a.	16.317	10.265	49.63	n.a.	BMb*
2	24.58	n.a.	15.483	10.419	50.37	n.a.	bMB*
Total:			31.800	20.683	100.00	0.000	



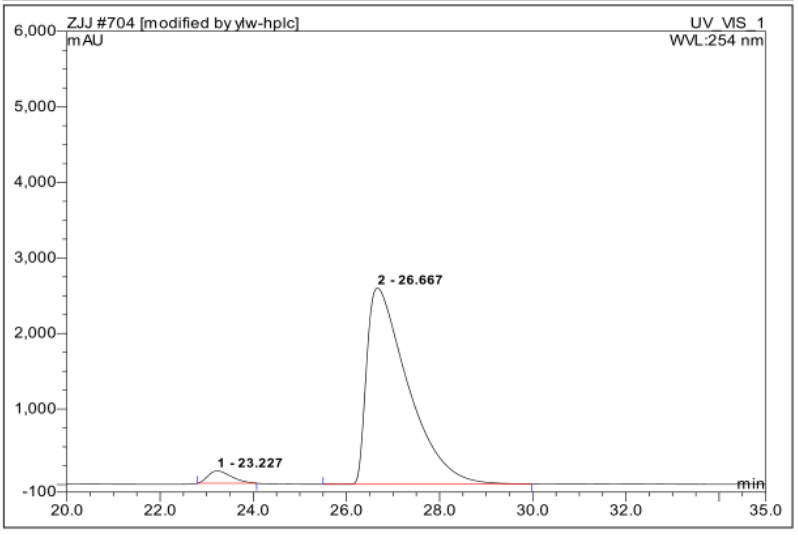
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	21.76	n.a.	150.818	99.839	97.43	n.a.	BMB*
2	23.59	n.a.	4.870	2.633	2.57	n.a.	BMB*
Total:			155.688	102.472	100.00	0.000	

(+)-2ae: IB, *n*-hexane/2-propanol = 90/10, v = 1.0 mL·min^{-1}, λ = 254 nm



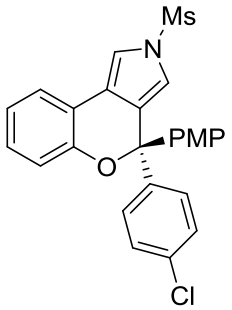


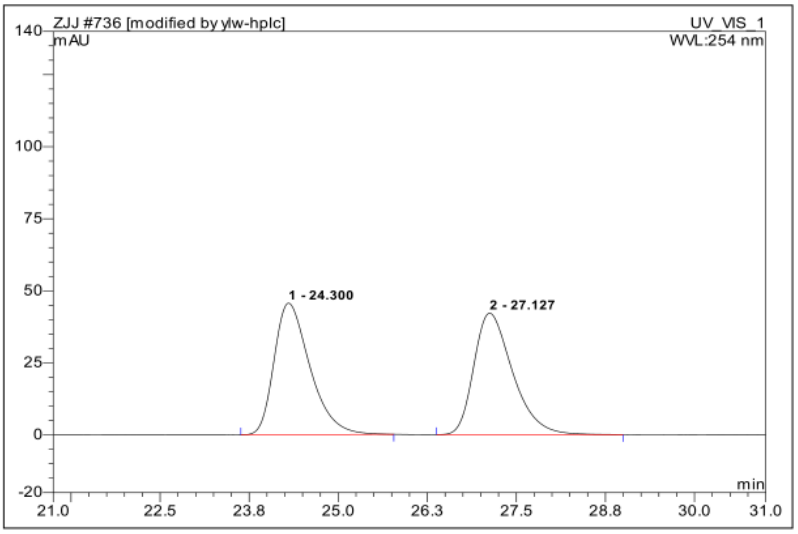
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	24.23	n.a.	254.055	183.114	50.06	n.a.	BMB*
2	28.82	n.a.	207.500	182.662	49.94	n.a.	BMB*
Total:			461.555	365.775	100.00	0.000	



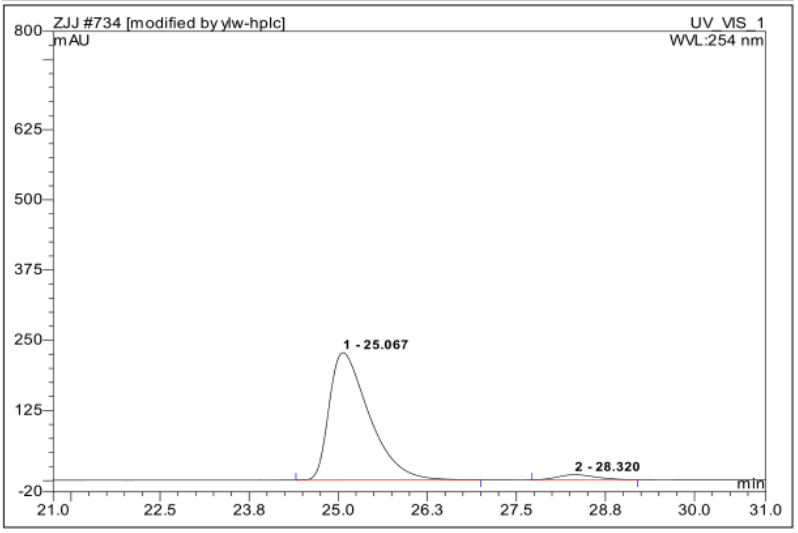
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	23.23	n.a.	163.549	95.505	3.46	n.a.	BMB*
2	26.67	n.a.	2598.095	2665.034	96.54	n.a.	BMB*
Total:			2761.643	2760.540	100.00	0.000	

(+)-2af: IB, *n*-hexane/2-propanol = 95/5, v = 1.0 mL min^{-1}, λ = 254 nm



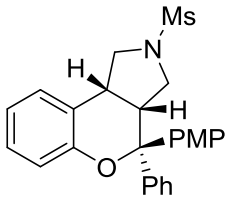


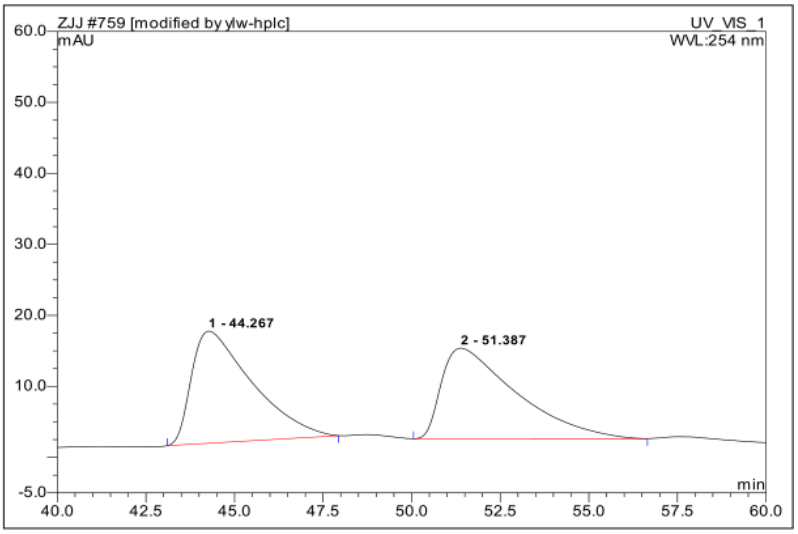
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	24.30	n.a.	45.627	26.677	50.08	n.a.	BMB*
2	27.13	n.a.	42.147	26.597	49.92	n.a.	BMB*
Total:			87.775	53.275	100.00	0.000	



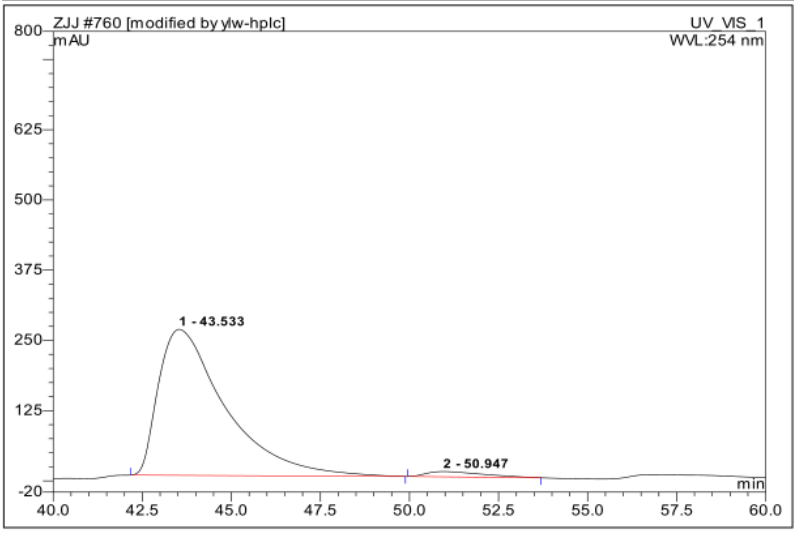
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	25.07	n.a.	226.787	147.640	96.29	n.a.	BMB*
2	28.32	n.a.	9.051	5.682	3.71	n.a.	BMB*
Total:			235.838	153.322	100.00	0.000	

(-)-6a: IA, *n*-hexane/2-propanol = 95/5, v = 1.0 mL min^{-1}, λ = 254 nm

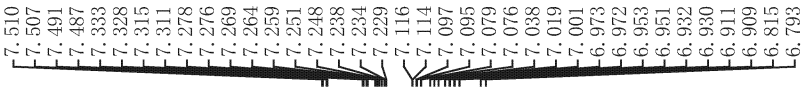




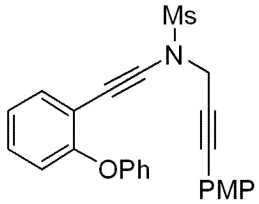
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	44.27	n.a.	15.778	31.160	50.08	n.a.	BMB*
2	51.39	n.a.	12.746	31.063	49.92	n.a.	BMB*
Total:			28.524	62.223	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	43.53	n.a.	259.710	565.065	97.06	n.a.	BMB*
2	50.95	n.a.	9.325	17.123	2.94	n.a.	BMB*
Total:			269.035	582.188	100.00	0.000	



Parameter	Value
1 Title	zjj-13-178-Ms-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-12T13:59:52
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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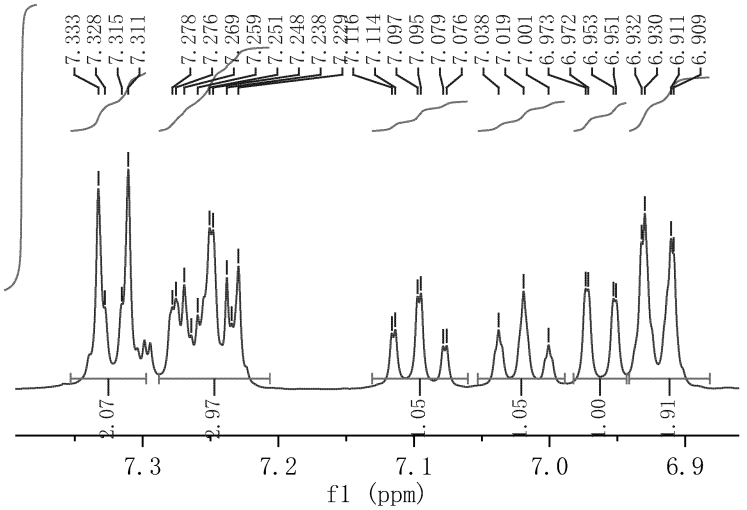
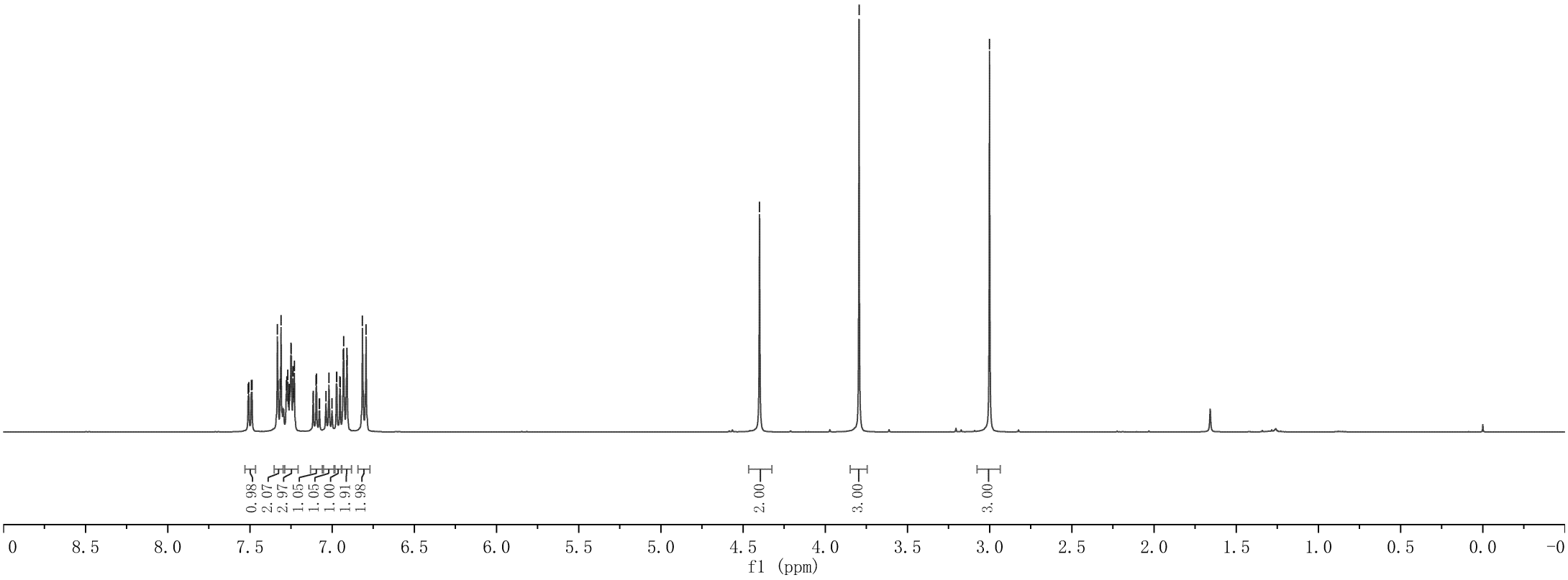
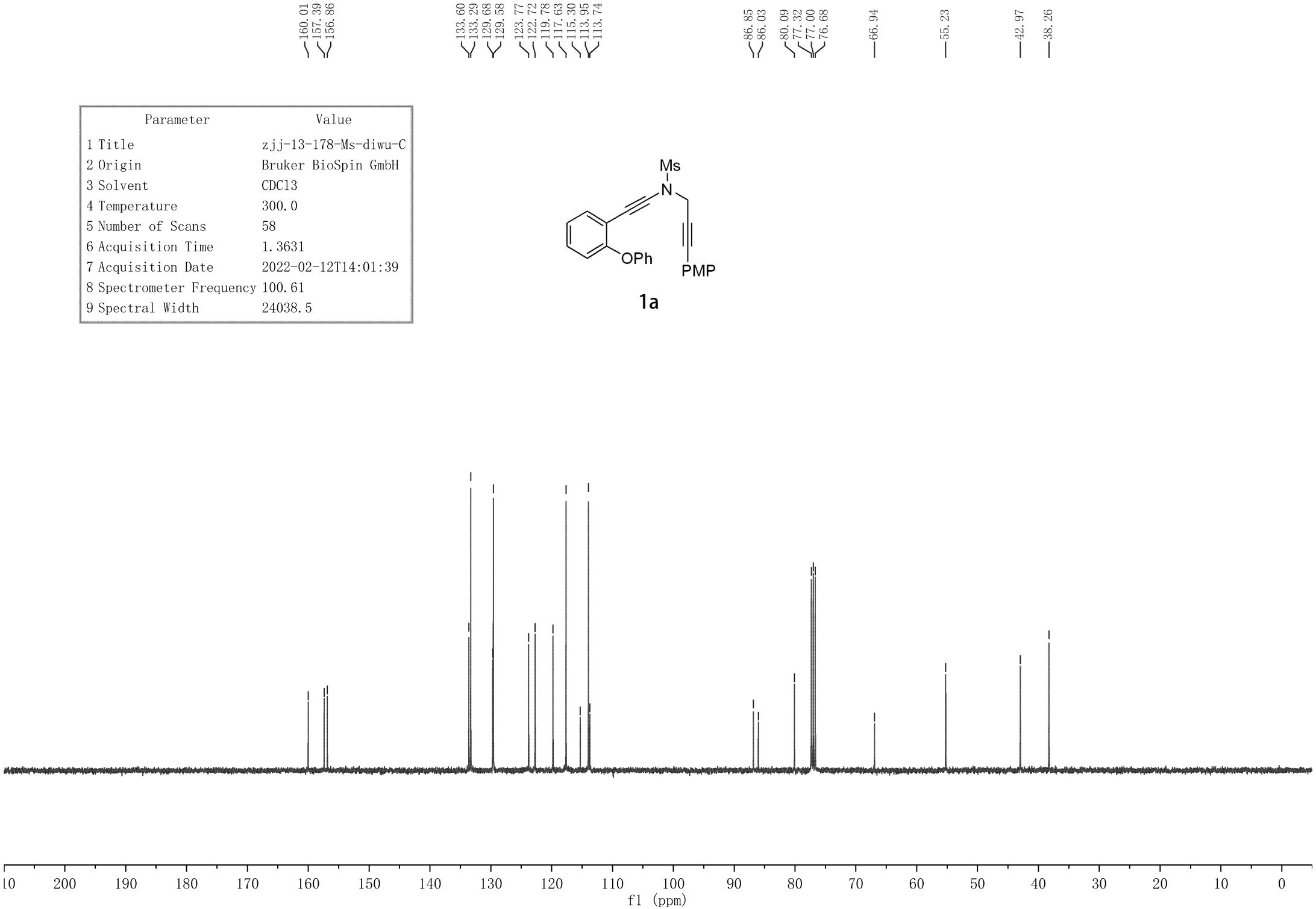
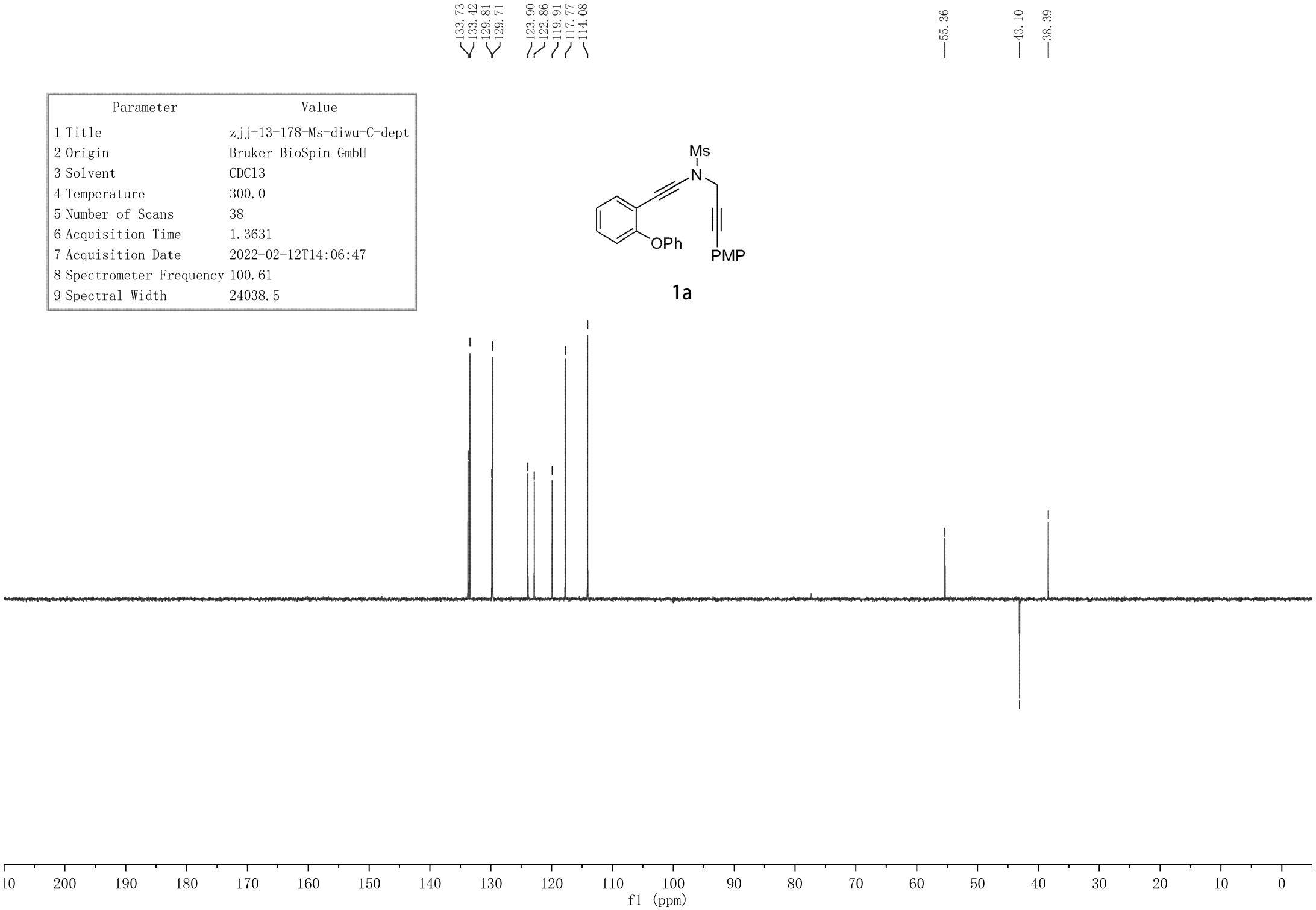


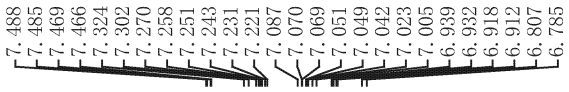


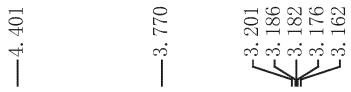


Parameter	Value
1 Title	zjj-13-178-Ms-diwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	58
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-12T14:01:39
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

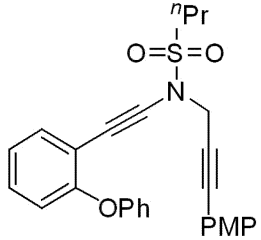


Parameter	Value
1 Title	zjj-13-178-Ms-diwu-C-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	38
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-12T14:06:47
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5





Parameter	Value
1 Title	LFS-2-145-H-nPrSO2
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.4
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-07T11:35:48
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



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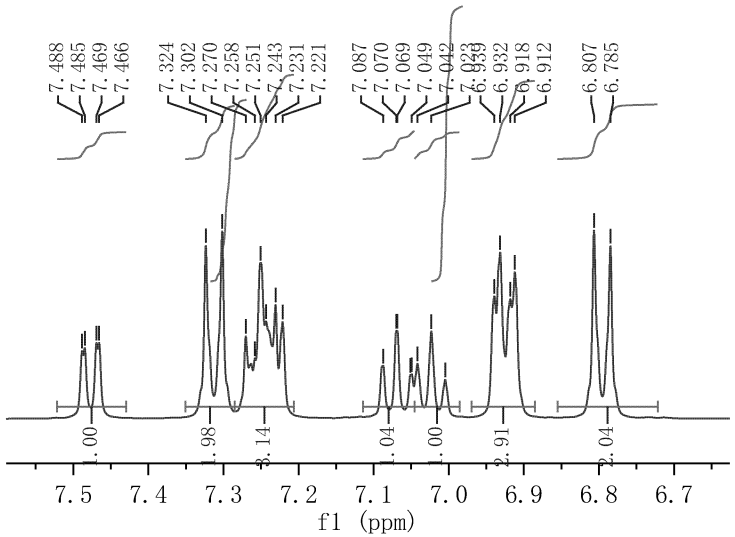

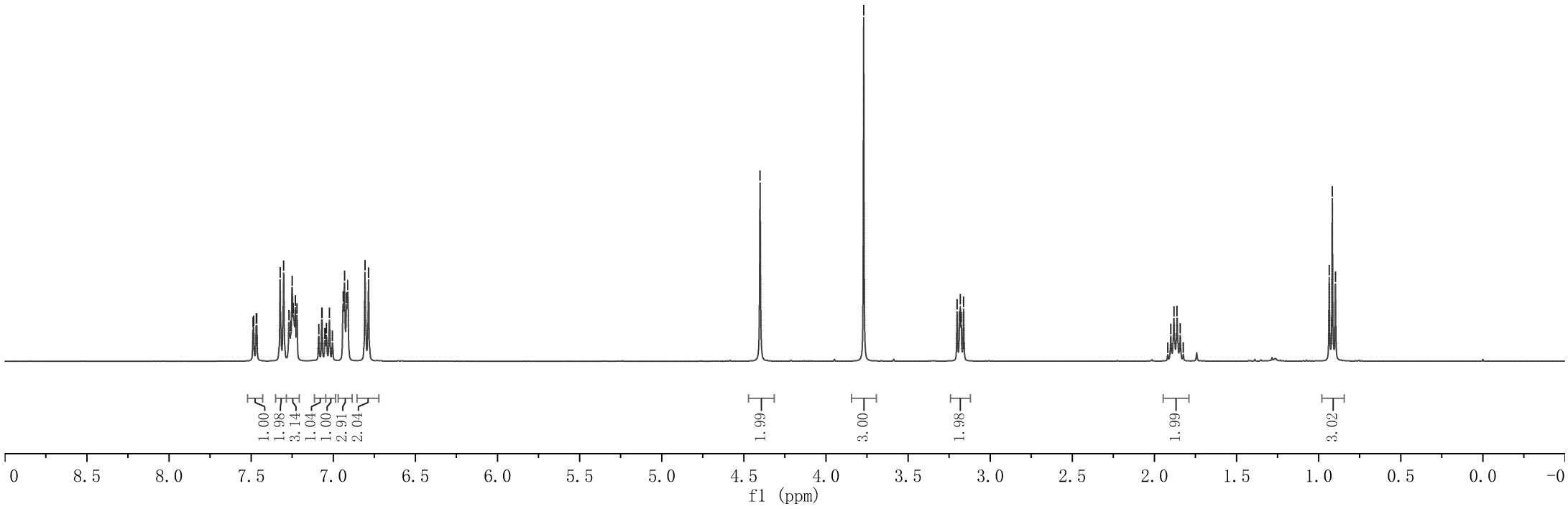

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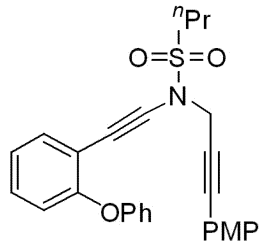
Parameter	Value
1 Title	LFS-2-145-C-nPrSO2
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-07T11:44:37
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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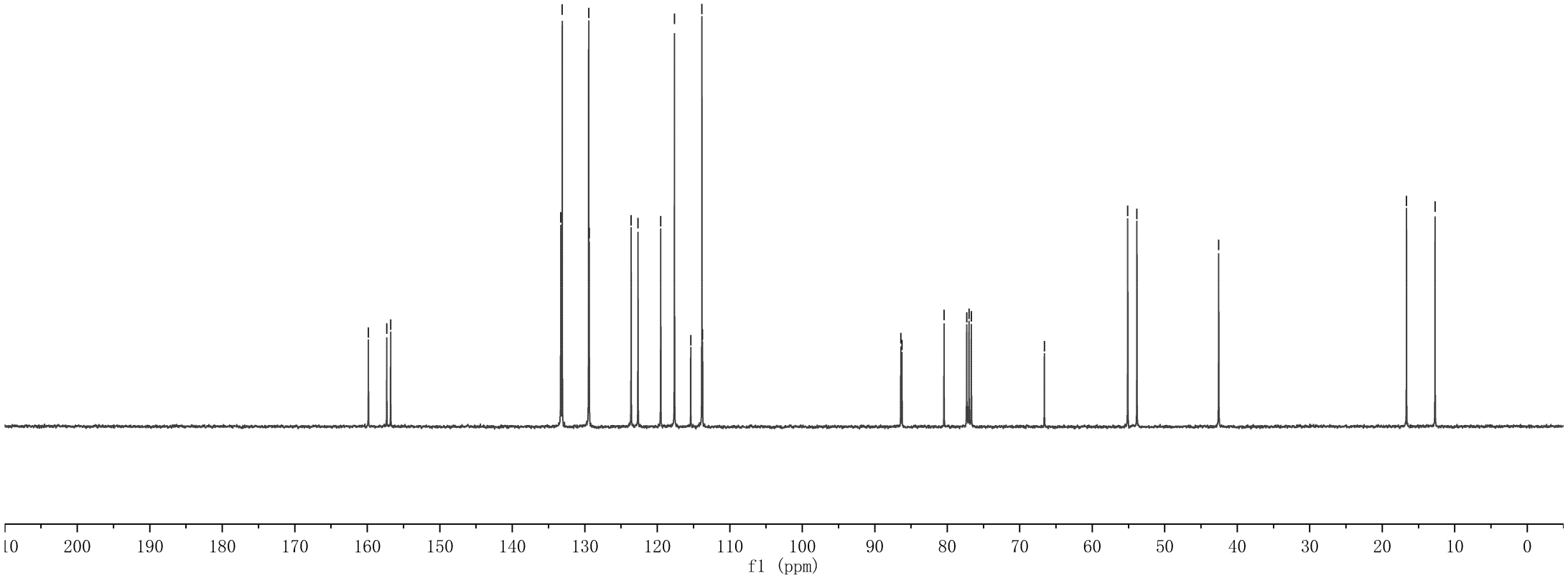
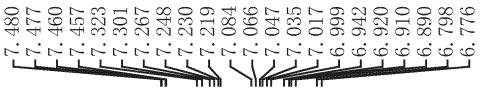
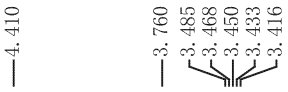
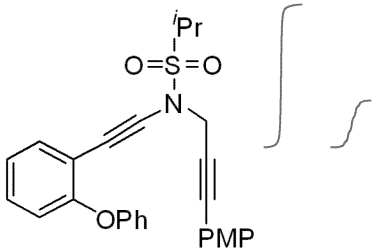






Parameter	Value
1 Title	LFS-2-146-H-IPrSO2
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-07T11:48:58
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



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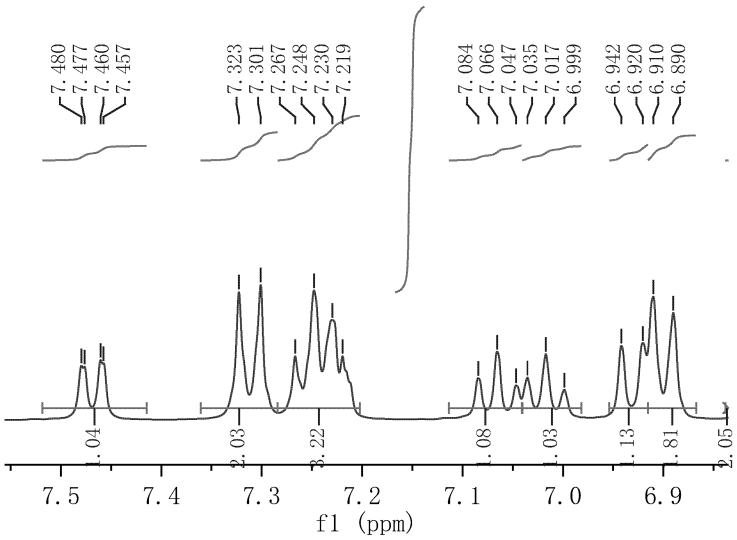

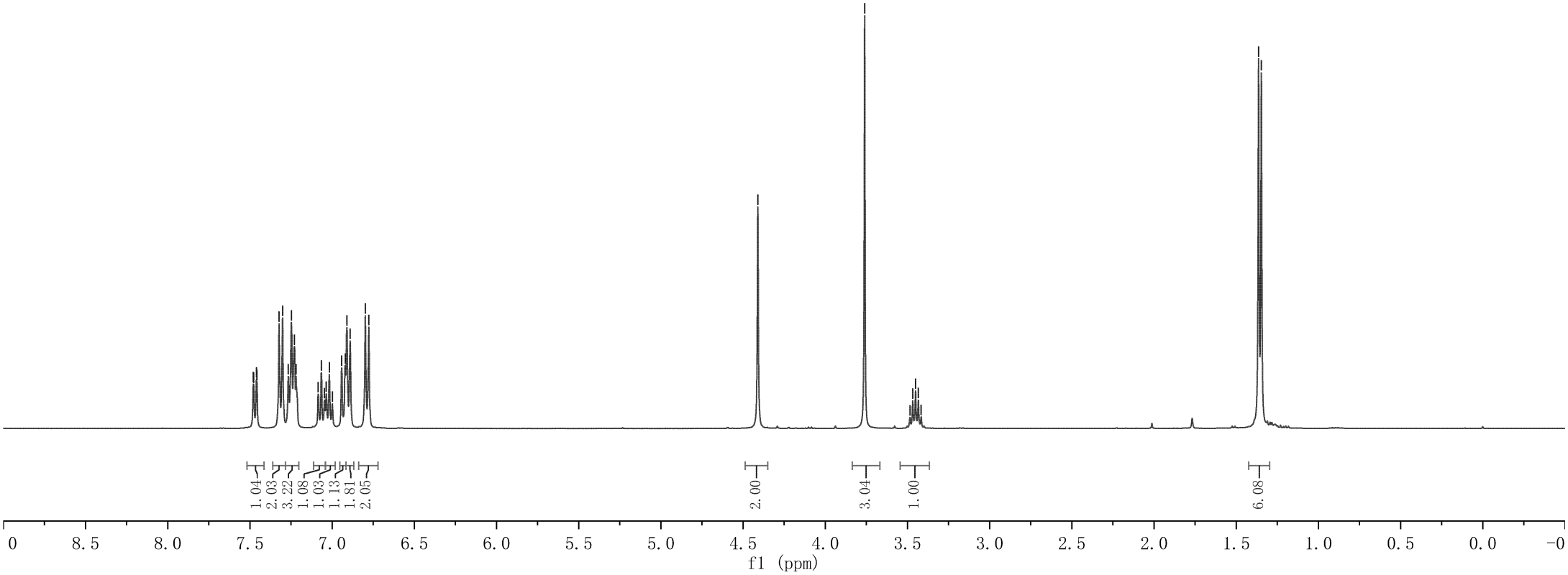

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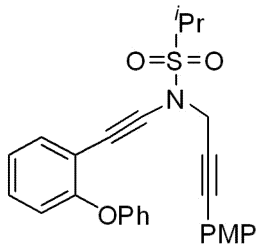
77.32
77.00
76.68
66.38
55.09
54.65
42.61
16.21

Parameter	Value
1 Title	LFS-2-146-C-IPrSO2
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-07T11:58:06
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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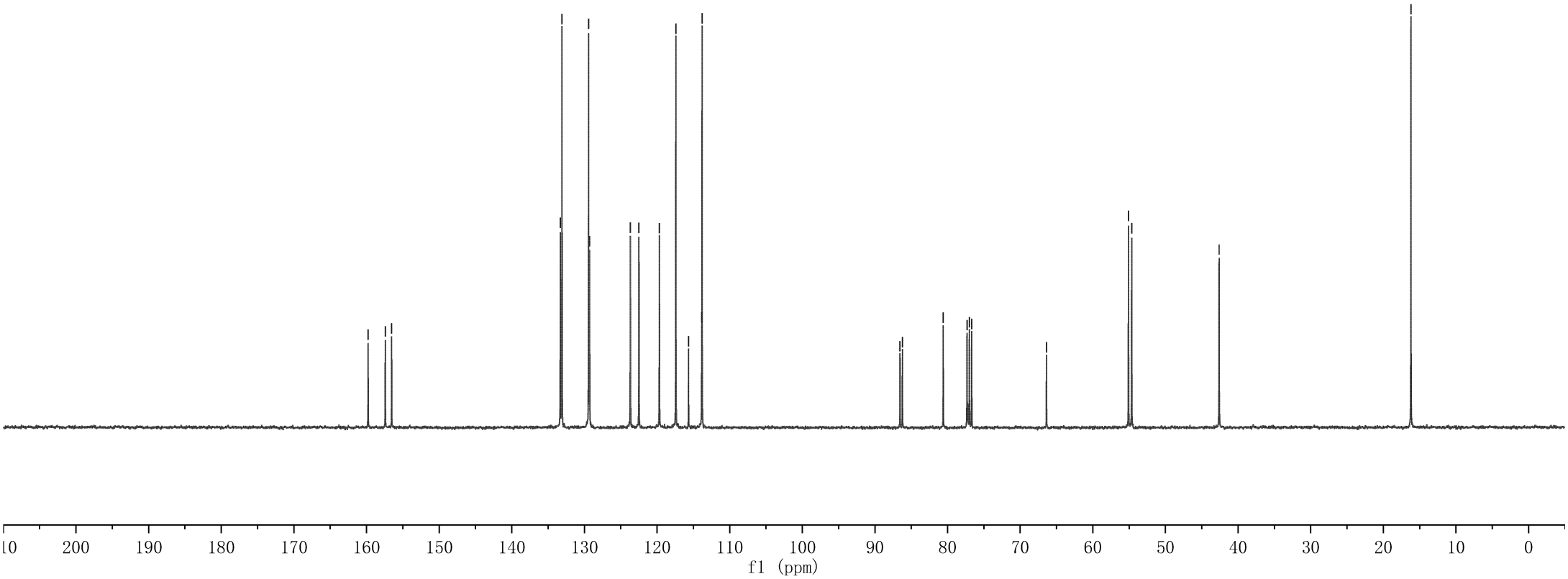
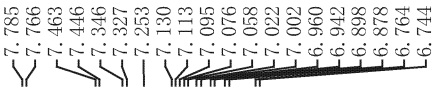
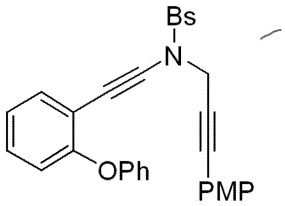




Parameter	Value
1 Title	zjj-13-226-Bs-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-27T17:23:08
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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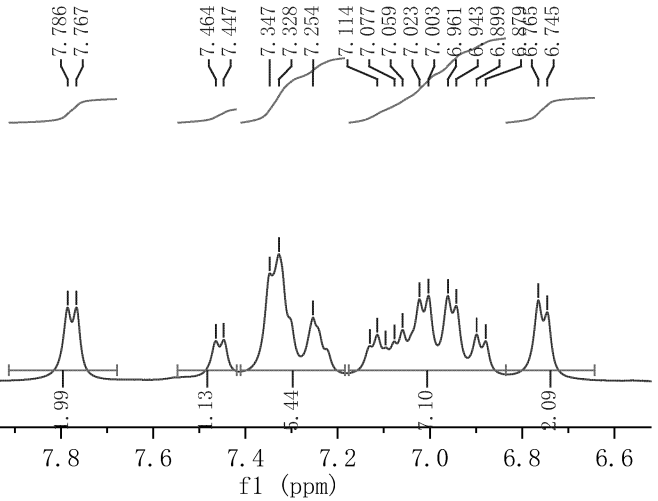

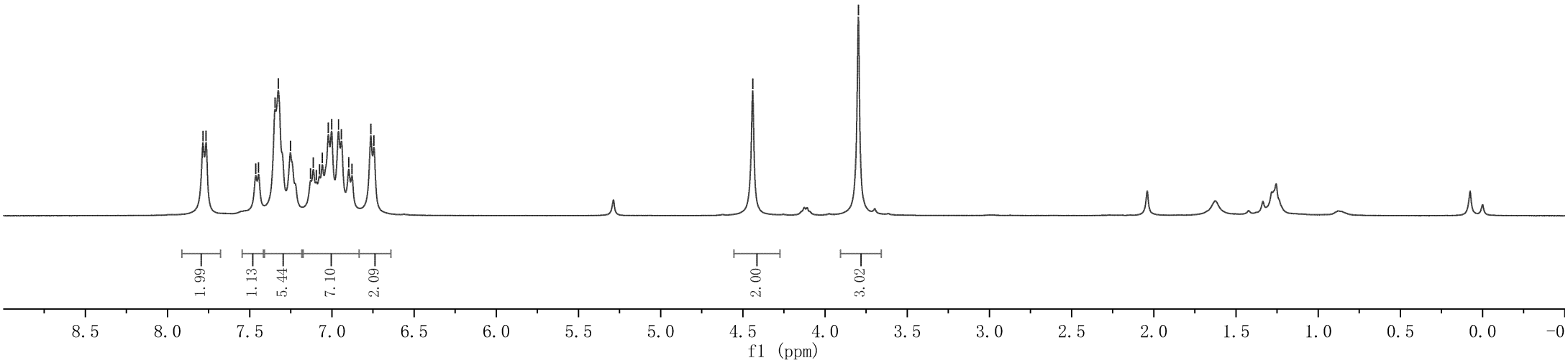

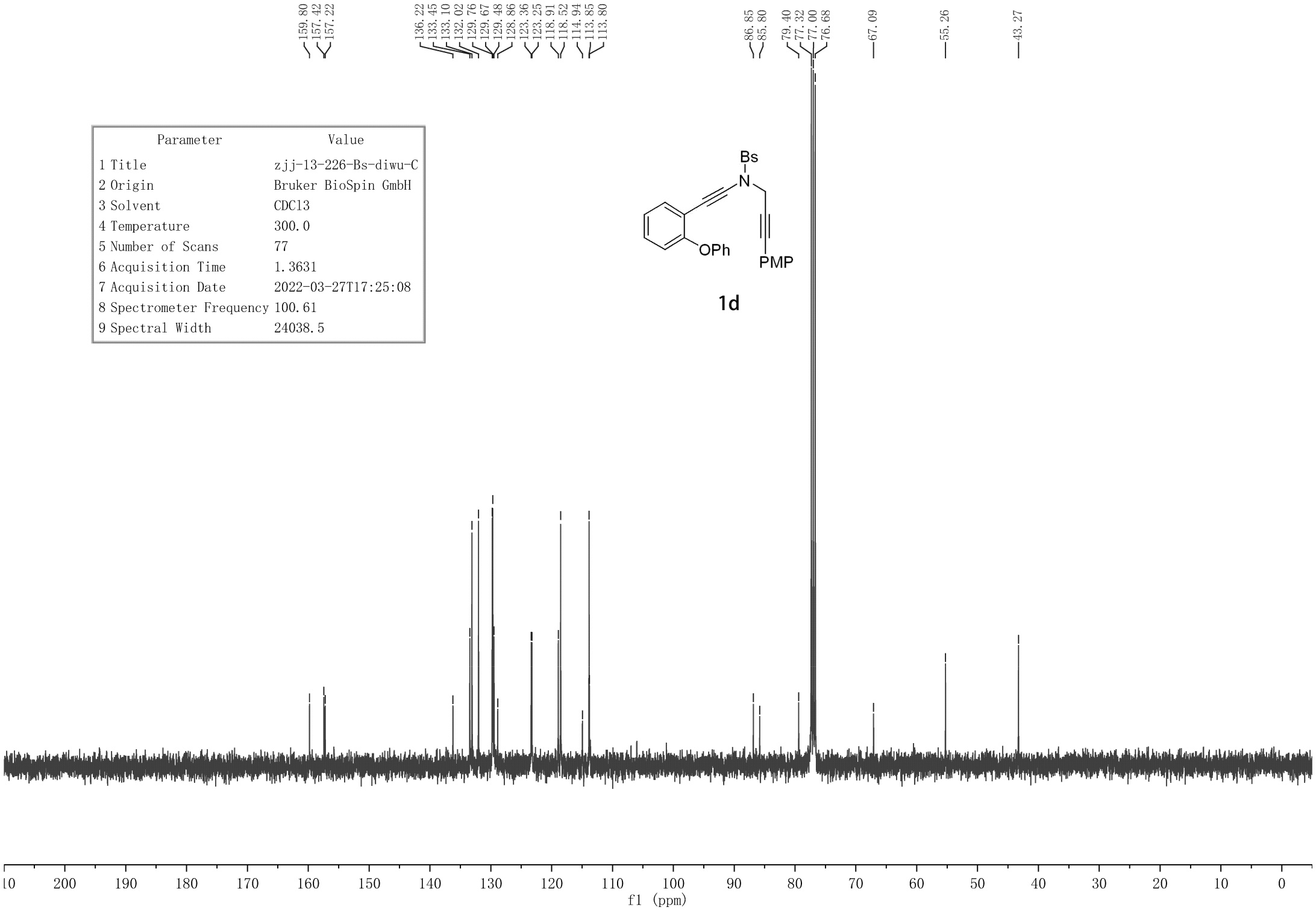
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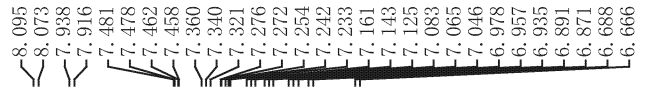
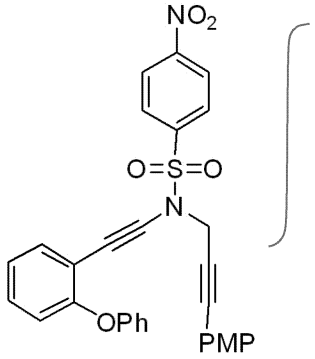
133.10
132.02
129.76
129.67
129.48
128.86
123.36
123.25
118.91
118.52
114.94
113.85
113.80
86.85
85.80
79.40
77.32
77.00
76.68
67.09
55.26
43.27
Parameter Value
1 Title zjj-13-226-Bs-diwu-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 77
6 Acquisition Time 1.3631
7 Acquisition Date 2022-03-27T17:25:08
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Bs
N
OPh
PMP
1d
f1 (ppm)



Parameter	Value
1 Title	zjj-14-2-sub-4-Ns-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-07T15:09:10
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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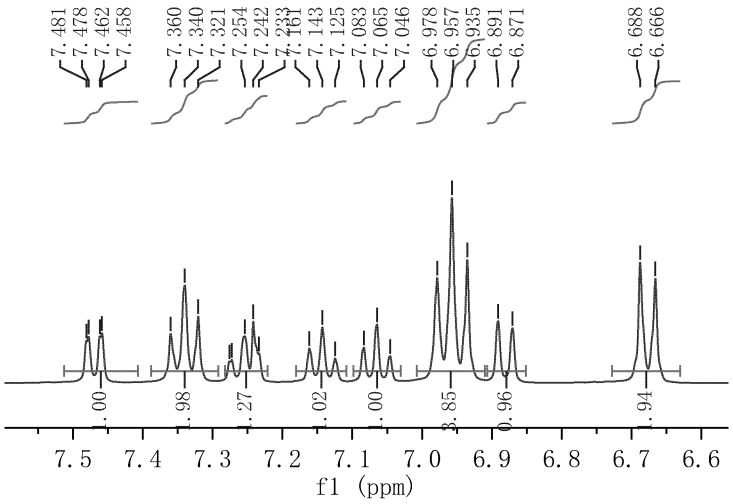

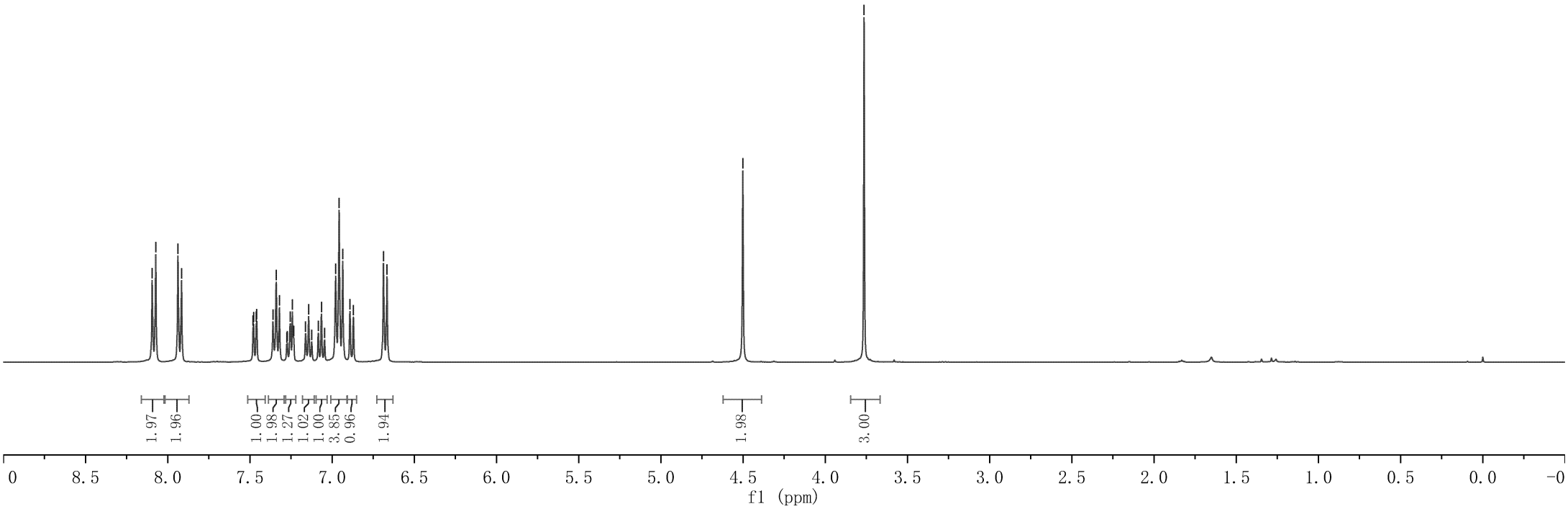

159.95
157.62
157.00
150.14
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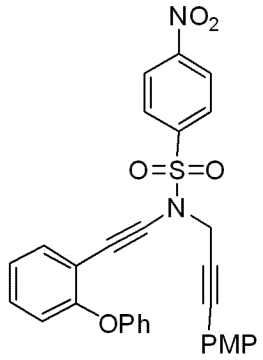
133.48
132.89
129.86
129.82
129.41
123.72
123.36
118.74
118.50
114.35
113.81
113.24
87.23
85.04
79.15
77.32
77.00
76.68
67.27
55.21
43.60

Parameter	Value
1 Title	zjj-14-2-sub-4-Ns-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	8
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-07T15:10:34
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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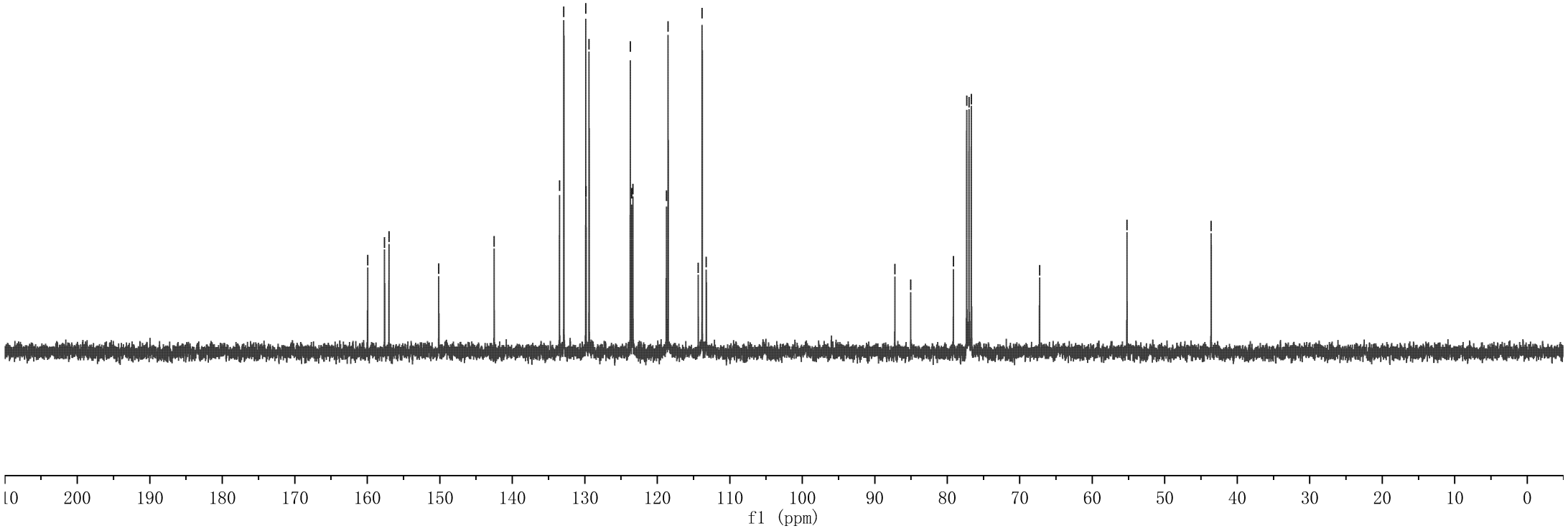
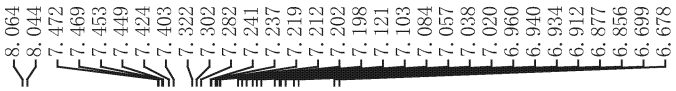
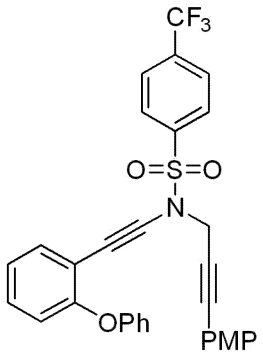




Parameter	Value
1 Title	LFS-2-141-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	296.8
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-05T18:49:34
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



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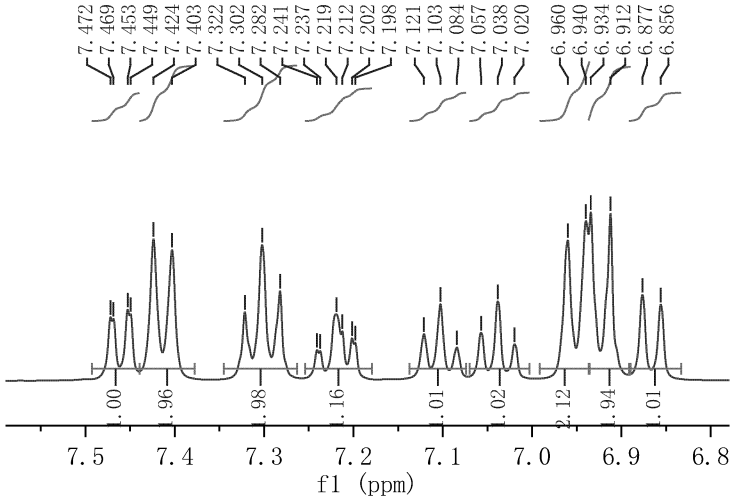
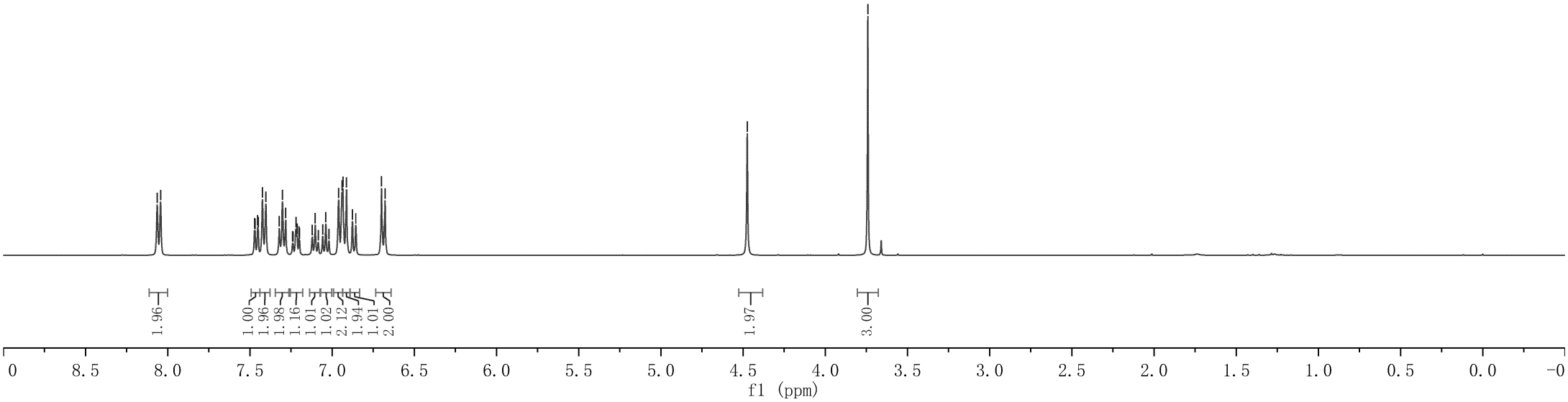
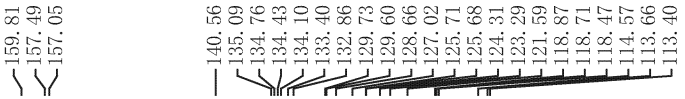
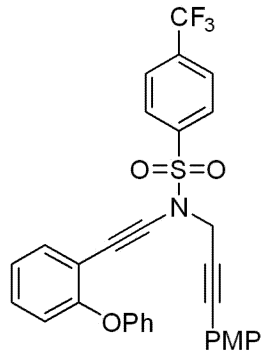






Parameter	Value
1 Title	LFS-2-141-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-05T18:58:30
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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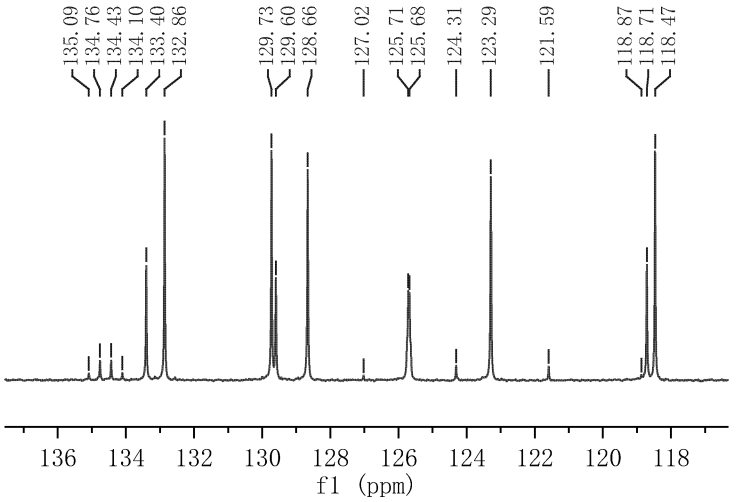
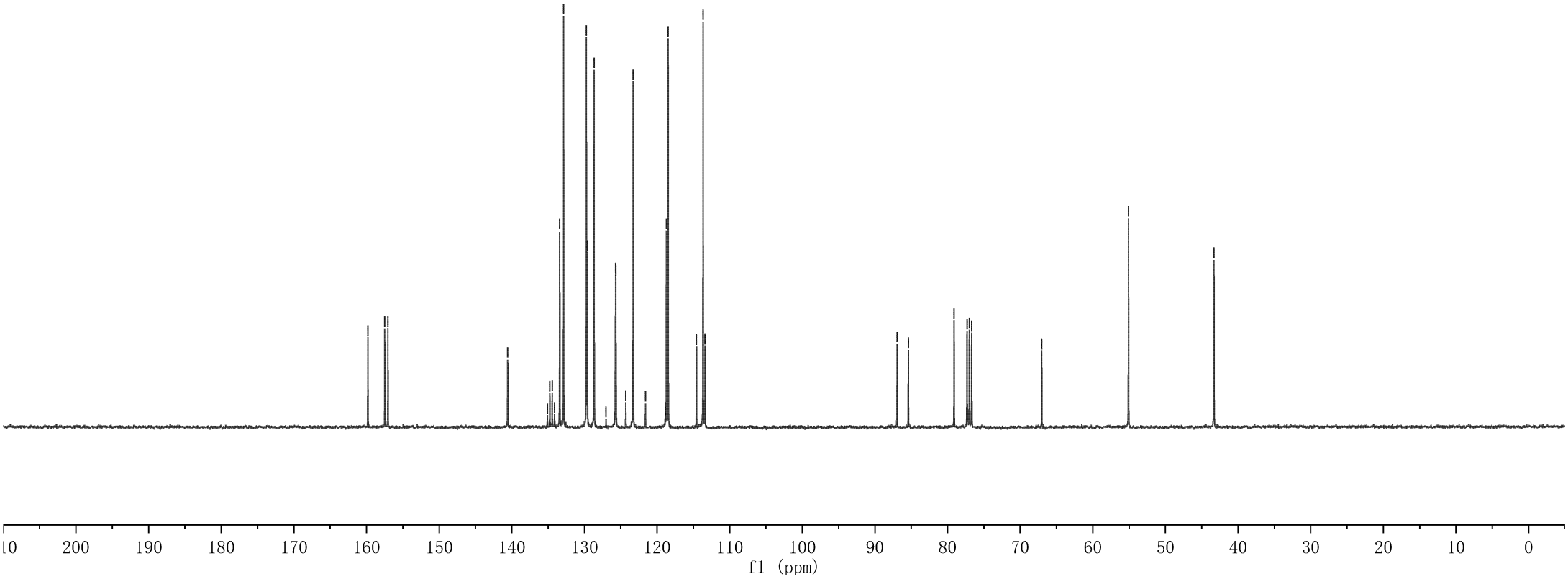
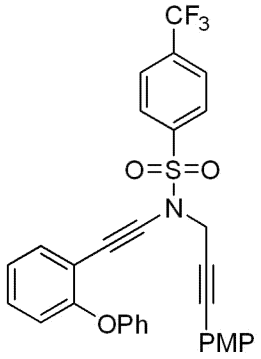




Parameter	Value
1 Title	zjj-14-CF3-sub-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	11
6 Acquisition Time	0.7340
7 Acquisition Date	2022-04-07T10:27:47
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



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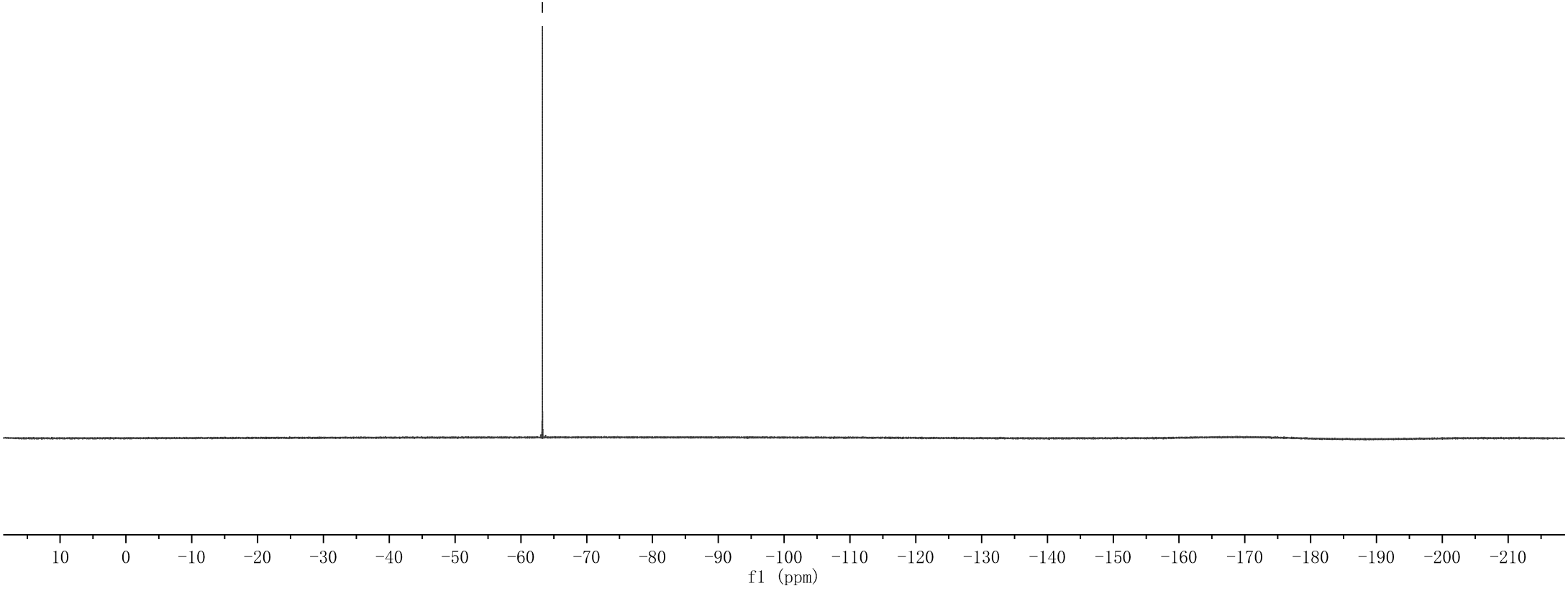
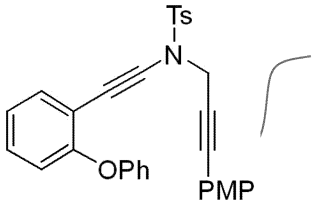
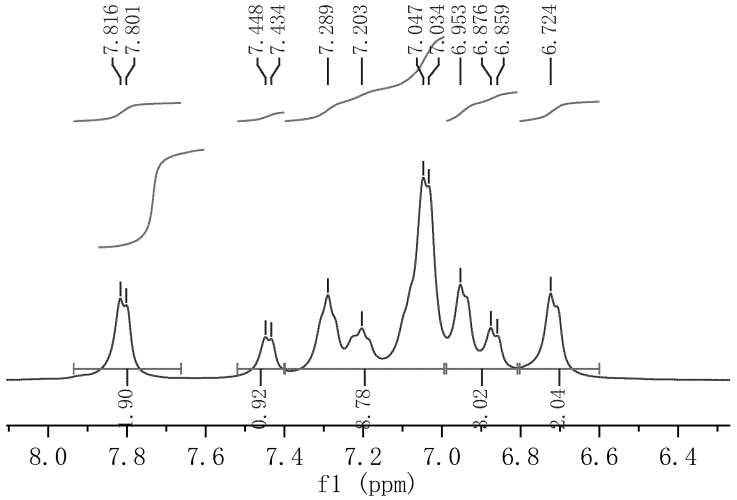
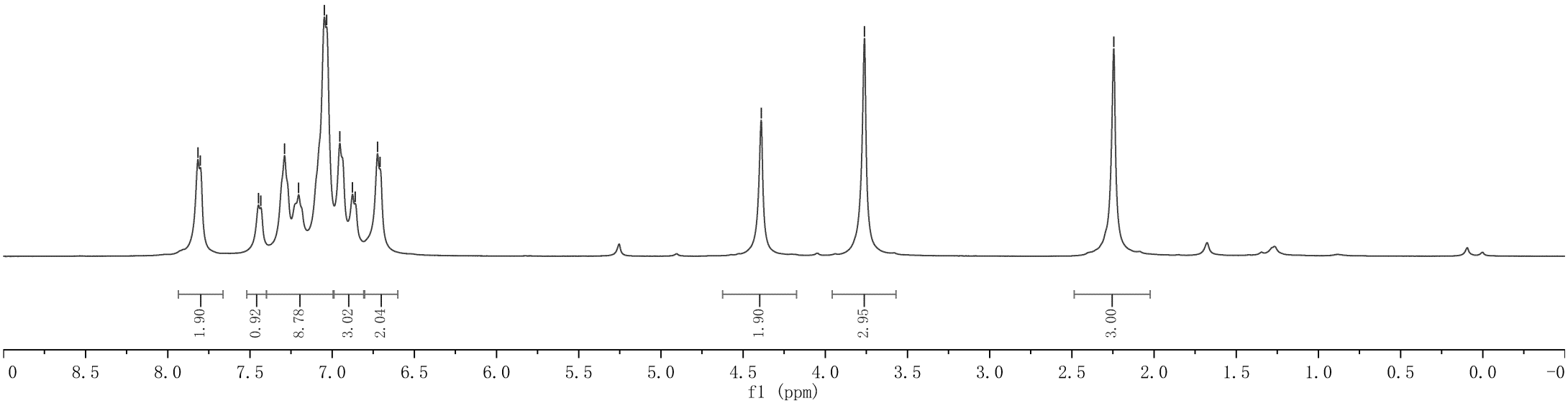


Parameter	Value
1 Title	zjj-13-Ts-H-re
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-28T15:52:50
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



1g





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134.18
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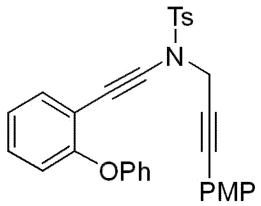
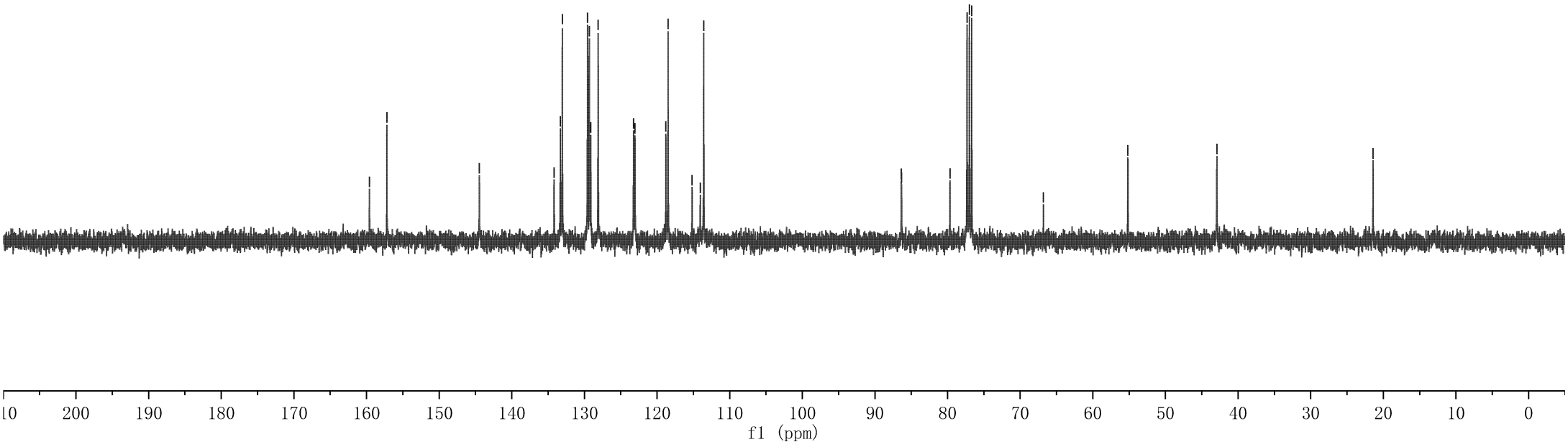
133.04
129.57
129.33
129.13
128.11
123.23
123.03
118.78
118.48
115.17
114.05
113.57
86.36
86.33
79.67
77.32
77.00
76.68
66.80
55.17
42.92
21.41

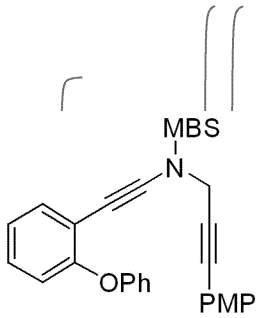
Parameter	Value
1 Title	zjj-13-Ts-C-re
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	15
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-28T15:53:54
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



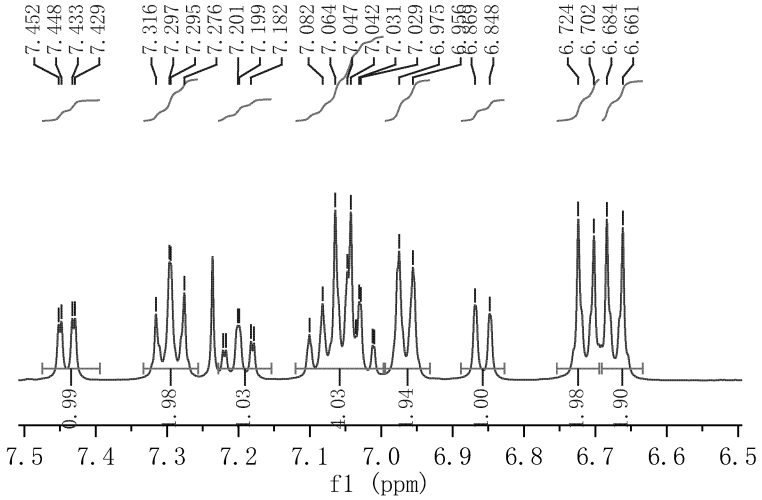
1g

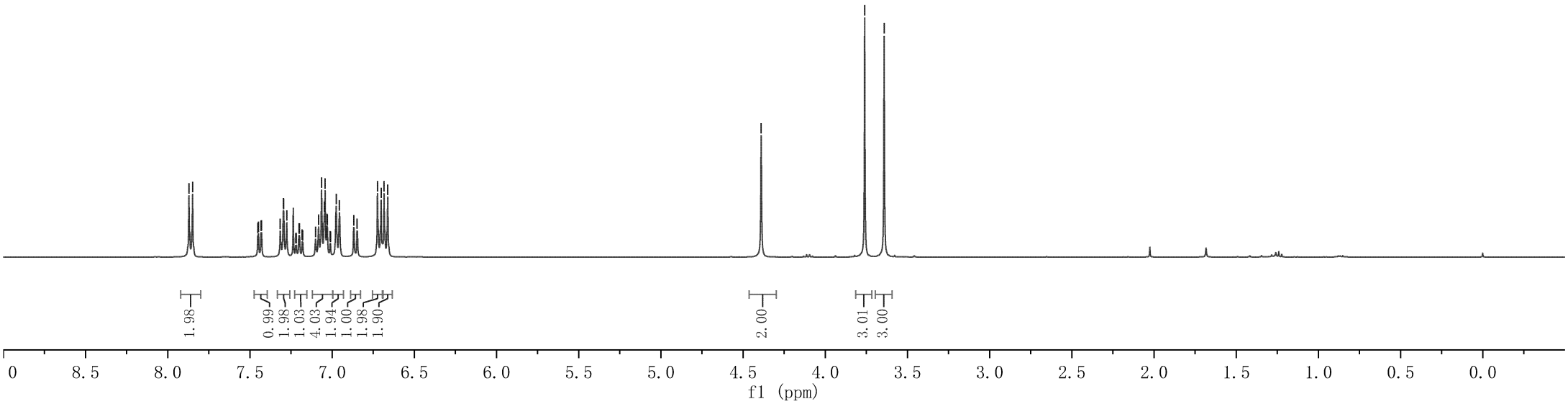


Parameter	Value
1 Title	zjj-13-229-Mbs-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-27T17:03:05
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



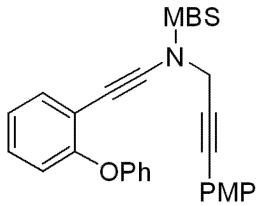
1h



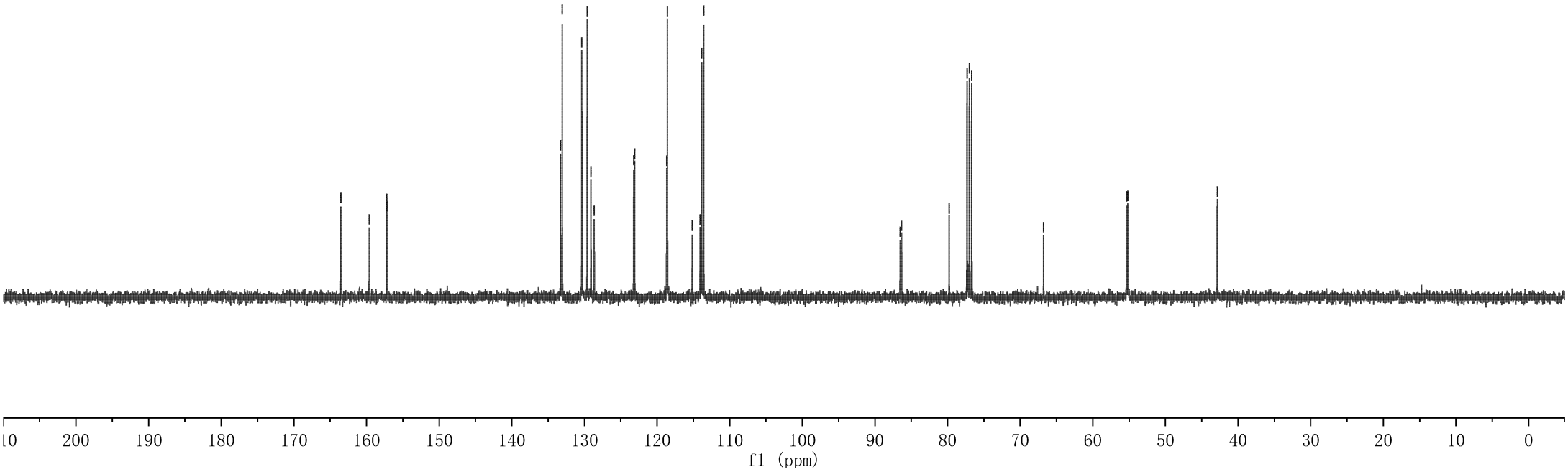


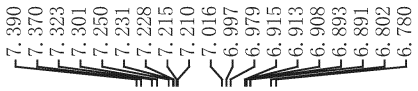
163.52
159.62
157.23
157.19
133.28
133.06
130.36
129.62
129.10
128.65
123.22
123.09
118.67
118.58
115.16
114.08
113.86
113.58
86.53
86.33
79.78
77.32
77.00
76.68
66.79
55.34
55.17
42.86

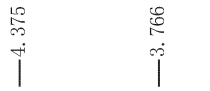
Parameter	Value
1 Title	zjj-13-229-Mbs-diwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	12
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-27T17:04:40
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



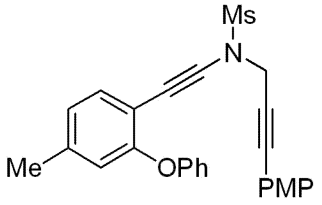
1h



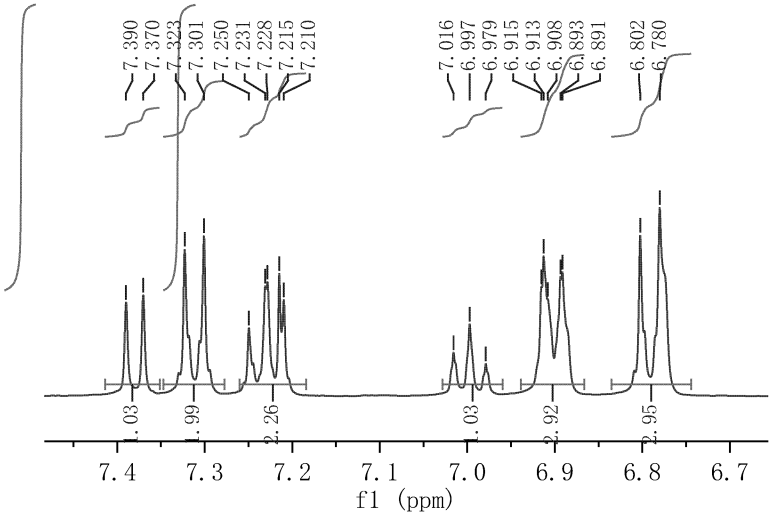


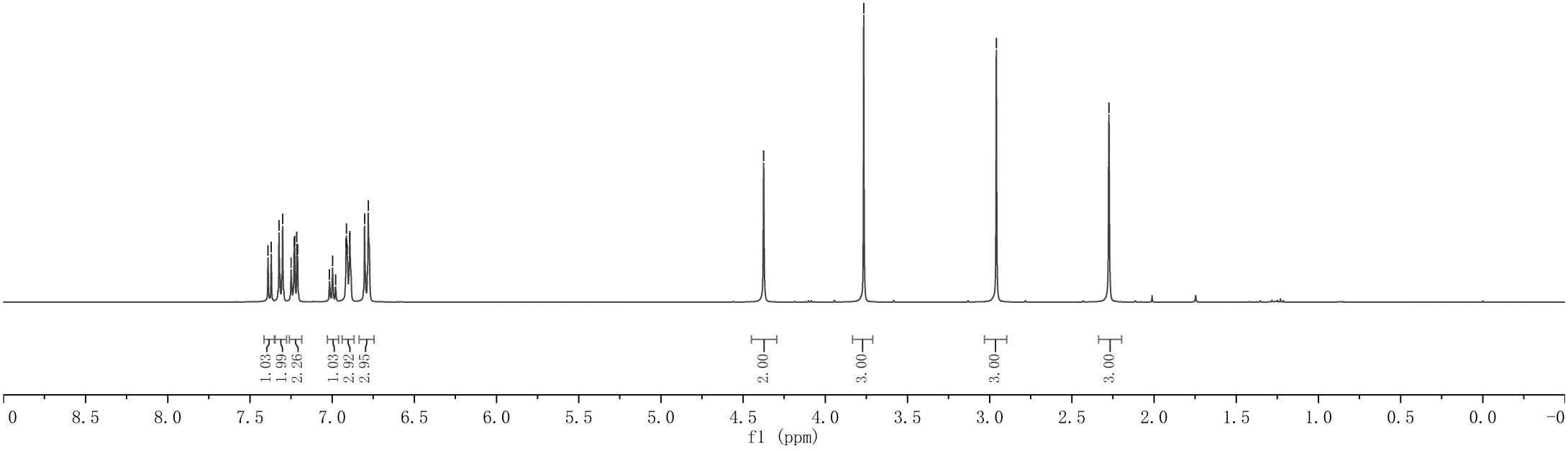


Parameter	Value
1 Title	zjj-13-217-5-Me-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-04T17:02:32
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



1i





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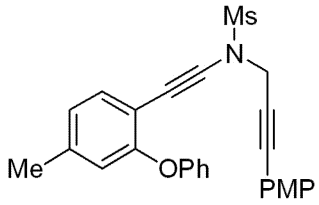
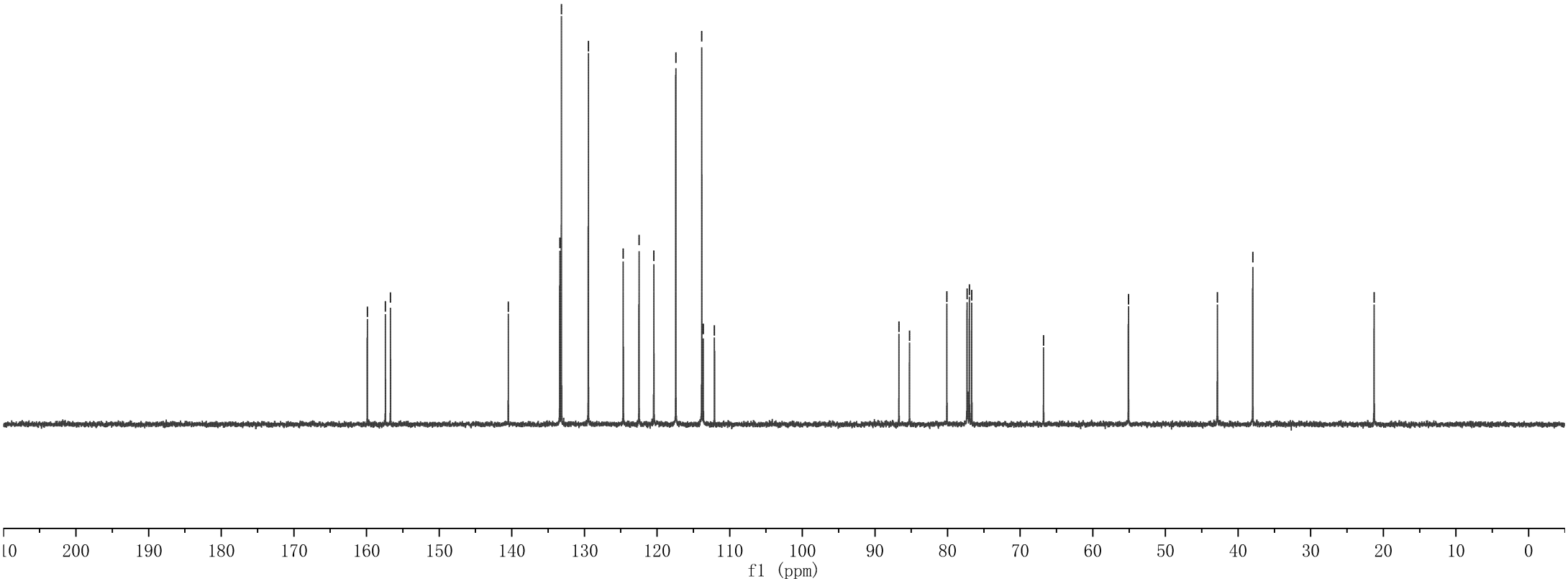
156.70
140.48
133.39
133.16
129.46
124.66
122.48
120.44
117.42
113.84
113.63
112.10
86.69
85.24
80.09
77.32
77.00
76.68
66.78
55.10
42.85
37.98
21.28

Parameter	Value
1 Title	zjj-13-217-5-Me-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	29
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-04T17:03:35
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

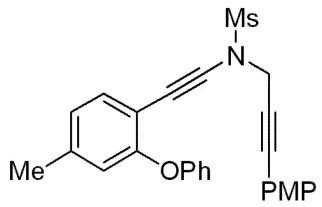


1i



133.66
133.44
129.73
124.93
122.76
120.71
117.69
114.12
55.37
43.12
38.26
21.55

Parameter	Value
1 Title	zjj-13-217-5-Me-C-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	5
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-04T17:05:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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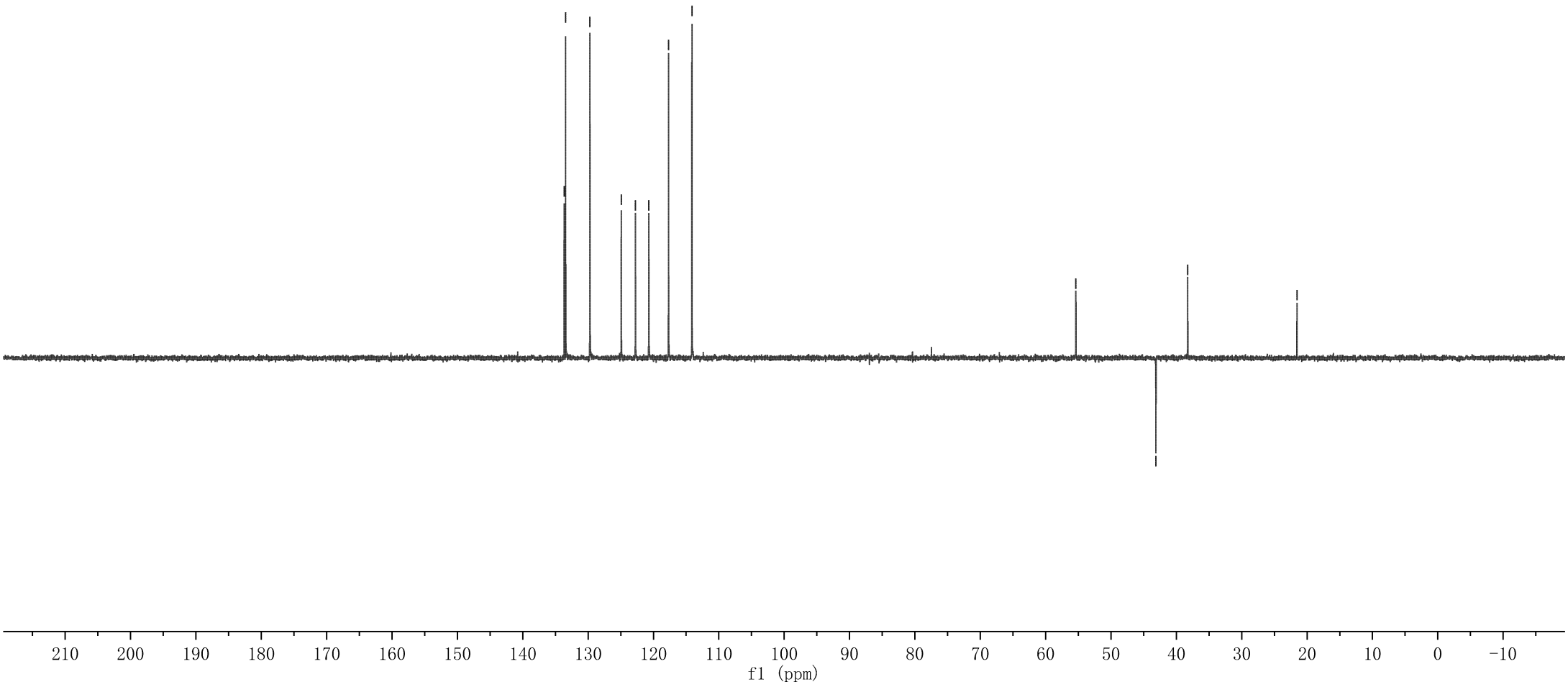
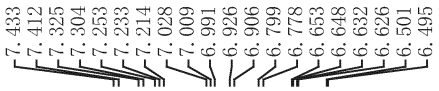
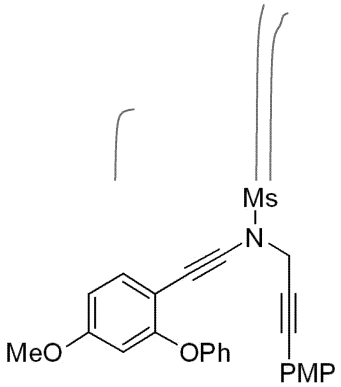




Parameter	Value
1 Title	ZJJ-13-222-5-OMe-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	16
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-15T14:12:30
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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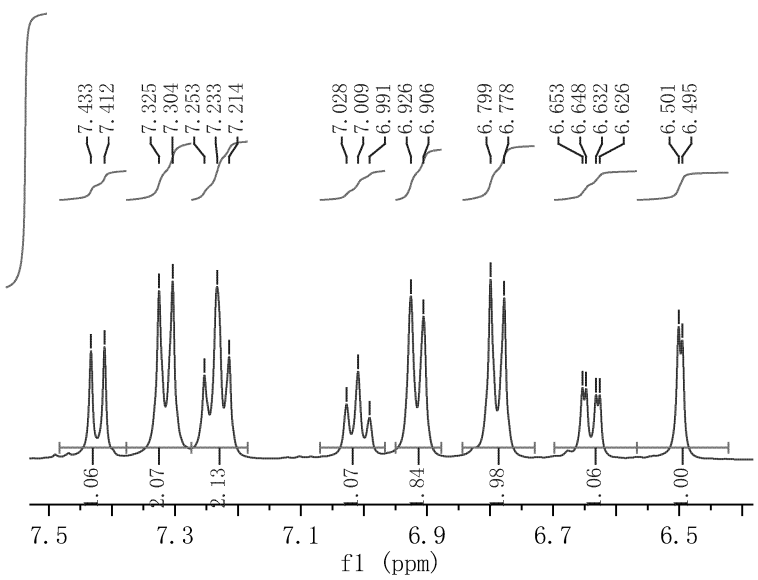

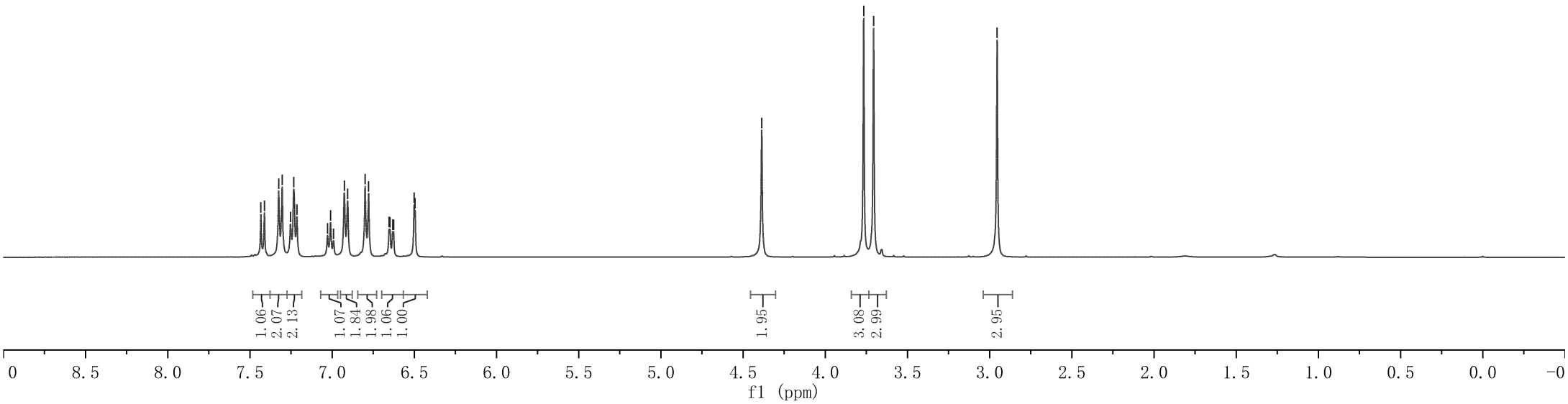

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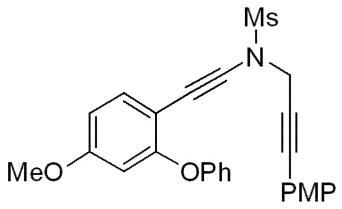
86.63
84.48
80.15
77.32
77.00
76.68
66.48
55.26
55.07
42.87
37.84

Parameter	Value
1 Title	ZJJ-13-222-5-OMe-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	23
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-15T14:16:30
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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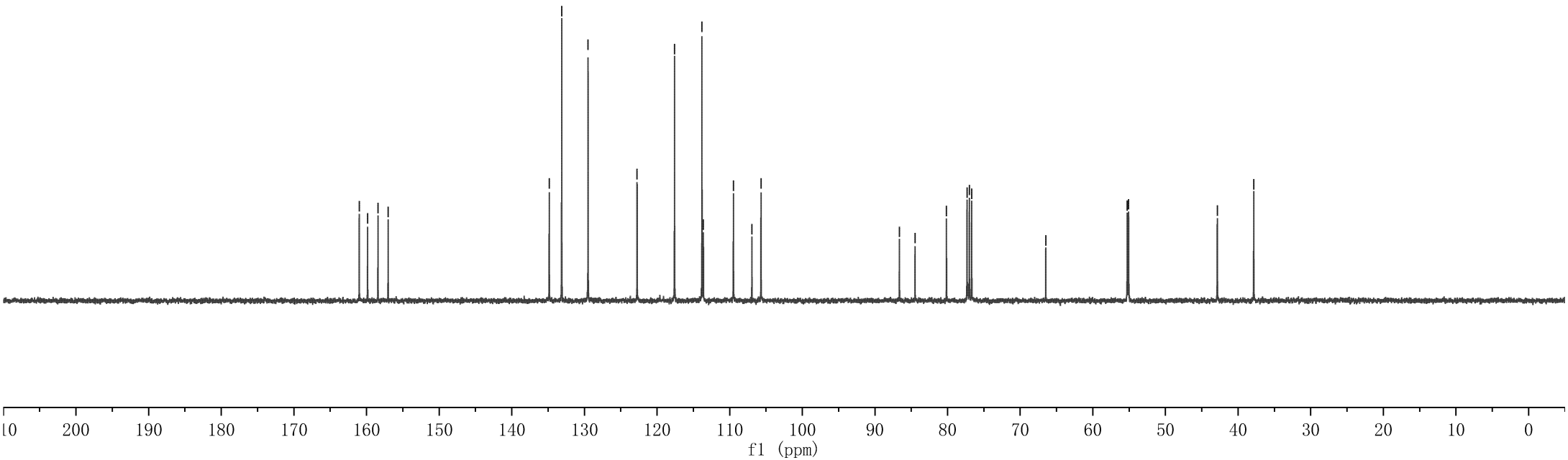
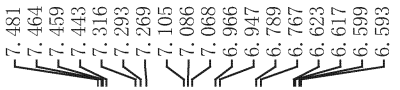
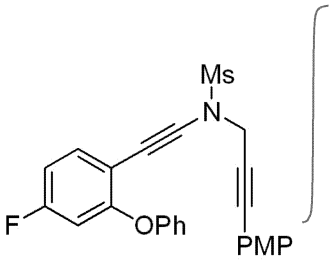




Parameter	Value
1 Title	LFS-2-140-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.8
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-05T18:35:49
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



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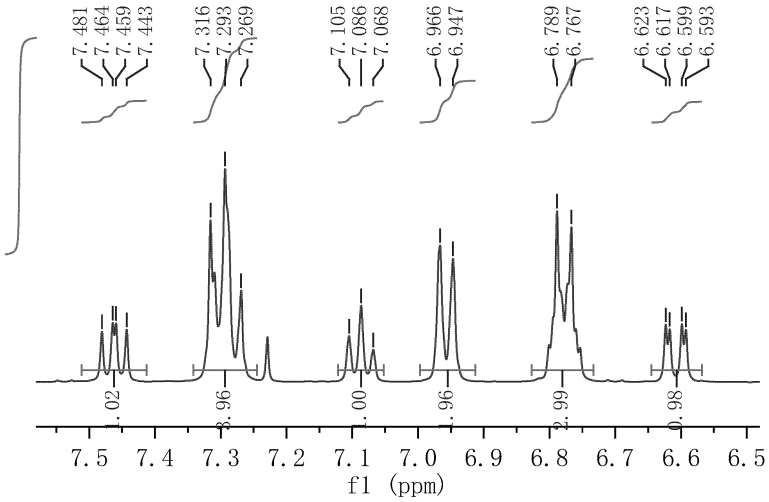
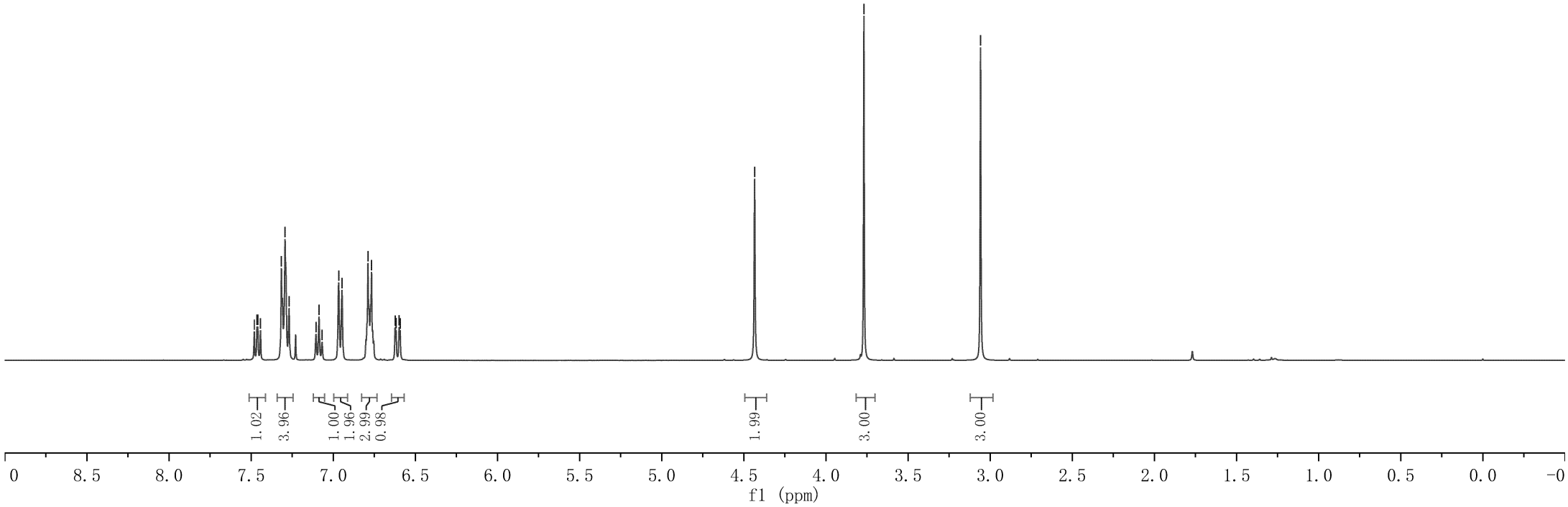
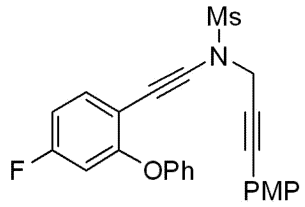




Parameter	Value
1 Title	zjj-14-5-F-diwu-C-LFS-2-140-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.8
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-05T18:44:46
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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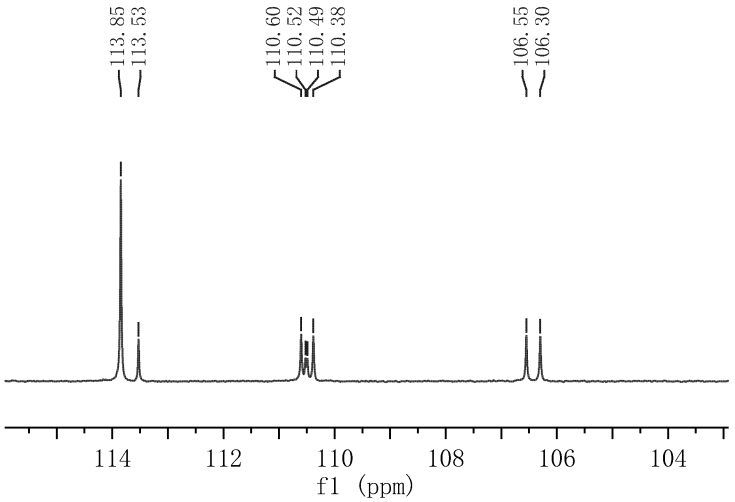
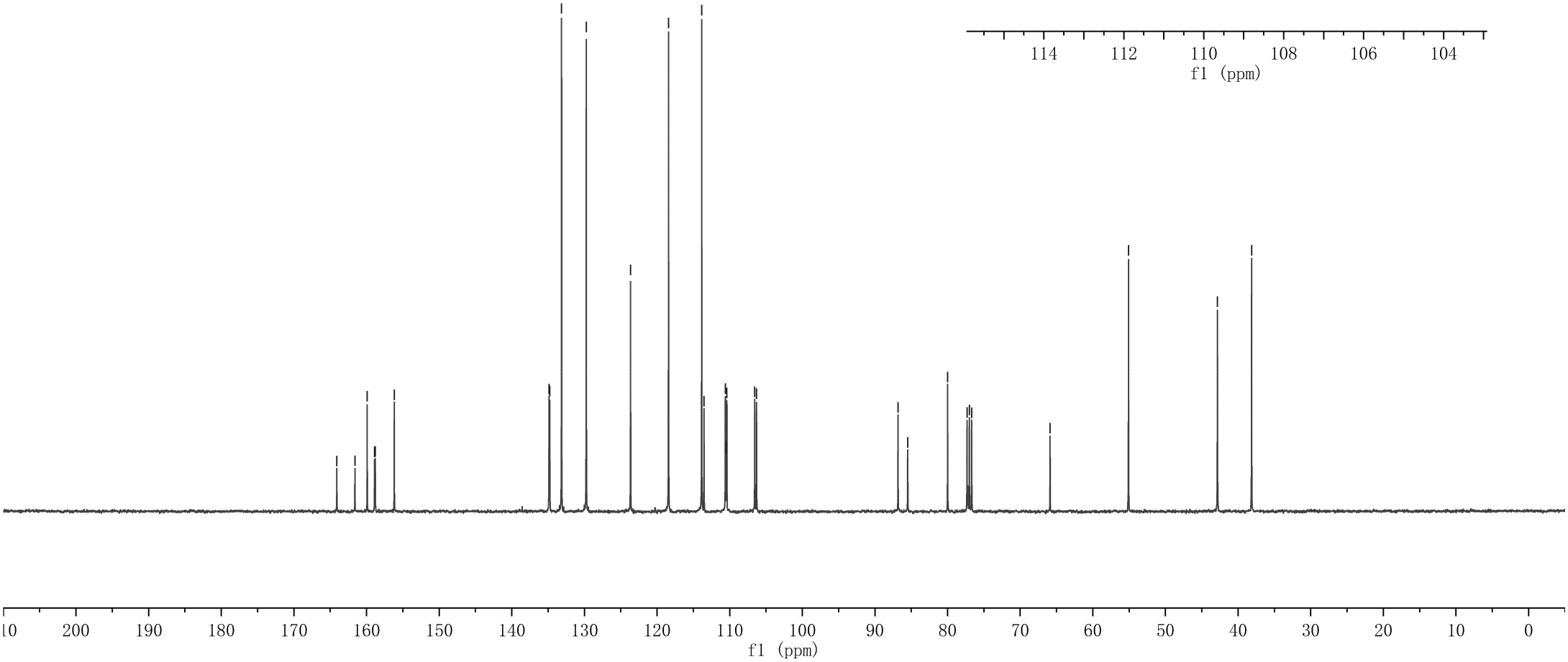
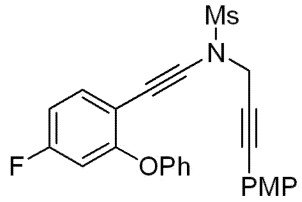


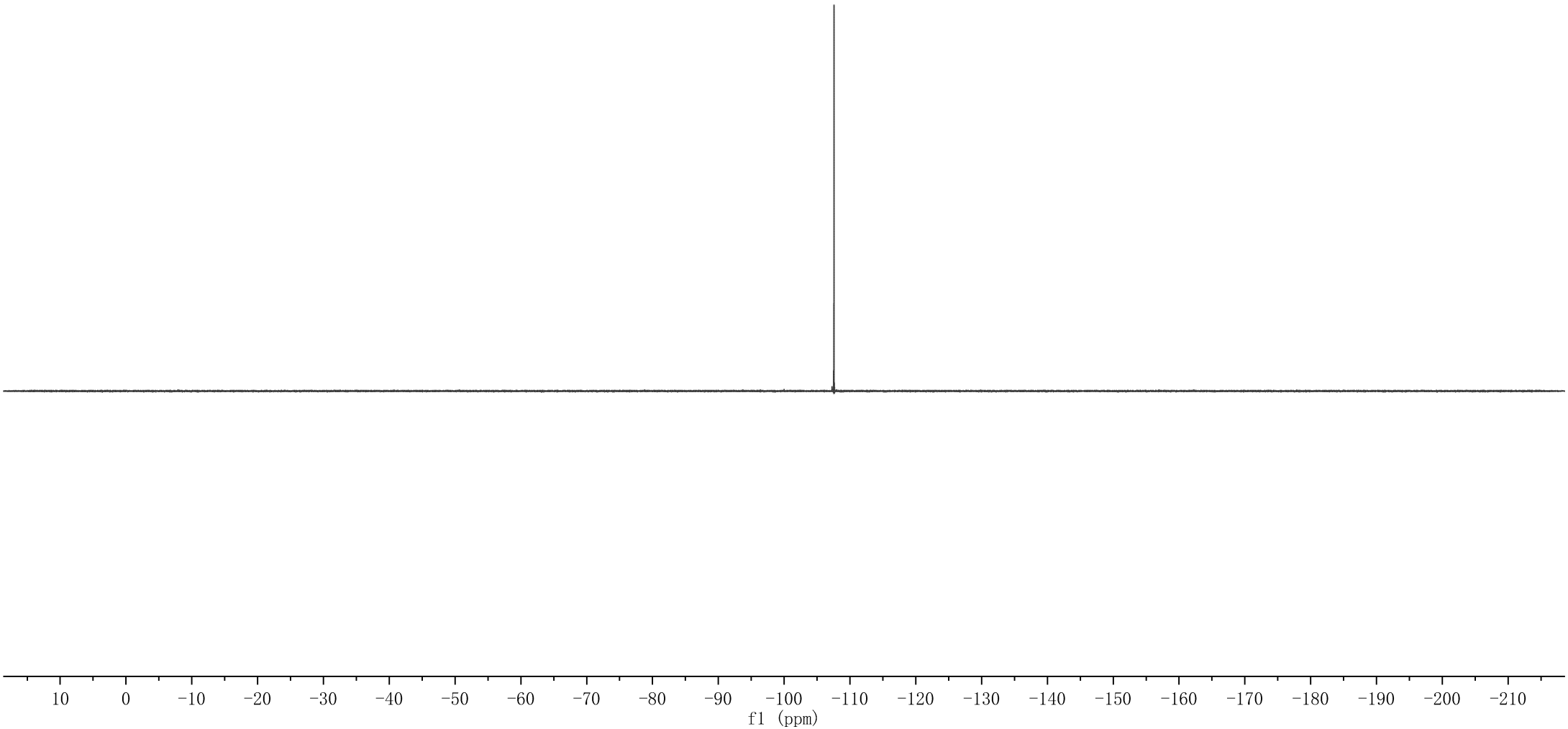


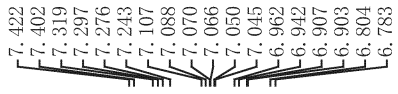
Parameter	Value
1 Title	zjj-14-5-F-sub-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	13
6 Acquisition Time	0.7340
7 Acquisition Date	2022-04-07T10:26:11
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



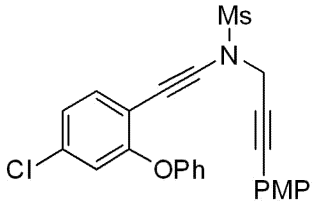
1k

-107.58





Parameter	Value
1 Title	zjj-14-22-5-Cl-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-08T14:49:45
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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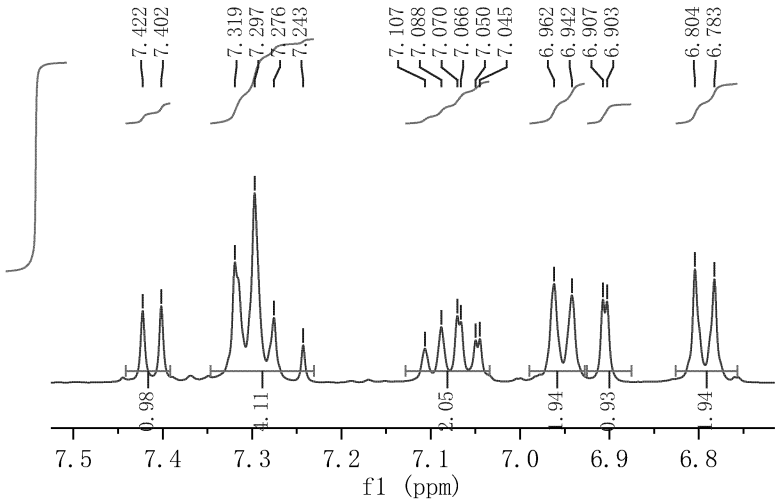

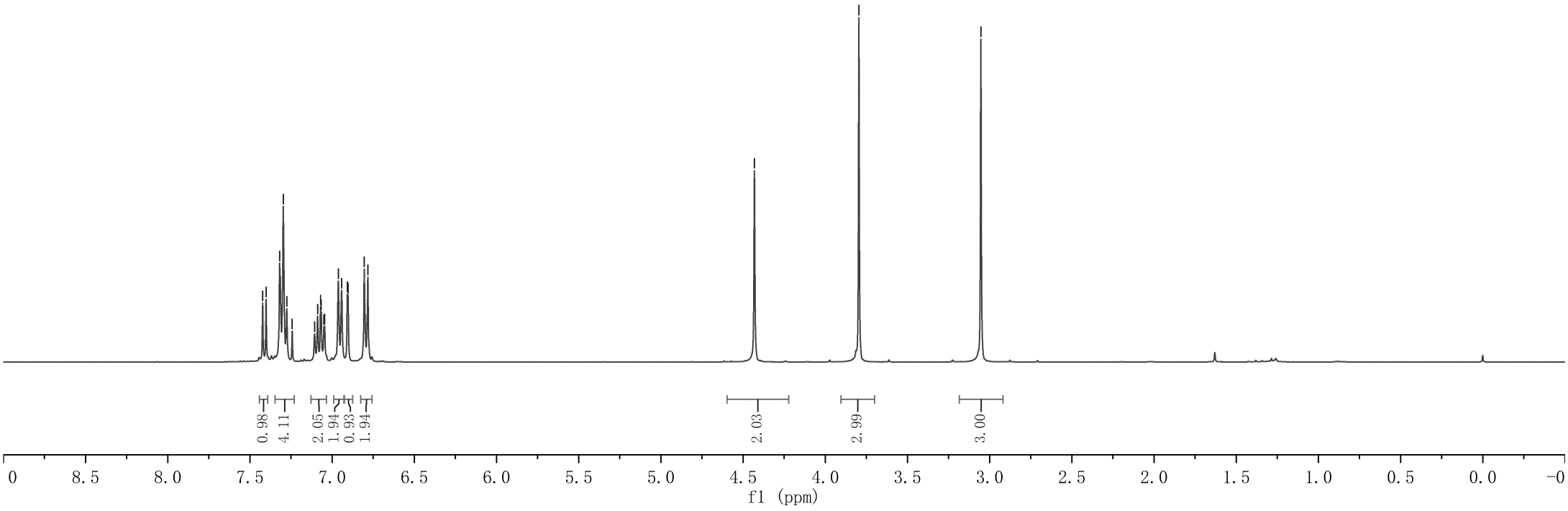

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134.85
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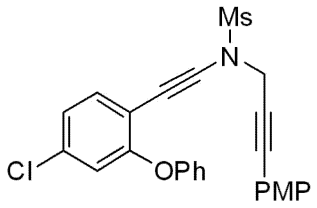
133.27
129.82
123.75
123.60
119.32
118.33
113.95
113.64
113.44
86.96
86.73
79.98
77.32
77.00
76.68
66.17
55.23
42.97
38.41

Parameter	Value
1 Title	zjj-14-22-5-Cl-diwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	32
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-08T14:50:54
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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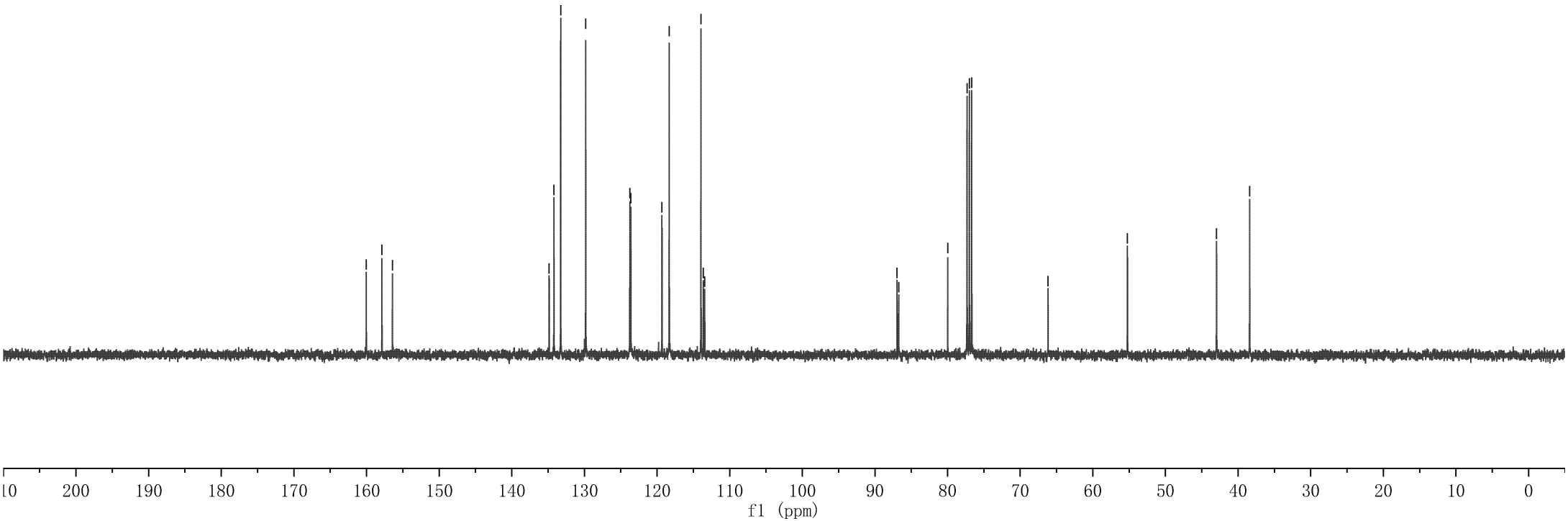
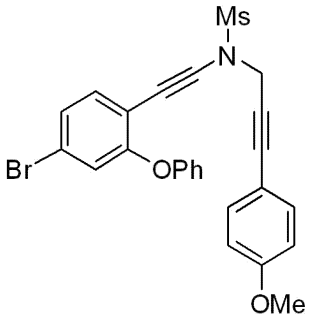


Parameter	Value
1 Title	ZJJ-13-157-5-Br-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2022-01-21T17:39:51
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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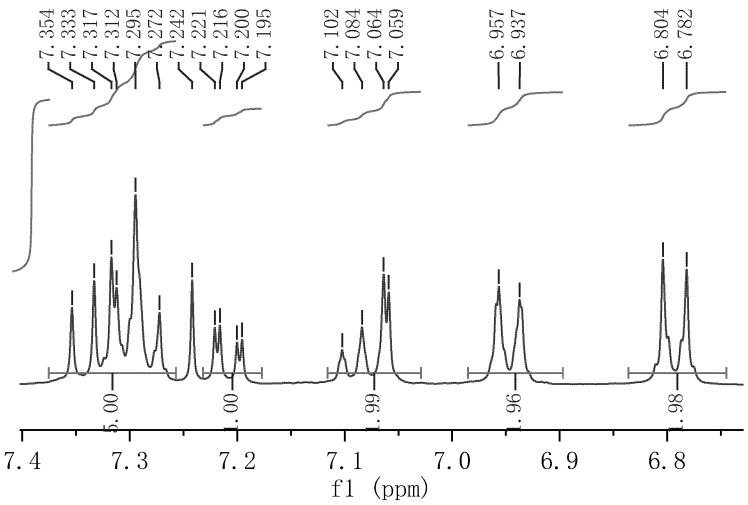

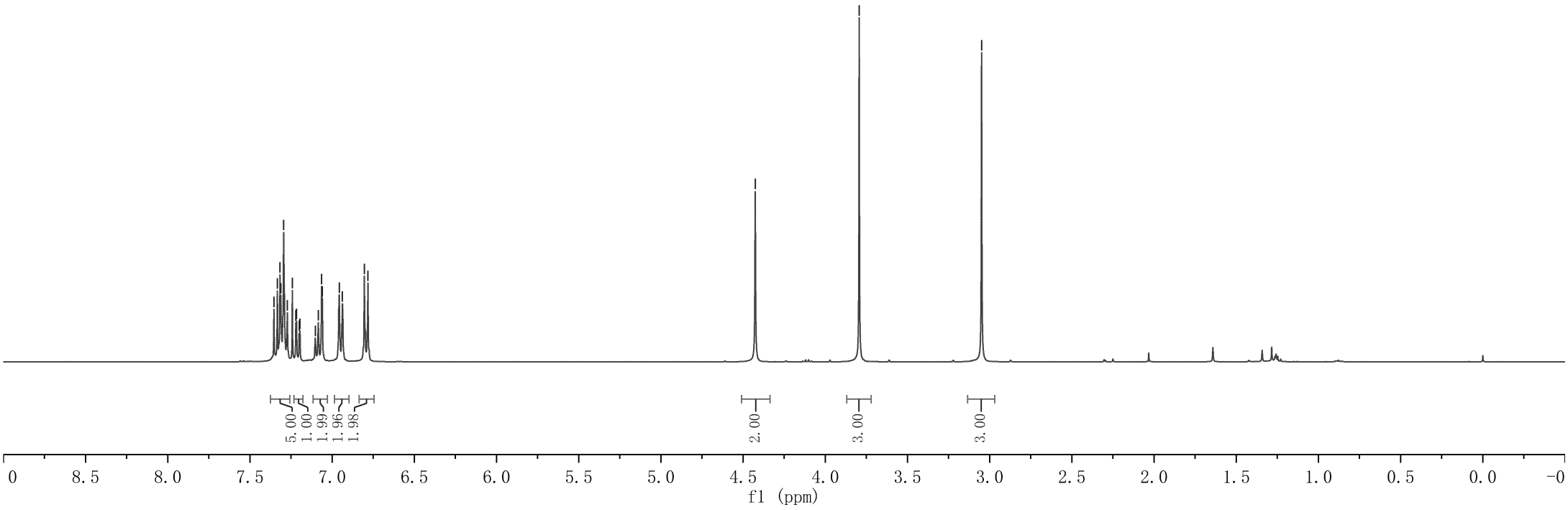

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134.33
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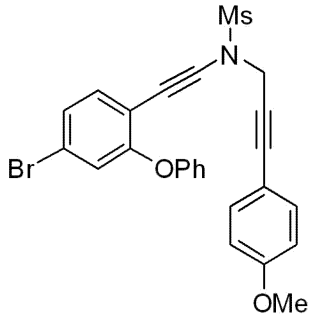
113.63
86.97
86.94
79.96
77.32
77.00
76.68
66.28
55.23
42.94
38.43

Parameter	Value
1 Title	ZJJ-13-157-5-Br-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2022-01-21T17:39:51
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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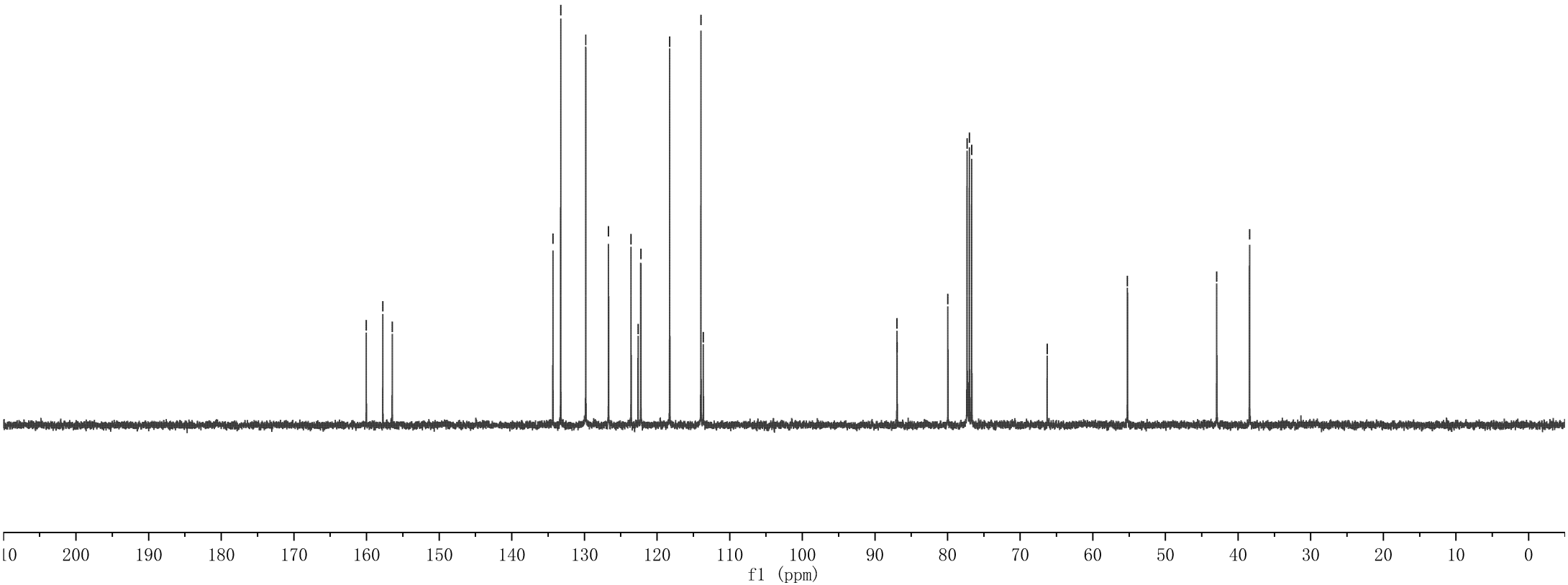
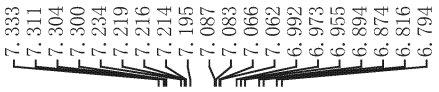
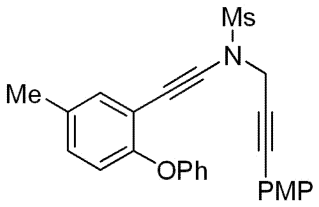




Parameter	Value
1 Title	zjj-13-191-4-Me-diwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-22T17:02:43
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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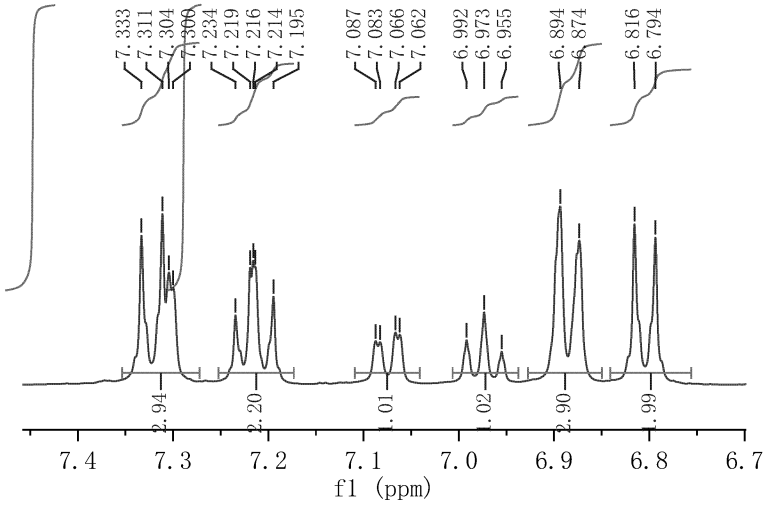

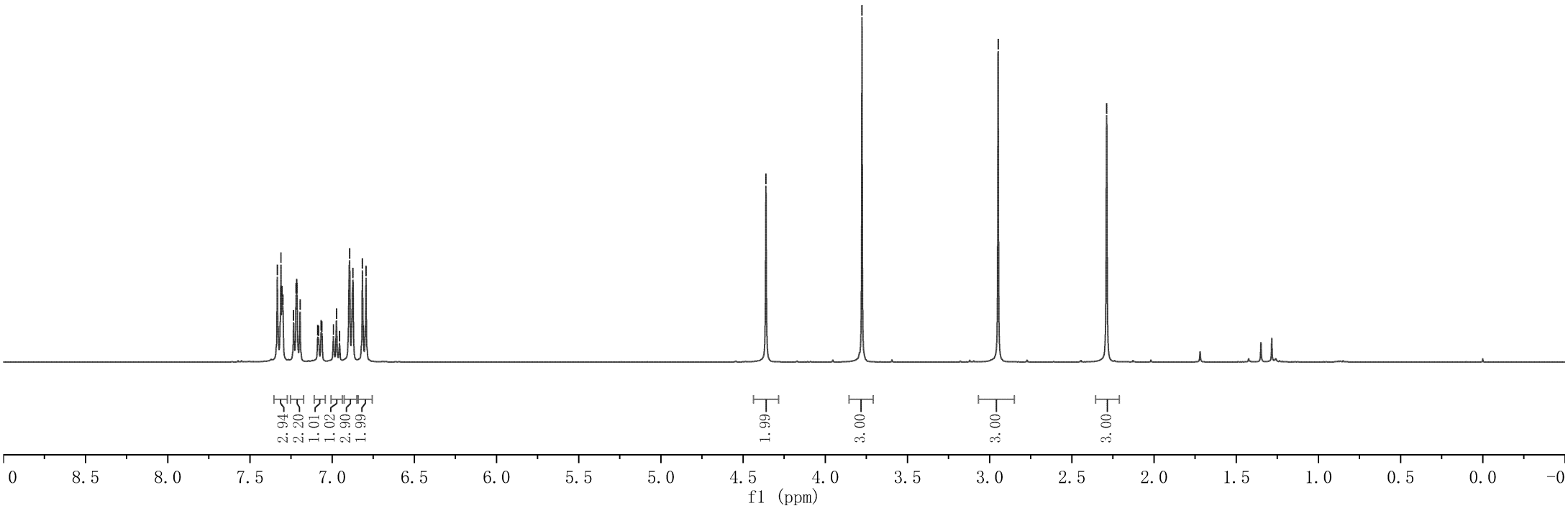

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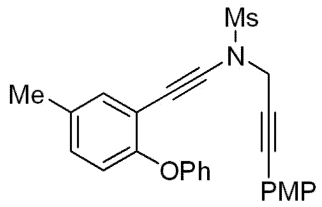
113.65
86.75
85.70
80.05
77.32
77.00
76.68
66.97
55.14
42.86
38.10
20.37

Parameter	Value
1 Title	zjj-13-191-4-Me-diwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	23
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-22T17:04:44
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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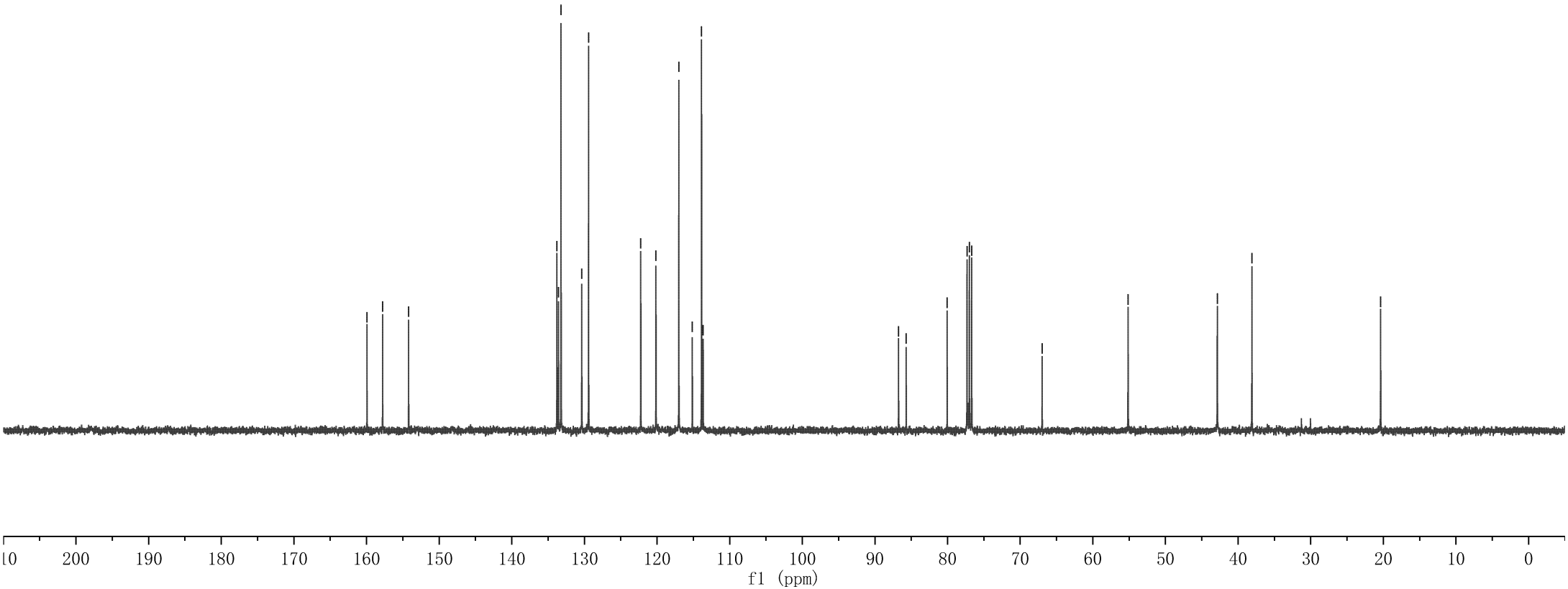
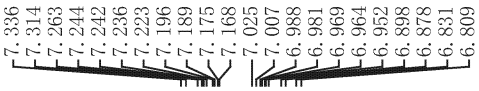
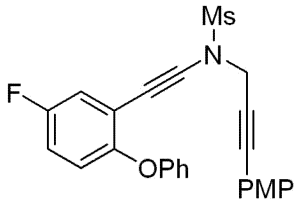




Parameter	Value
1 Title	ZJJ-13-18000-4-F-DIWU-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.3
5 Number of Scans	12
6 Acquisition Time	3.9846
7 Acquisition Date	2022-01-19T17:40:21
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7



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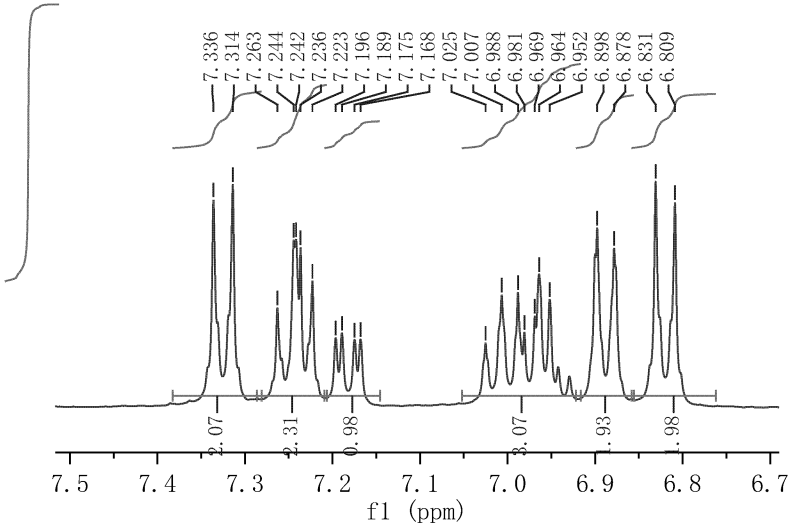
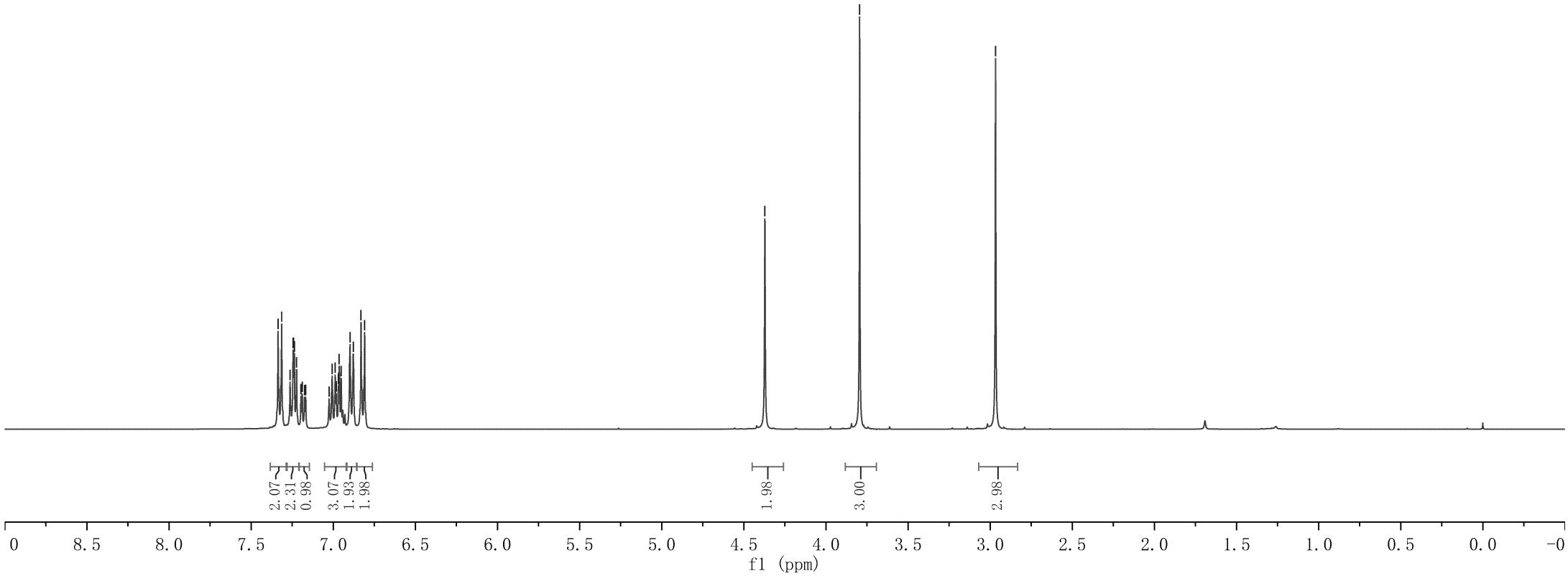
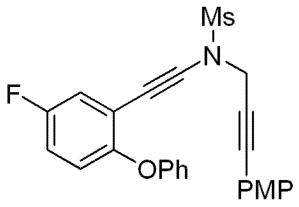




Parameter	Value
1 Title	ZJJ-13-4-F-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.3
5 Number of Scans	12
6 Acquisition Time	3.9846
7 Acquisition Date	2022-01-19T17:40:21
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7



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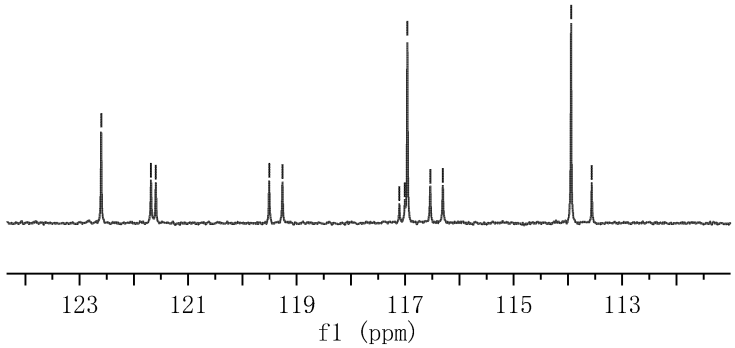
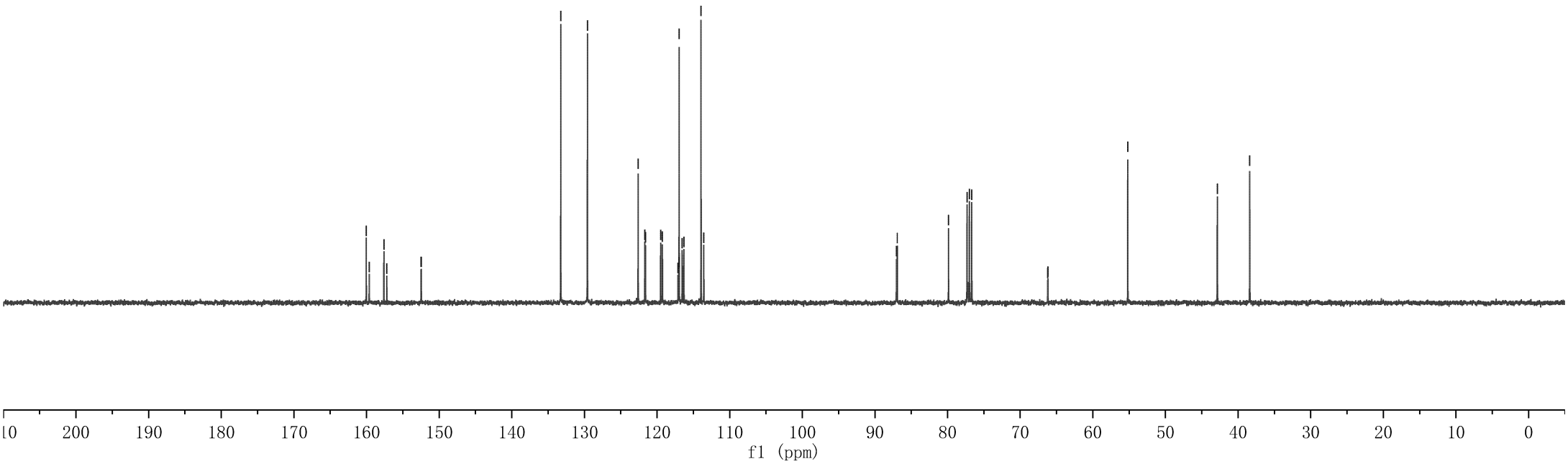
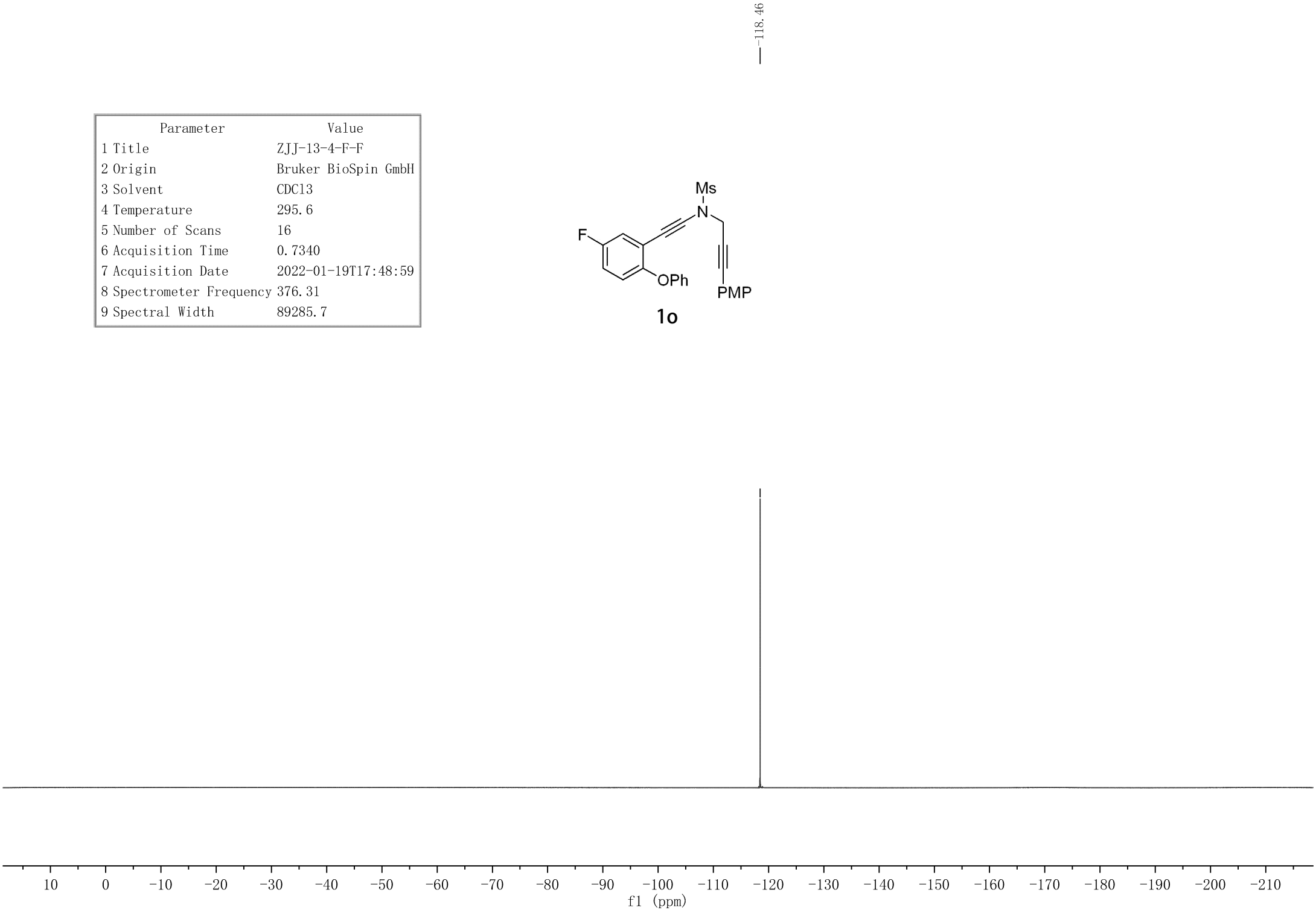
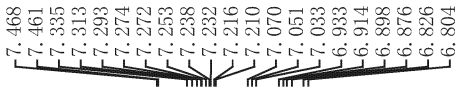




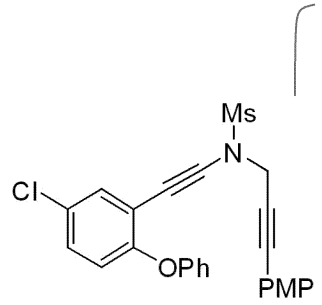
Parameter	Value
1 Title	ZJJ-13-4-F-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-19T17:48:59
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

1o





Parameter	Value
1 Title	ZJJ-13-124-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2022-01-05T20:09:51
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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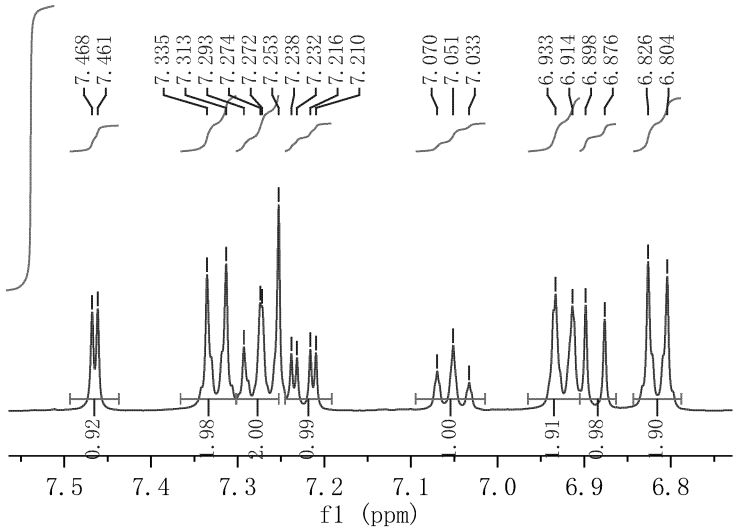

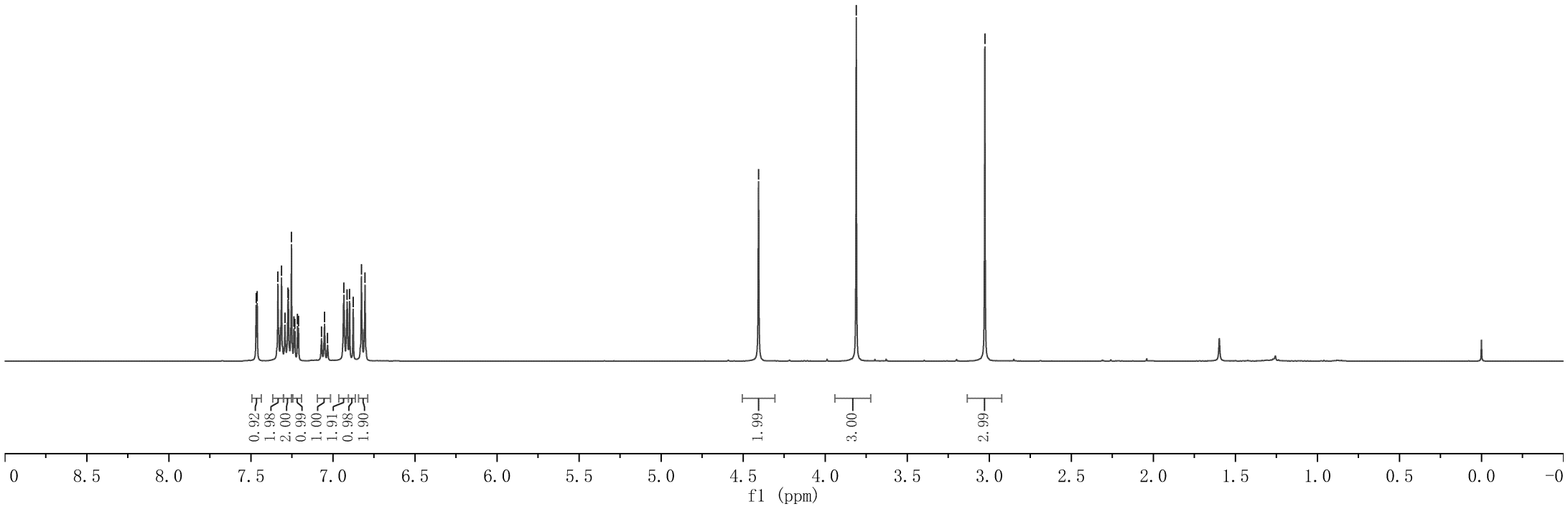

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157.07
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129.74
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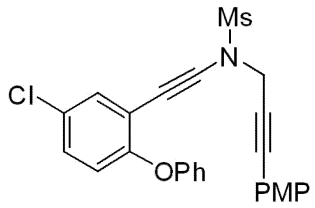
120.82
117.75
116.91
114.02
113.67
87.21
87.04
79.93
77.32
77.00
76.68
66.16
55.29
42.99
38.56

Parameter	Value
1 Title	ZJJ-13-124-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	44
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-05T20:11:10
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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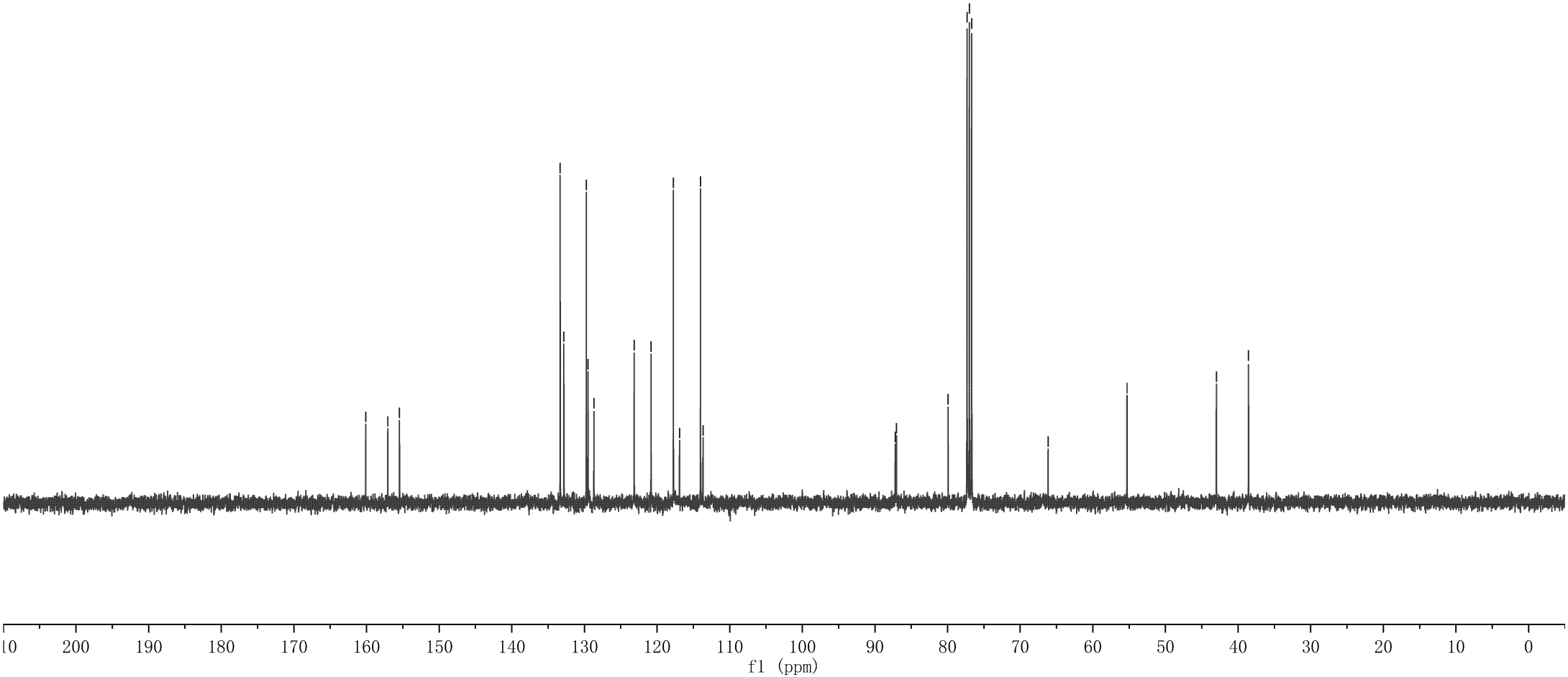
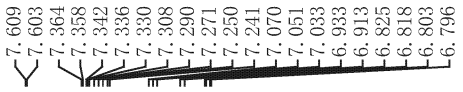
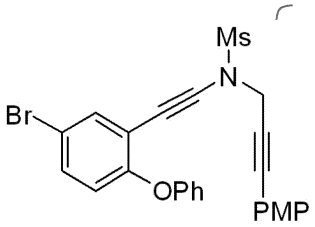




Parameter	Value
1 Title	zjj-13-205-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-27T16:55:27
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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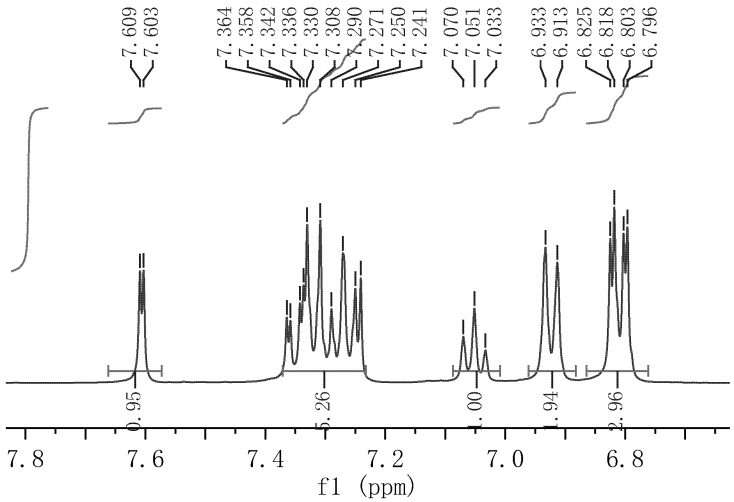
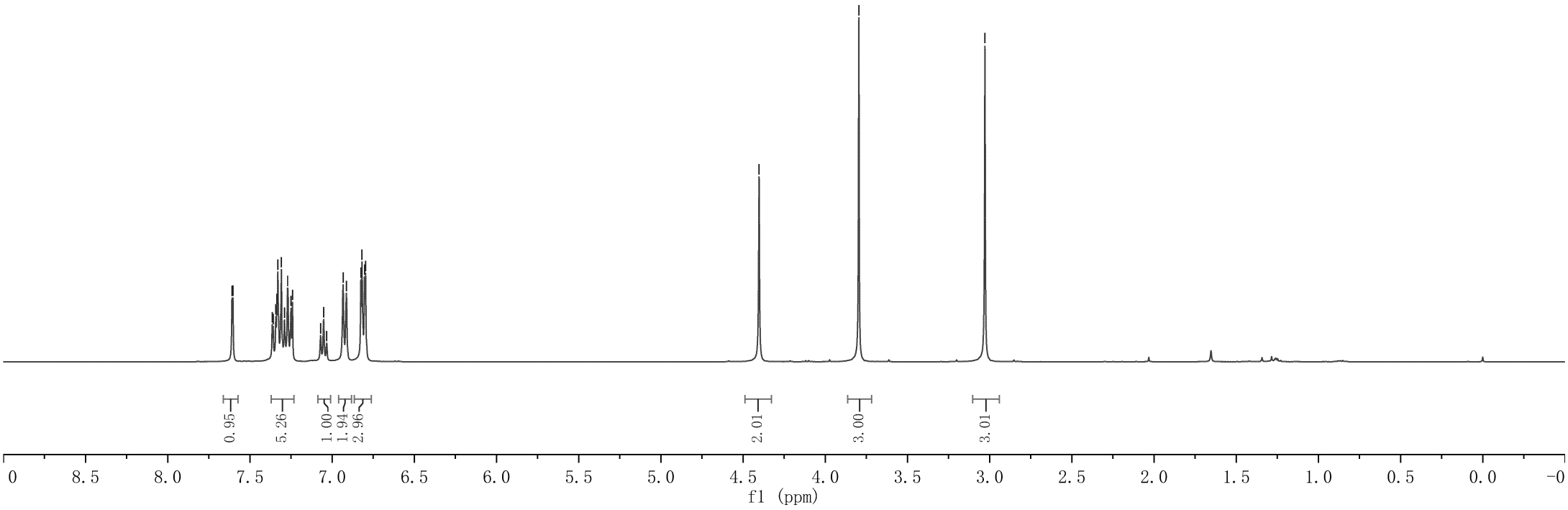
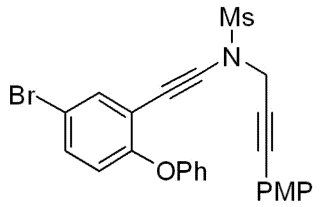




160.04
156.85
155.98
135.65
133.27
132.36
129.70
123.18
121.00
117.79
117.22
115.85
113.96
113.58
87.28
87.01
79.88
77.32
77.20
77.00
76.68
65.98
55.23
42.92
38.50

Parameter	Value
1 Title	zjj-13-205-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	28
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-27T16:57:32
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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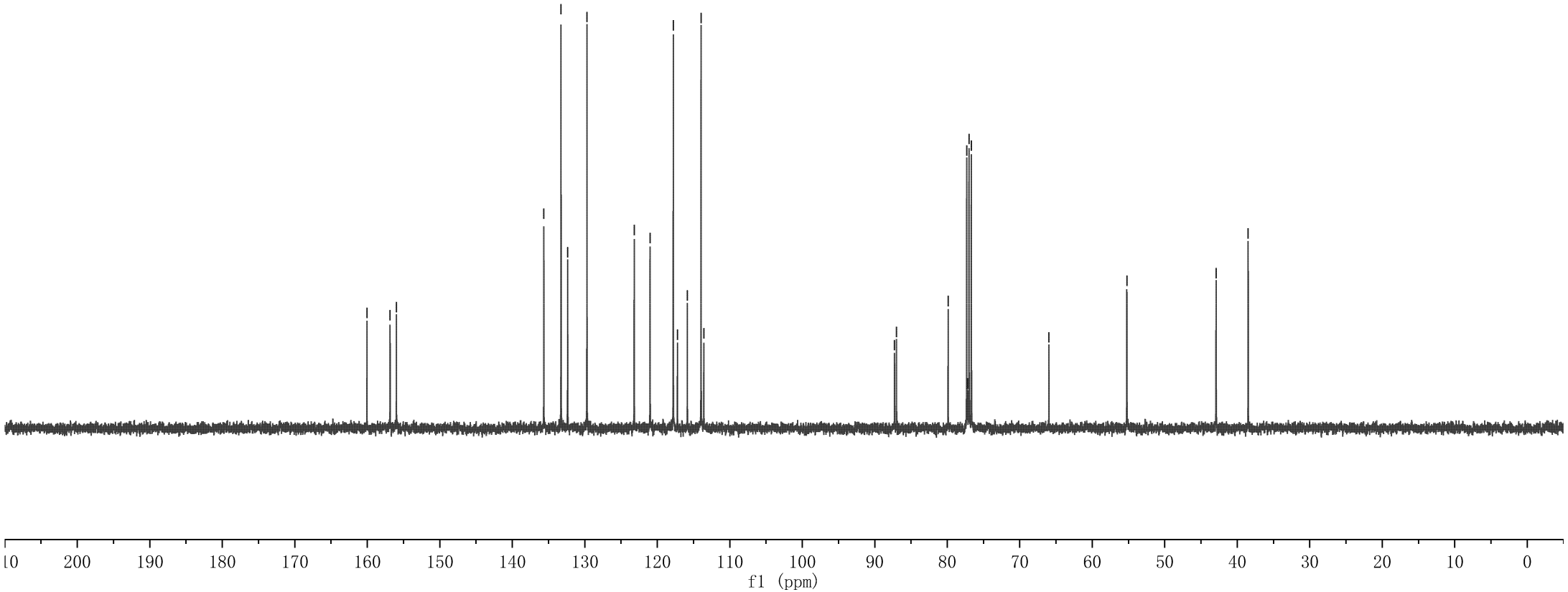
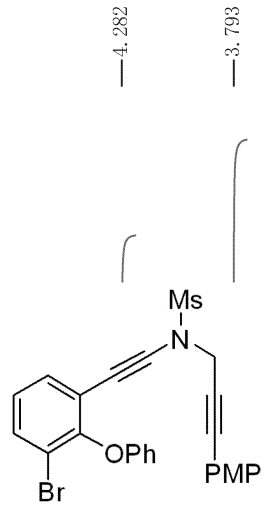


Parameter	Value
1 Title	LFS-2-133-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-02T15:01:05
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



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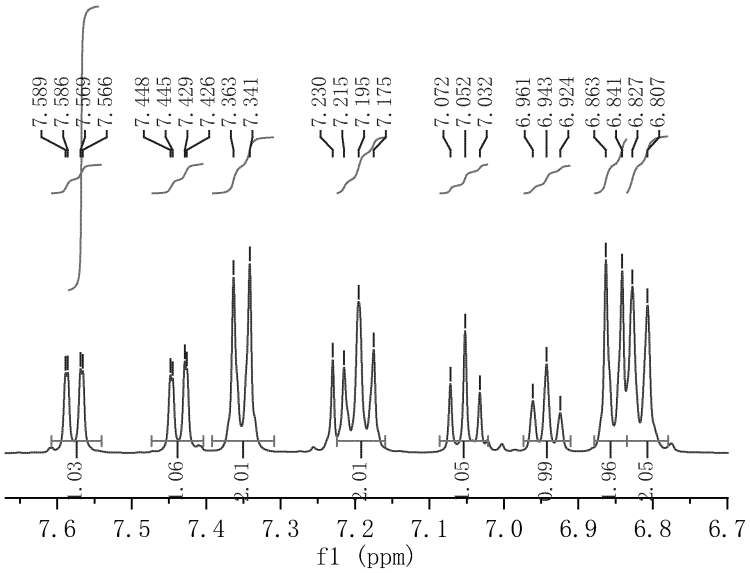

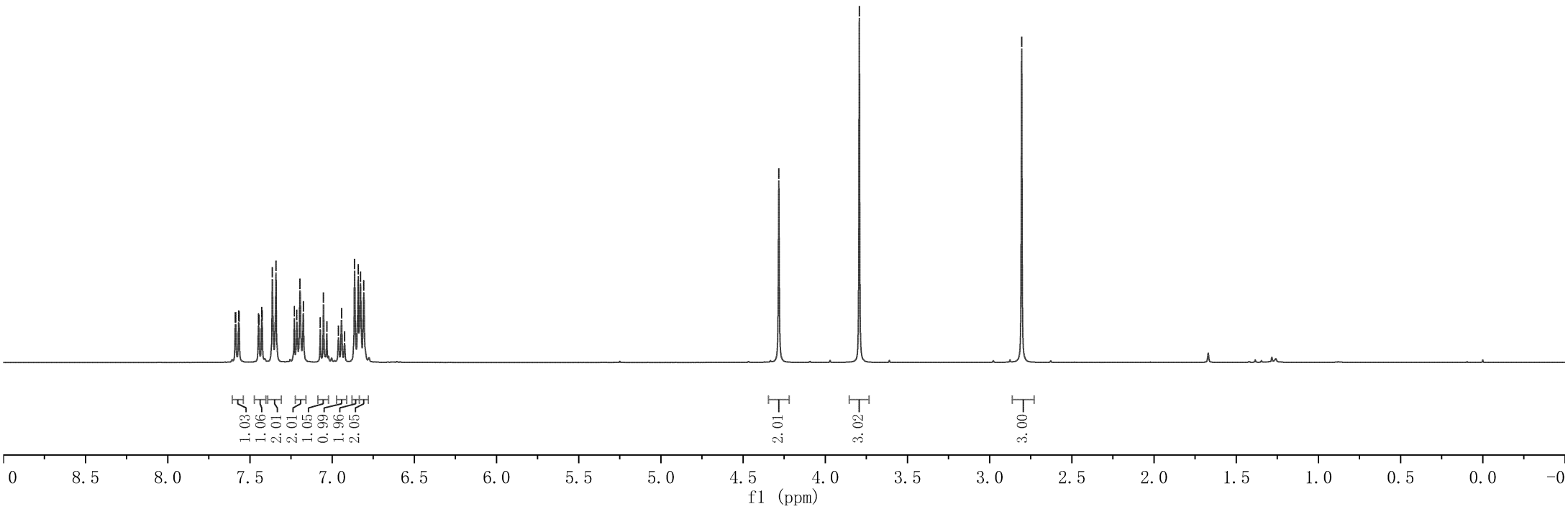

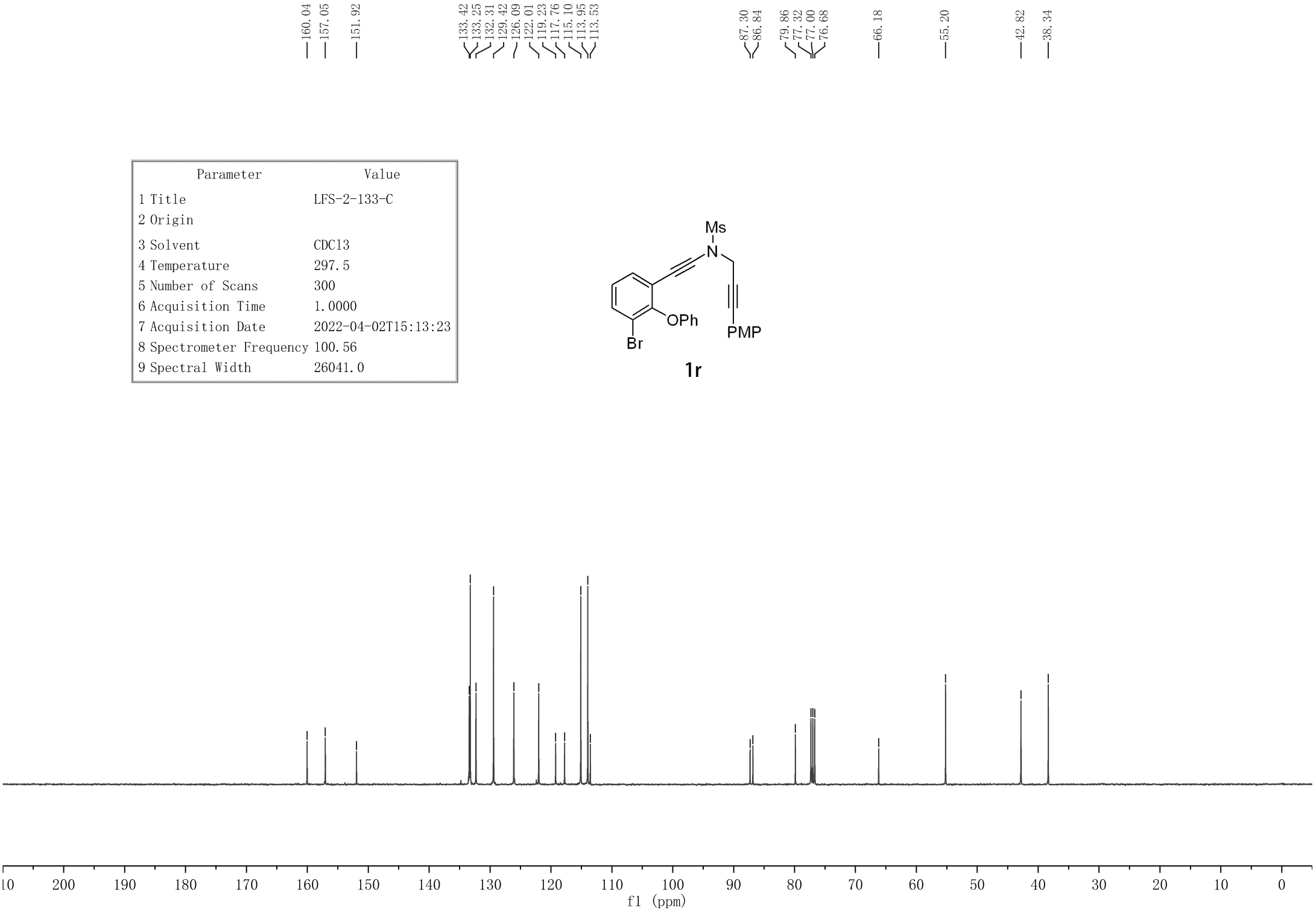
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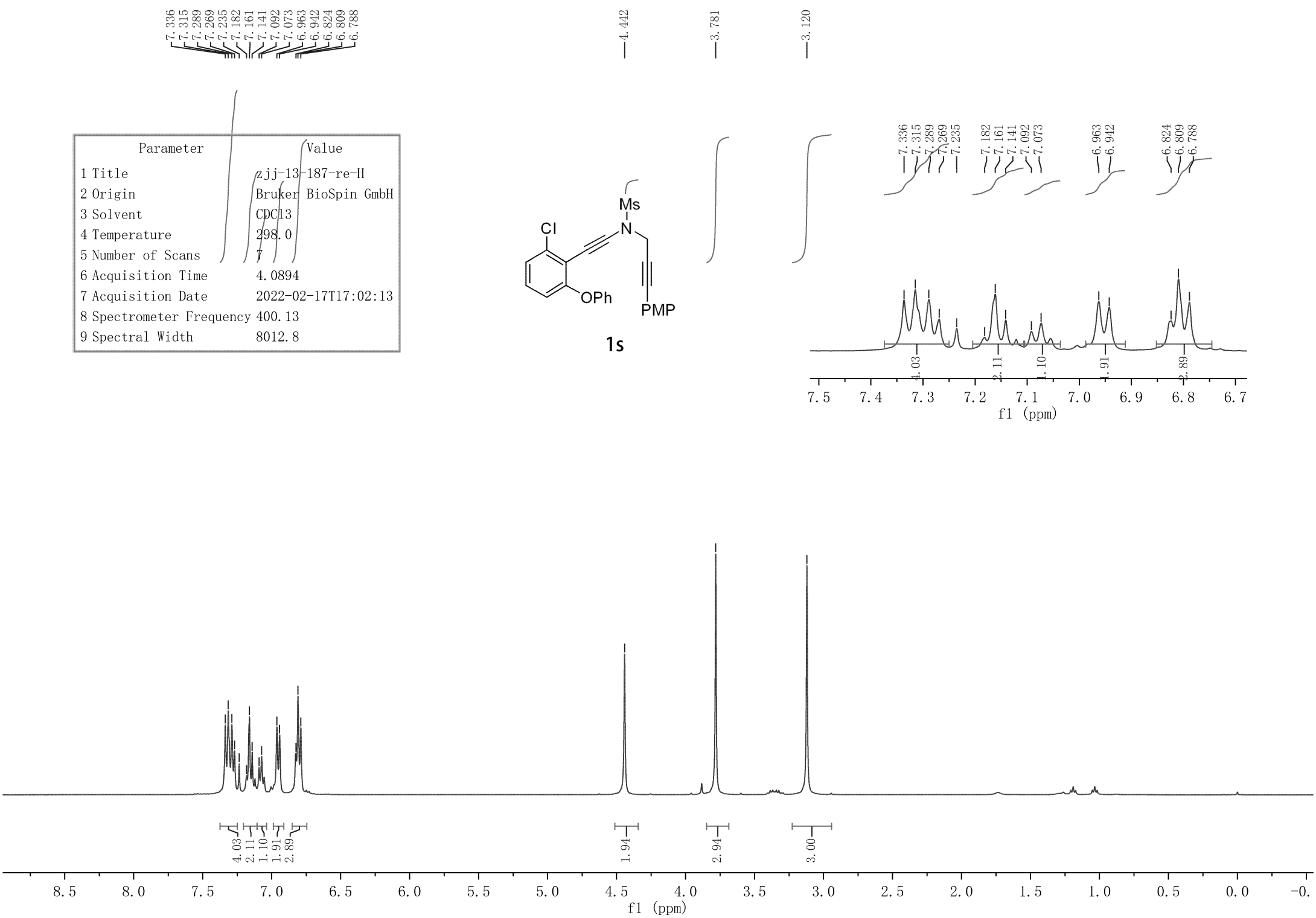
132.31
129.42
126.09
122.01
119.23
117.76
115.10
113.95
113.53
87.30
86.84
79.86
77.32
77.00
76.68
66.18
55.20
42.82
38.34
Parameter
Value
1 Title
LFS-2-133-C
2 Origin
3 Solvent
CDCl3
4 Temperature
297.5
5 Number of Scans
300
6 Acquisition Time
1.0000
7 Acquisition Date
2022-04-02T15:13:23
8 Spectrometer Frequency
100.56
9 Spectral Width
26041.0
Ms
N
OPh
Br
PMP
1r
f1 (ppm)

Parameter	Value
1 Title	zjj-13-187-re-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-17T17:02:13
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

1s



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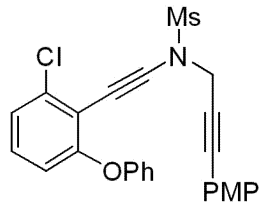
129.01
124.18
123.38
118.18
117.11
115.52
113.90
113.63
90.96
86.91
79.93
77.32
77.00
76.68
64.68
55.18
42.96
38.48

Parameter	Value
1 Title	zjj-13-187-re-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	12
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-17T17:03:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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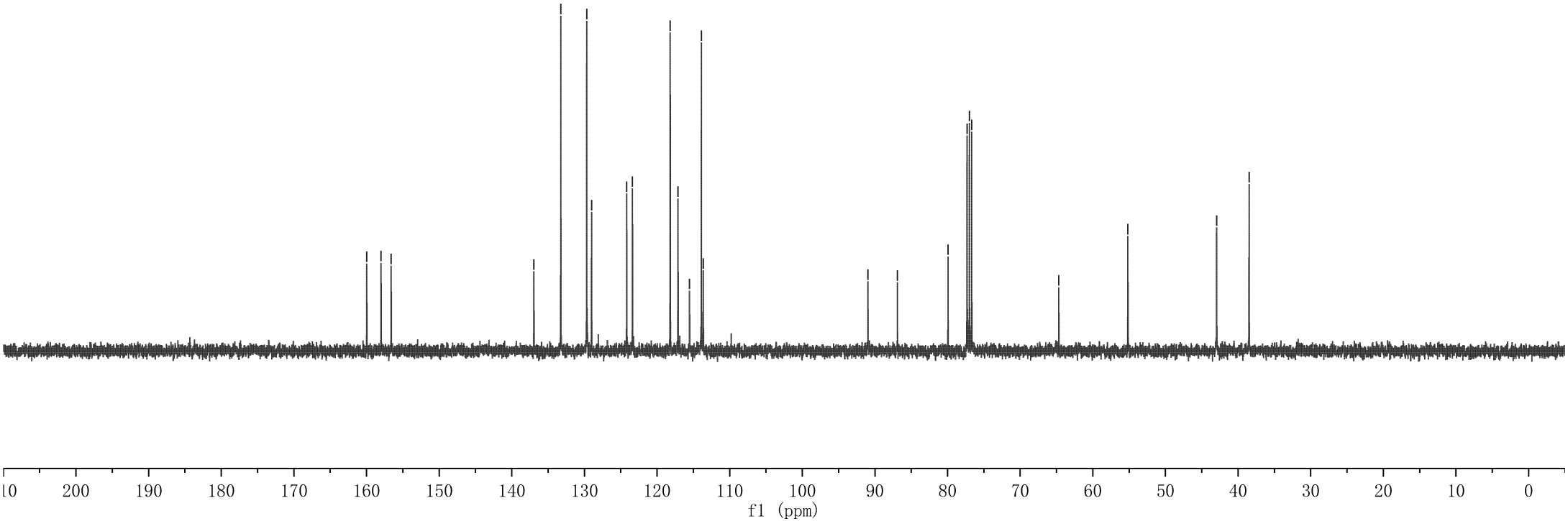
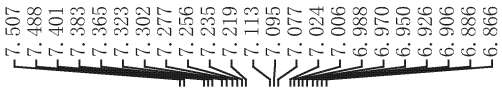
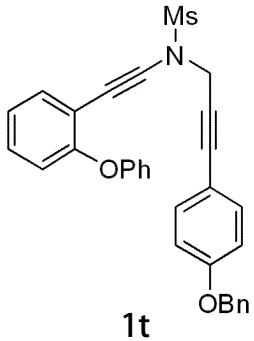




Parameter	Value
1 Title	zjj-13-ph-4-OBn-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-28T15:45:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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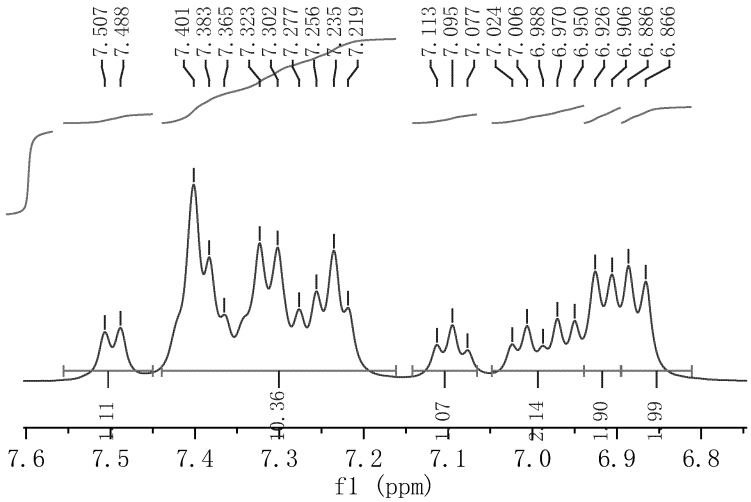

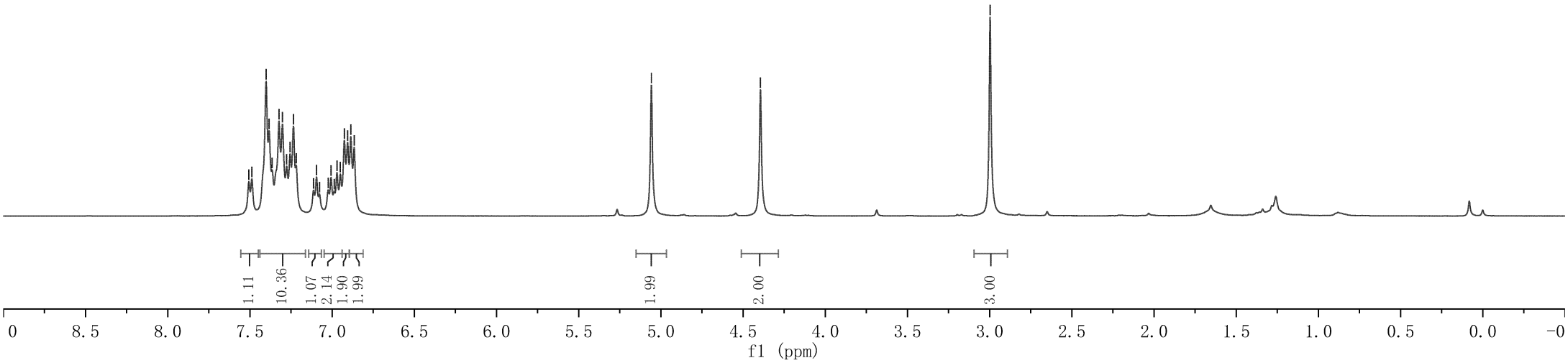

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133.33
129.70
129.60
128.60
128.10
127.38
123.79
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117.66
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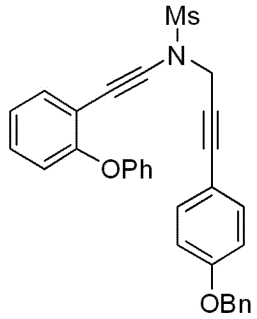
114.88
114.05
86.81
86.03
80.21
77.32
77.00
76.68
69.97
66.97
42.99
38.29

Parameter	Value
1 Title	zjj-13-Ph-4-OBn-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	36
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-28T15:47:14
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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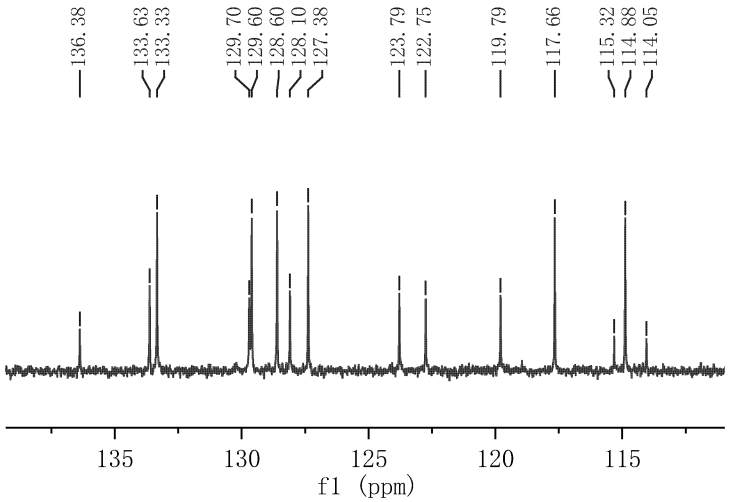
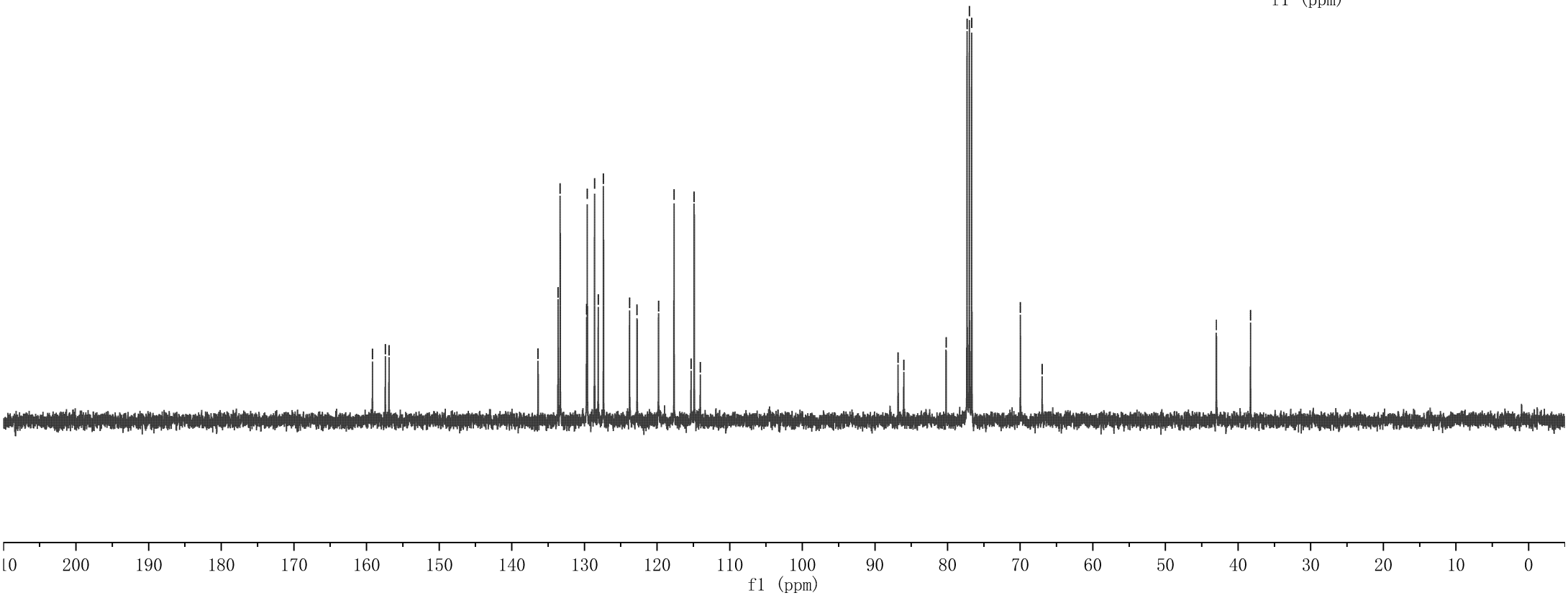
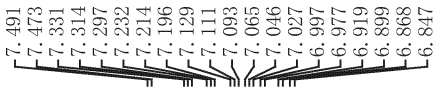
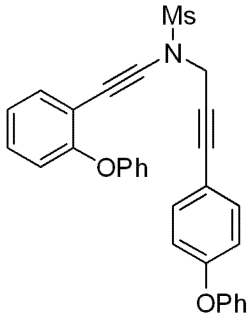






Parameter	Value
1 Title	LFS-2-152-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-10T13:43:52
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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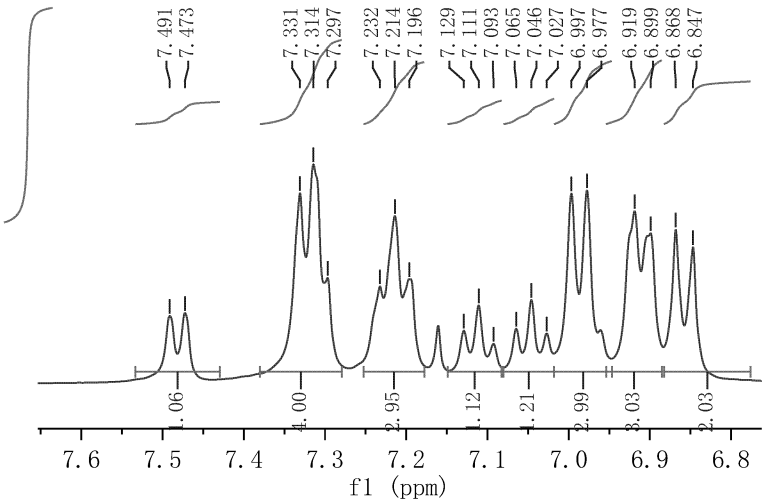
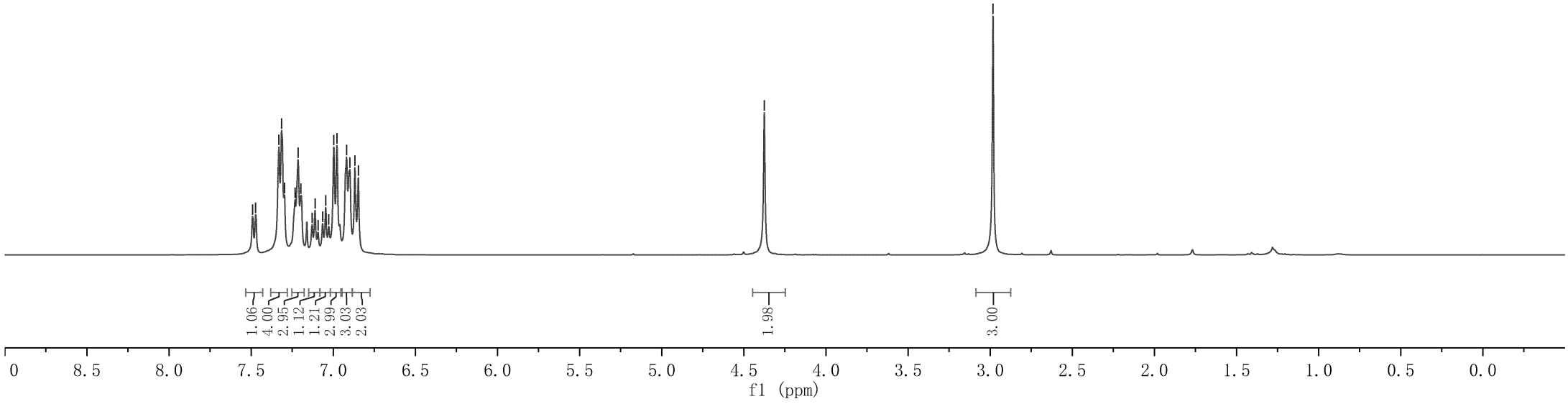
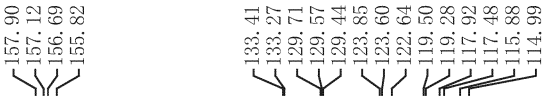
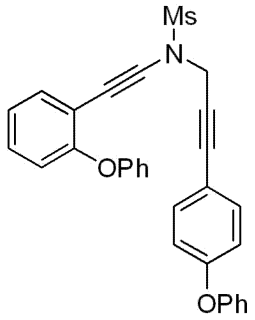






Parameter	Value
1 Title	LFS-2-152-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	48
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-10T13:47:18
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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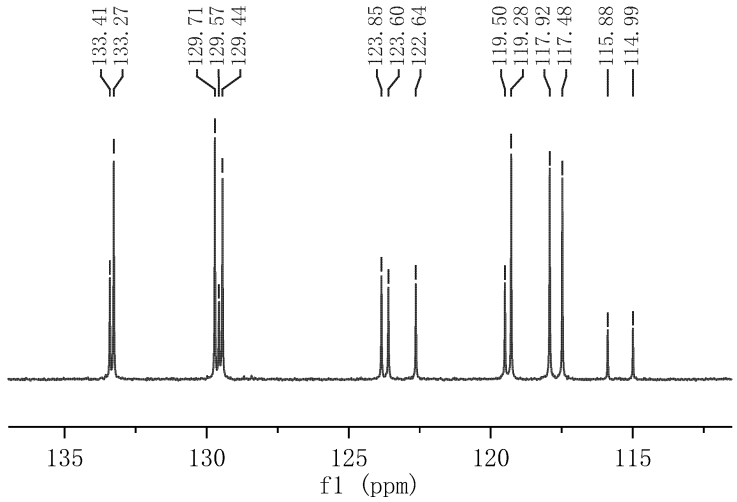
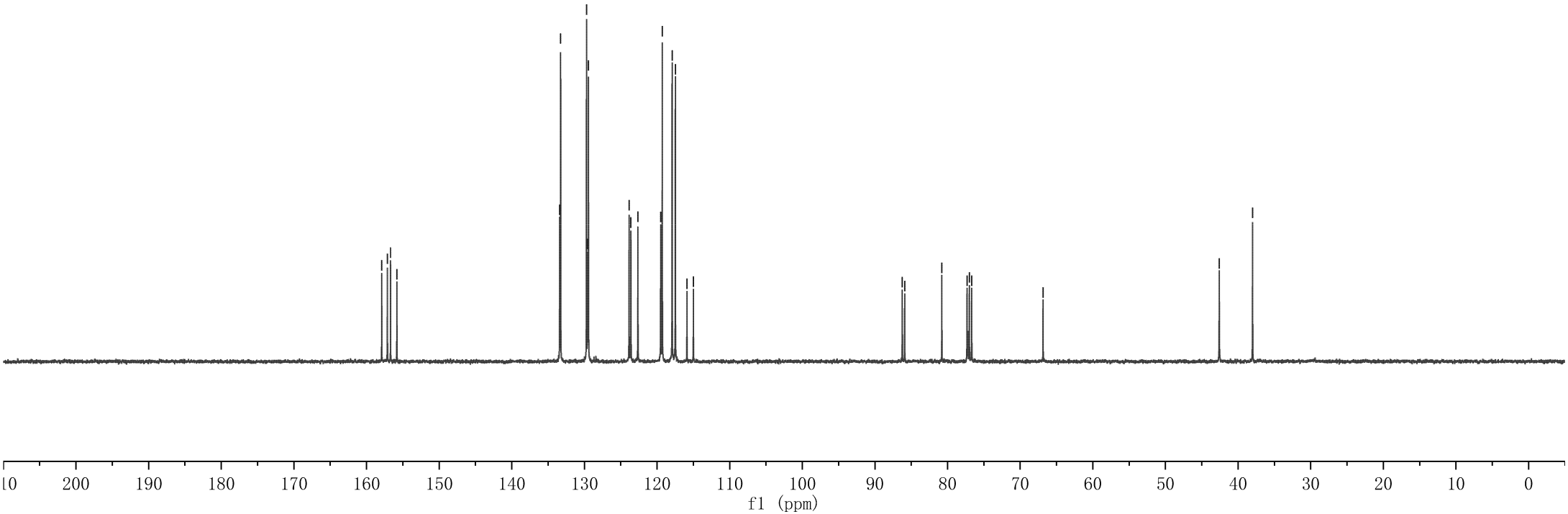
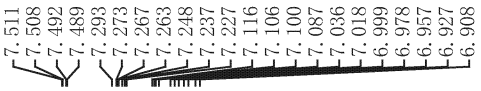
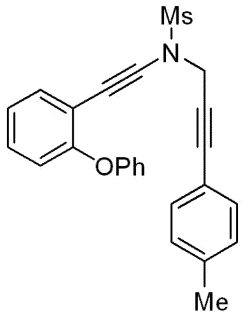


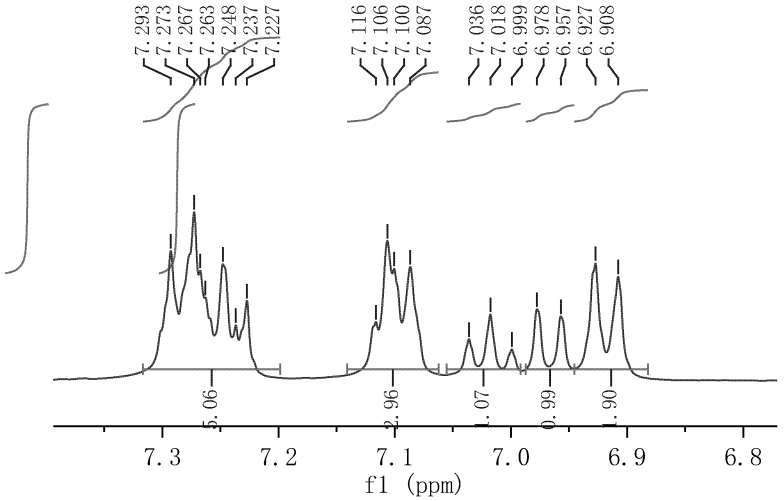


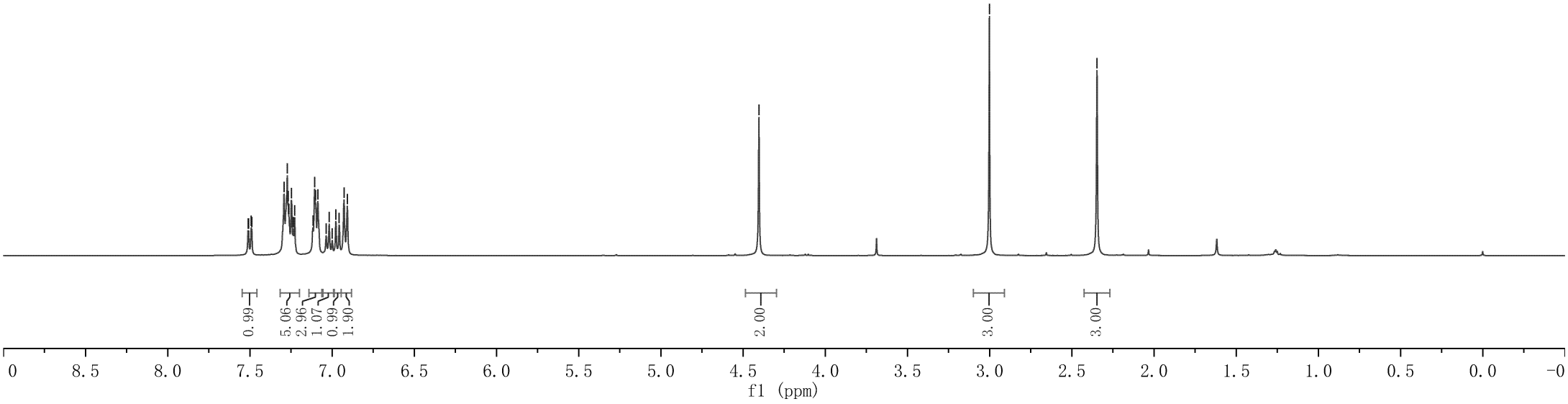


Parameter	Value
1 Title	zjj-Ph-4-Me-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-11T19:39:20
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



1v





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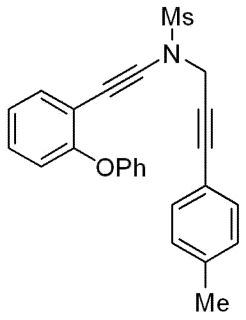
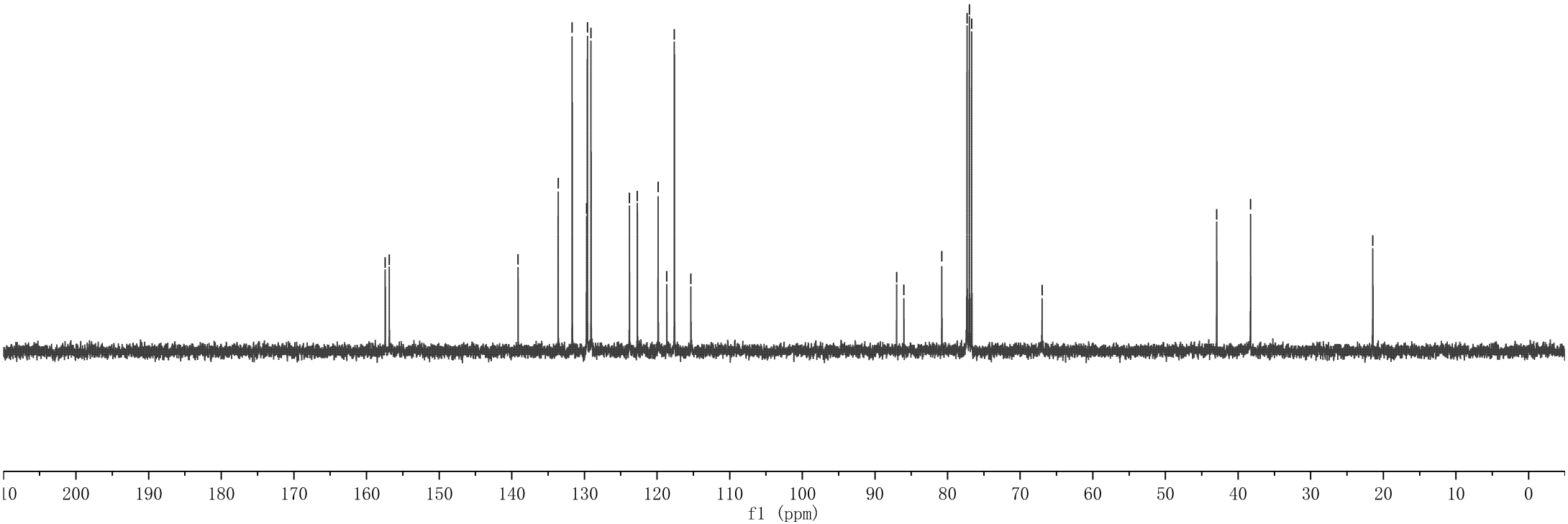
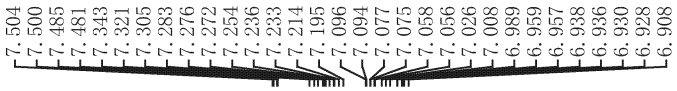
117.61
115.34
87.01
86.01
80.79
77.32
77.00
76.68
66.98
42.94
38.28
21.45

Parameter	Value
1 Title	zjj-Ph-4-Me-diwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	24
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-11T19:40:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

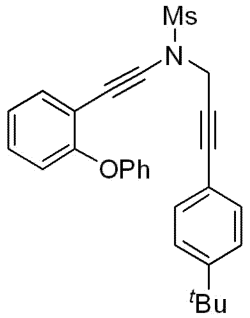


1v

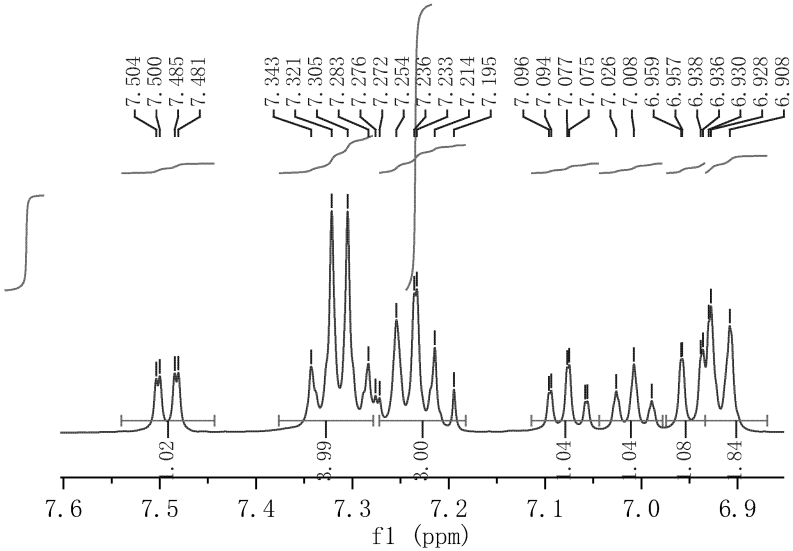


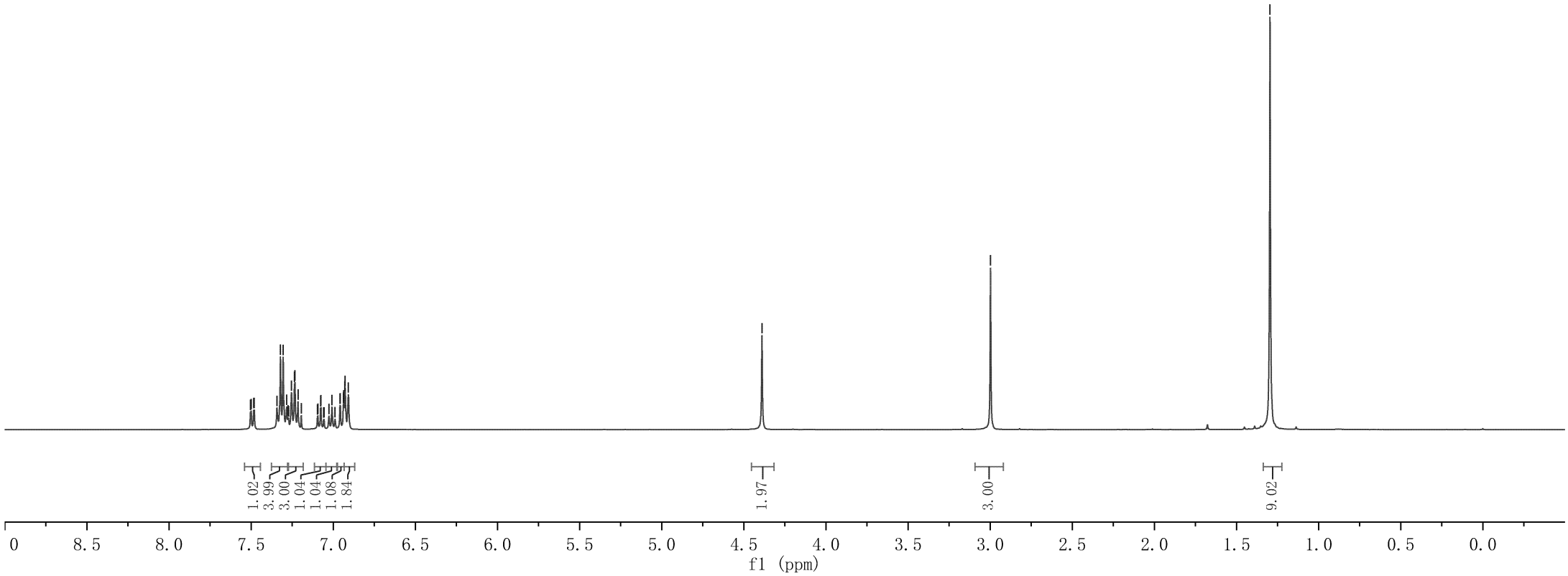


Parameter	Value
1 Title	LFS-2-175-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-18T22:12:31
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



1w





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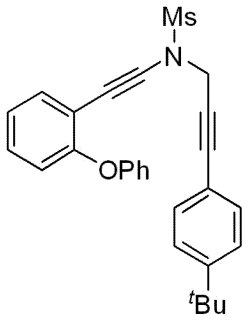
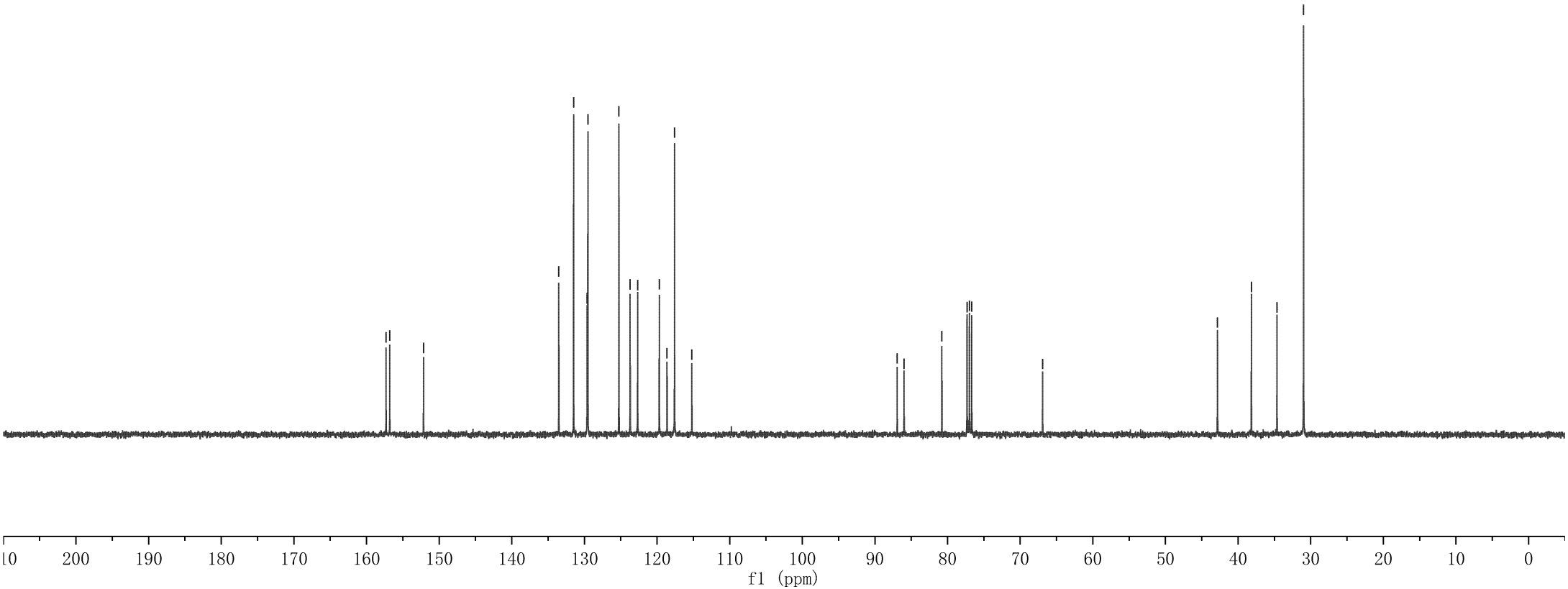
122.67
119.69
118.63
117.59
115.21
86.94
85.99
80.78
77.32
77.00
76.68
66.91
42.84
38.16
34.65
30.98

Parameter	Value
1 Title	LFS-2-175-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	22
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-18T22:14:17
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

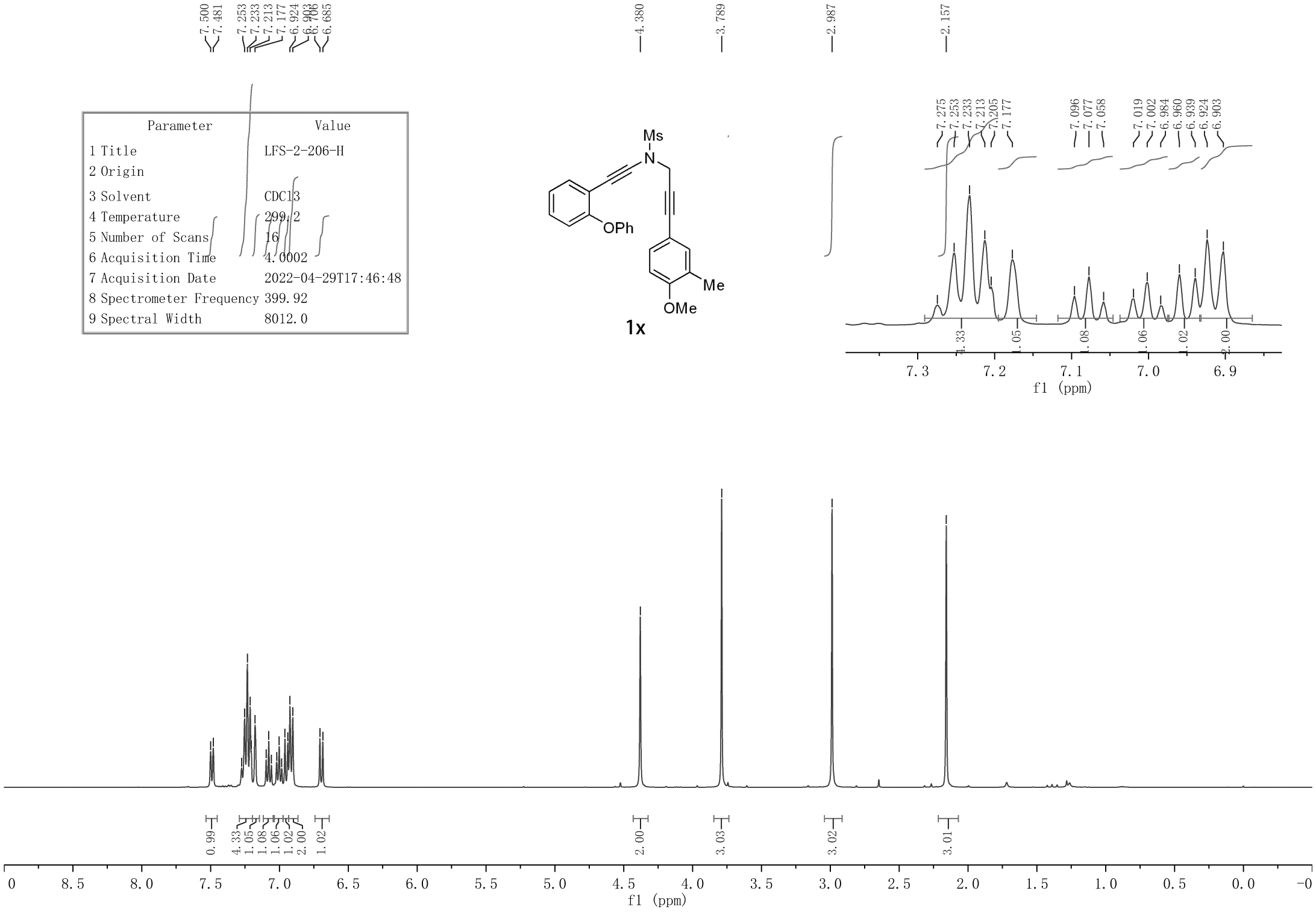


1w



Parameter	Value
1 Title	LFS-2-206-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.2
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-29T17:46:48
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0

1x



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122.62
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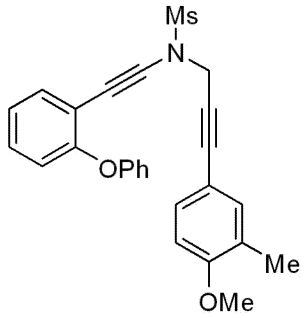
113.07
109.61
87.11
86.10
79.66
77.32
77.00
76.68
66.83
55.17
42.93
38.16
15.86

Parameter	Value
1 Title	LFS-2-206-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.2
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-29T17:55:53
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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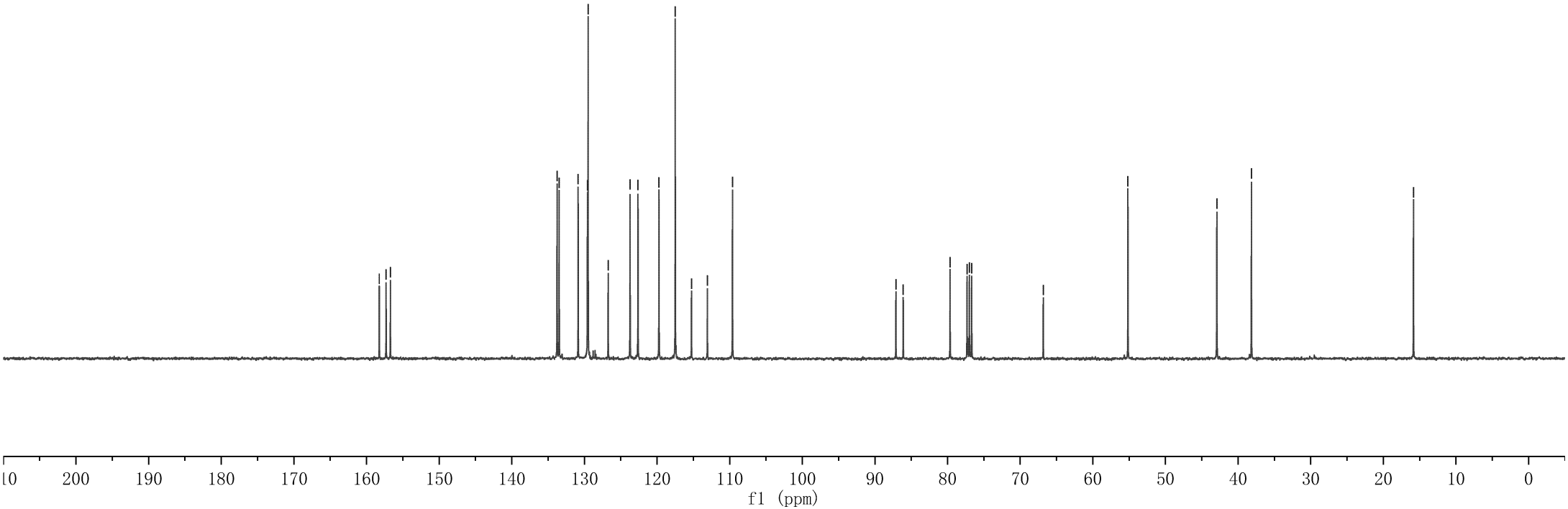
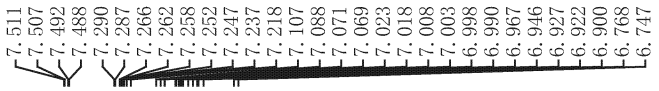
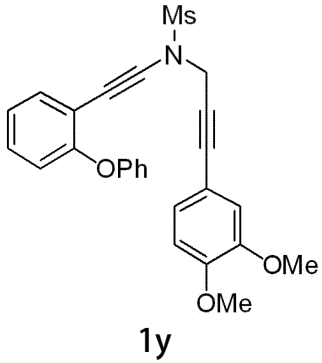




Parameter	Value
1 Title	LFS-2-170-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	15
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-17T17:41:40
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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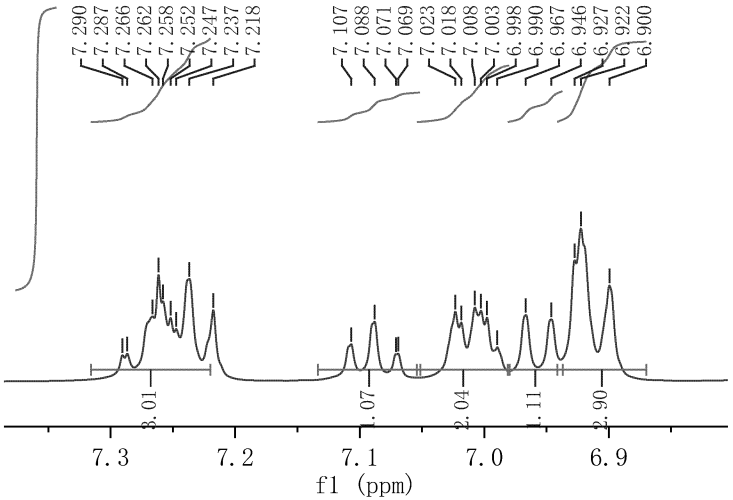
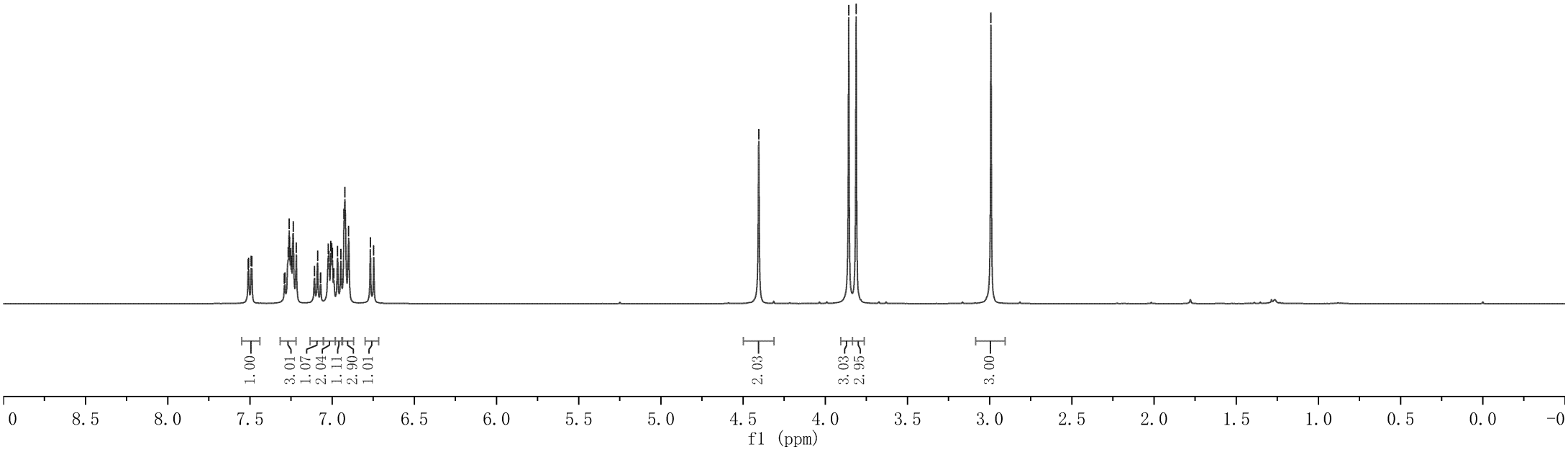
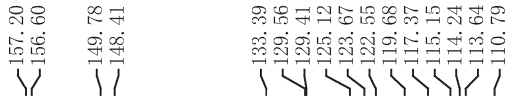
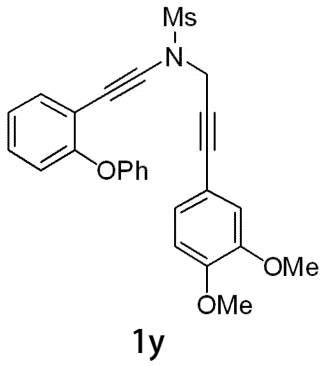






Parameter	Value
1 Title	LFS-2-170-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	33
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-17T17:44:47
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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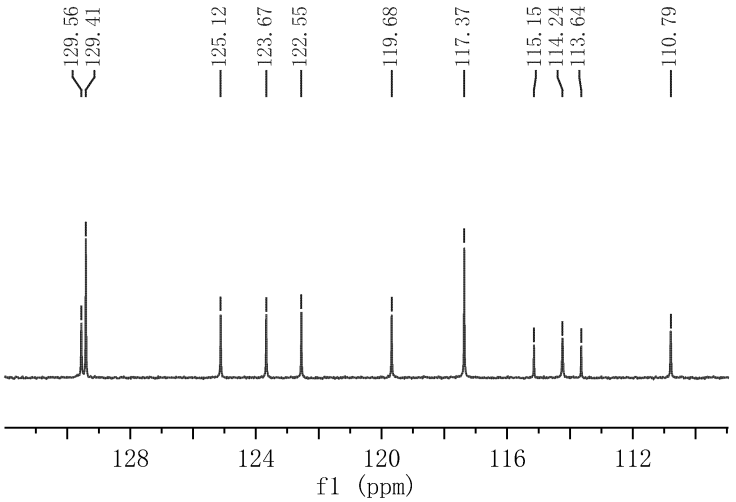
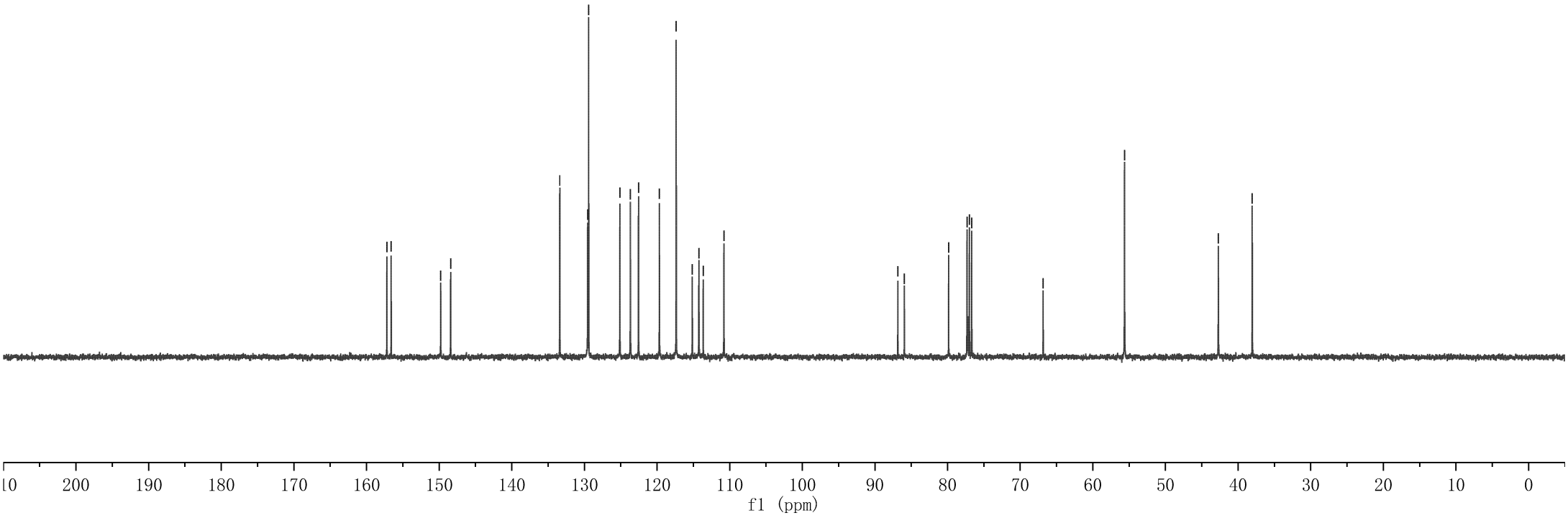
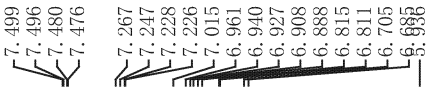
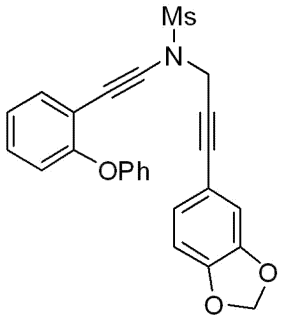


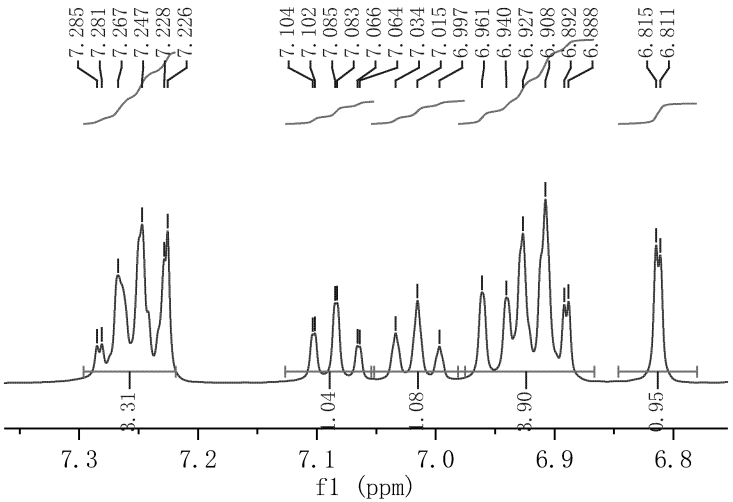


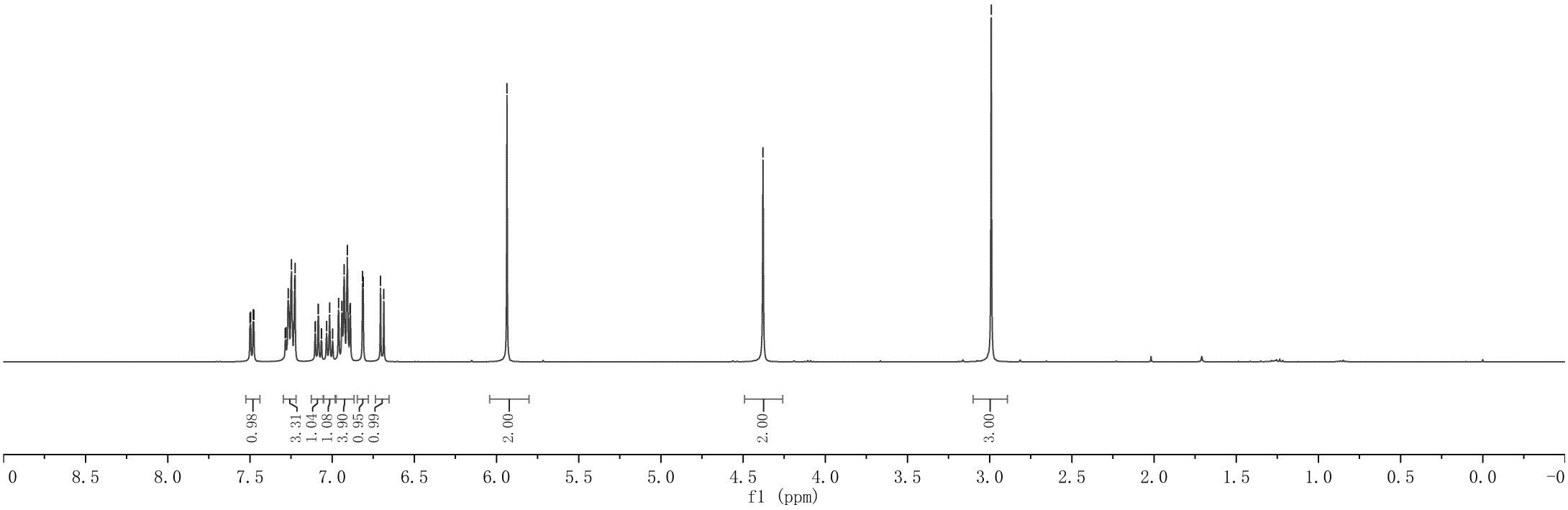


Parameter	Value
1 Title	zjj-14-32-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-14T19:46:26
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



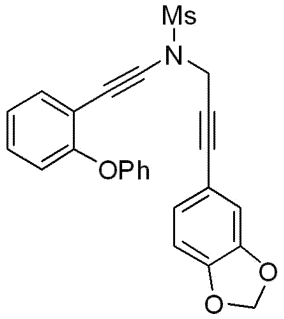
1z



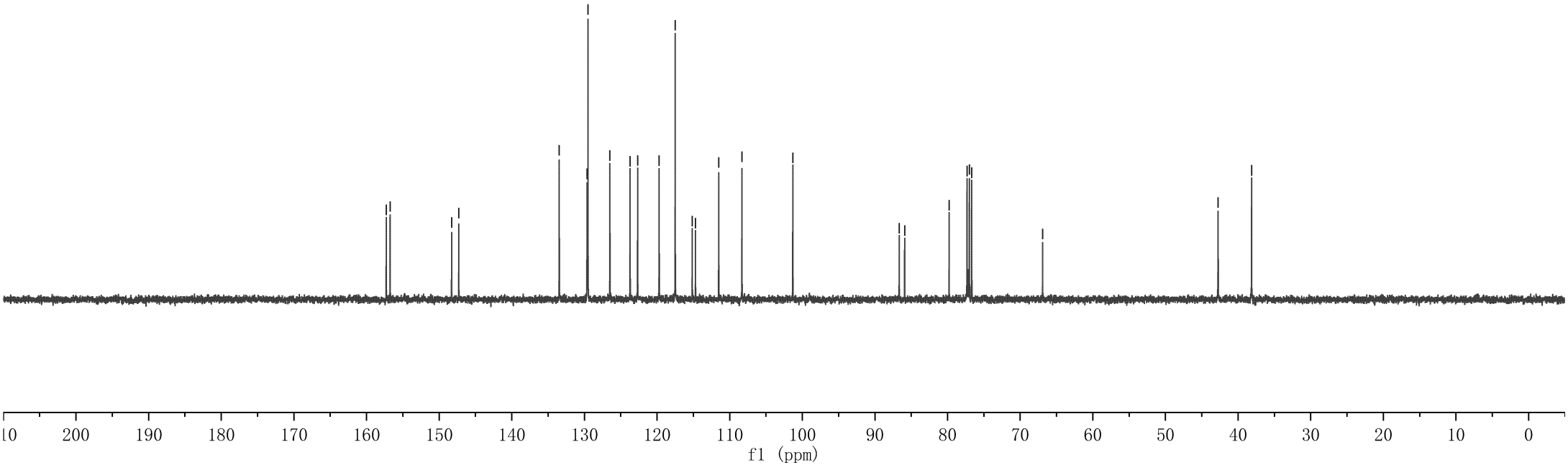


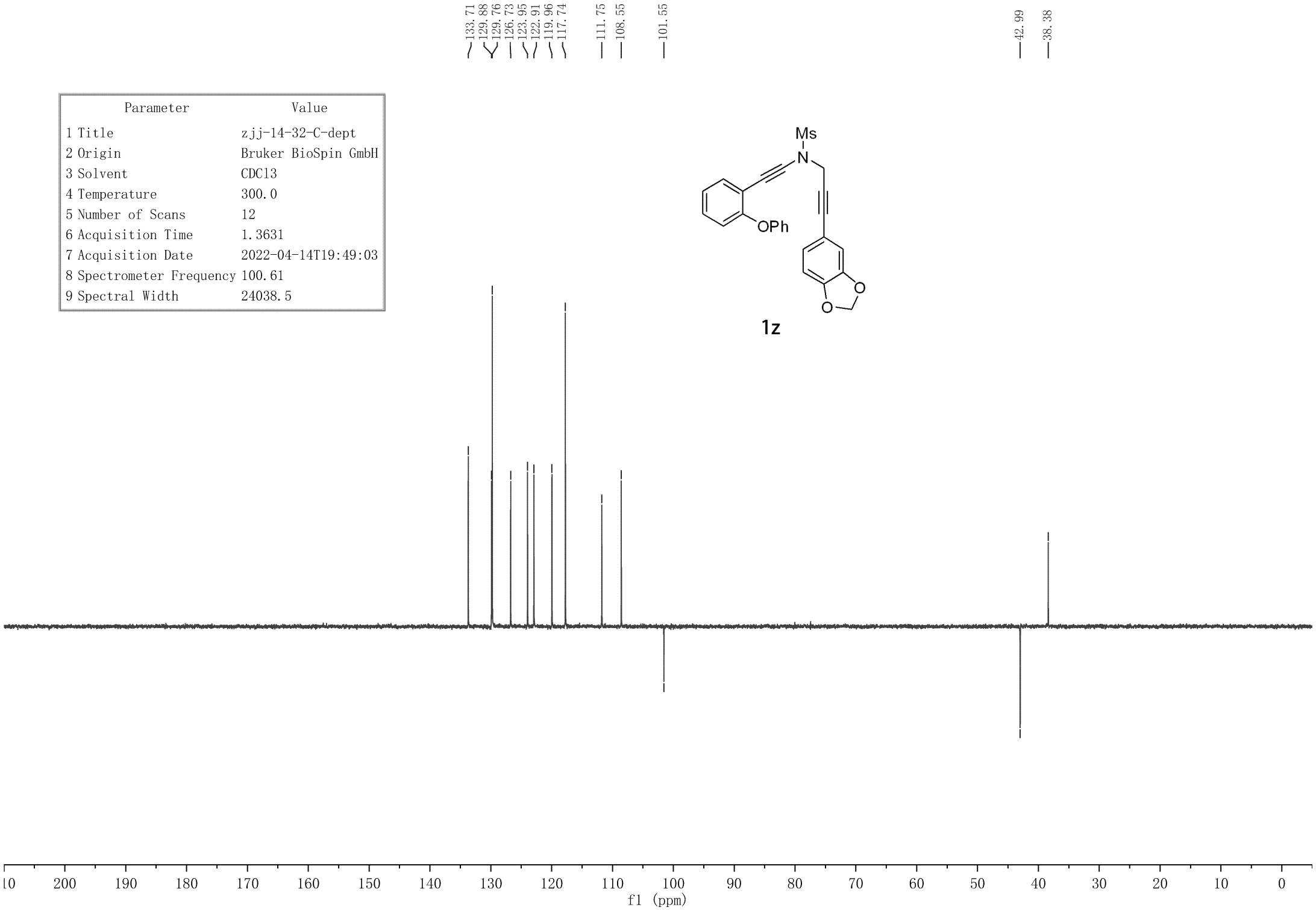
157.28
156.75
148.28
147.30
133.47
129.64
129.51
126.49
123.71
122.67
119.71
117.50
115.16
114.71
111.51
108.31
101.31
86.66
85.91
79.78
77.32
77.00
76.68
66.91
42.75
38.14

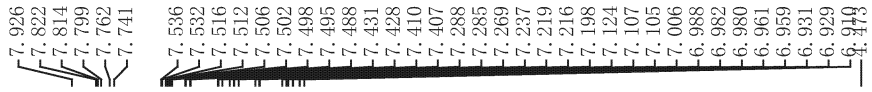
Parameter	Value
1 Title	zjj-14-32-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	9
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-14T19:47:35
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



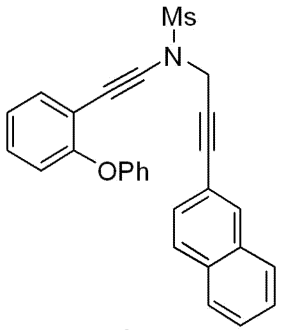
1z




133.71
129.88
129.76
126.73
123.95
122.91
119.96
117.74
111.75
108.55
101.55
42.99
38.38
Parameter Value
1 Title zjj-14-32-C-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 12
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-14T19:49:03
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
OPh
O
O
1z
f1 (ppm)



Parameter	Value
1 Title	zjj-14-37-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-16T21:01:29
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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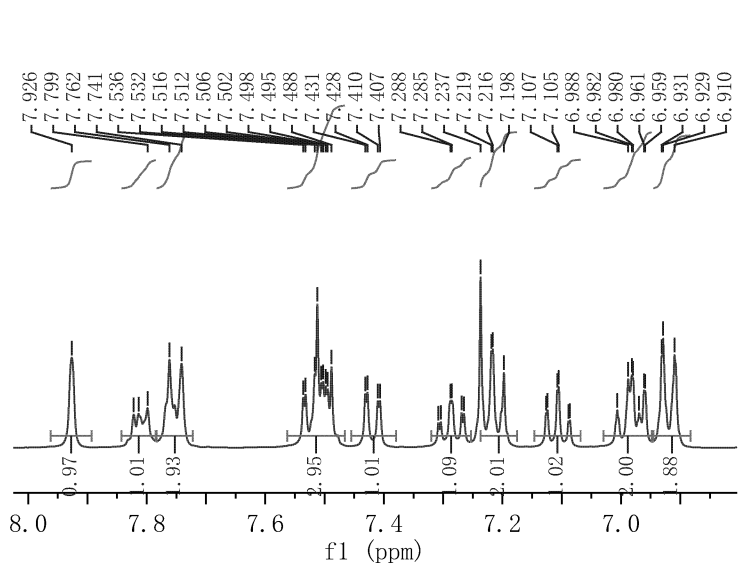
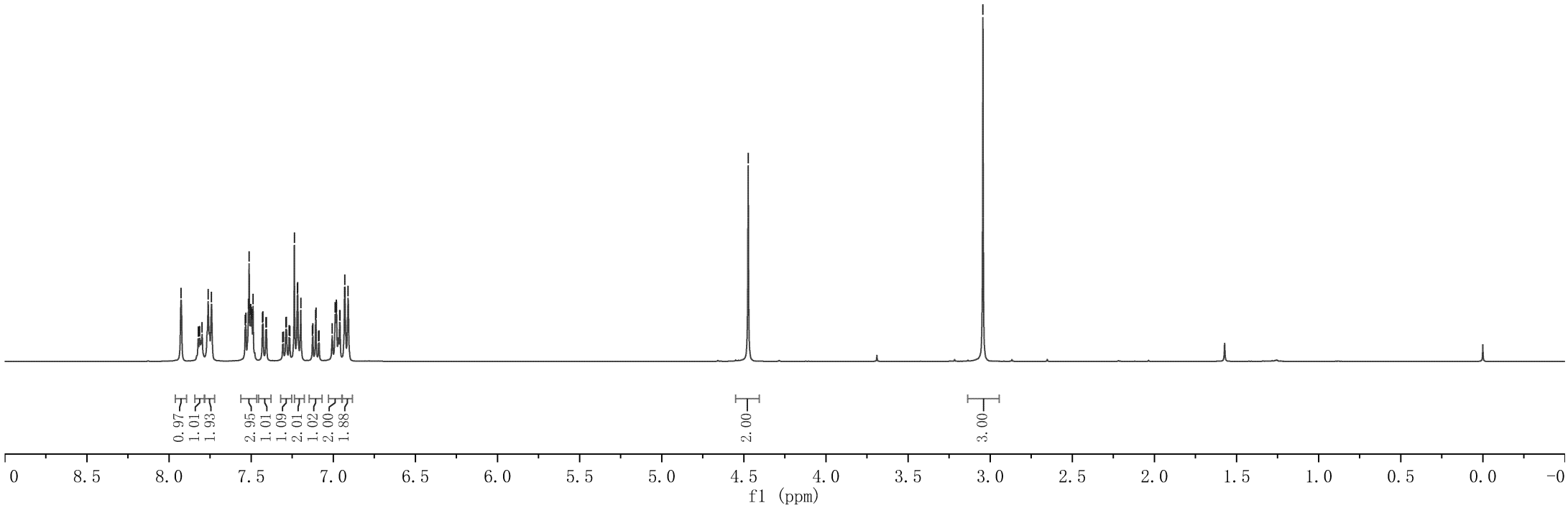
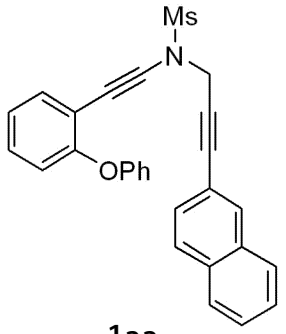


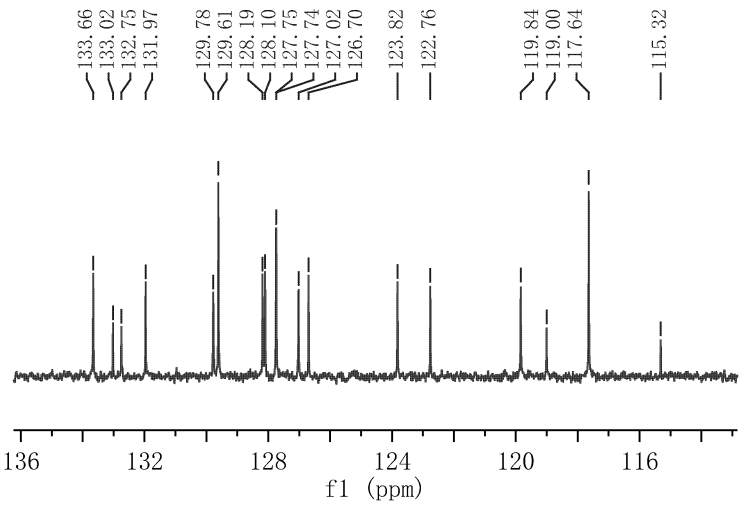


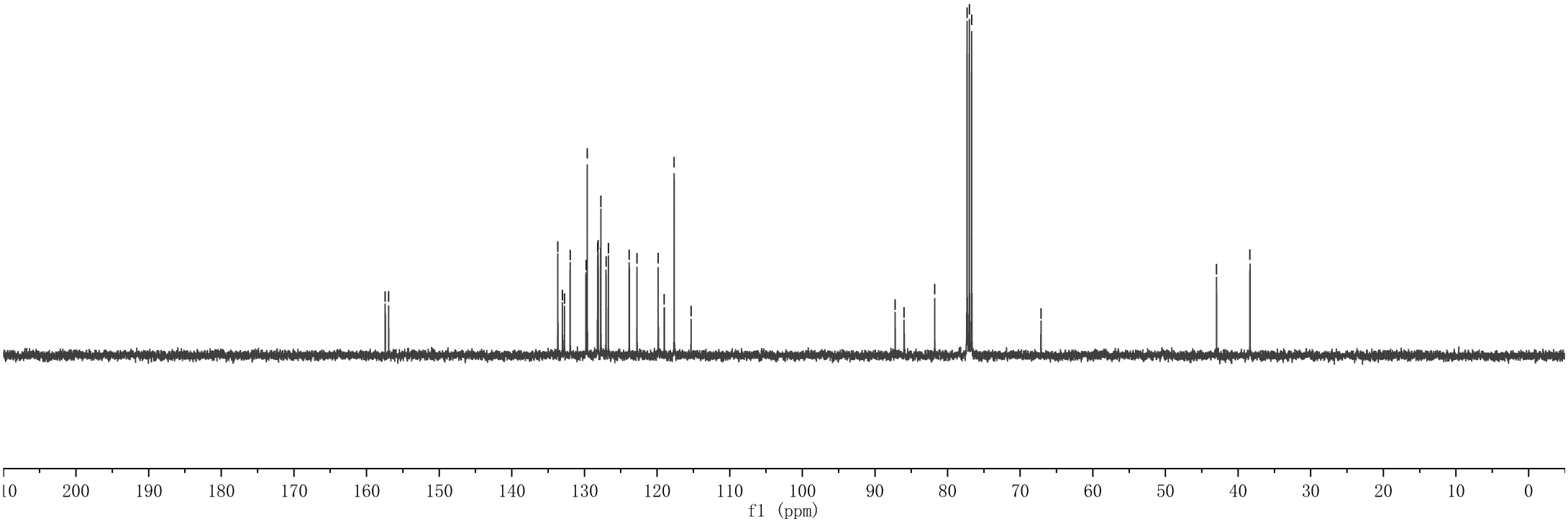
157.42
156.95
133.66
133.02
132.75
131.97
129.78
129.61
128.19
128.10
127.75
127.74
127.02
126.70
123.82
122.76
119.84
119.00
117.64
115.32
87.22
85.98
81.77
77.32
77.00
76.68
67.14
42.97
38.37

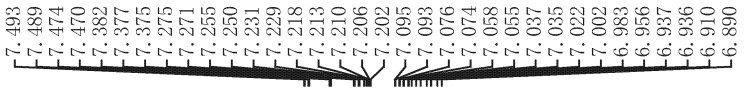
Parameter	Value
1 Title	zjj-14-37-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	34
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-16T21:03:19
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



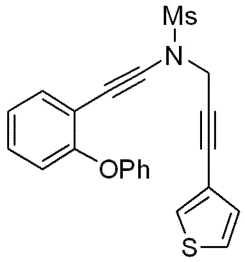
1aa







Parameter	Value
1 Title	LFS-2-174-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-18T22:07:14
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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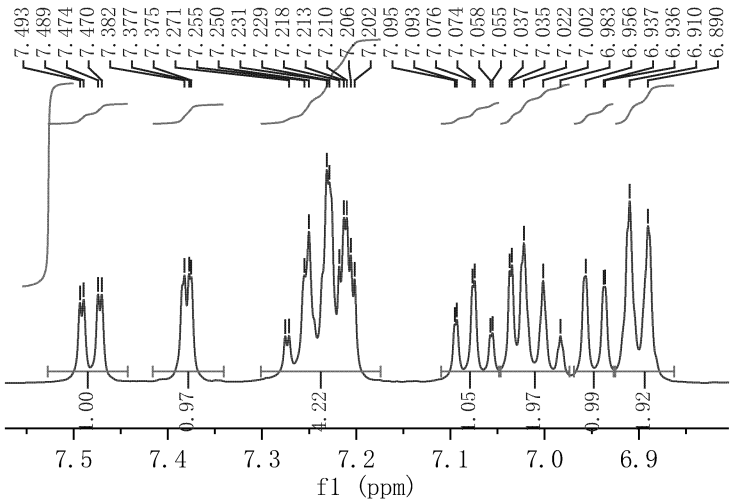
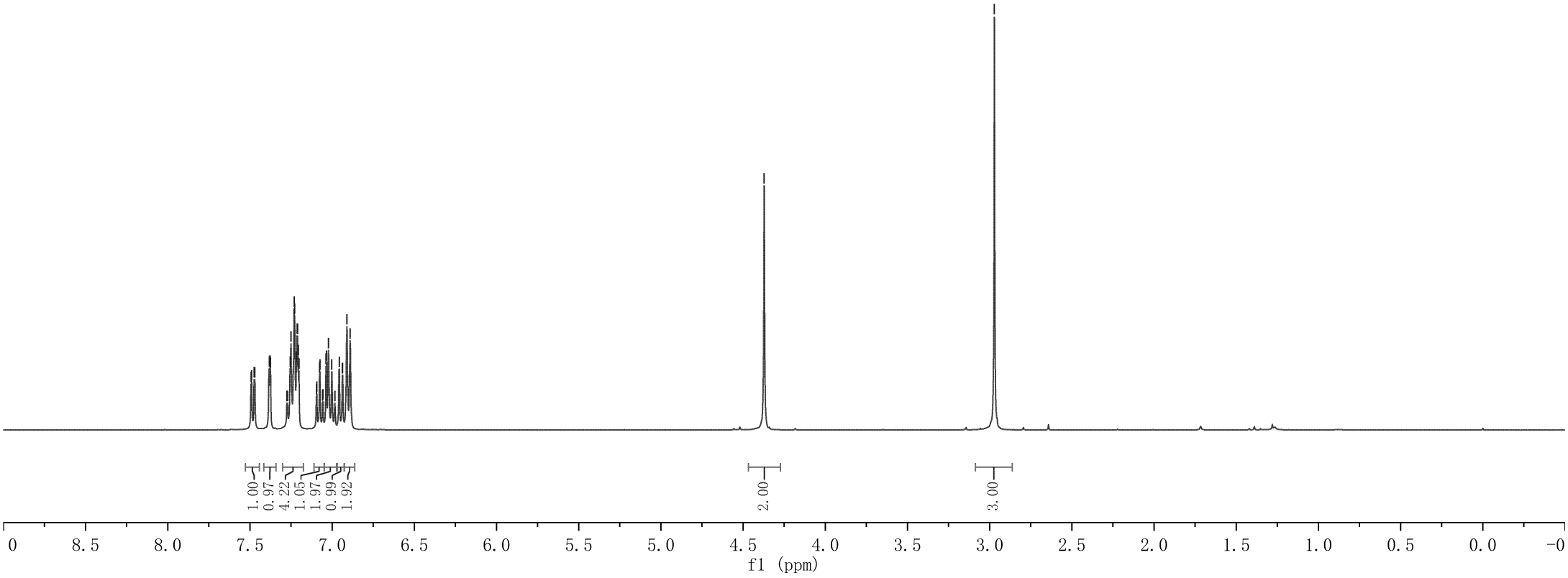
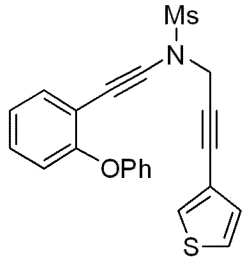


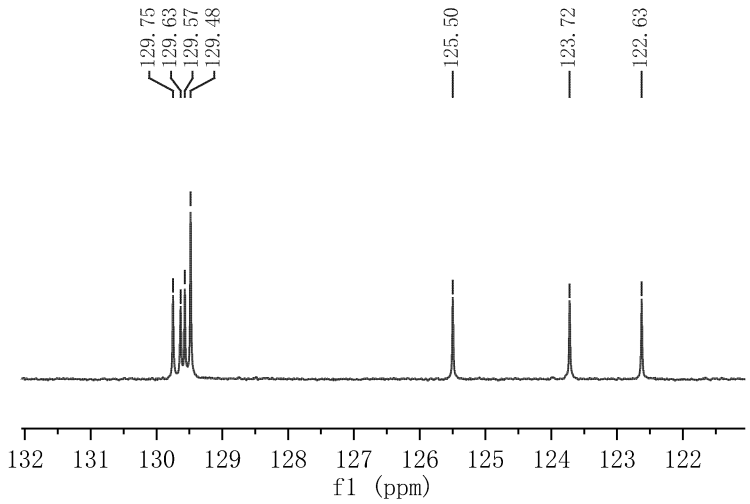


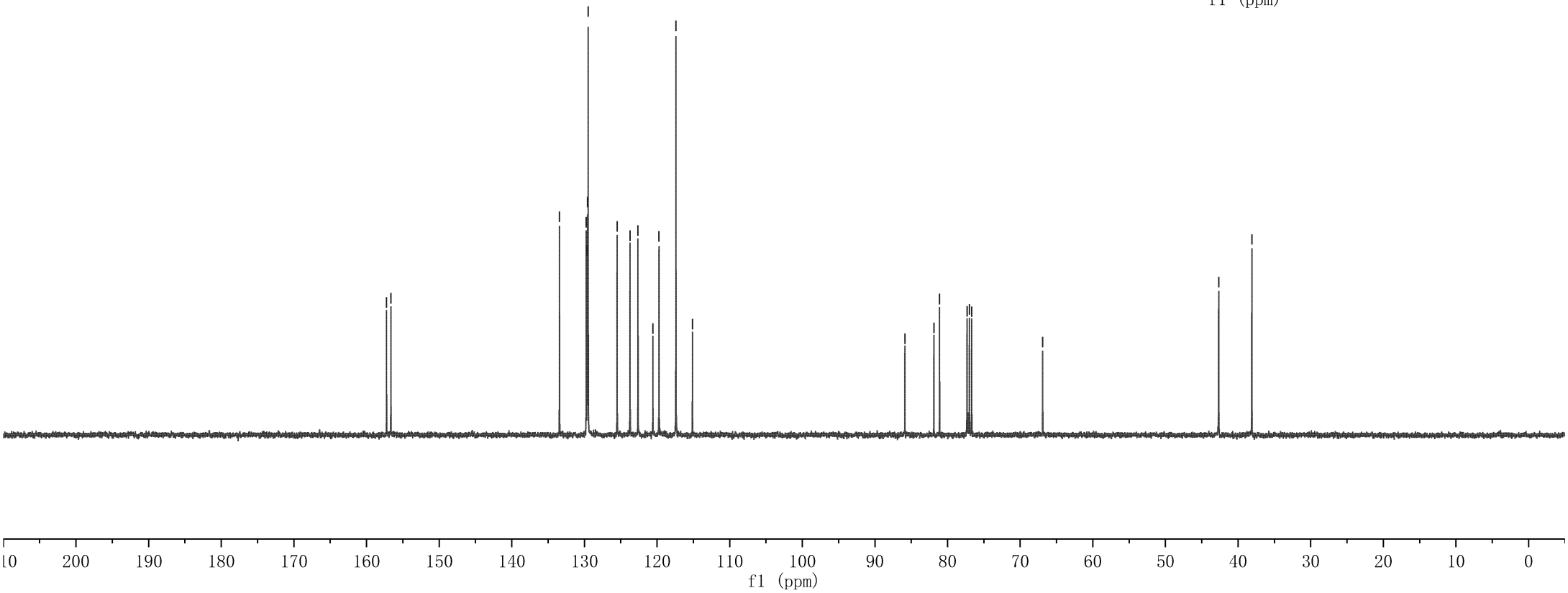
157.24
156.64
133.43
129.75
129.63
129.57
129.48
125.50
123.72
122.63
120.57
119.73
117.40
115.12
85.88
81.88
81.10
77.32
77.00
76.68
66.91
42.67
38.11

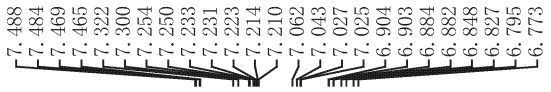
Parameter	Value
1 Title	LFS-2-174-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	22
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-18T22:08:44
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



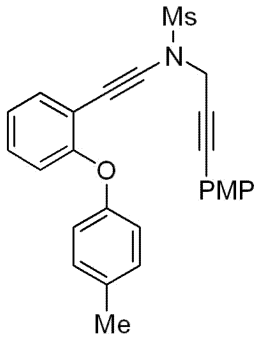
1ab



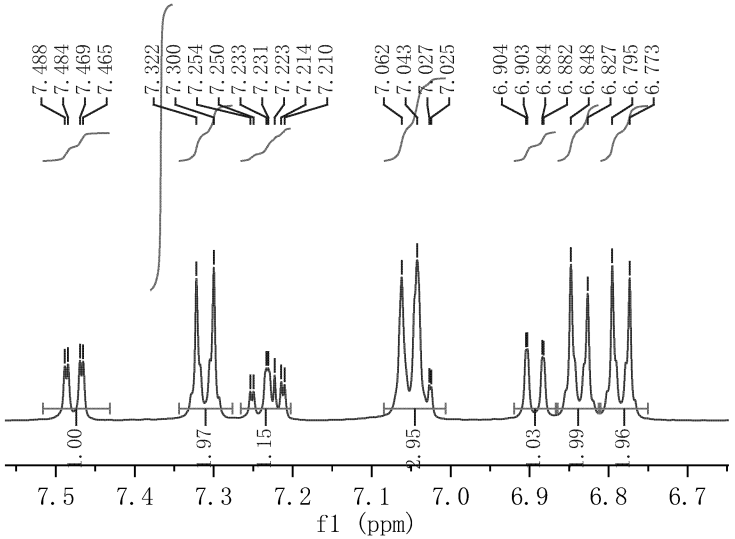


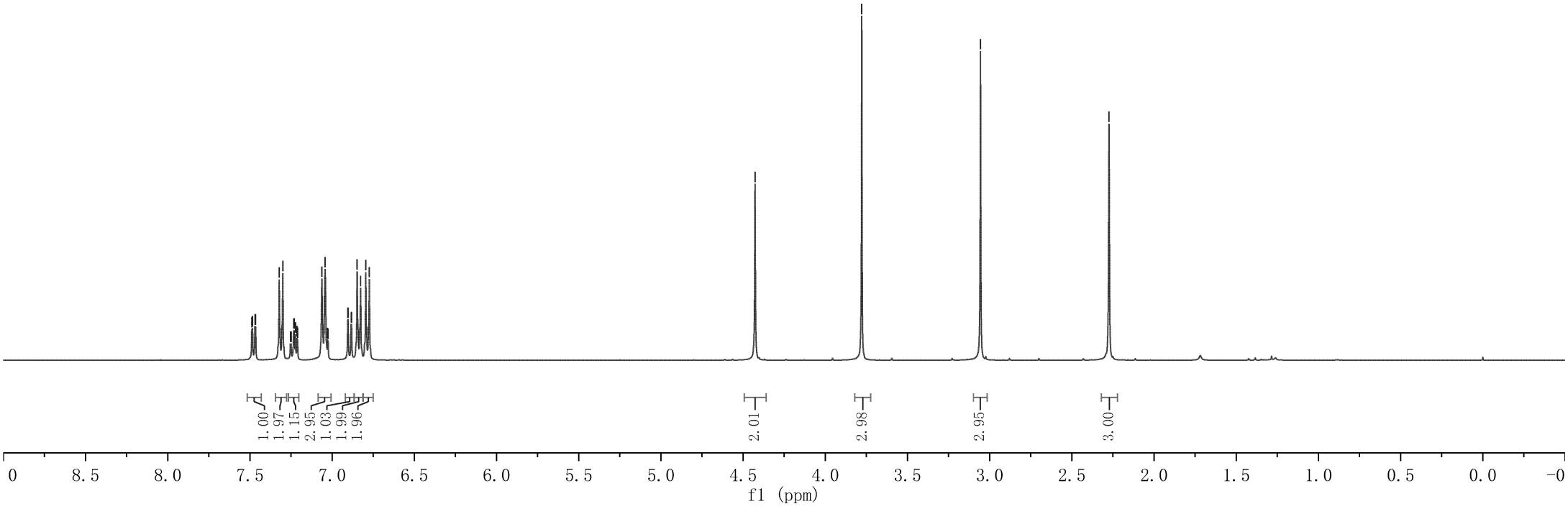


Parameter	Value
1 Title	LFS-2-195-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-26T09:33:33
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



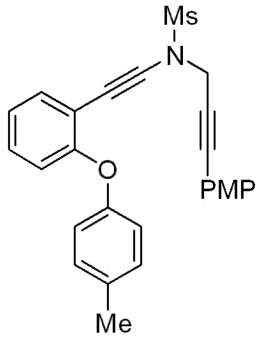
1ac



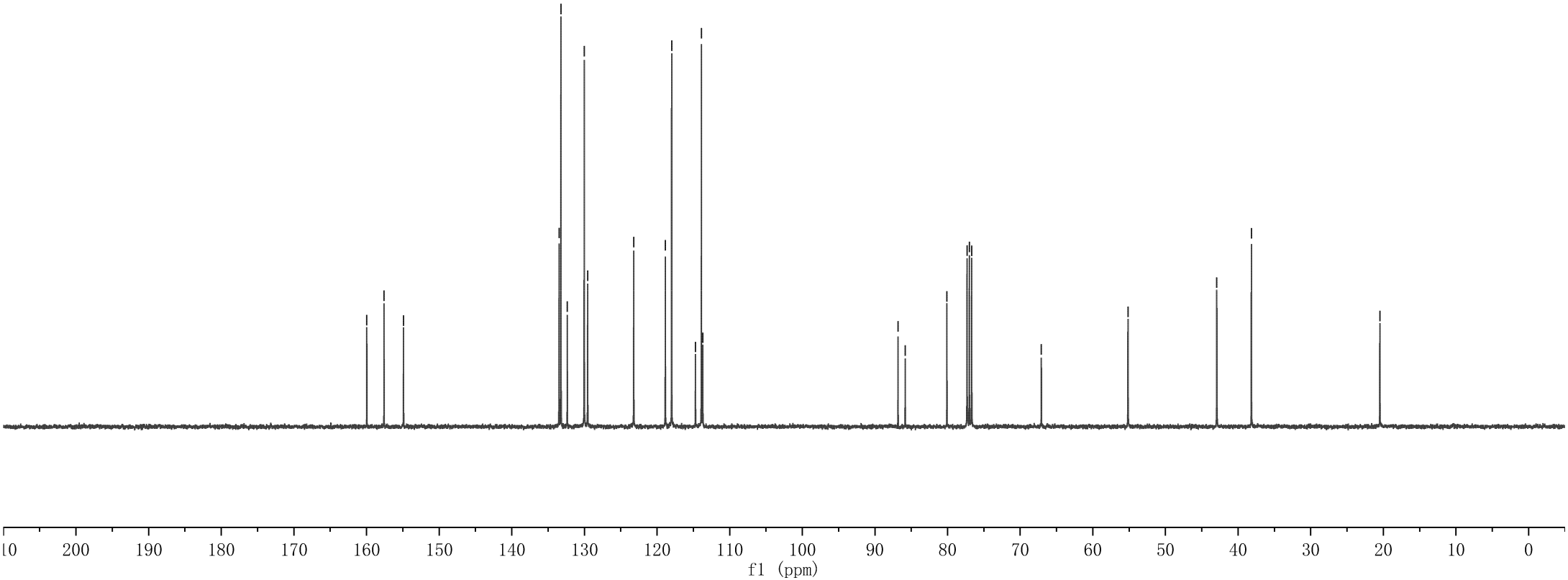


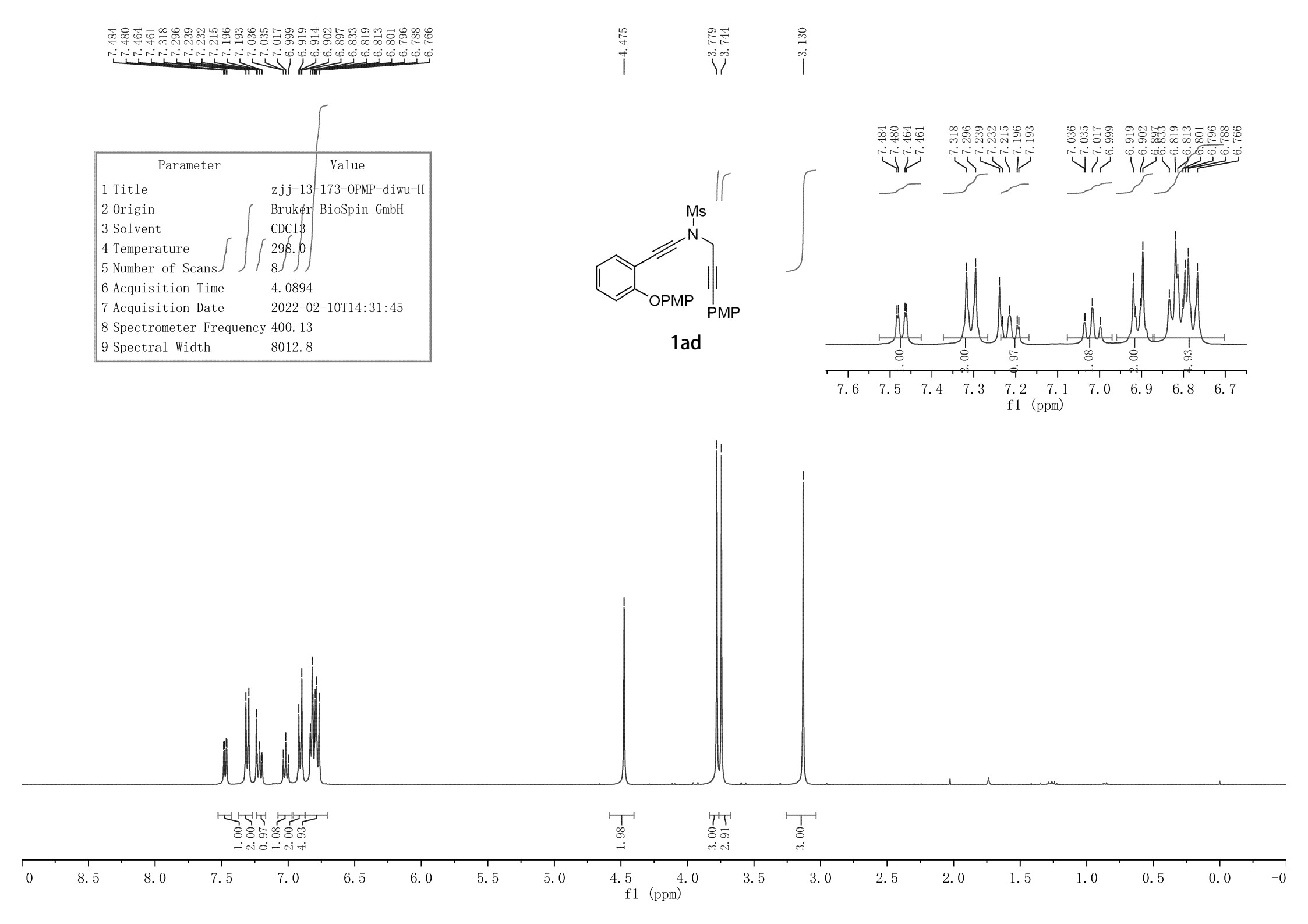
159.96
157.58
154.91
133.48
133.23
132.36
130.02
129.55
123.21
118.86
117.99
114.72
113.89
113.70
86.82
85.83
80.09
77.32
77.00
76.68
67.09
55.16
42.93
38.17
20.48

Parameter	Value
1 Title	LFS-2-195-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	103
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-26T09:35:52
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

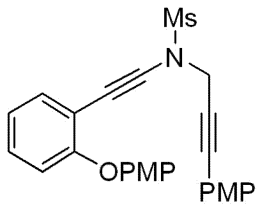


1ac




7.484
7.480
7.464
7.461
7.318
7.296
7.239
7.232
7.215
7.196
7.193
7.036
7.035
7.017
6.999
6.919
6.914
6.902
6.897
6.833
6.819
6.813
6.801
6.796
6.788
6.766
4.475
3.779
3.744
3.130
Parameter Value
1 Title zjj-13-173-OPMP-diwu-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-10T14:31:45
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
OPMP
PMP
1ad
1.00
2.00
0.97
1.08
2.00
4.93
1.98
3.00
2.91
3.00
f1 (ppm)

Parameter	Value
1 Title	zjj-13-173-OPMP-diwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	20
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-10T14:33:09
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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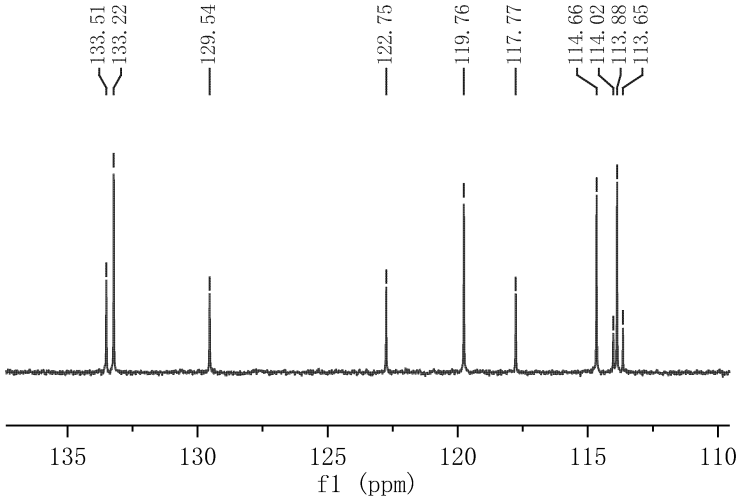
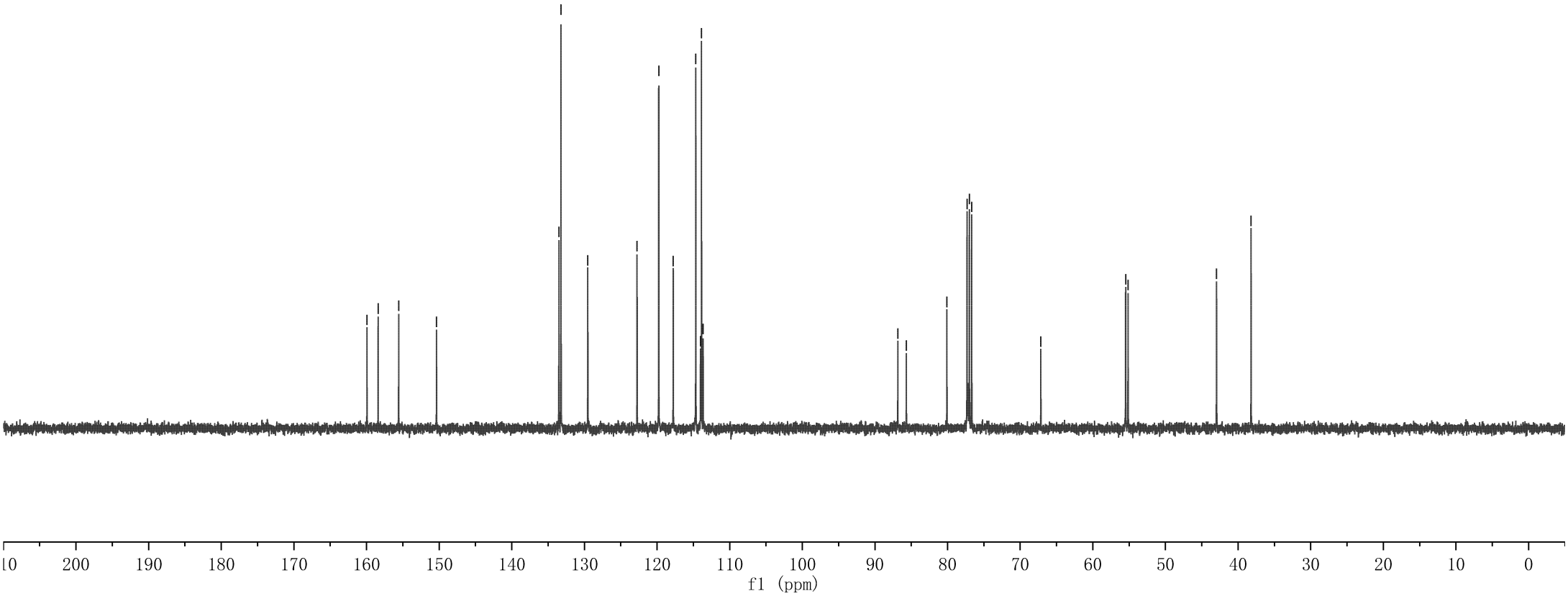
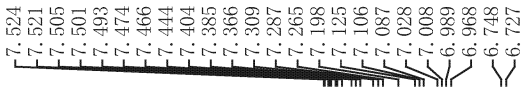
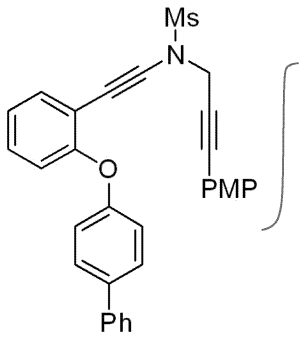






Parameter	Value
1 Title	LFS-2-191-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-25T09:47:33
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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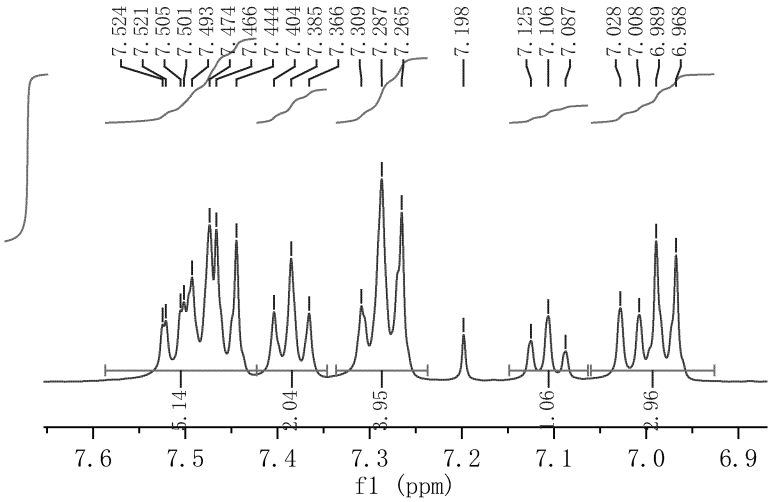

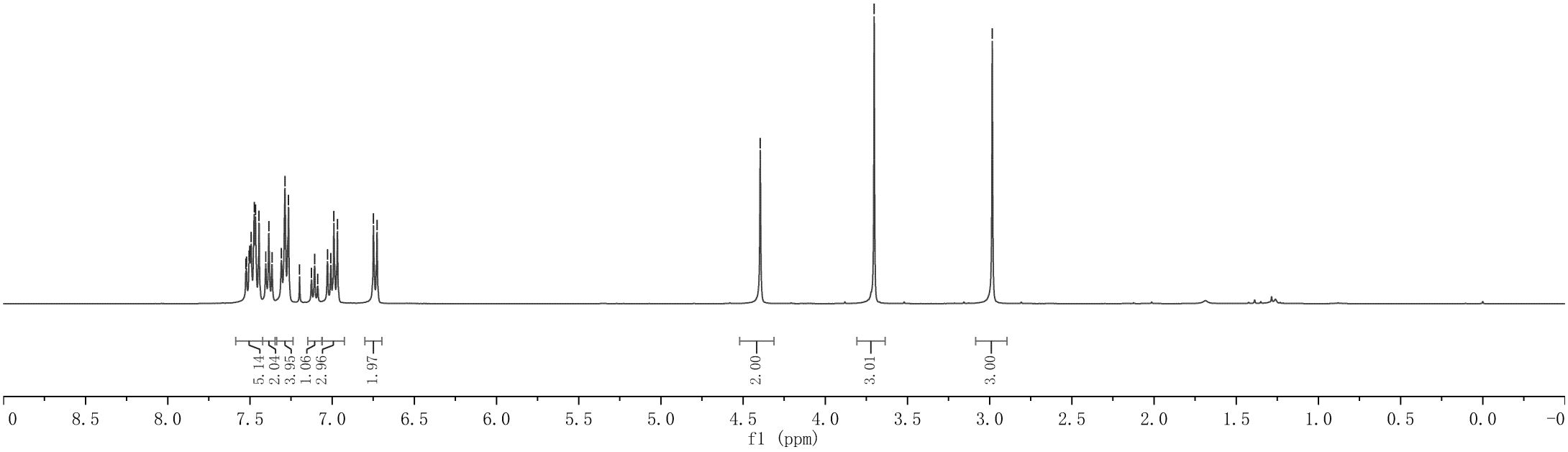

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156.68
140.20
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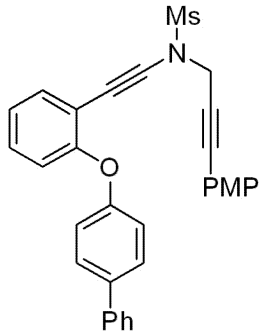
133.61
133.21
129.71
128.71
128.15
126.93
126.62
123.94
119.96
117.76
115.39
113.90
113.62
86.84
86.20
80.05
77.32
77.00
76.68
66.87
55.11
42.93
38.20

Parameter	Value
1 Title	LFS-2-191-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	30
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-25T09:49:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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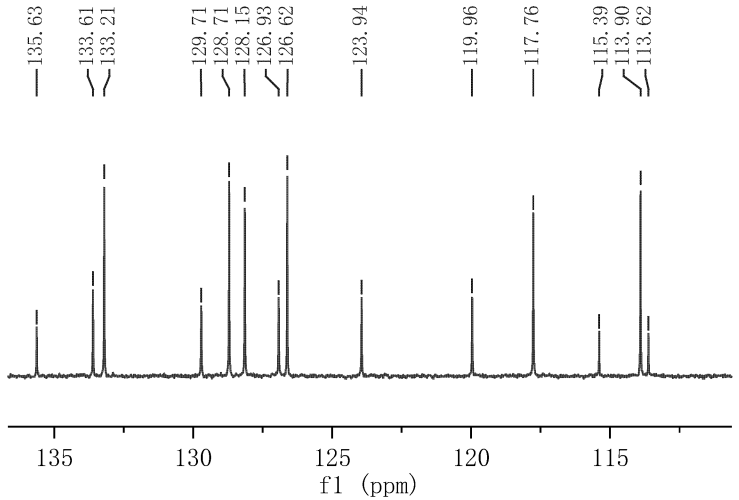

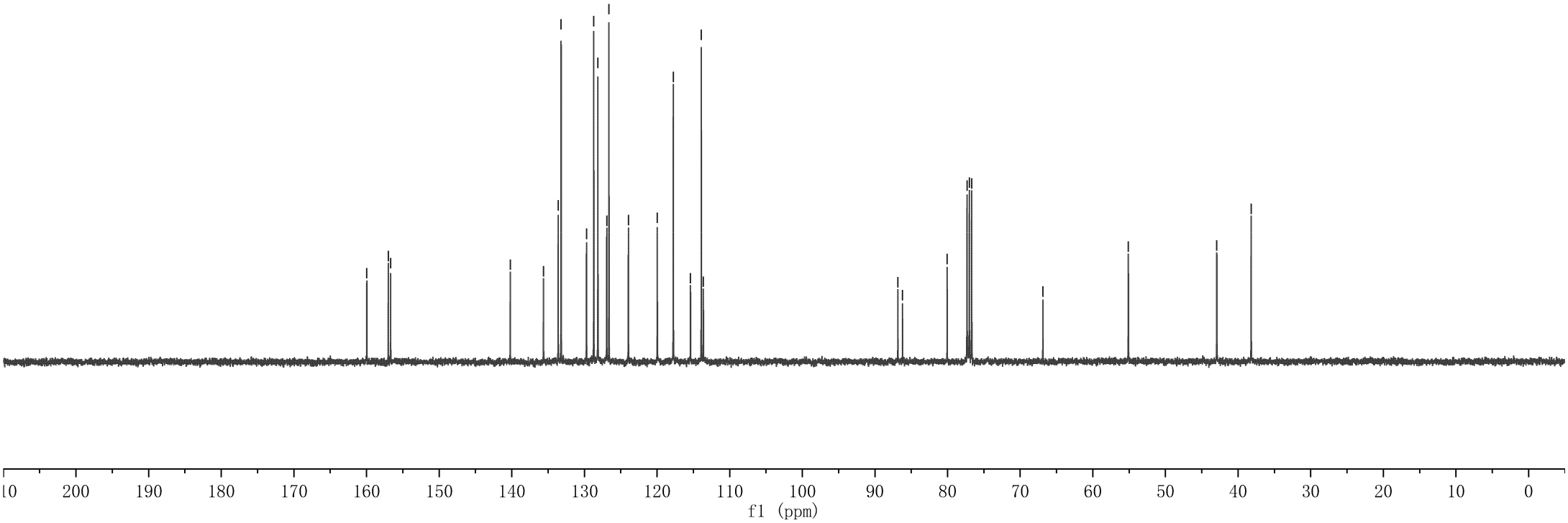

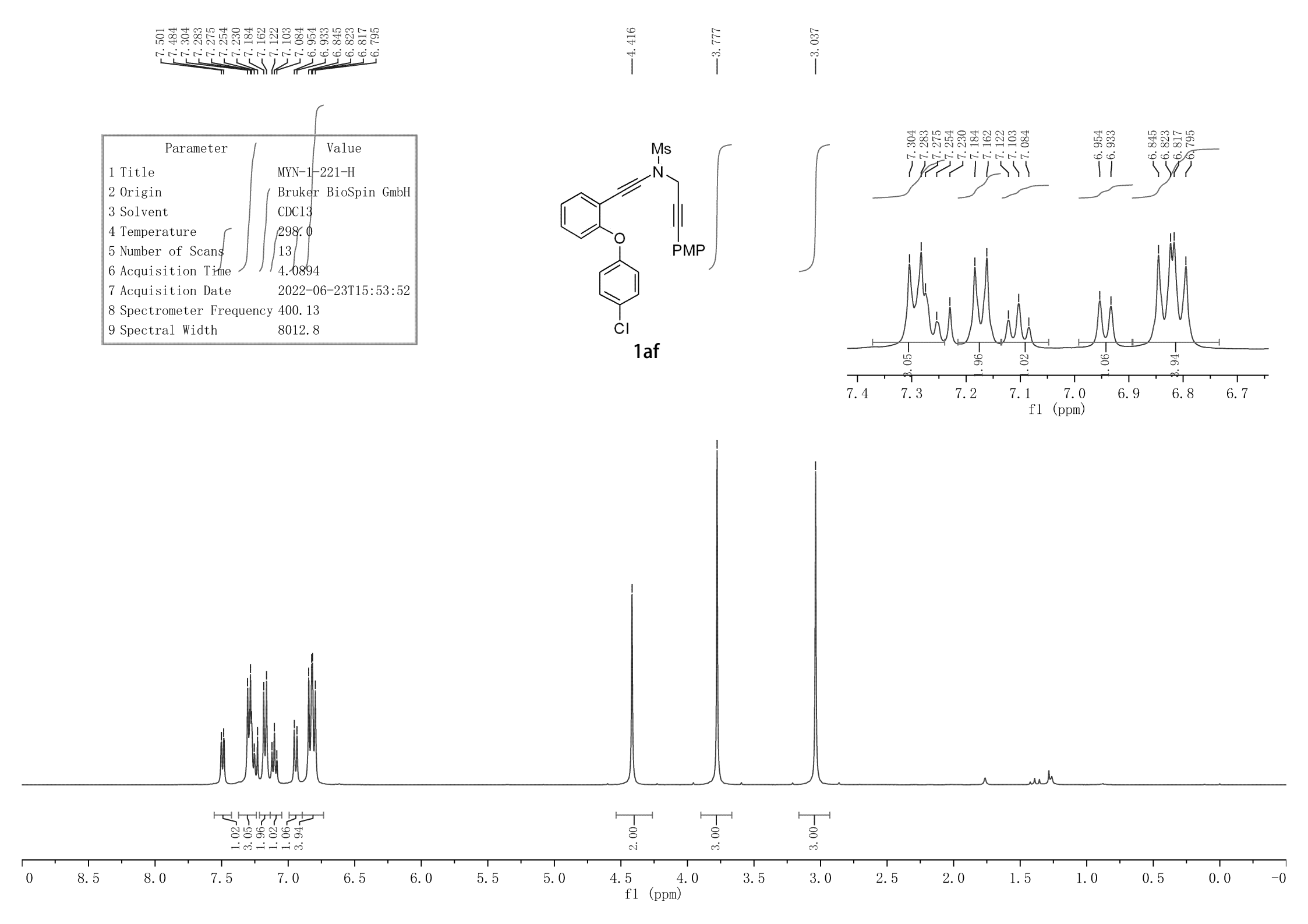
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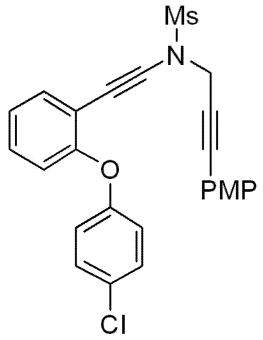
7.254
7.230
7.184
7.162
7.122
7.103
7.084
6.954
6.933
6.845
6.823
6.817
6.795
4.416
3.777
3.037
Parameter
Value
1 Title
MYN-1-221-H
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
298.0
5 Number of Scans
13
6 Acquisition Time
4.0894
7 Acquisition Date
2022-06-23T15:53:52
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
Ms
N
O
PMP
Cl
1af
1.02
3.05
1.96
1.02
1.06
3.94
2.00
3.00
3.00
f1 (ppm)

159.95
156.24
156.01
133.54
133.11
129.65
129.37
127.48
124.12
119.78
118.70
115.30
113.89
113.48
86.81
86.20
79.91
77.32
77.00
76.68
66.65
55.11
42.82
38.18

Parameter	Value
1 Title	MYN-1-221-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	13
6 Acquisition Time	1.3631
7 Acquisition Date	2022-06-23T15:56:25
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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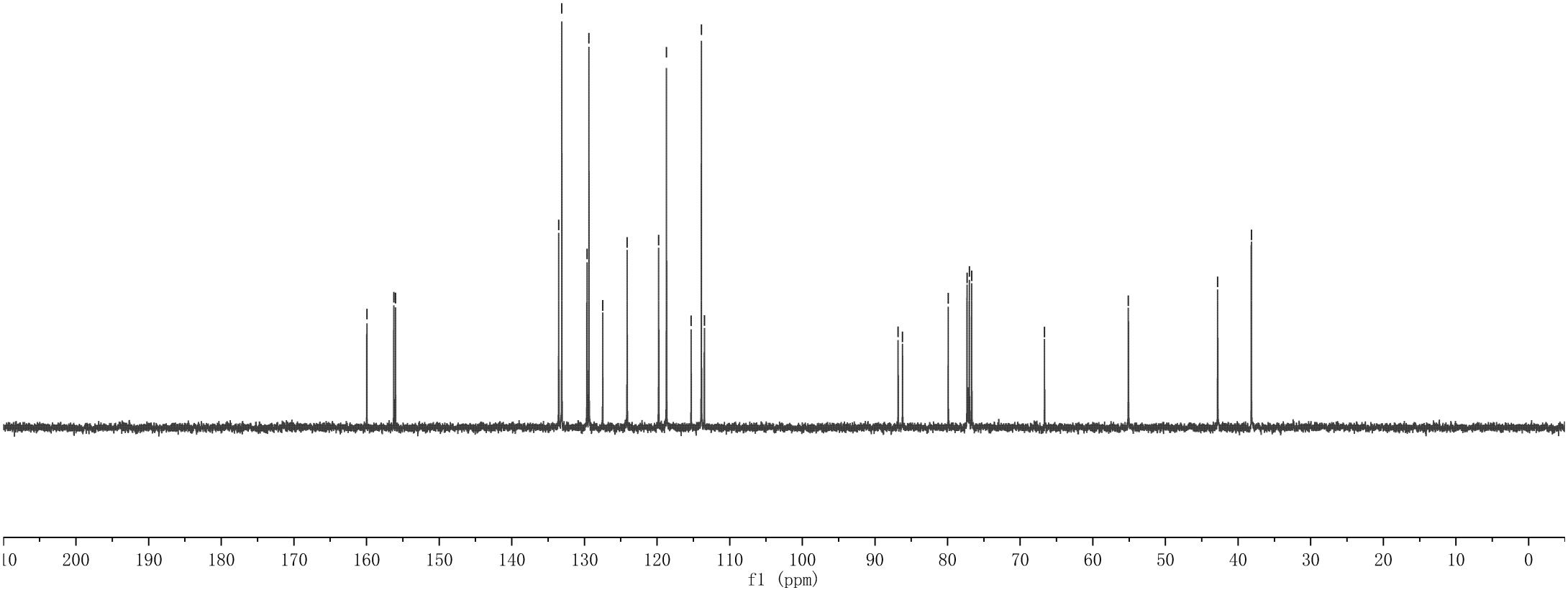
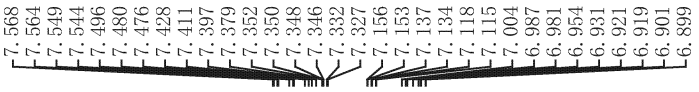
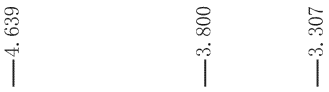
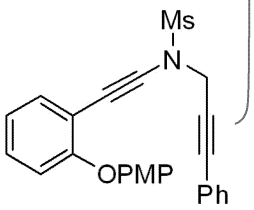






Parameter	Value
1 Title	MYN-1-218-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	Acetone
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2022-06-21T17:44:04
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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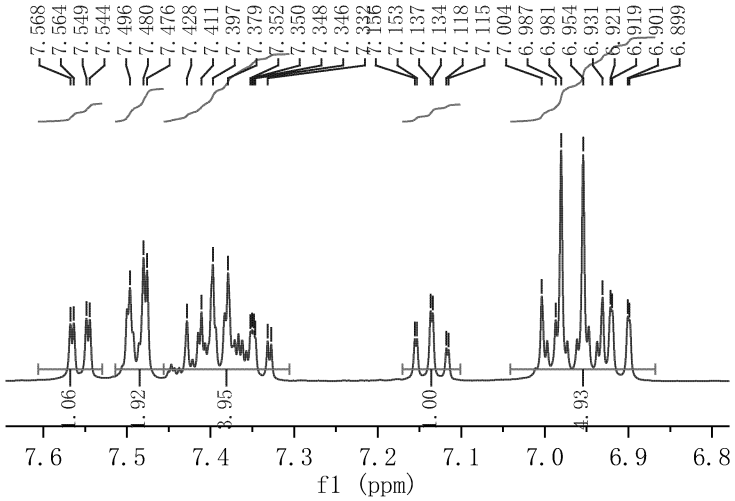

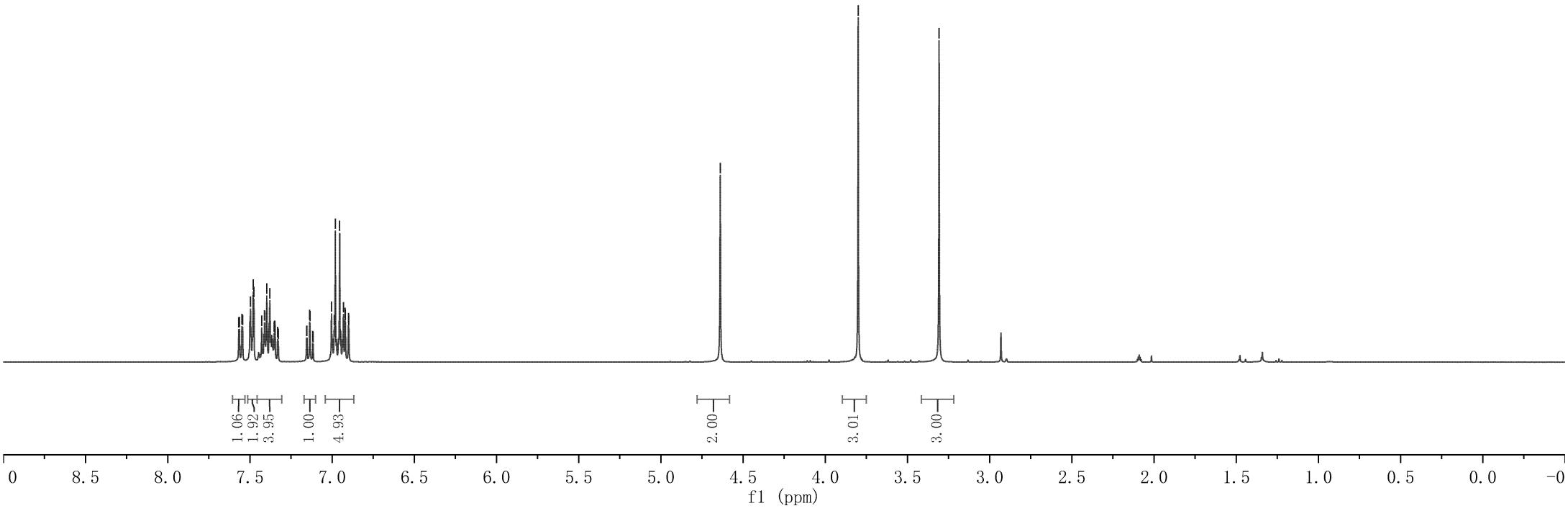

206.26
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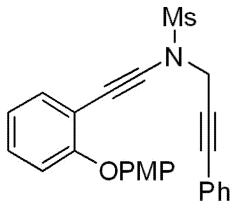
156.75
151.13
134.26
132.46
130.57
129.75
129.31
123.82
122.63
120.60
118.71
115.66
114.98
87.13
87.04
82.93
67.68
55.86
43.29
38.58
30.43
30.24
30.05
29.85
29.66
29.47
29.28

Parameter	Value
1 Title	MYN-1-218-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	Acetone
4 Temperature	300.0
5 Number of Scans	24
6 Acquisition Time	1.3631
7 Acquisition Date	2022-06-21T17:46:34
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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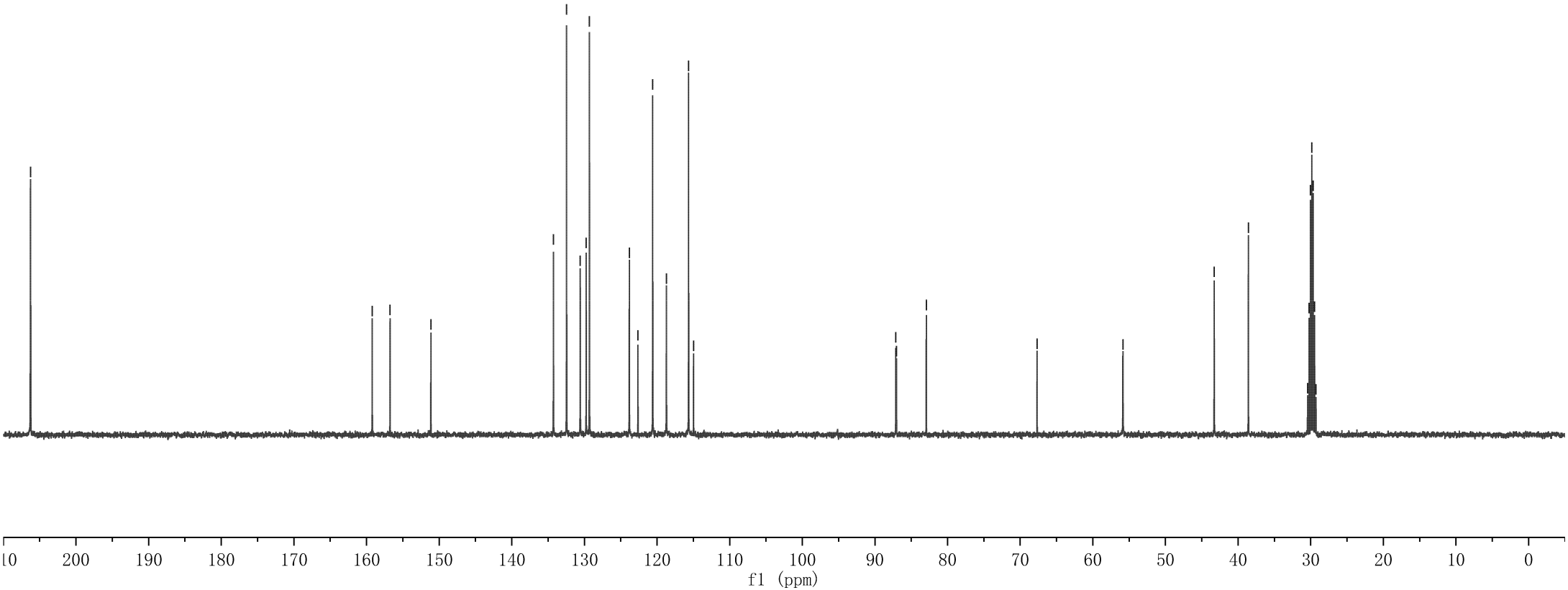
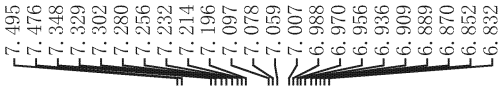
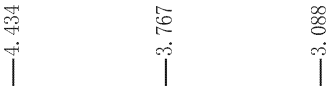
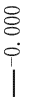
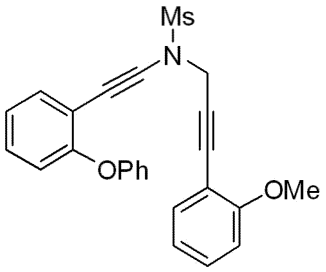








Parameter	Value
1 Title	LFS-2-205-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.4
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-29T17:33:21
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0



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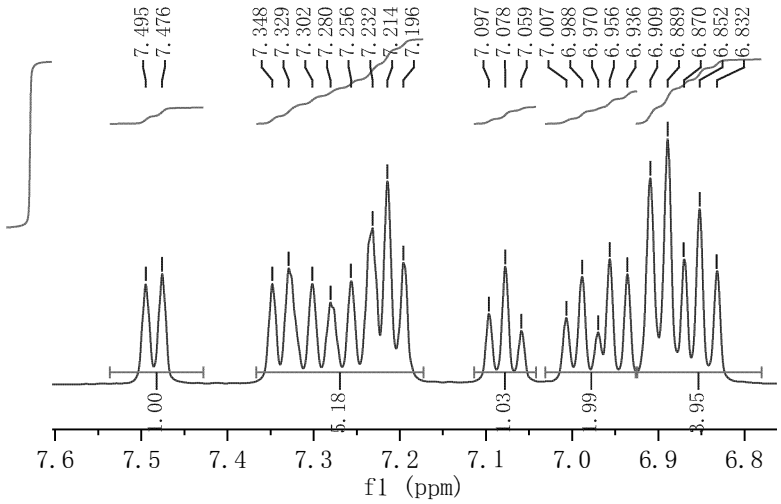
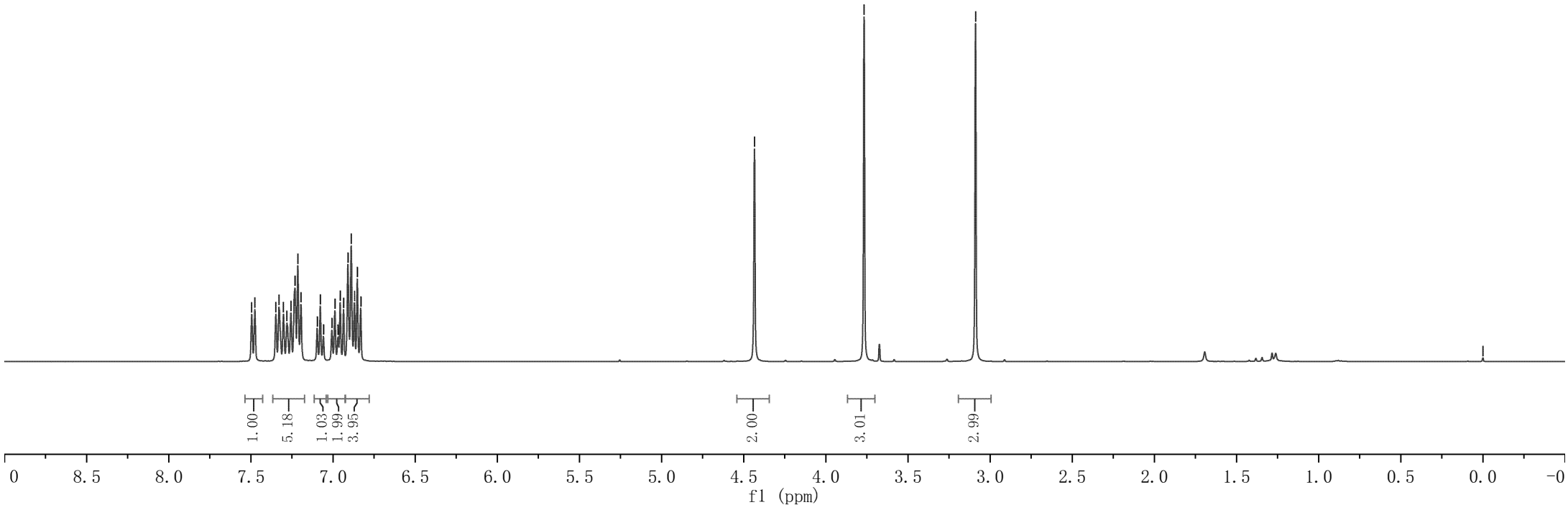
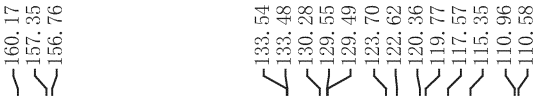
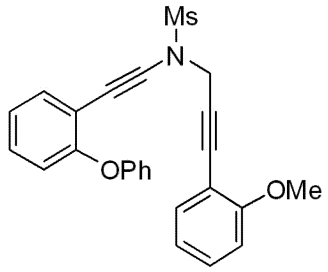


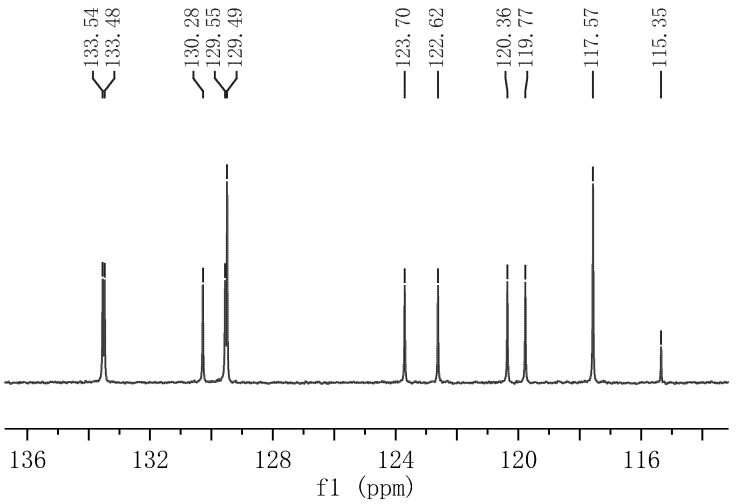


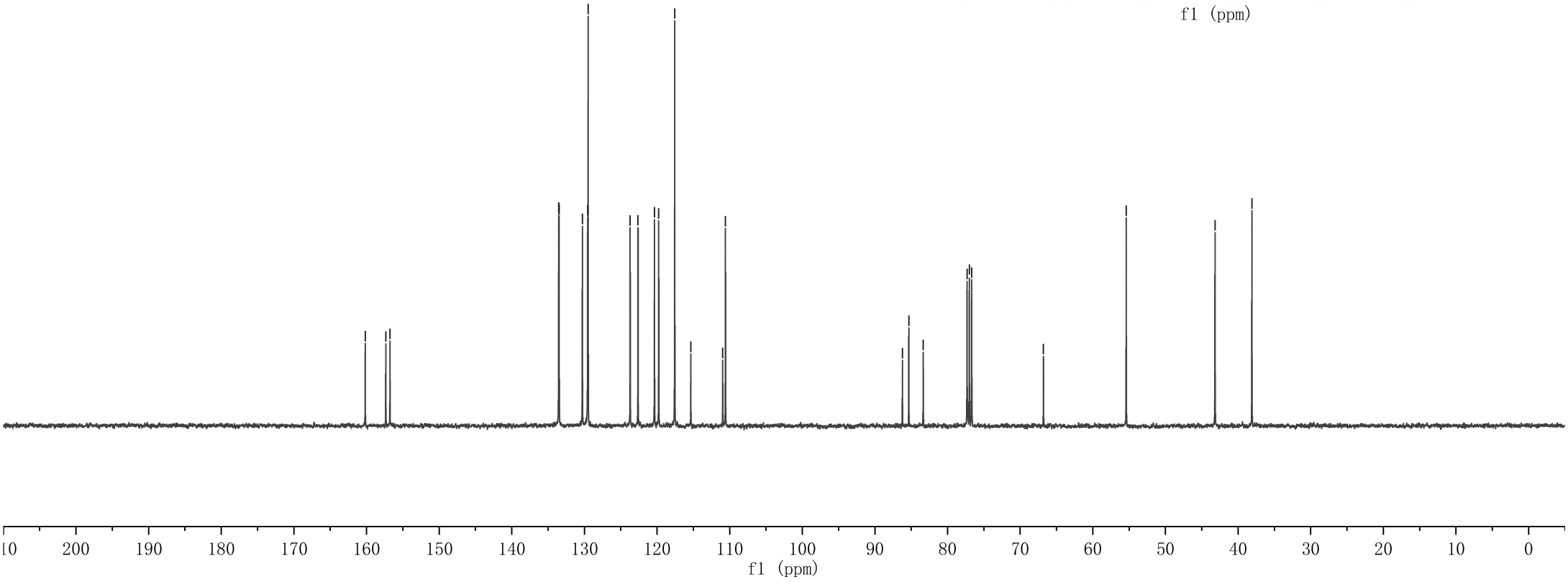


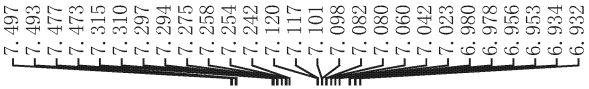
Parameter	Value
1 Title	LFS-2-205-C-2-OMe
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.2
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-29T17:42:15
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



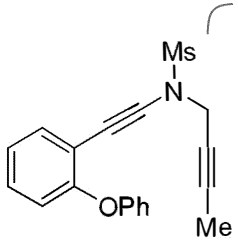
1ah



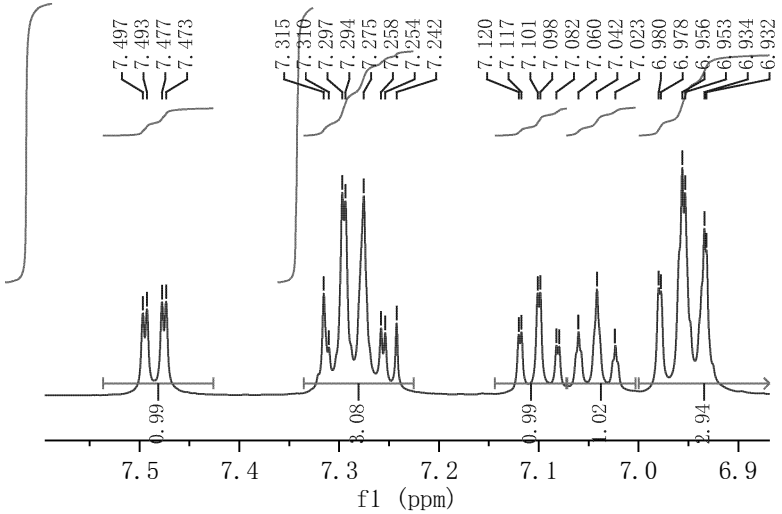


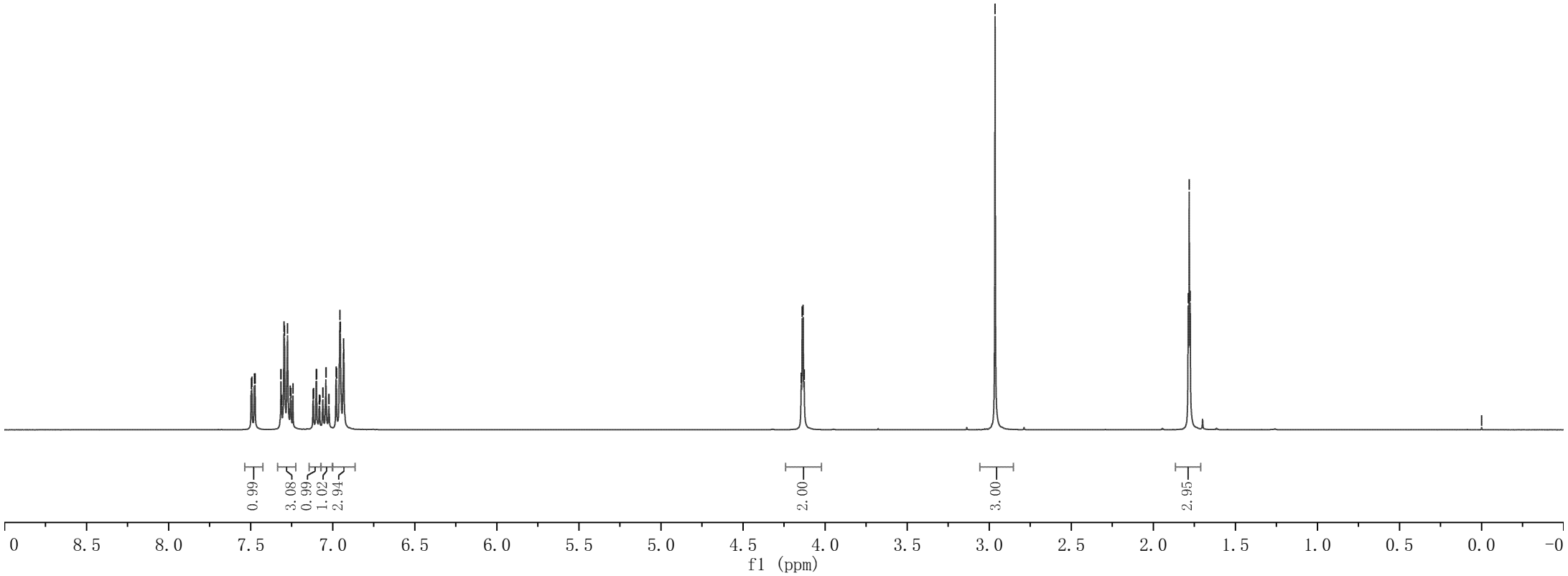


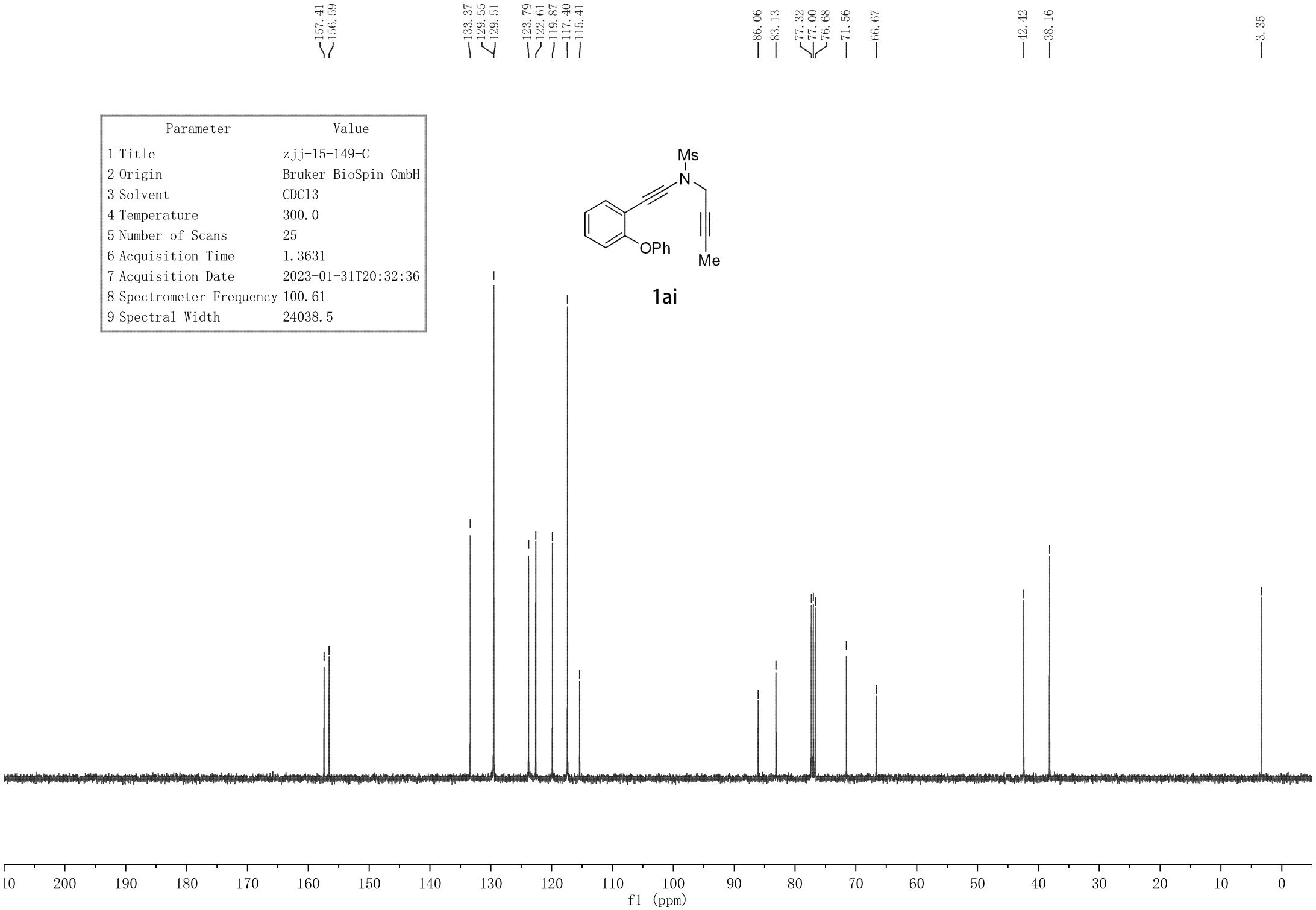
Parameter	Value
1 Title	zjj-15-149-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2023-01-31T20:28:19
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



1ai



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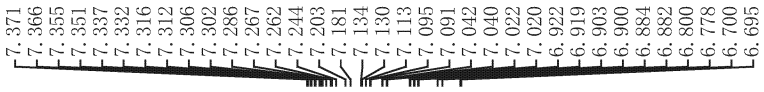
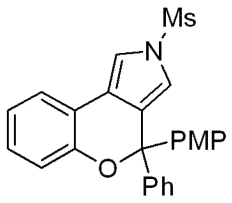
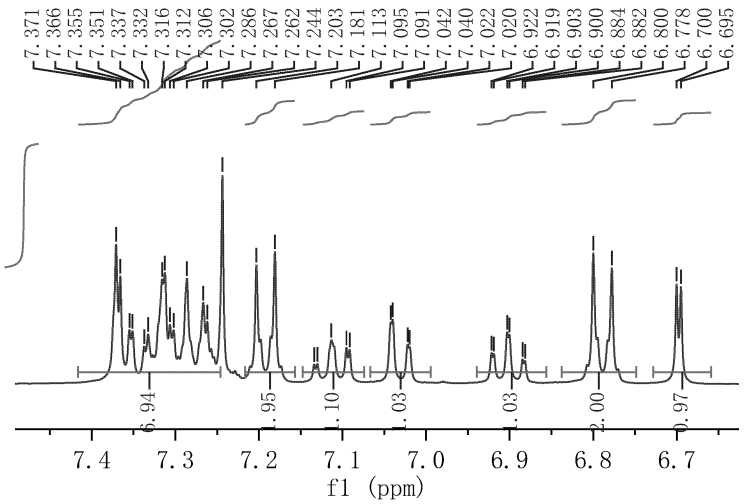
123.79
122.61
119.87
117.40
115.41
86.06
83.13
77.32
77.00
76.68
71.56
66.67
42.42
38.16
3.35
Parameter Value
1 Title zjj-15-149-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 25
6 Acquisition Time 1.3631
7 Acquisition Date 2023-01-31T20:32:36
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
OPh
Me
1ai
f1 (ppm)

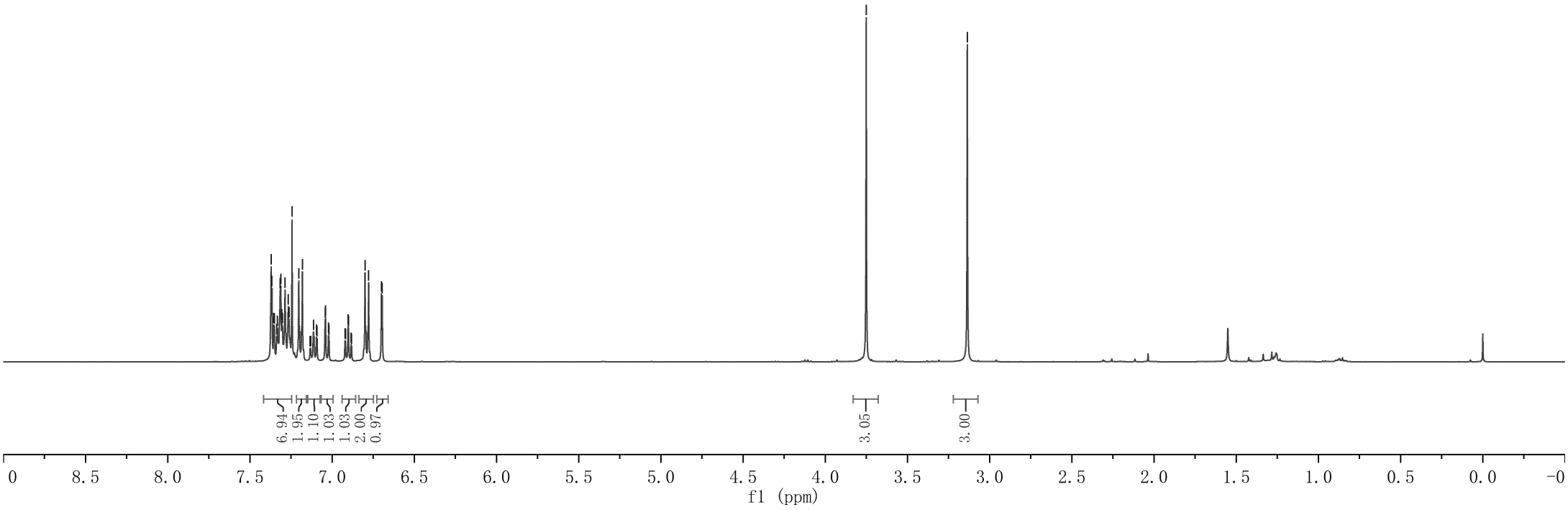


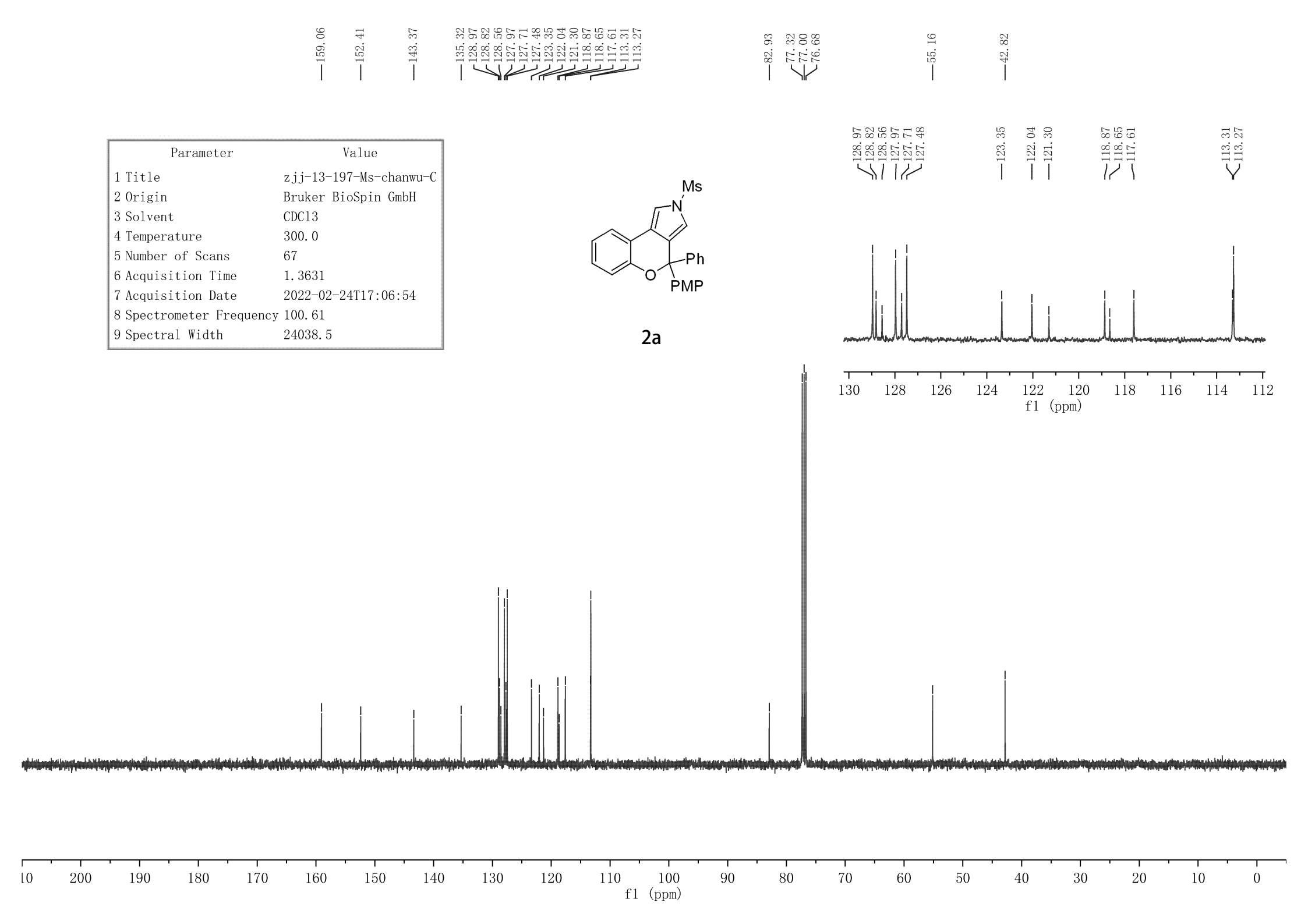
Parameter	Value
1 Title	zjj-13-197-Ms-chanwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-24T17:04:25
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2a



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143.37
135.32
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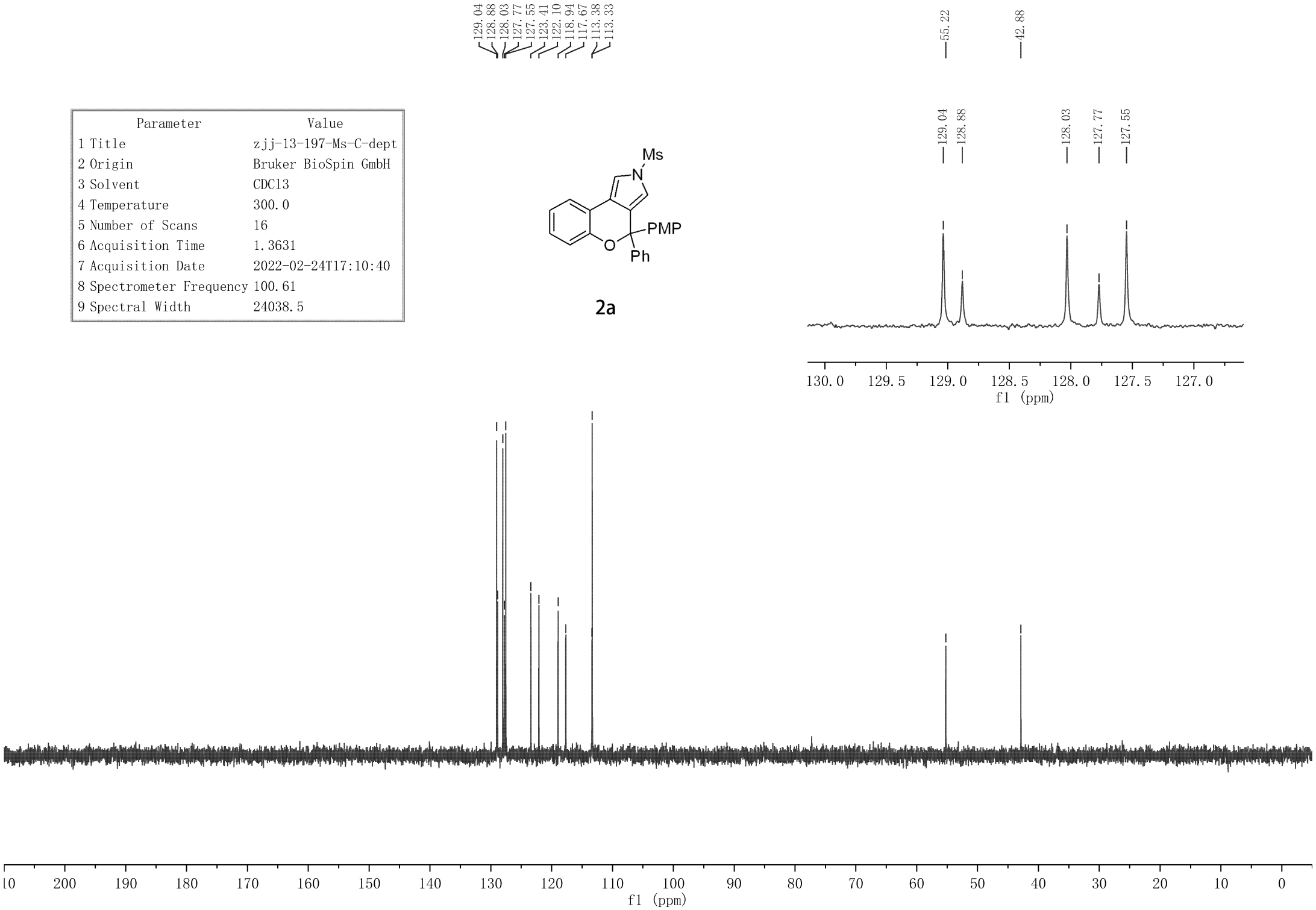
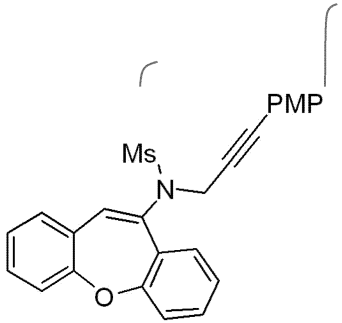
128.82
128.56
127.97
127.71
127.48
123.35
122.04
121.30
118.87
118.65
117.61
113.31
113.27
82.93
77.32
77.00
76.68
55.16
42.82
Parameter Value
1 Title zjj-13-197-Ms-chanwu-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 67
6 Acquisition Time 1.3631
7 Acquisition Date 2022-02-24T17:06:54
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Ph
O
PMP
2a
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	zjj-13-197-Ms-C-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	16
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-24T17:10:40
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

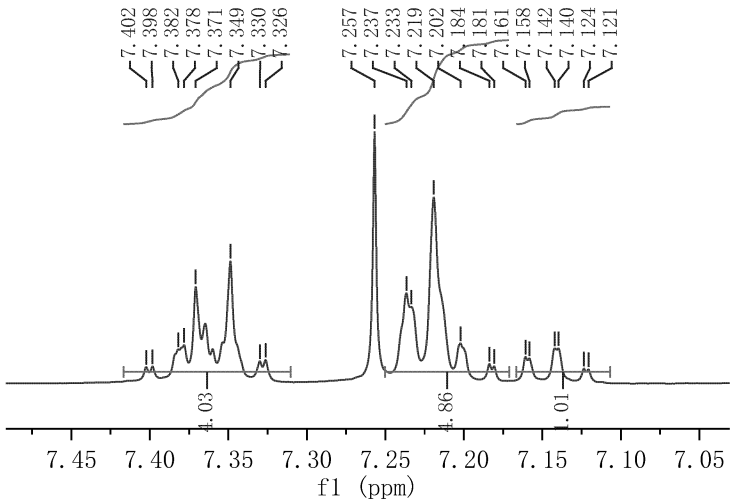
2a

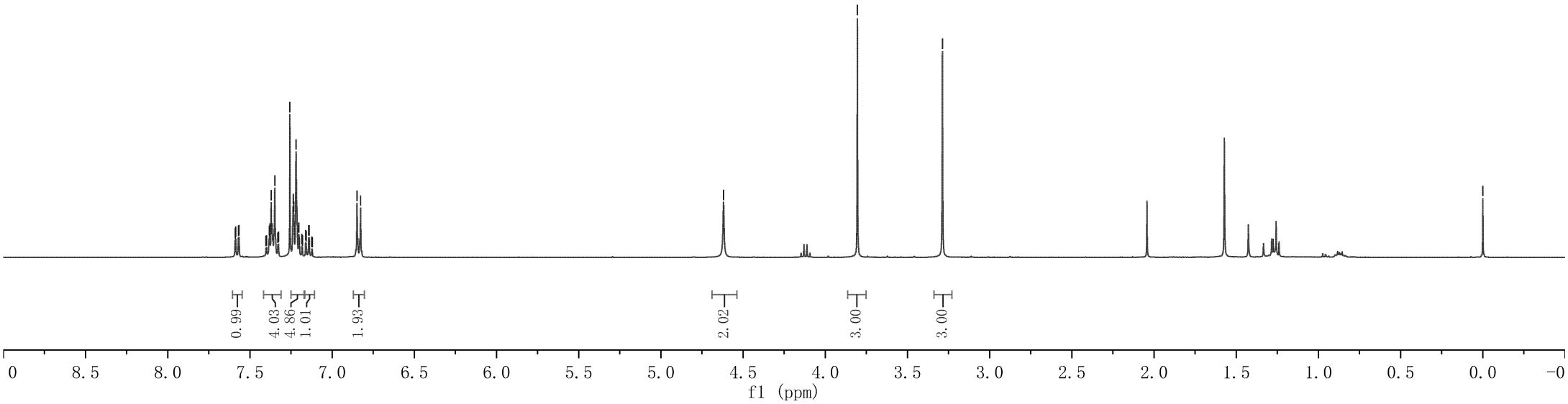


Parameter	Value
1 Title	zjj-12-218-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2021-11-07T20:29:32
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



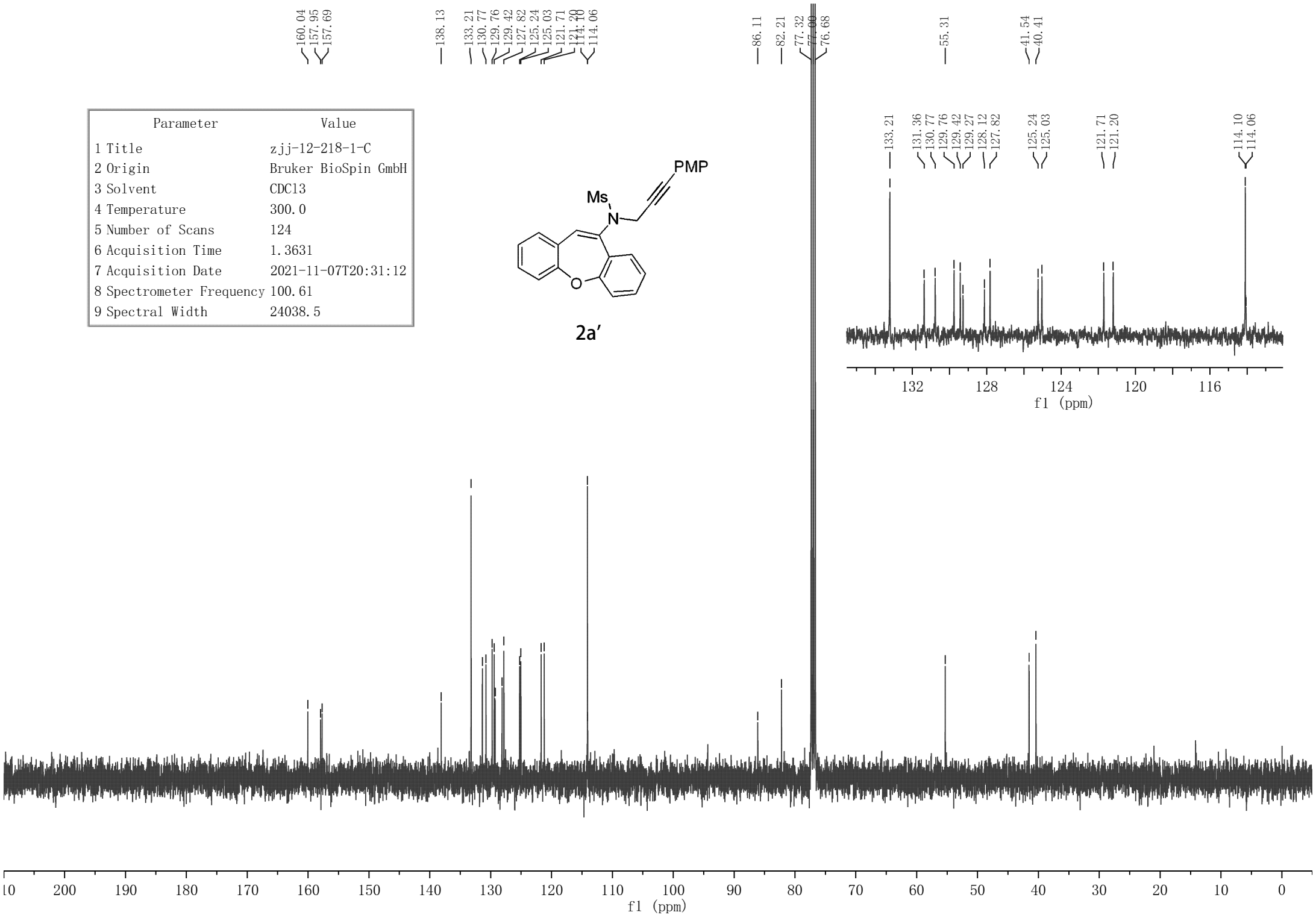
2a′

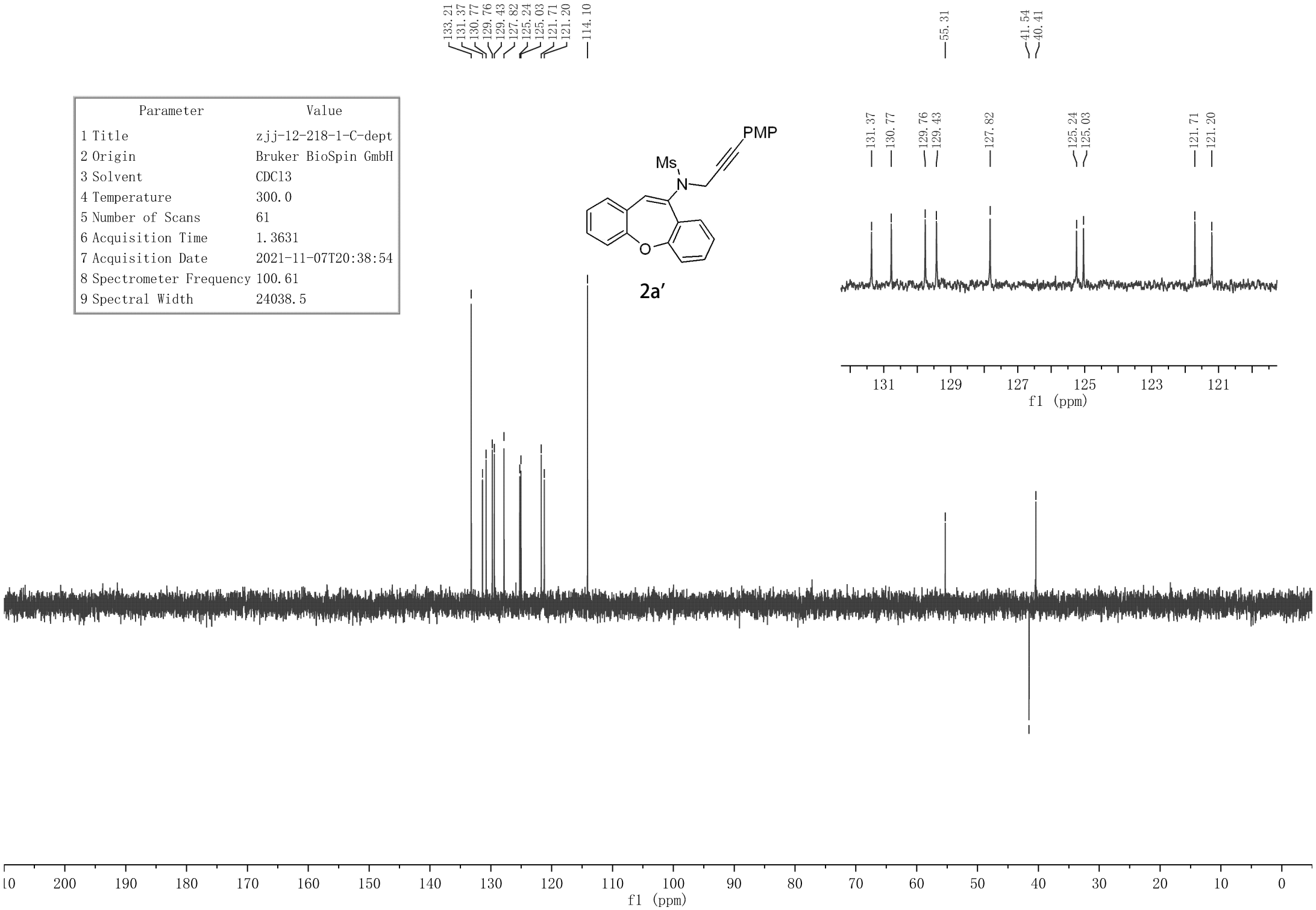




Parameter	Value
1 Title	zjj-12-218-1-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	124
6 Acquisition Time	1.3631
7 Acquisition Date	2021-11-07T20:31:12
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

2a'

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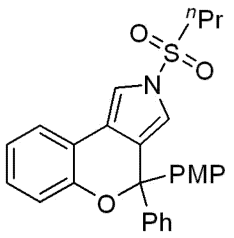
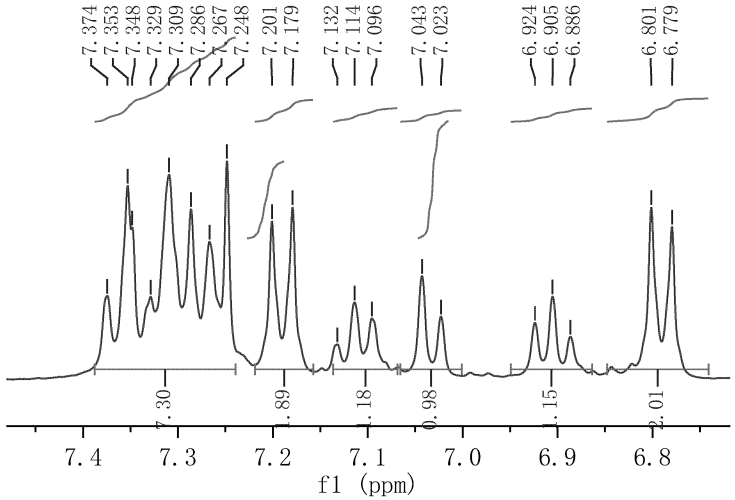
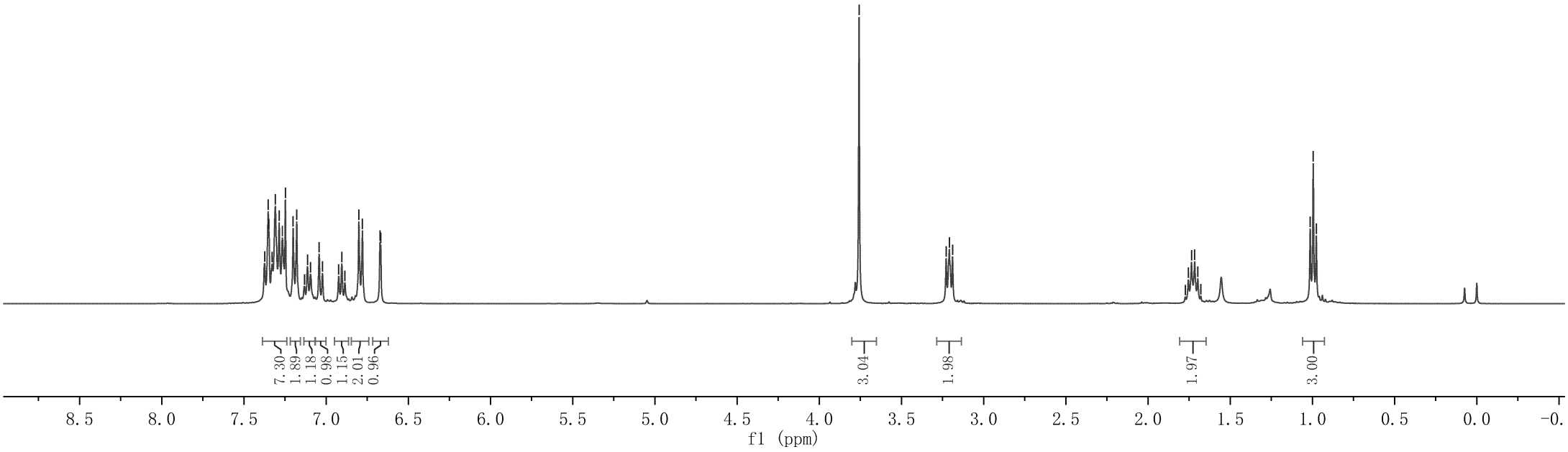
131.37
130.77
129.76
129.43
127.82
125.24
125.03
121.71
121.20
114.10
55.31
41.54
40.41
Parameter Value
1 Title zjj-12-218-1-C-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 61
6 Acquisition Time 1.3631
7 Acquisition Date 2021-11-07T20:38:54
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
PMP
Ms
N
O
2a'
131.37
130.77
129.76
129.43
127.82
125.24
125.03
121.71
121.20
131
129
127
125
123
121
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	zjj-14-15-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-09T21:16:11
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

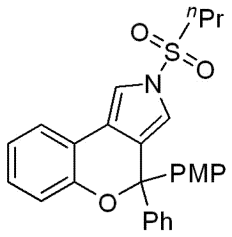


2b



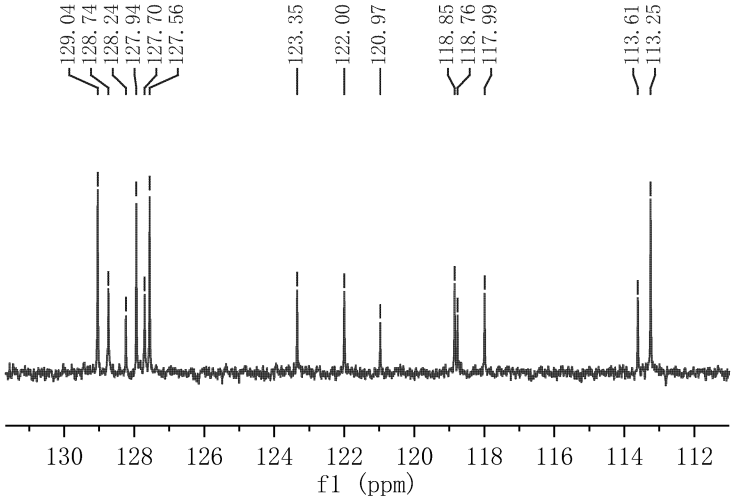


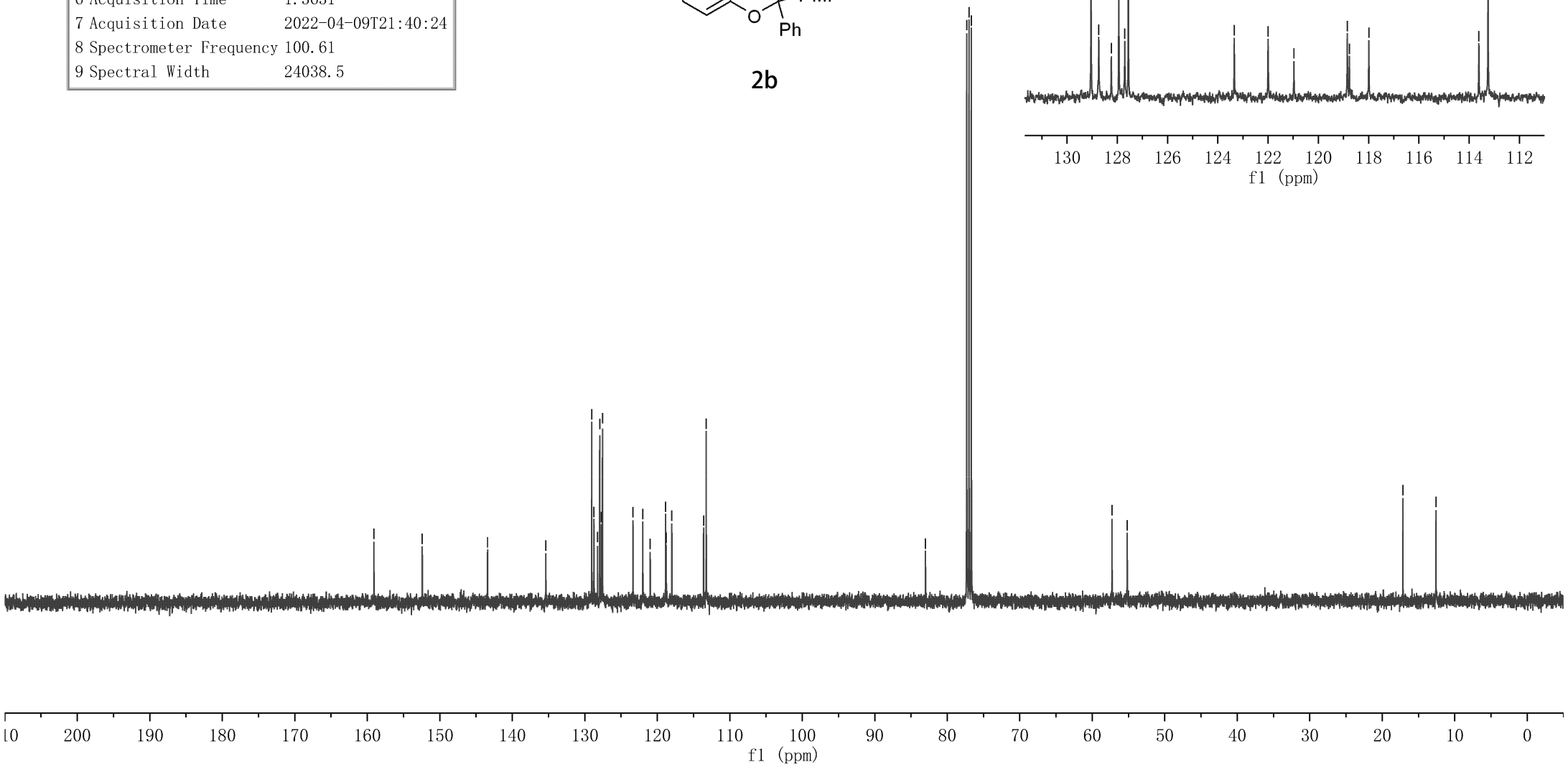
Parameter	Value
1 Title	zjj-14-15-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	73
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-09T21:40:24
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

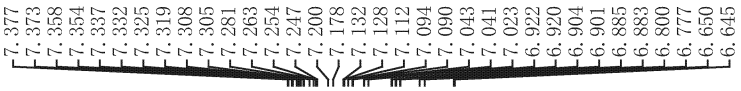


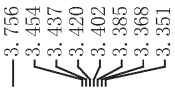
2b

159.08 152.41 143.41 135.37 129.04 128.74 127.94 127.56 123.35 122.00 118.85 117.99 113.61 113.25 83.00 77.32 77.00 76.68 57.27 55.18 17.15 12.59

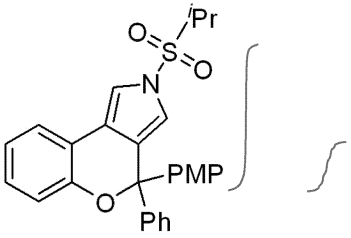








Parameter	Value
1 Title	zjj-14-16-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-09T21:28:06
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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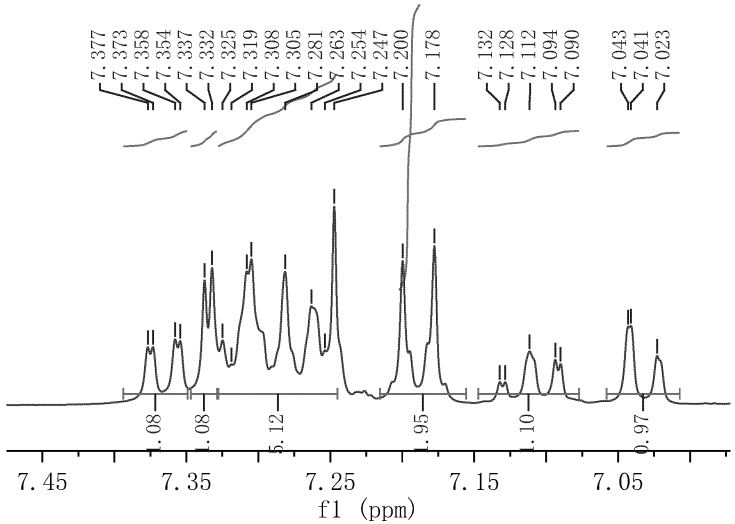
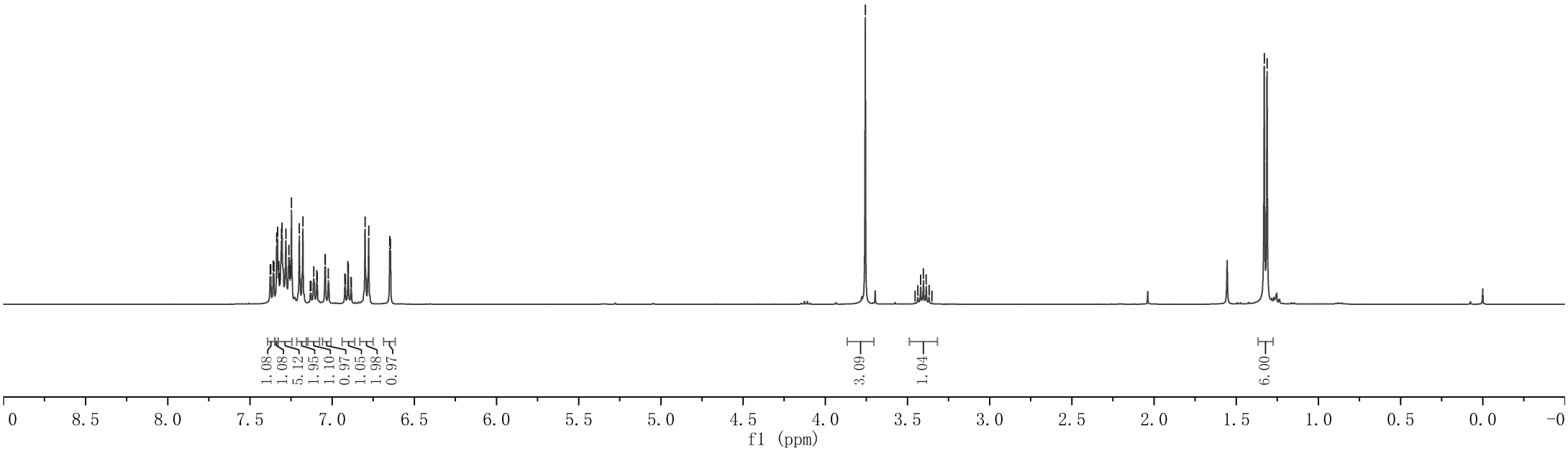
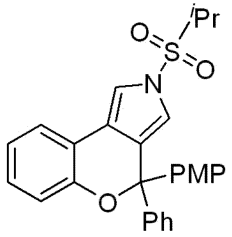


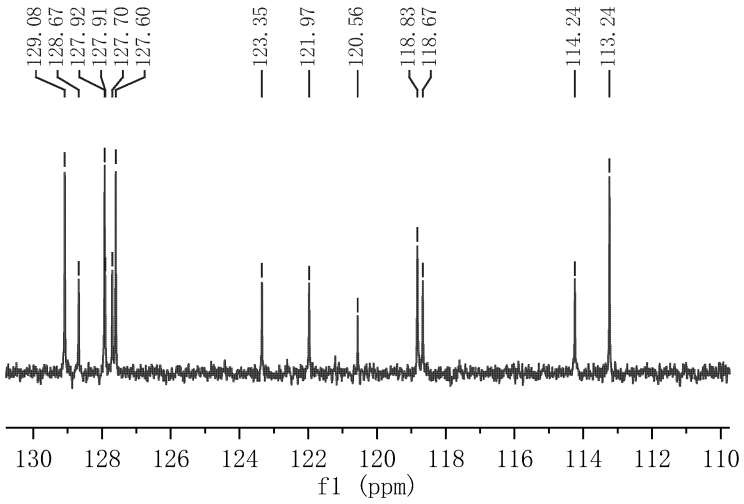


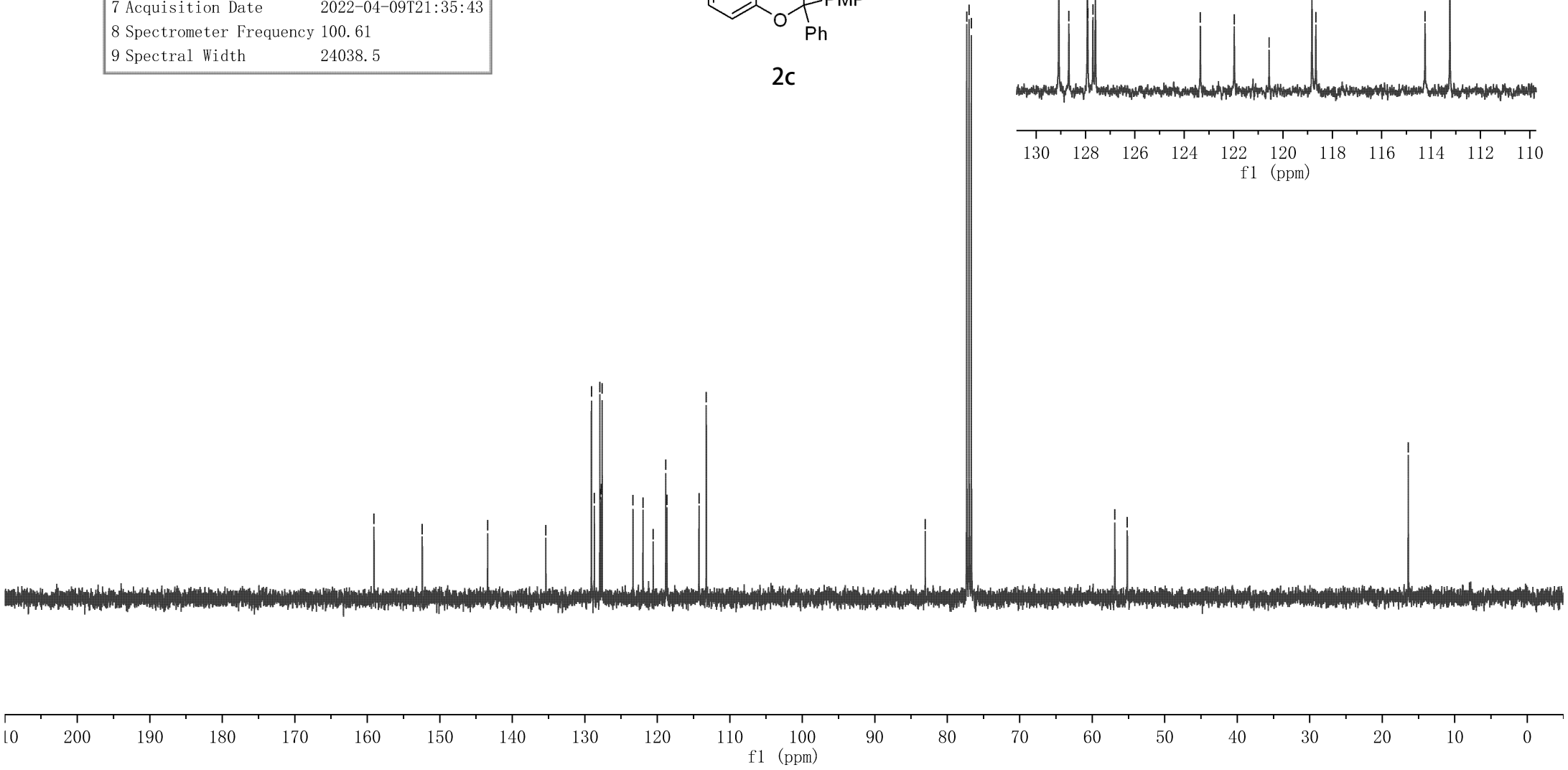
Parameter	Value
1 Title	zjj-14-16-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	38
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-09T21:35:43
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



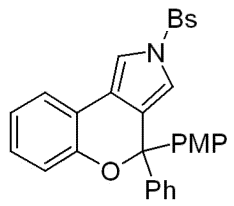
2c

159.07 152.41 143.40 135.37 129.08 128.67 127.92 127.91 127.70 127.60 118.83 118.67 114.24 113.24 83.04 77.32 77.00 76.68 56.89 55.17 16.42

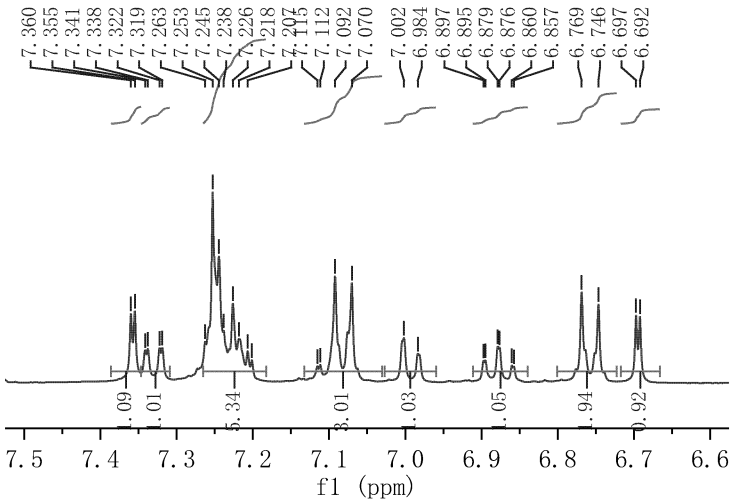


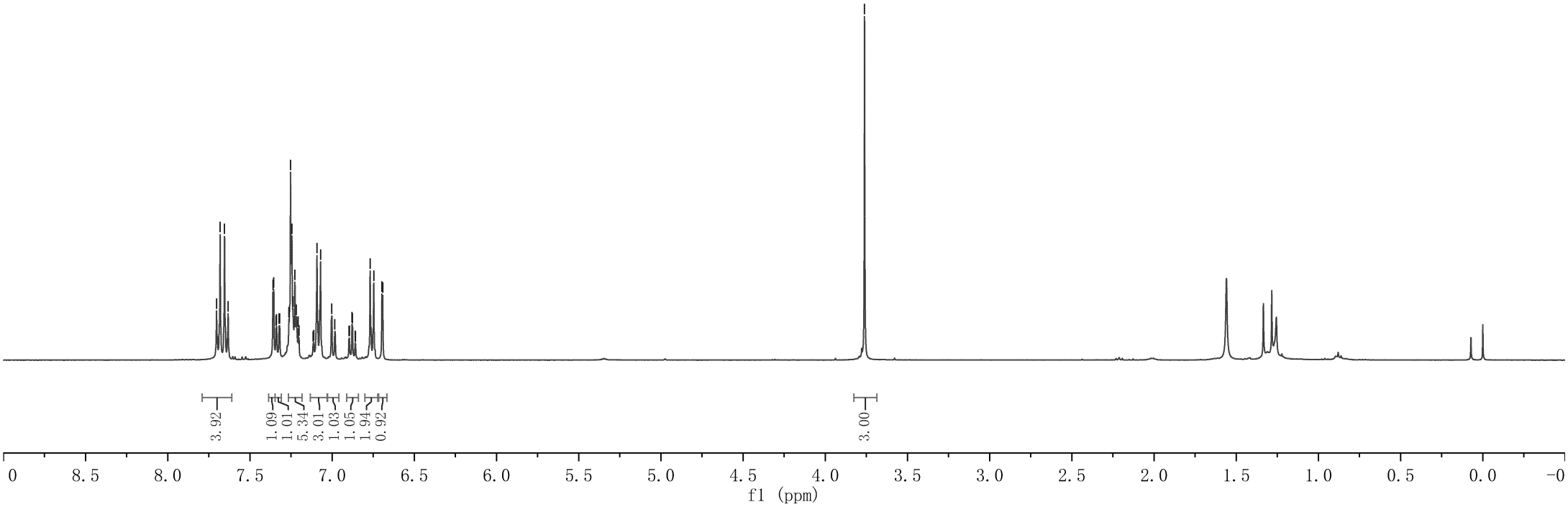


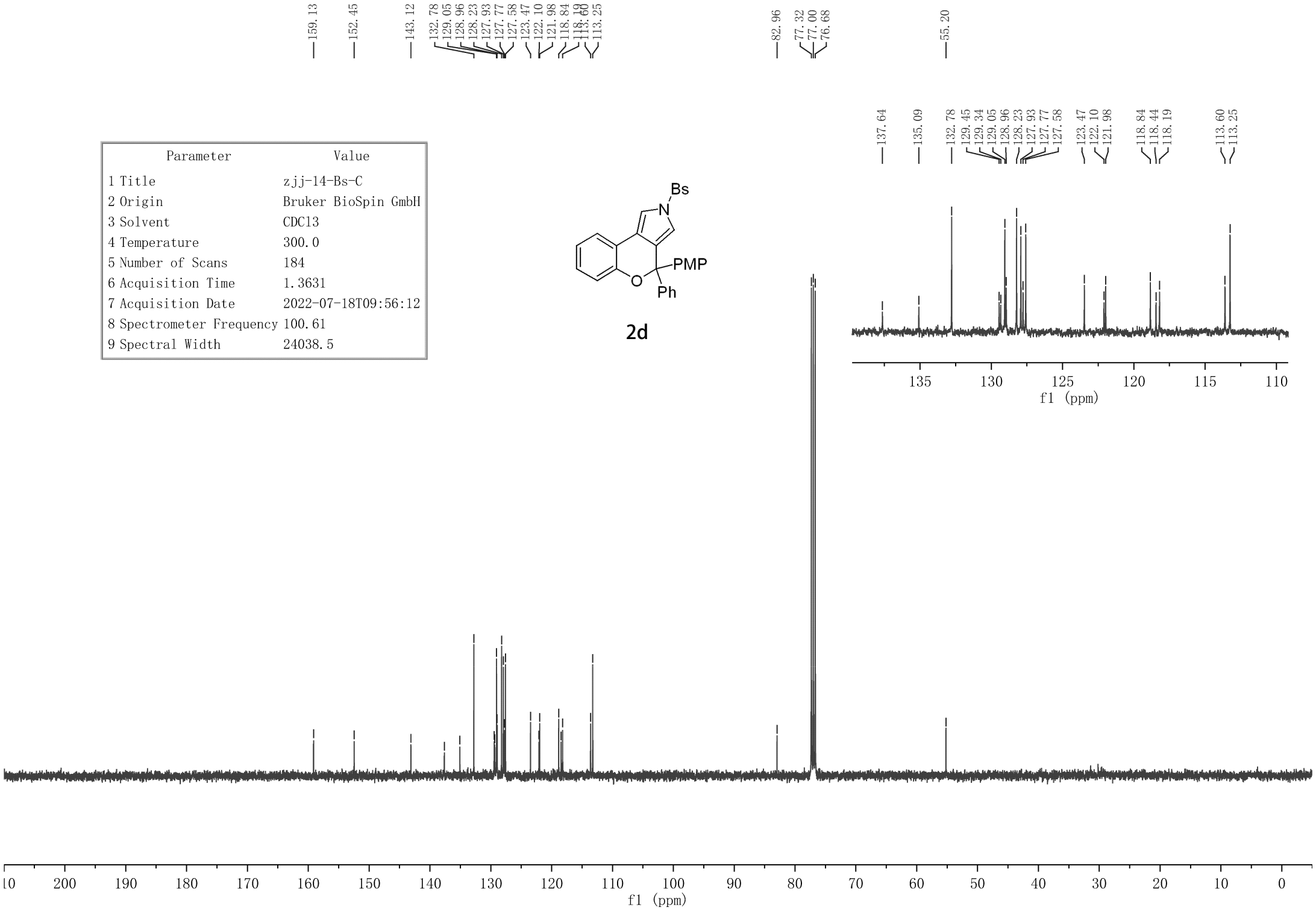
Parameter	Value
1 Title	ZJJ-14-Bs-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-07-15T11:36:30
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2d

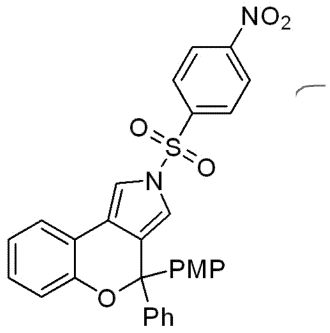




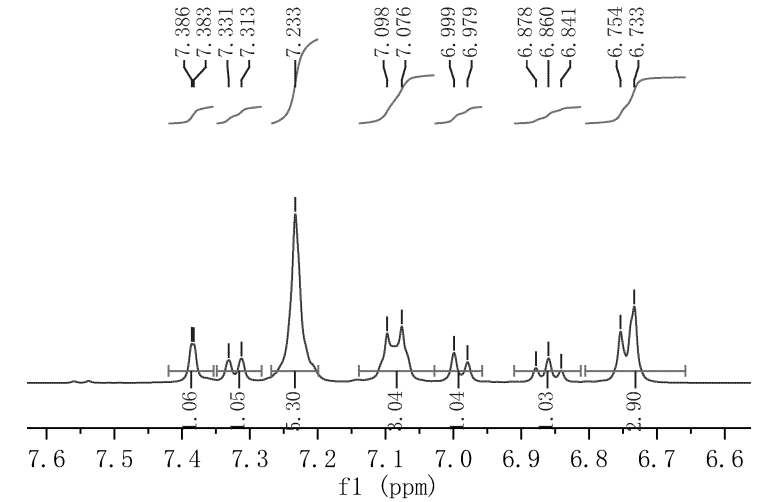

159.13
152.45
143.12
132.78
129.05
128.96
128.23
127.93
127.77
127.58
123.47
122.10
121.98
118.84
118.60
118.19
113.25
82.96
77.32
77.00
76.68
55.20
137.64
135.09
132.78
129.45
129.34
129.05
128.96
128.23
127.93
127.77
127.58
123.47
122.10
121.98
118.84
118.44
118.19
113.60
113.25
Bs
N
PMP
O
Ph
2d
Parameter Value
1 Title zjj-14-Bs-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 184
6 Acquisition Time 1.3631
7 Acquisition Date 2022-07-18T09:56:12
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
f1 (ppm)
f1 (ppm)

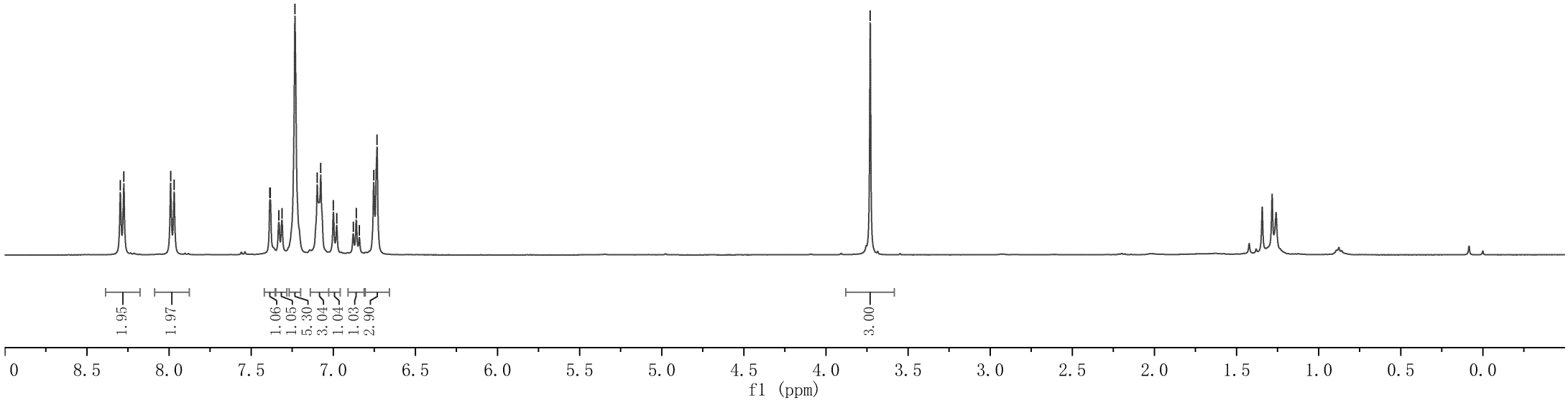
8.297
8.275
7.990
7.969
7.386
7.383
7.331
7.313
7.233
7.098
7.076
6.999
6.979
6.878
6.860
6.841
6.754
6.733
3.730

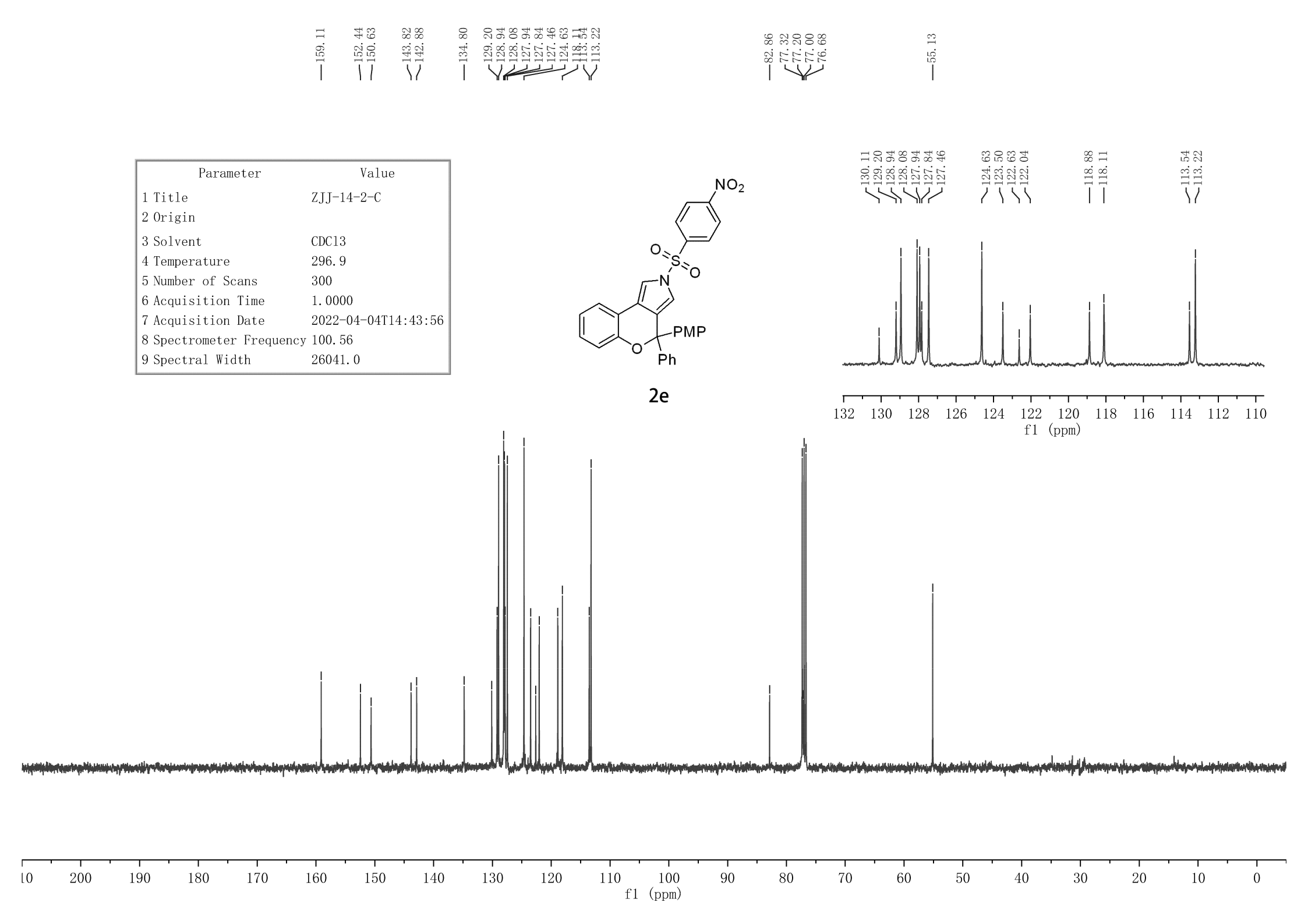
Parameter	Value
1 Title	ZJJ-14-2-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	296.6
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-04T14:31:42
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



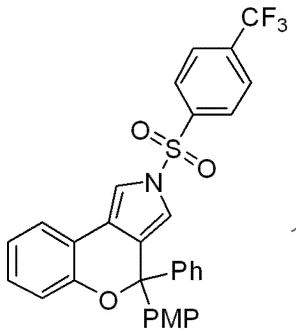
2e



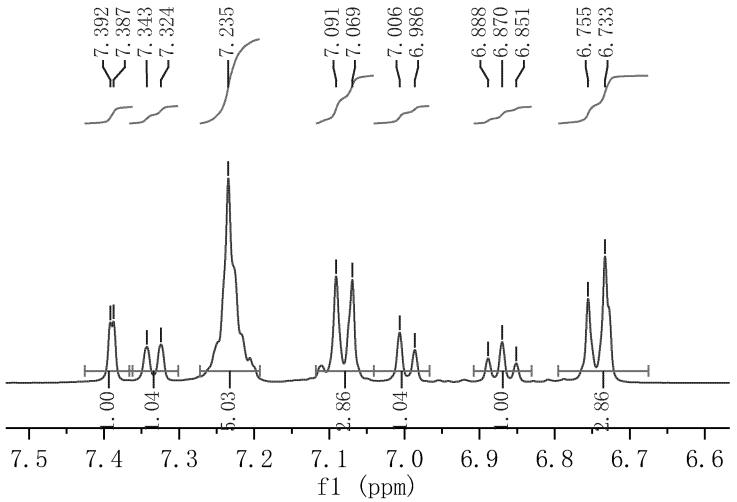


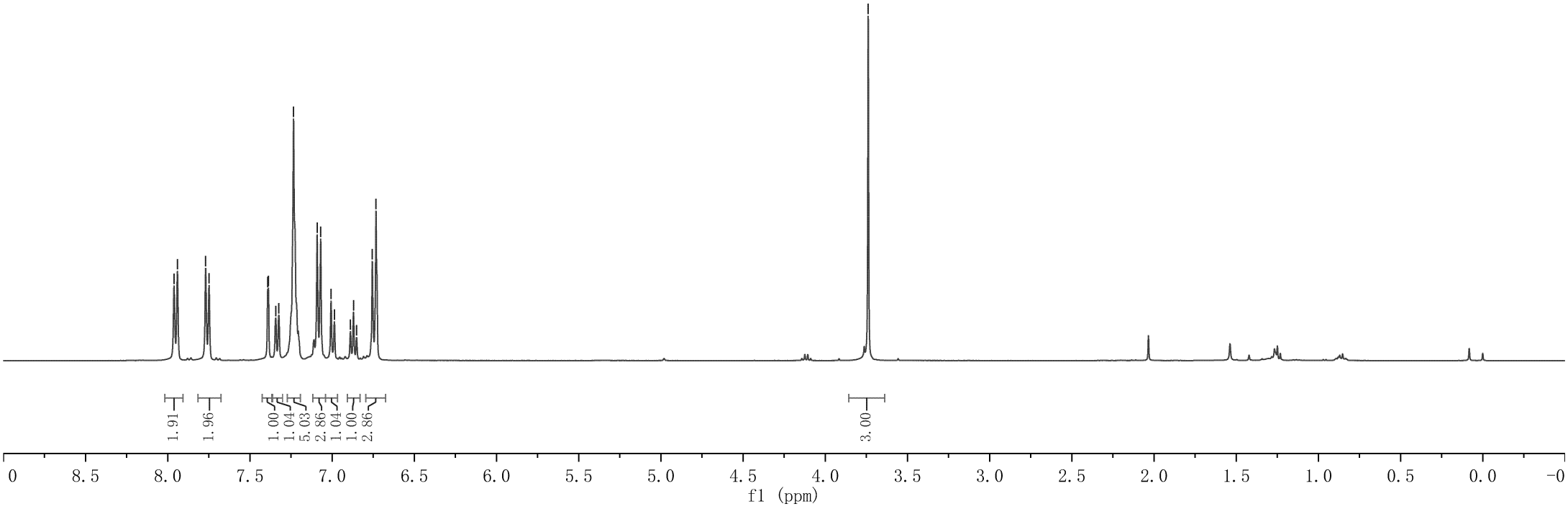

159.11
152.44
150.63
143.82
142.88
134.80
129.20
128.94
128.08
127.94
127.84
127.46
124.63
118.11
113.54
113.22
82.86
77.32
77.20
77.00
76.68
55.13
Parameter Value
1 Title ZJJ-14-2-C
2 Origin
3 Solvent CDCl3
4 Temperature 296.9
5 Number of Scans 300
6 Acquisition Time 1.0000
7 Acquisition Date 2022-04-04T14:43:56
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
NO2
O
S
O
N
PMP
O
Ph
2e
130.11
129.20
128.94
128.08
127.94
127.84
127.46
124.63
123.50
122.63
122.04
118.88
118.11
113.54
113.22
132 130 128 126 124 122 120 118 116 114 112 110
f1 (ppm)
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Parameter	Value
1 Title	zjj-14-12-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-08T14:56:46
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



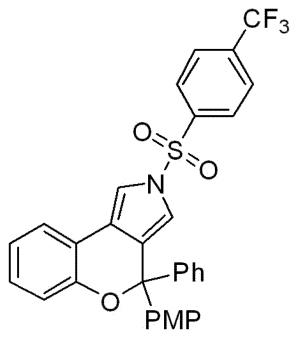
2f



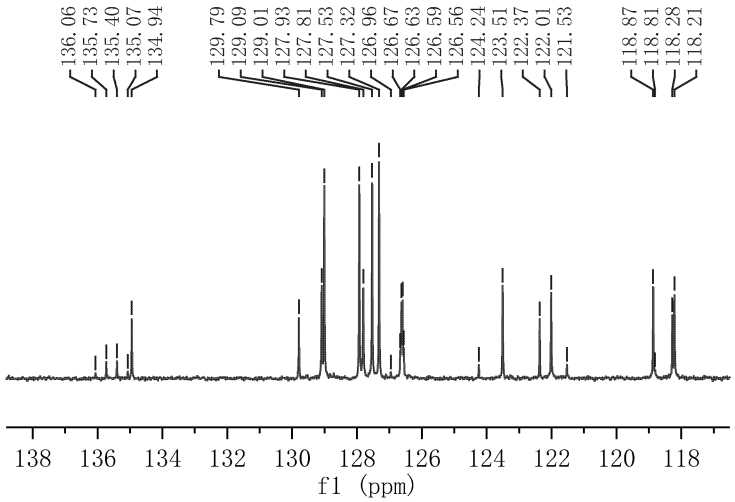


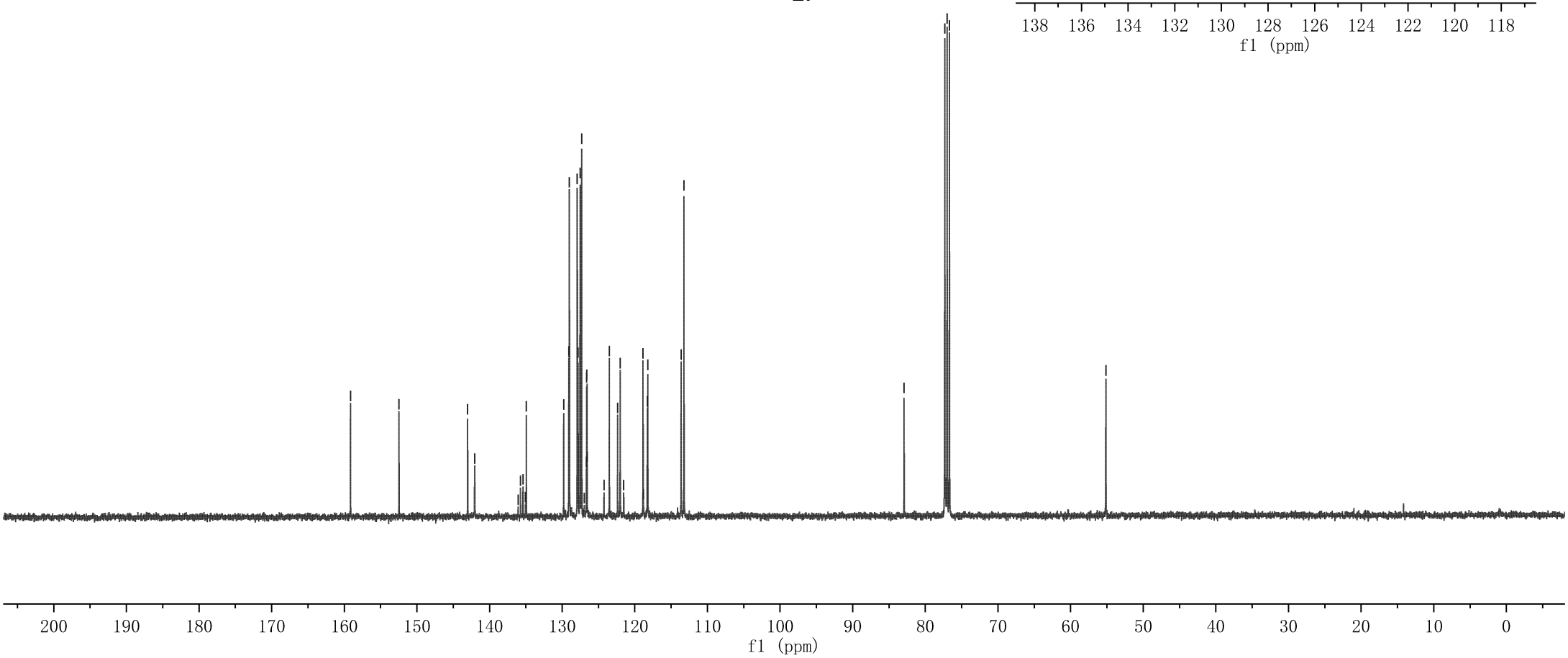
159.14
152.46
143.02
142.04
135.73
135.40
134.94
129.09
129.01
127.93
127.81
127.53
127.32
123.51
123.62
113.23
82.92
77.32
77.00
76.68
55.14

Parameter	Value
1 Title	zjj-14-12-CF3PhO2-chanwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	325
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-08T14:58:32
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

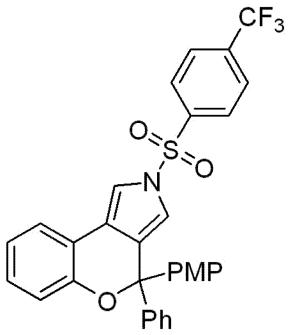


2f

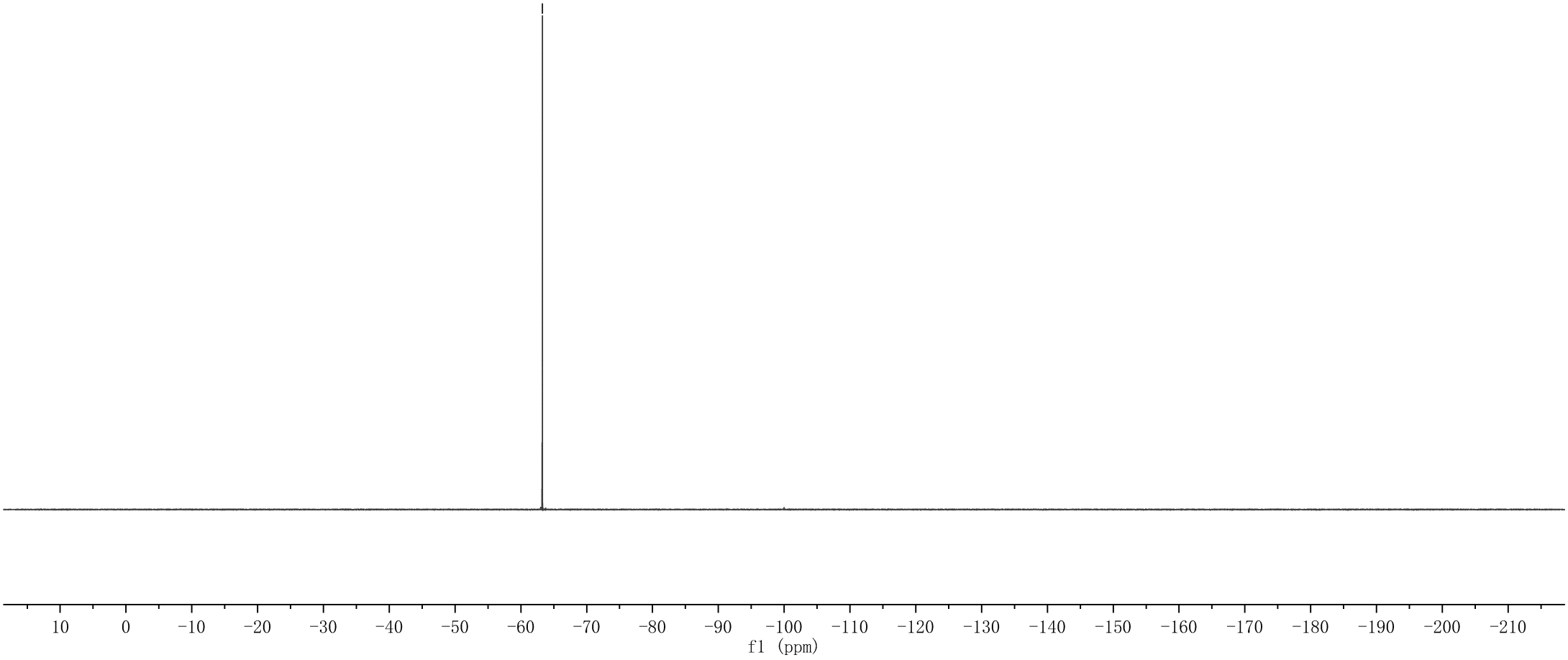


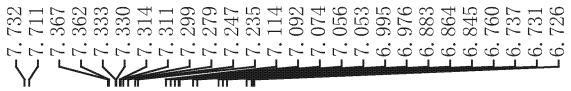


Parameter	Value
1 Title	zjj-14-4-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.3
5 Number of Scans	13
6 Acquisition Time	0.7340
7 Acquisition Date	2022-04-12T11:37:38
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

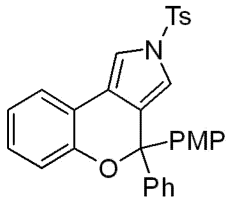


2f

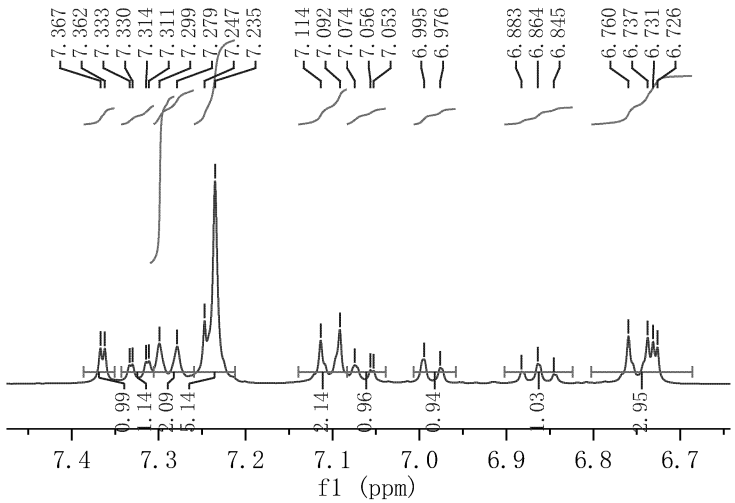


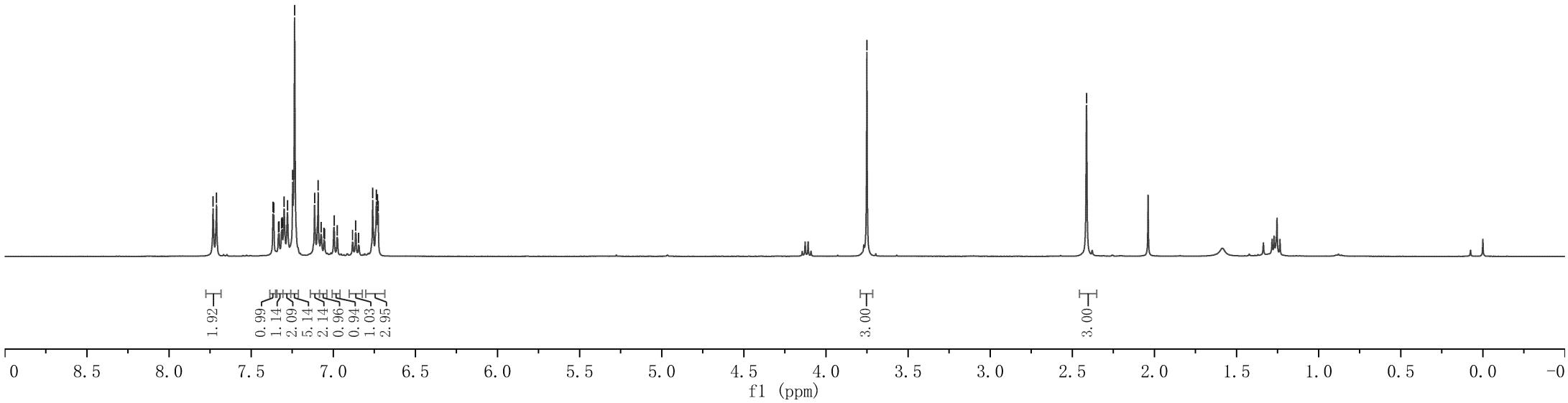


Parameter	Value
1 Title	LFS-127-T-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-27T17:12:27
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



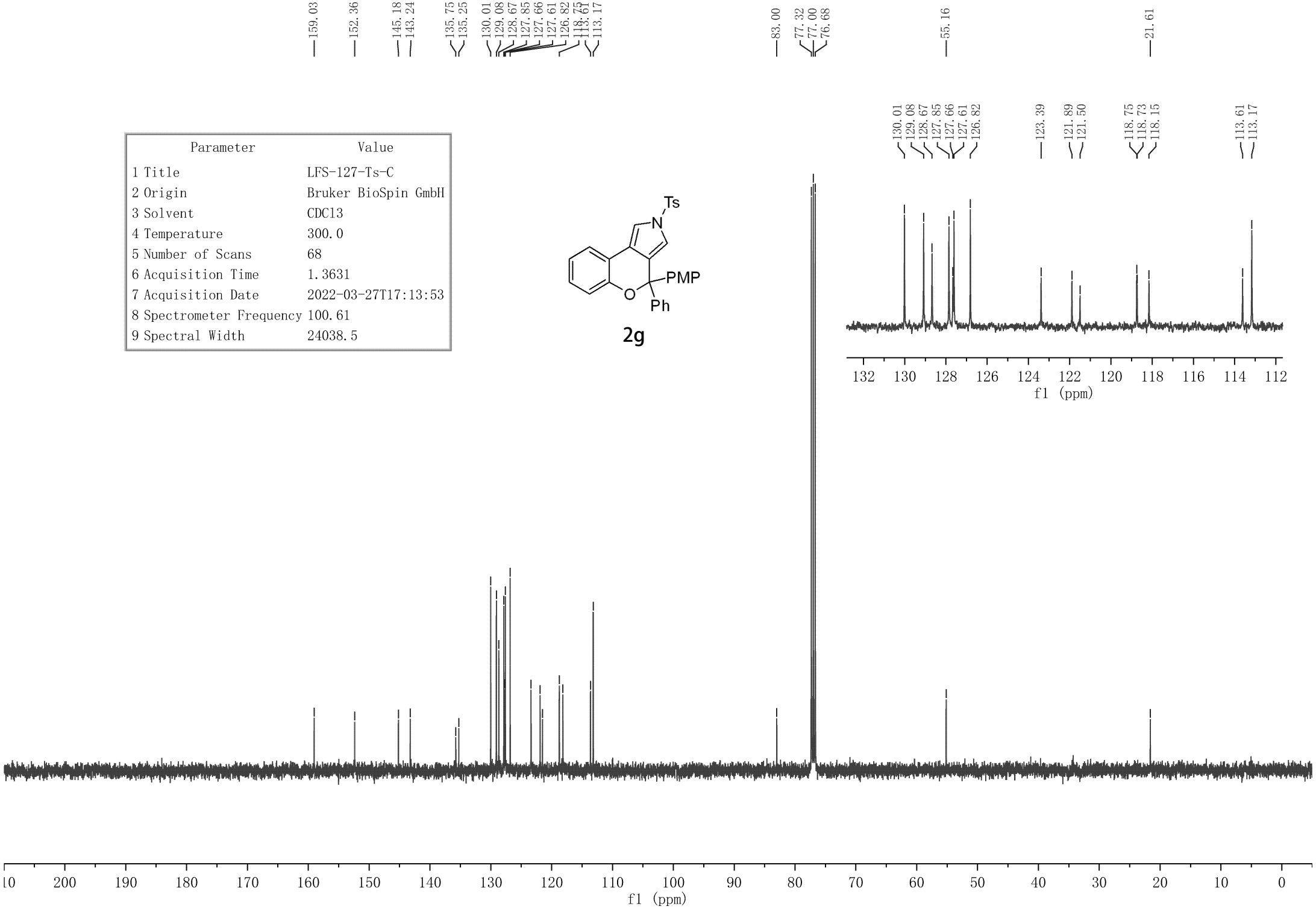
2g

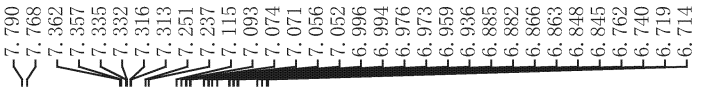




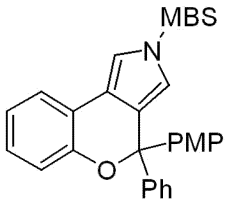
Parameter	Value
1 Title	LFS-127-Ts-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	68
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-27T17:13:53
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

2g

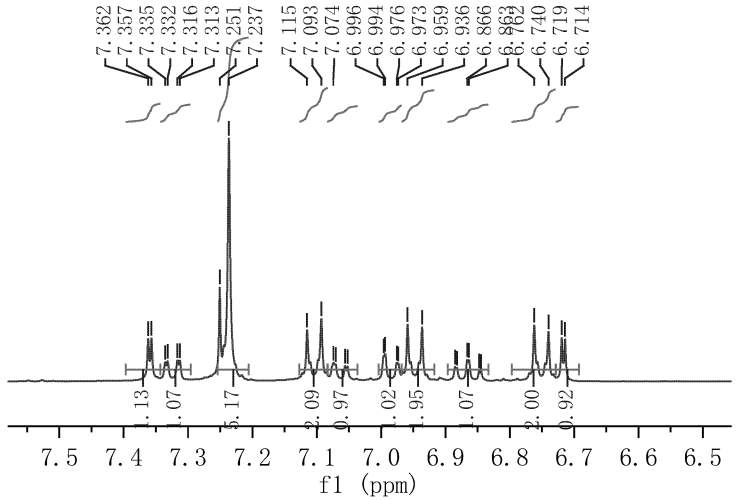


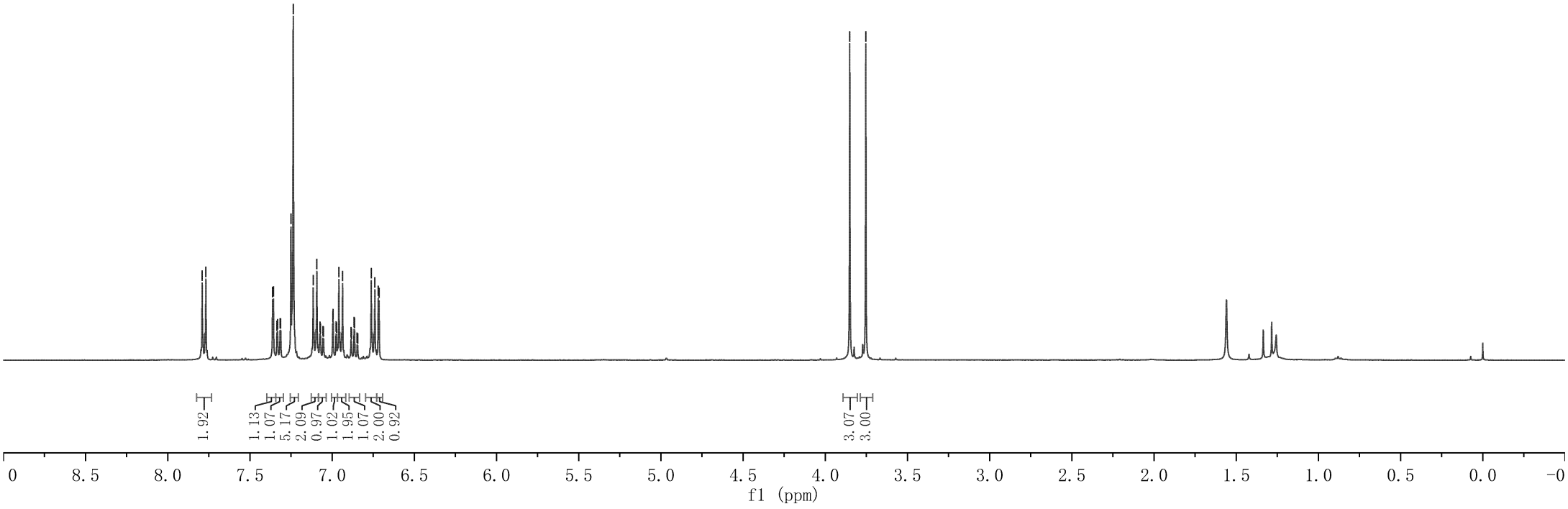


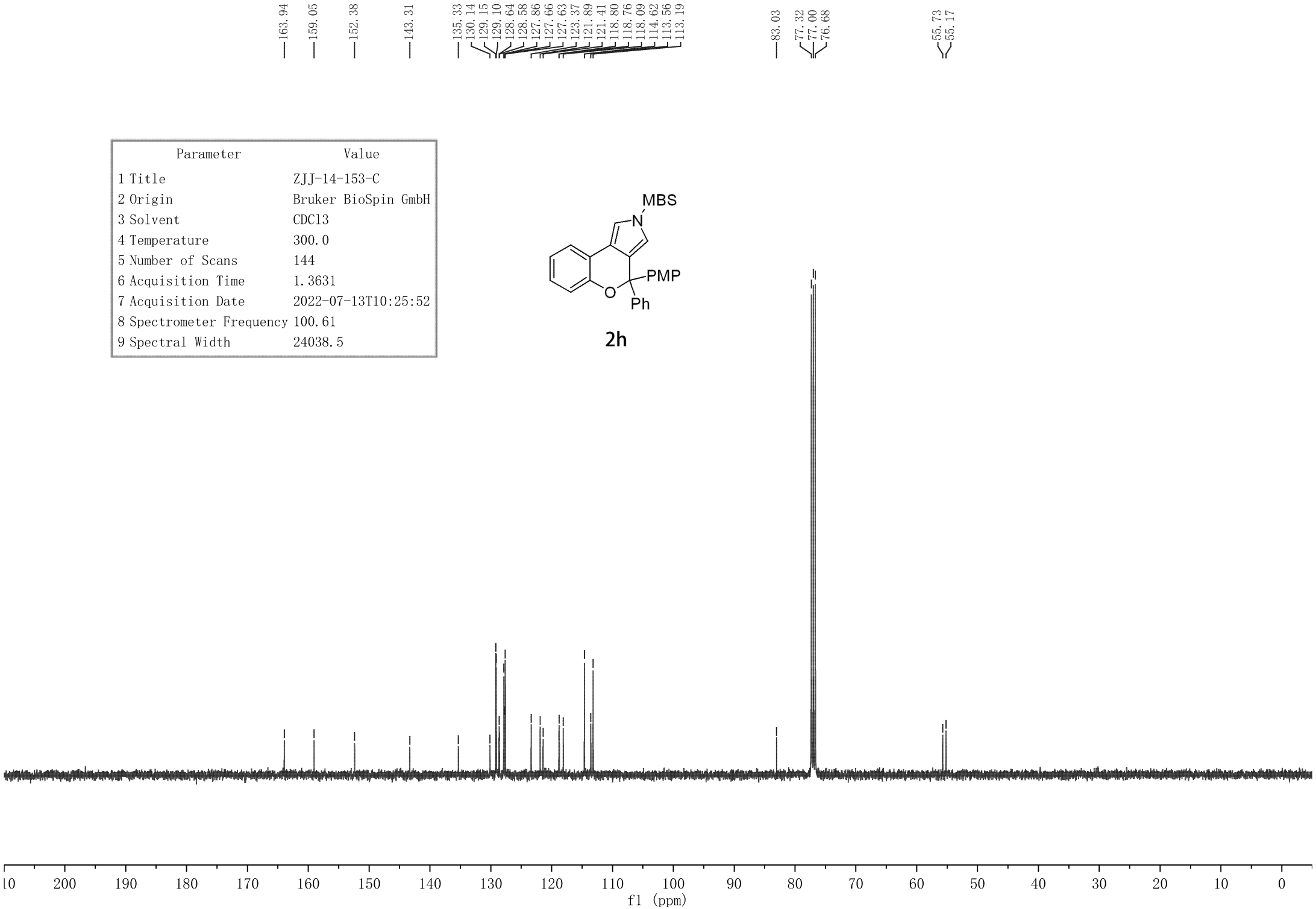
Parameter	Value
1 Title	ZJJ-14-153-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2022-07-13T10:24:36
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



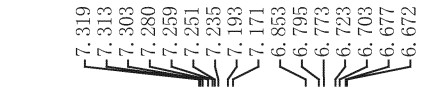
2h



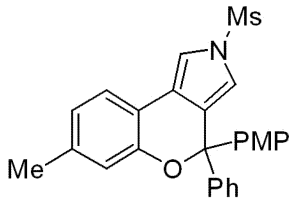




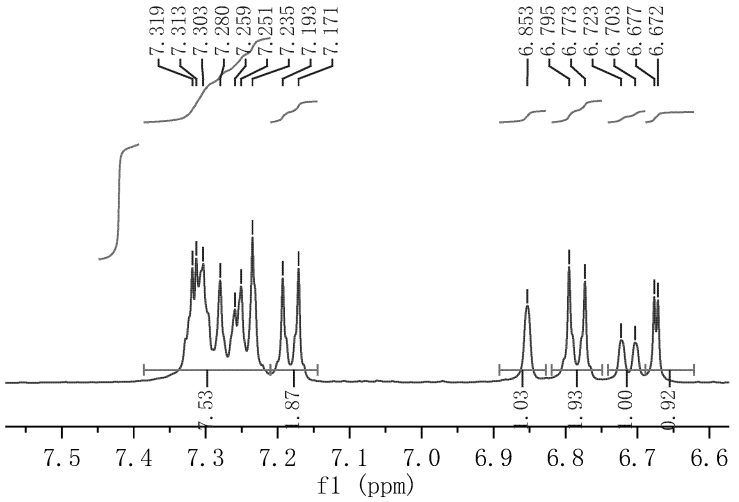
Parameter	Value
1 Title	ZJJ-14-153-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	144
6 Acquisition Time	1.3631
7 Acquisition Date	2022-07-13T10:25:52
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

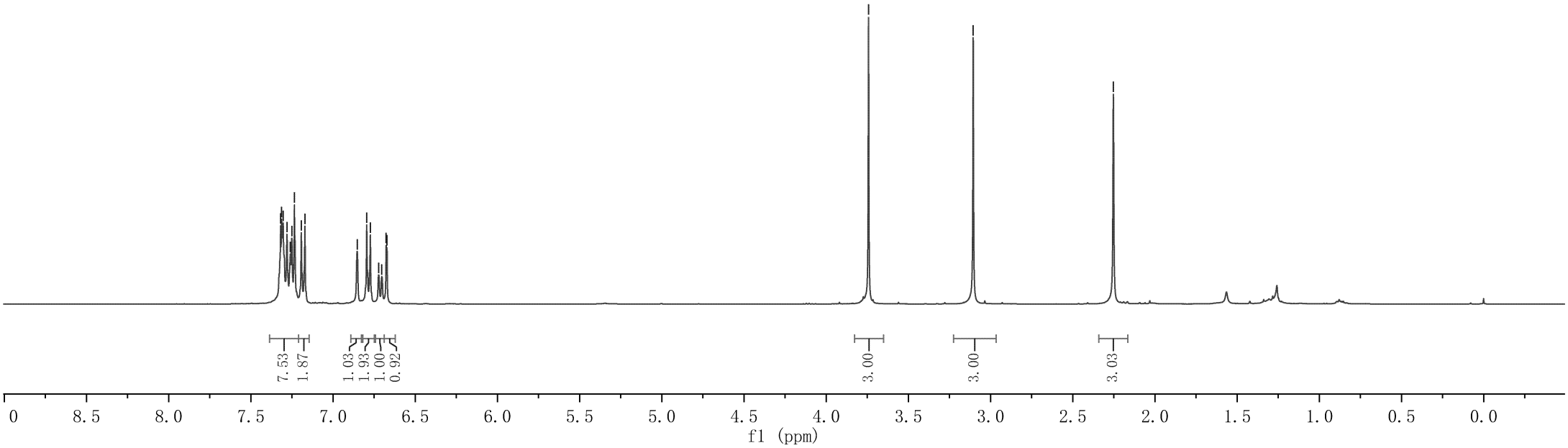


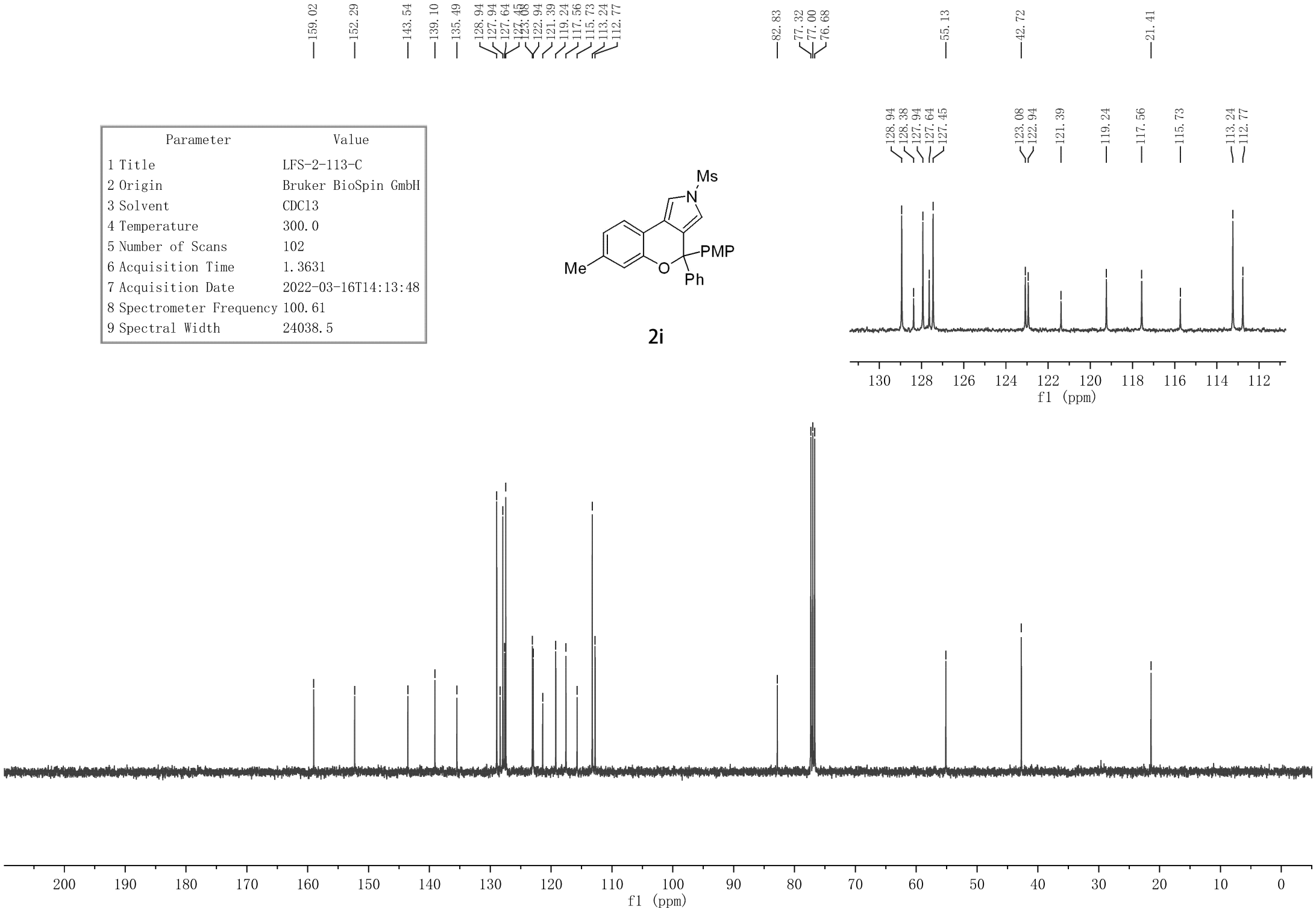
Parameter	Value
1 Title	LFS-2-113-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	17
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-16T14:10:10
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2i



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127.94
127.64
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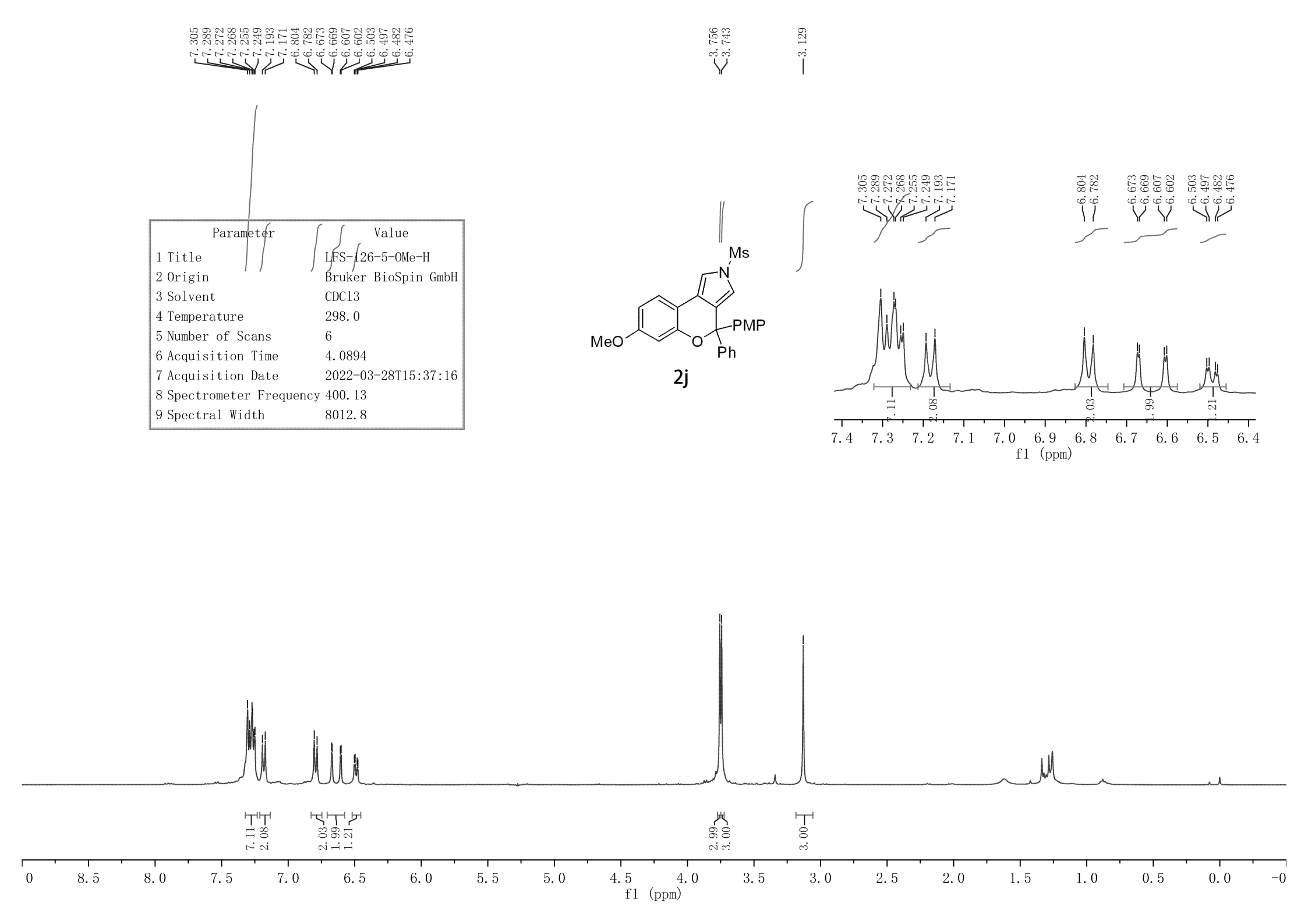
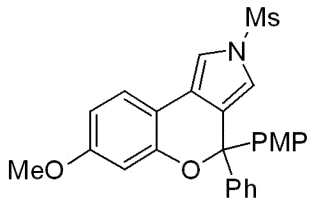
122.94
121.39
119.24
117.56
115.73
113.24
112.77
82.83
77.32
77.00
76.68
55.13
42.72
21.41
Parameter Value
1 Title LFS-2-113-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 102
6 Acquisition Time 1.3631
7 Acquisition Date 2022-03-16T14:13:48
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
PMP
Me
O
Ph
2i
f1 (ppm)
f1 (ppm)

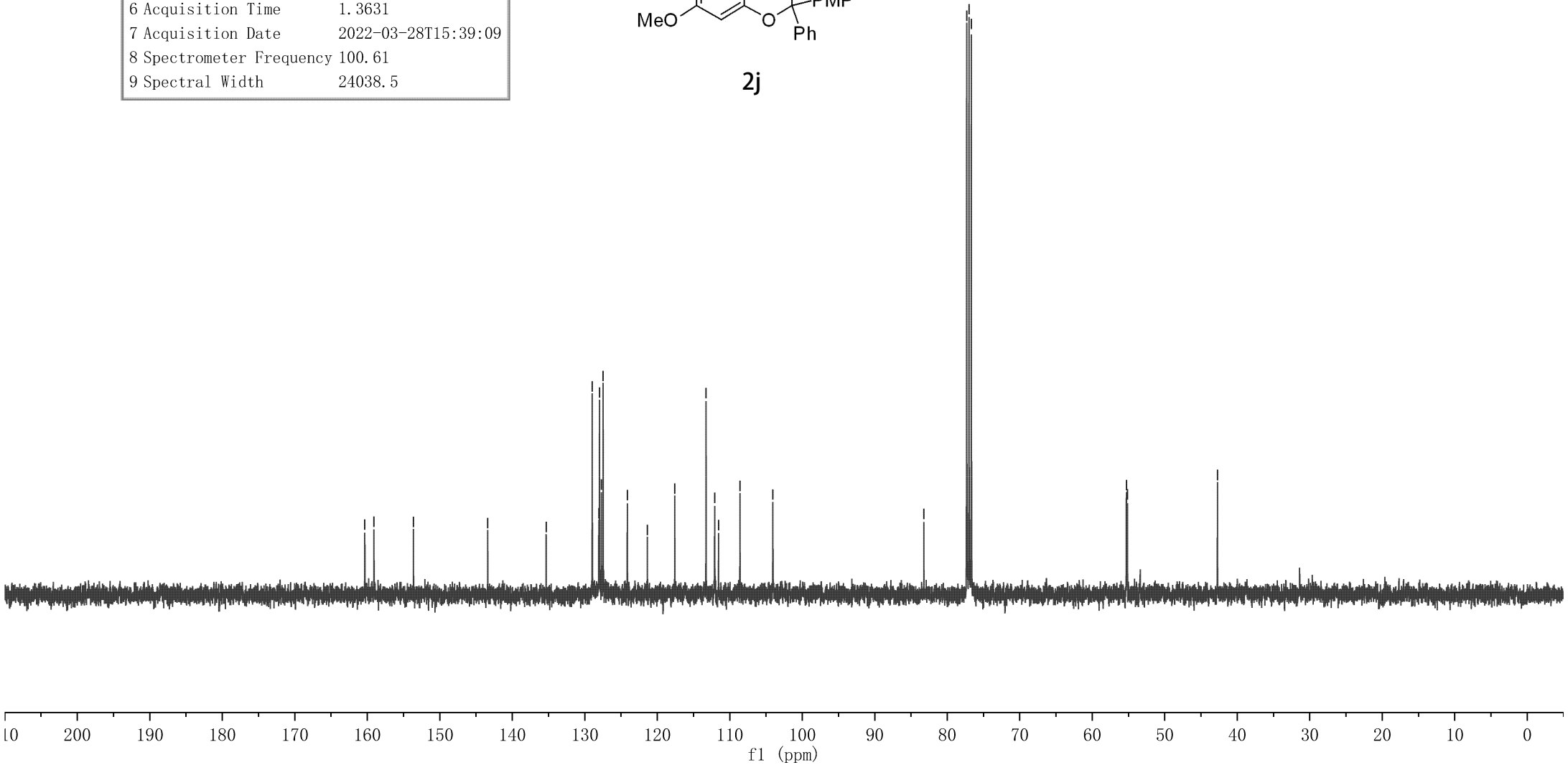

7.305
7.289
7.272
7.268
7.255
7.249
7.193
7.171
6.804
6.782
6.673
6.669
6.607
6.602
6.503
6.497
6.482
6.476
3.756
3.743
3.129
Parameter
Value
1 Title
LFS-126-5-OMe-H
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
298.0
5 Number of Scans
6
6 Acquisition Time
4.0894
7 Acquisition Date
2022-03-28T15:37:16
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
Ms
N
PMP
MeO
O
Ph
2j
7.11
2.08
2.03
1.99
1.21
2.99
3.00
3.00
f1 (ppm)

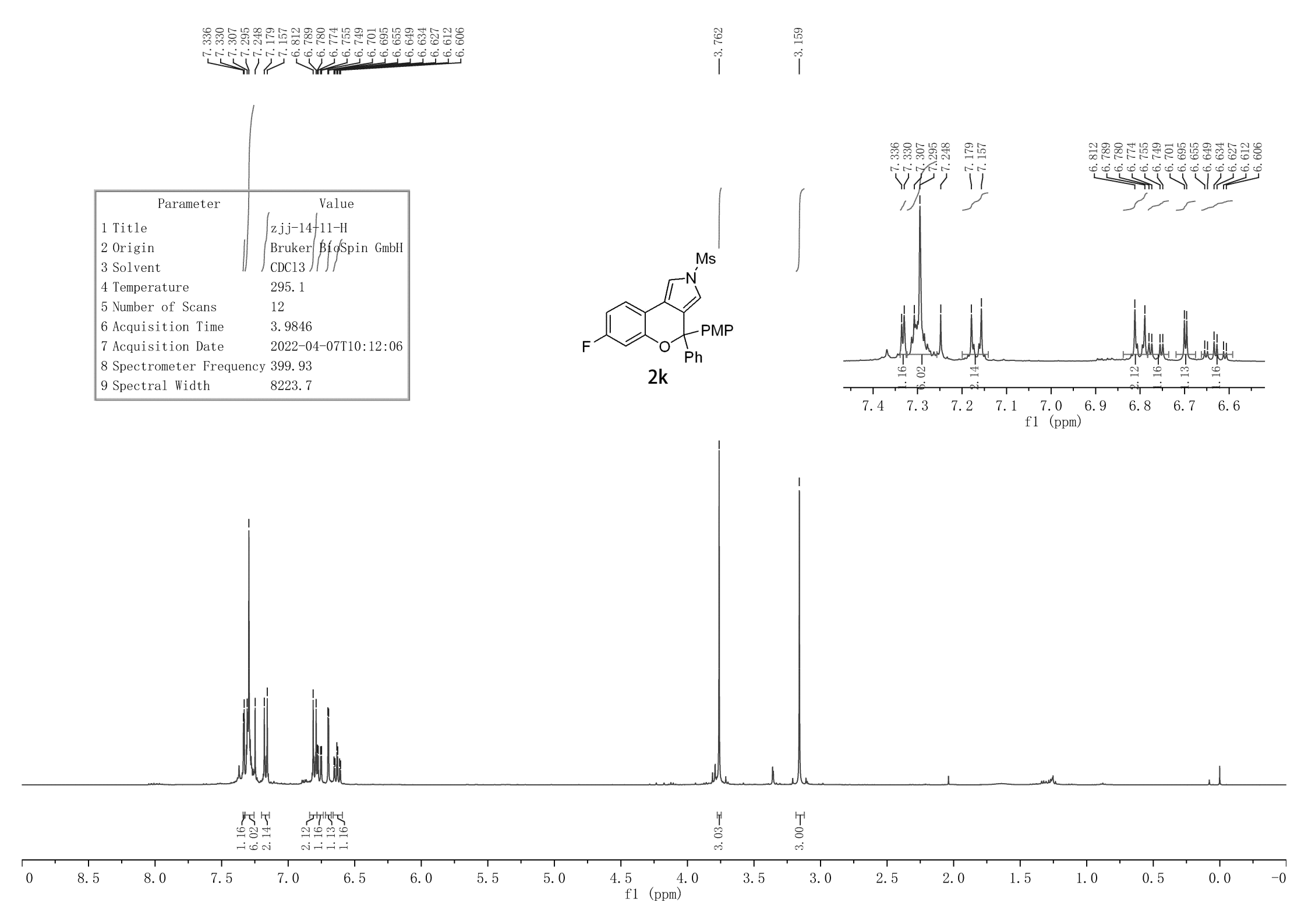
160.34
159.08
153.63
143.38
135.33
128.97
128.07
127.97
127.71
127.47
124.13
121.36
117.59
113.27
112.09
111.54
108.59
104.06
83.23
77.32
77.00
76.68
55.29
55.16
42.73

Parameter	Value
1 Title	LFS-126-5-OMe-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	47
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-28T15:39:09
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



2j

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7.307
7.295
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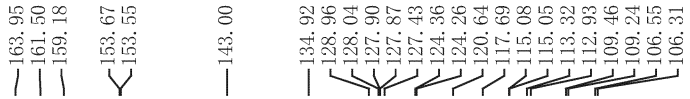
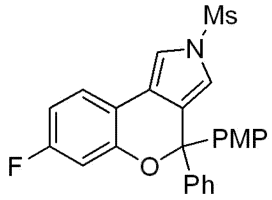
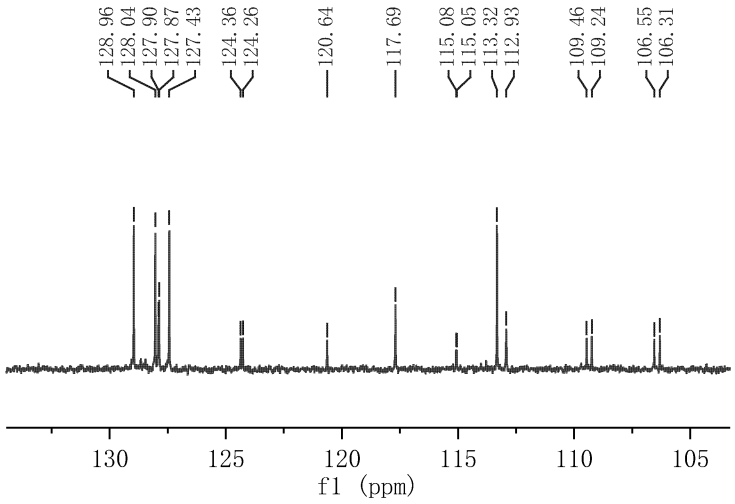
7.179
7.157
6.812
6.789
6.780
6.774
6.755
6.749
6.701
6.695
6.655
6.649
6.634
6.627
6.612
6.606
3.762
3.159
Parameter Value
1 Title zjj-14-11-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.1
5 Number of Scans 12
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-07T10:12:06
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
PMP
F
O
Ph
2k
1.16
6.02
2.14
2.12
1.16
1.13
1.16
3.03
3.00
f1 (ppm)

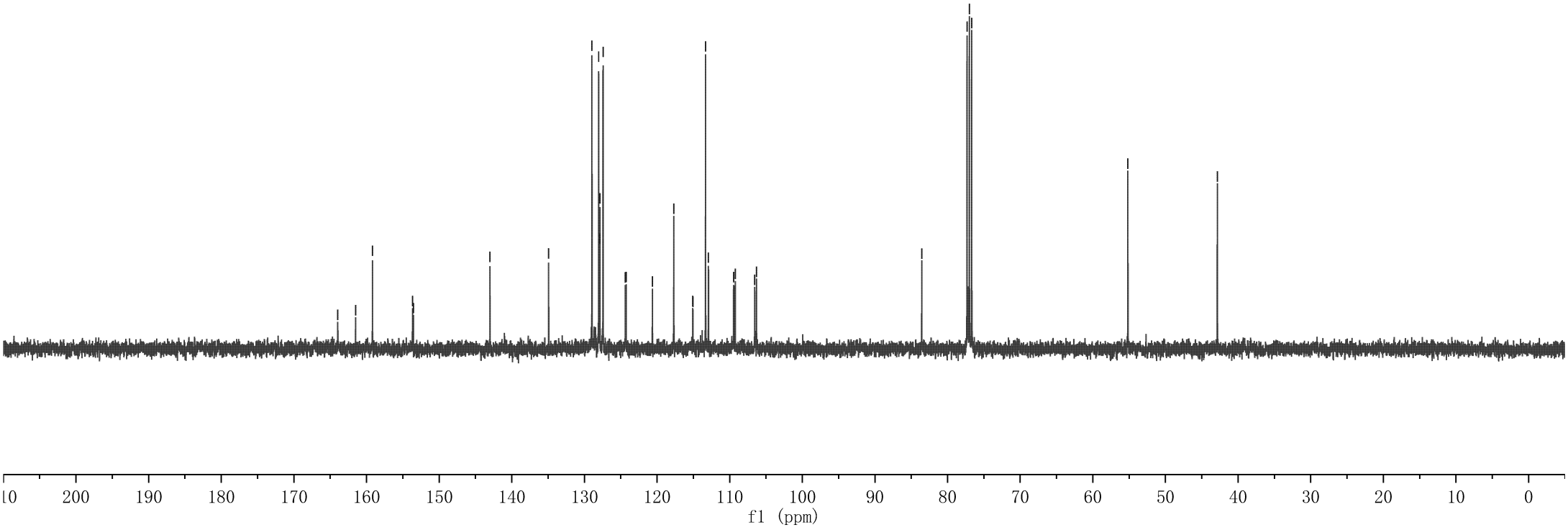


Parameter	Value
1 Title	zjj-14-11-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	96
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-07T10:15:13
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



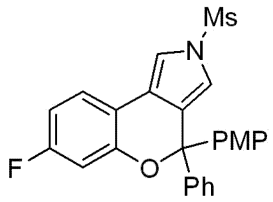
2k



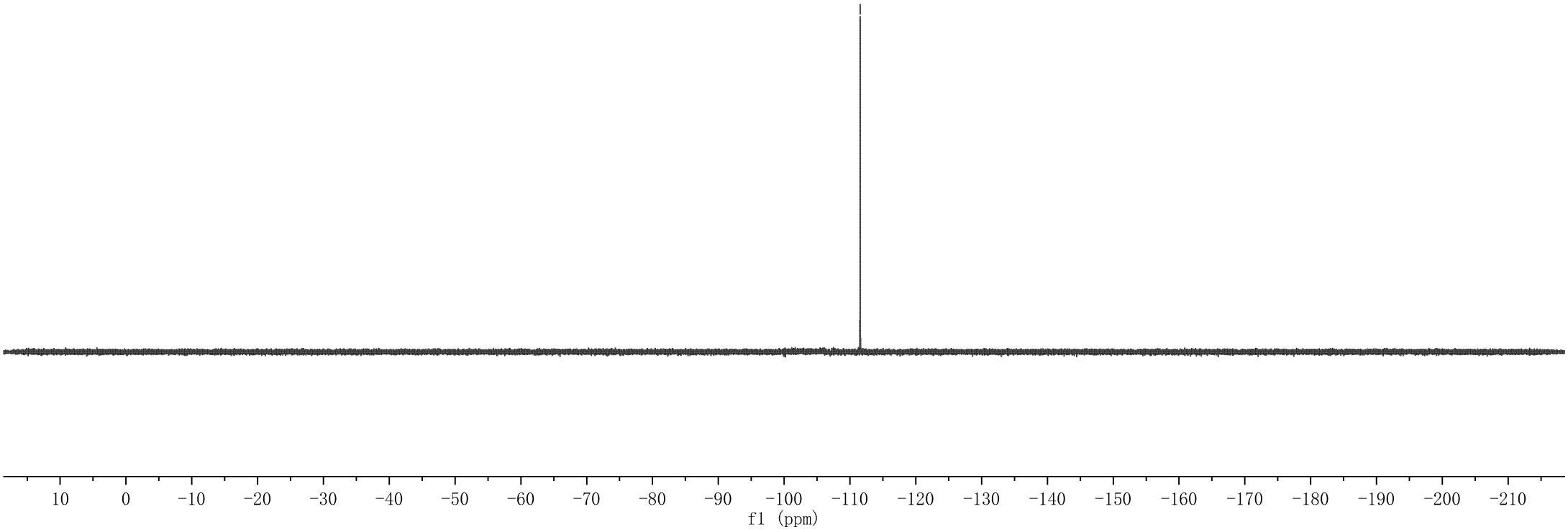


^{19}F NMR (376 MHz, $CDCl_3$) δ = -111.55.

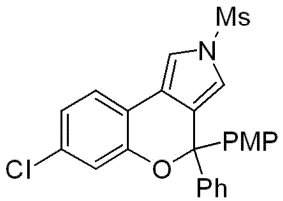
Parameter	Value
1 Title	zjj-14-11-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	10
6 Acquisition Time	0.7340
7 Acquisition Date	2022-04-07T10:22:47
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



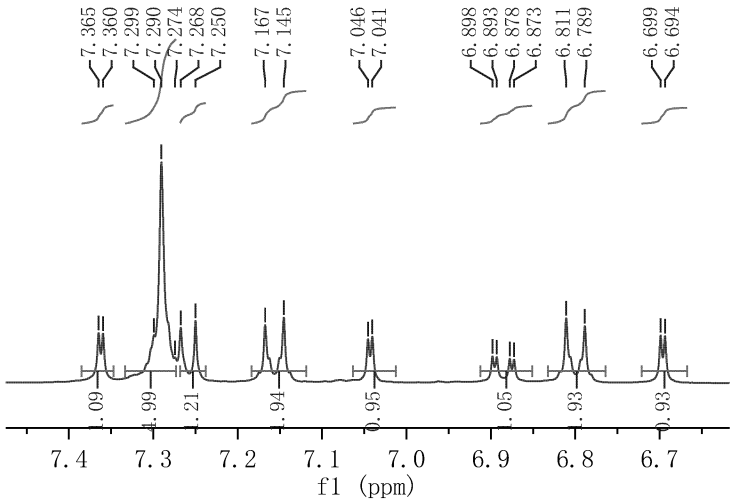
2k

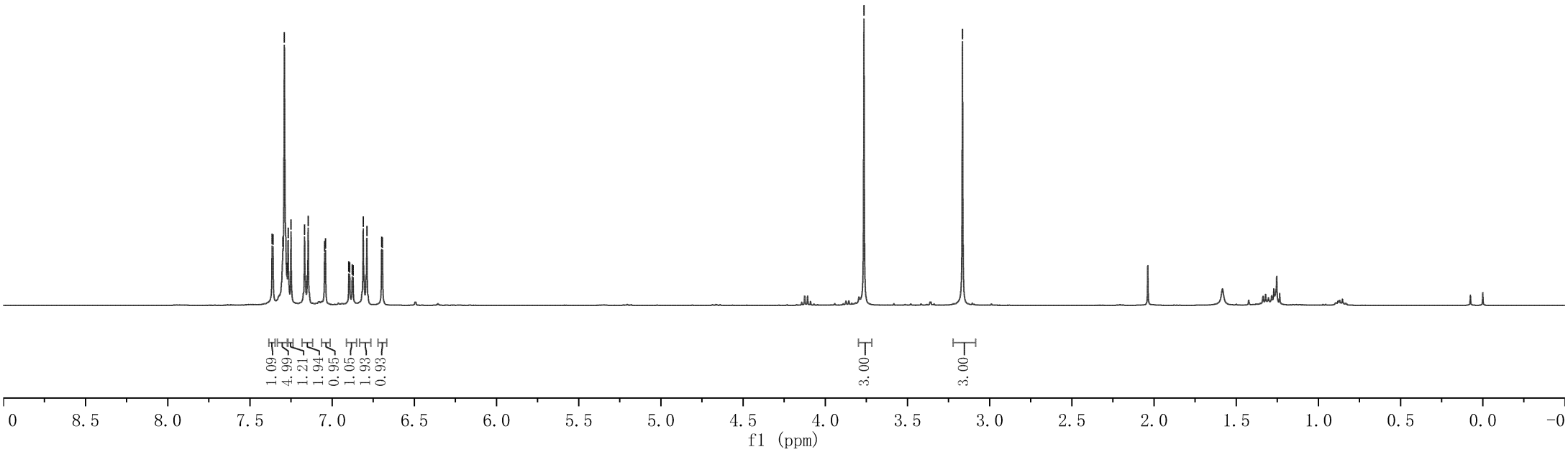


Parameter	Value
1 Title	zjj-14-22-5-Cl-chanwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	14
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-11T19:45:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



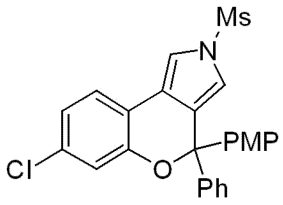
2l



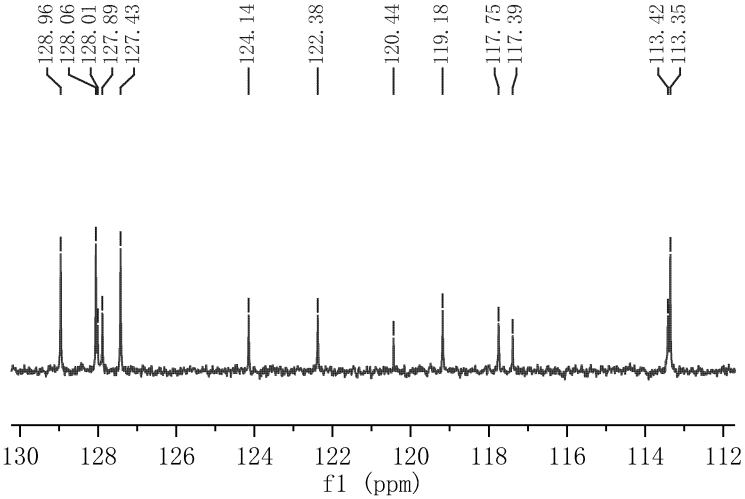


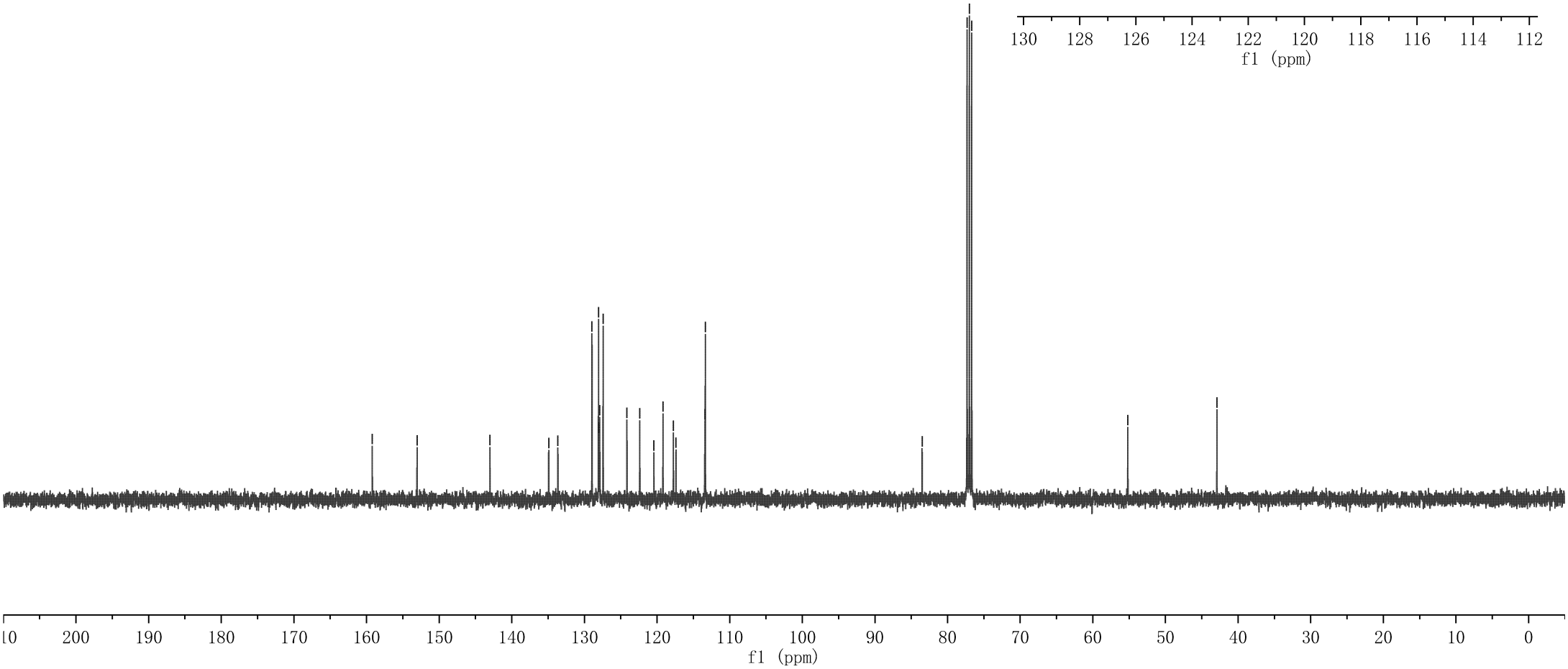
159.21
153.04
143.01
134.91
133.65
128.96
128.06
128.01
127.89
127.43
124.14
122.38
120.44
119.18
117.75
117.39
113.42
113.35
83.50
77.32
77.00
76.68
55.18
42.92

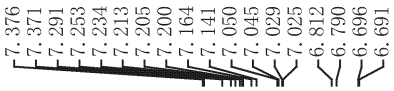
Parameter	Value
1 Title	zjj-14-22-5-Cl-chanwu-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	43
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-11T19:48:21
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



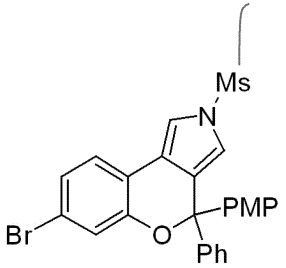
2l



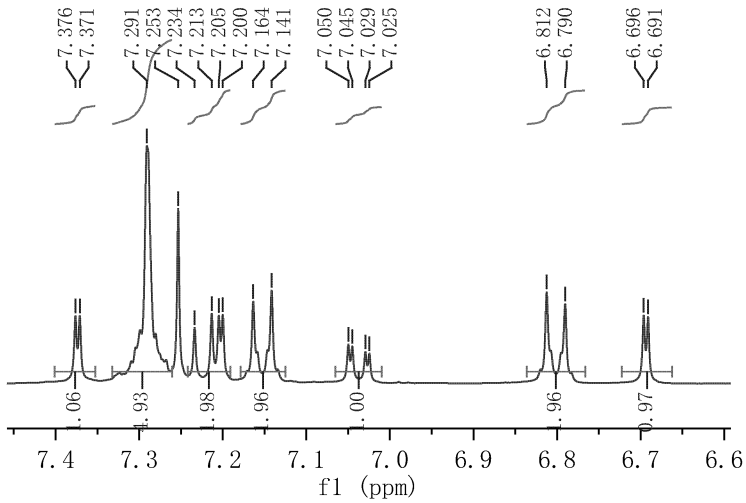


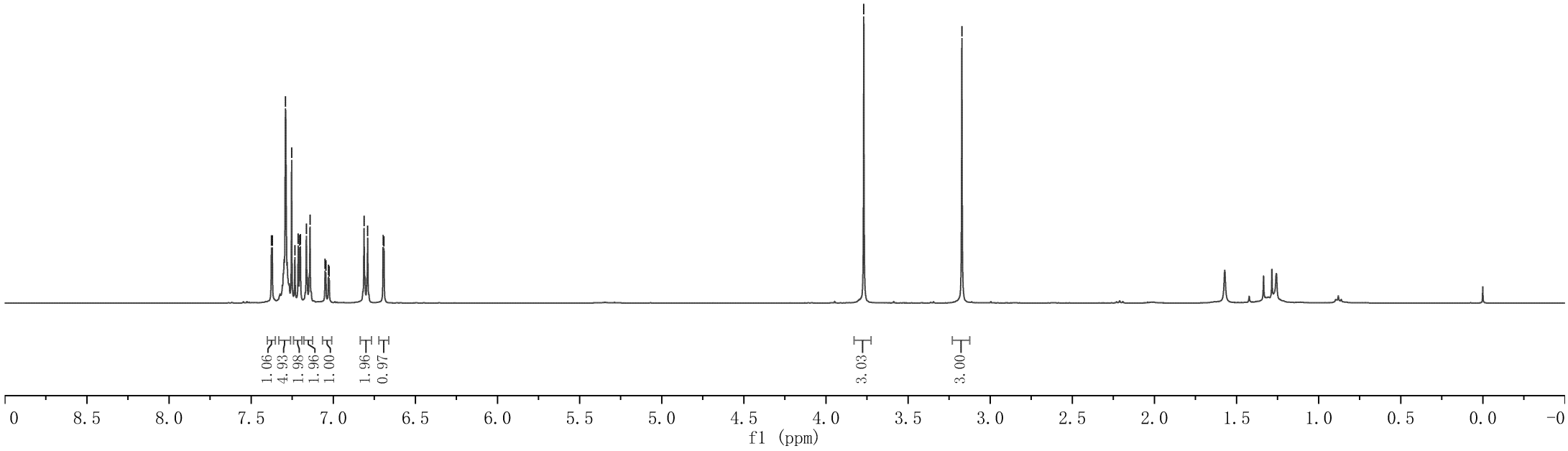


Parameter	Value
1 Title	LFS-2-123-H-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	17
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-01T08:54:13
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



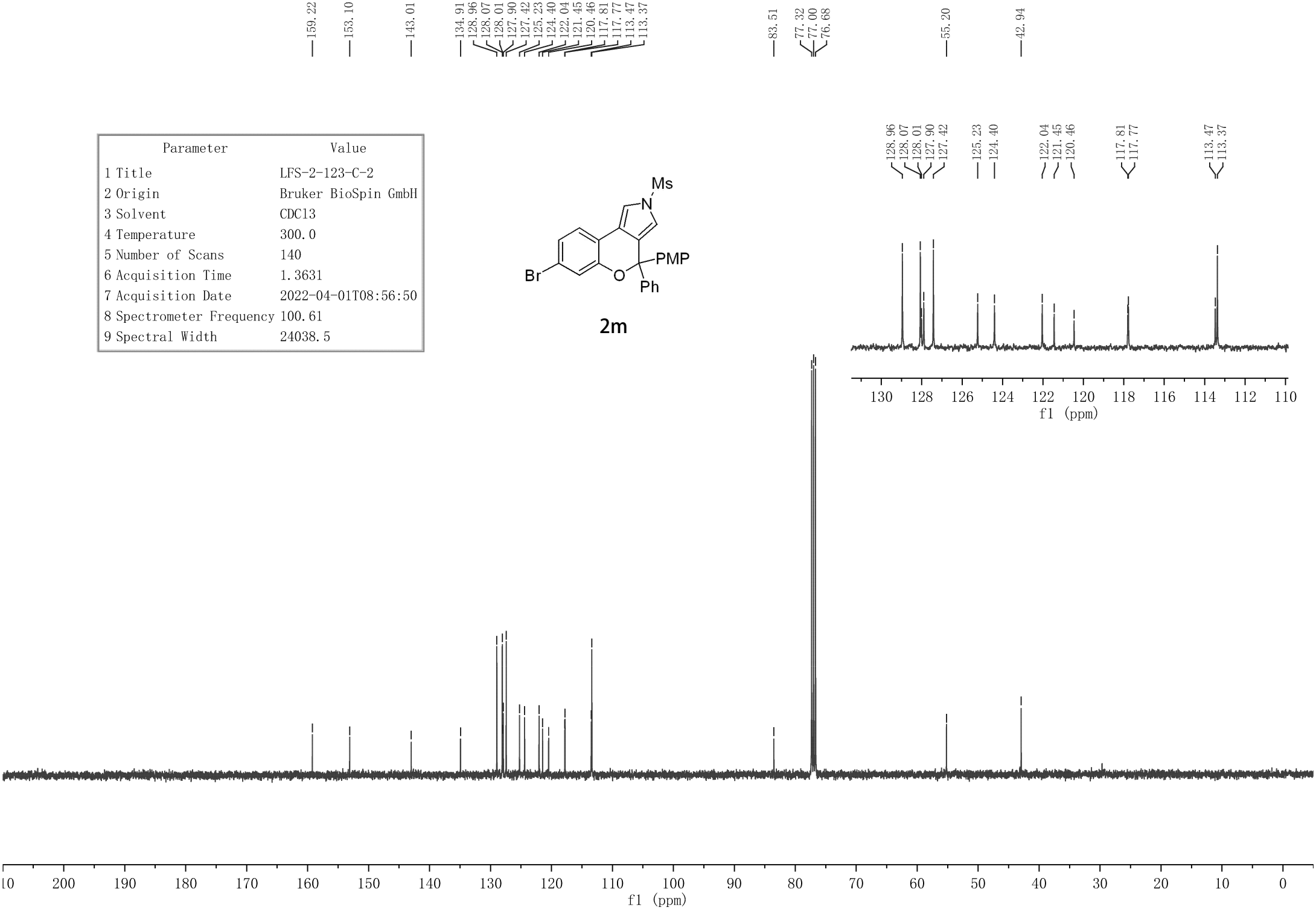
2m



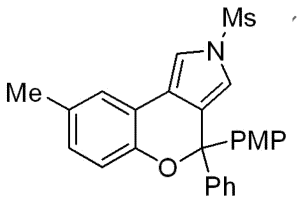


Parameter	Value
1 Title	LFS-2-123-C-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	140
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-01T08:56:50
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

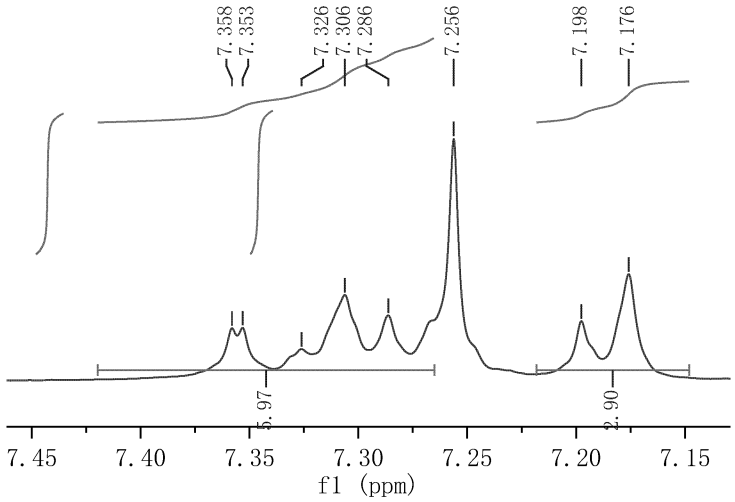
2m

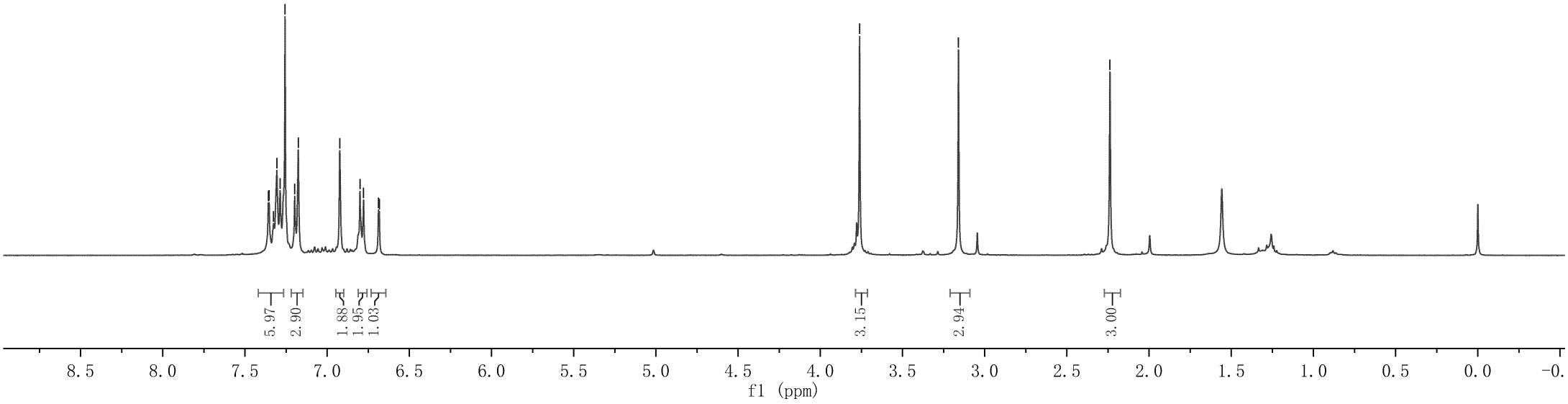


Parameter	Value
1 Title	zjj-13-198-4-Me-diwu-H-3
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-25T17:00:41
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



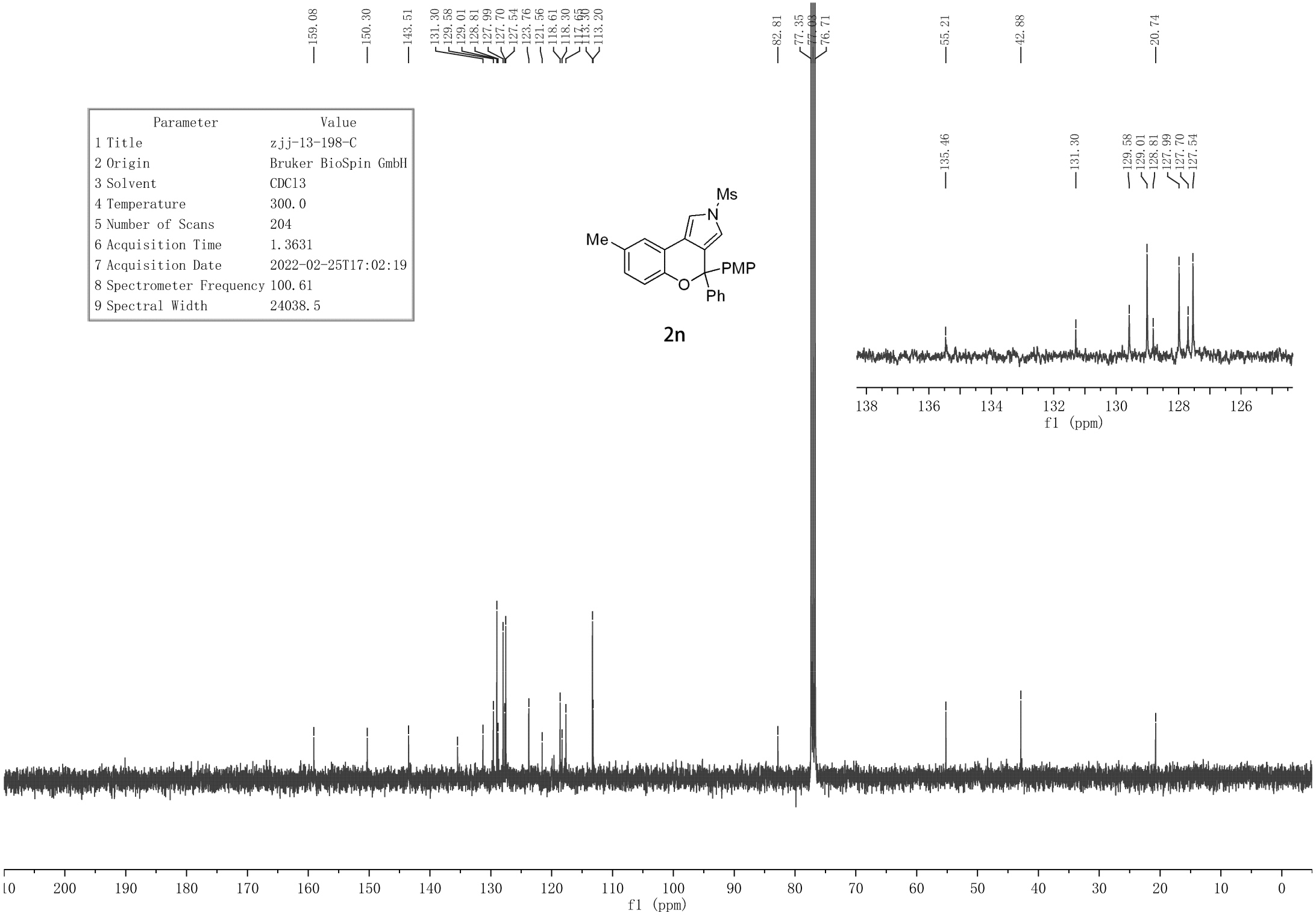
2n



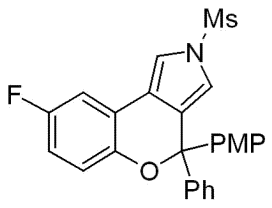


Parameter	Value
1 Title	zjj-13-198-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	204
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-25T17:02:19
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

2n



Parameter	Value
1 Title	LFS-2-114-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	21
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-16T14:21:36
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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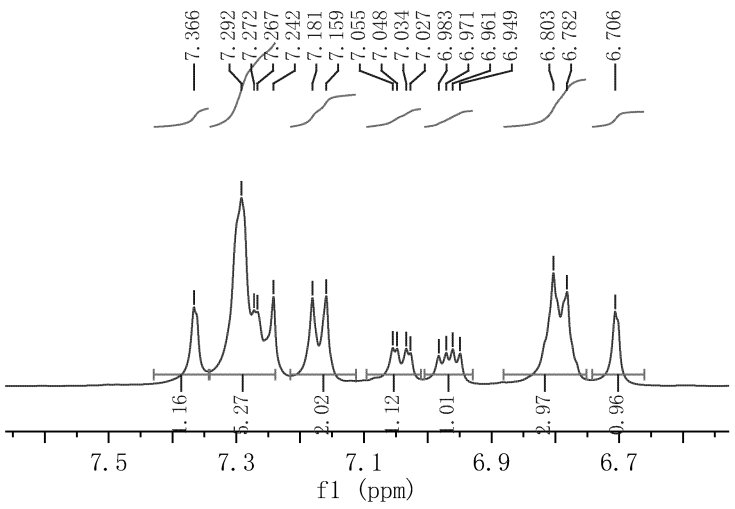

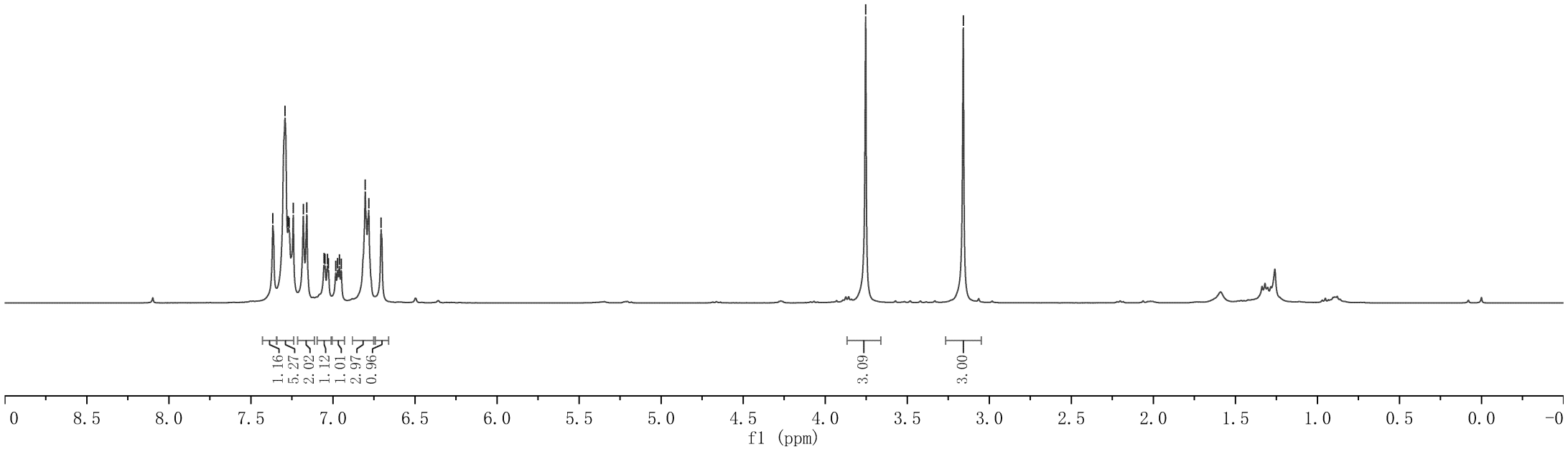

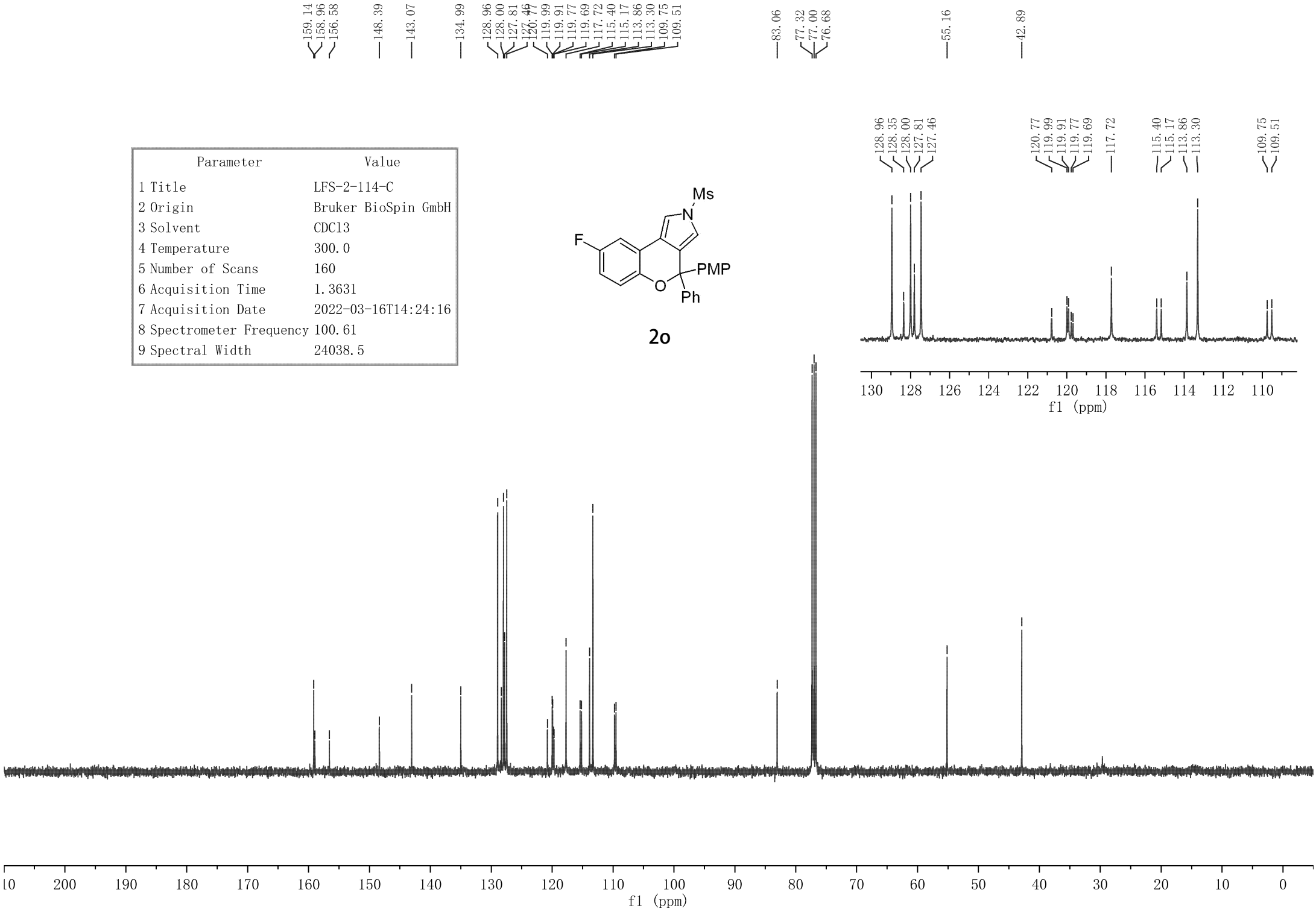
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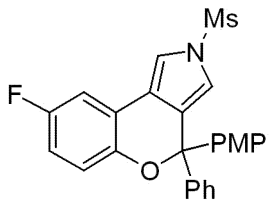
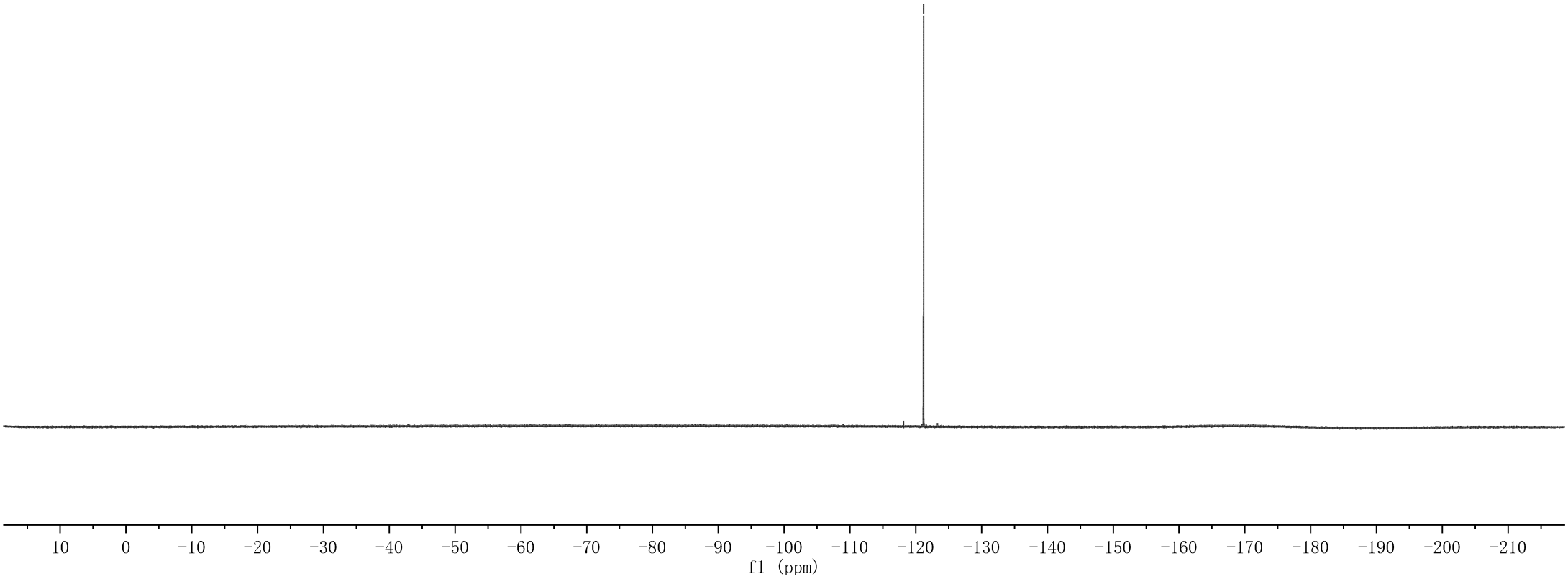
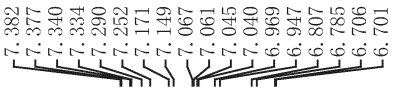
127.46
120.77
119.99
119.91
119.77
119.69
117.72
115.40
115.17
113.86
113.30
109.75
109.51
83.06
77.32
77.00
76.68
55.16
42.89
Parameter
Value
1 Title
LFS-2-114-C
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
300.0
5 Number of Scans
160
6 Acquisition Time
1.3631
7 Acquisition Date
2022-03-16T14:24:16
8 Spectrometer Frequency
100.61
9 Spectral Width
24038.5
Ms
N
F
PMP
O
Ph
2o
f1 (ppm)

Parameter	Value
1 Title	zjj-14-4-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-04-08T10:24:26
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

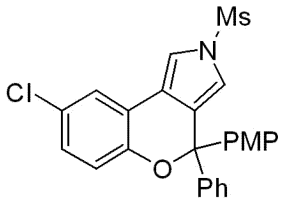


2o

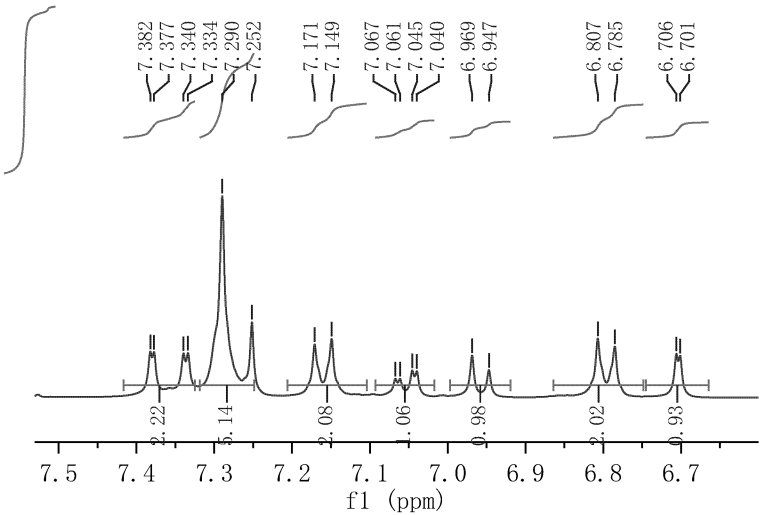


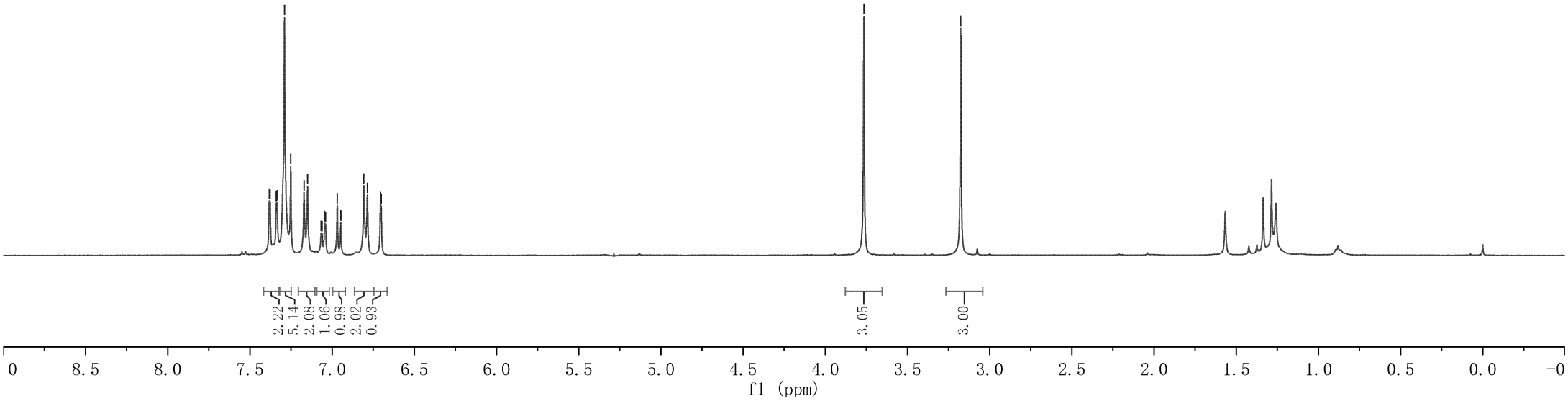


Parameter	Value
1 Title	LFS-2-124-H-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	14
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-01T08:43:14
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2p





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134.91
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128.04
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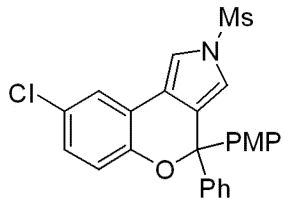
127.45
126.93
123.15
120.35
120.21
120.19
117.77
113.81
113.34
83.28
77.32
77.00
76.68
55.19
42.96

Parameter	Value
1 Title	LFS-2-124-C-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	91
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-01T08:45:37
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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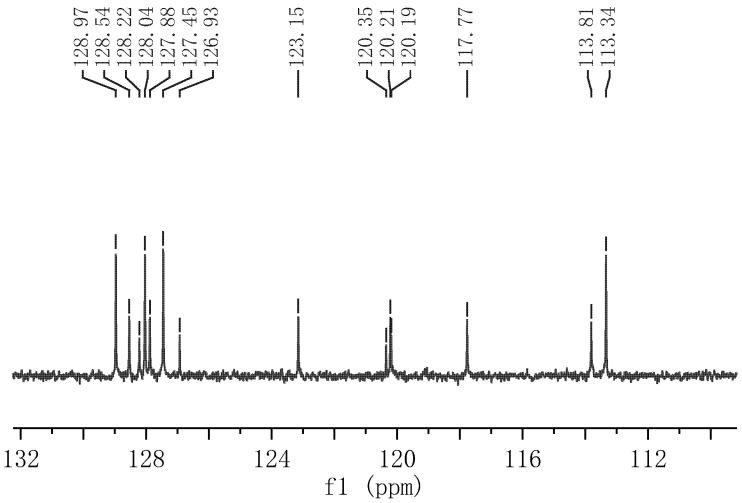
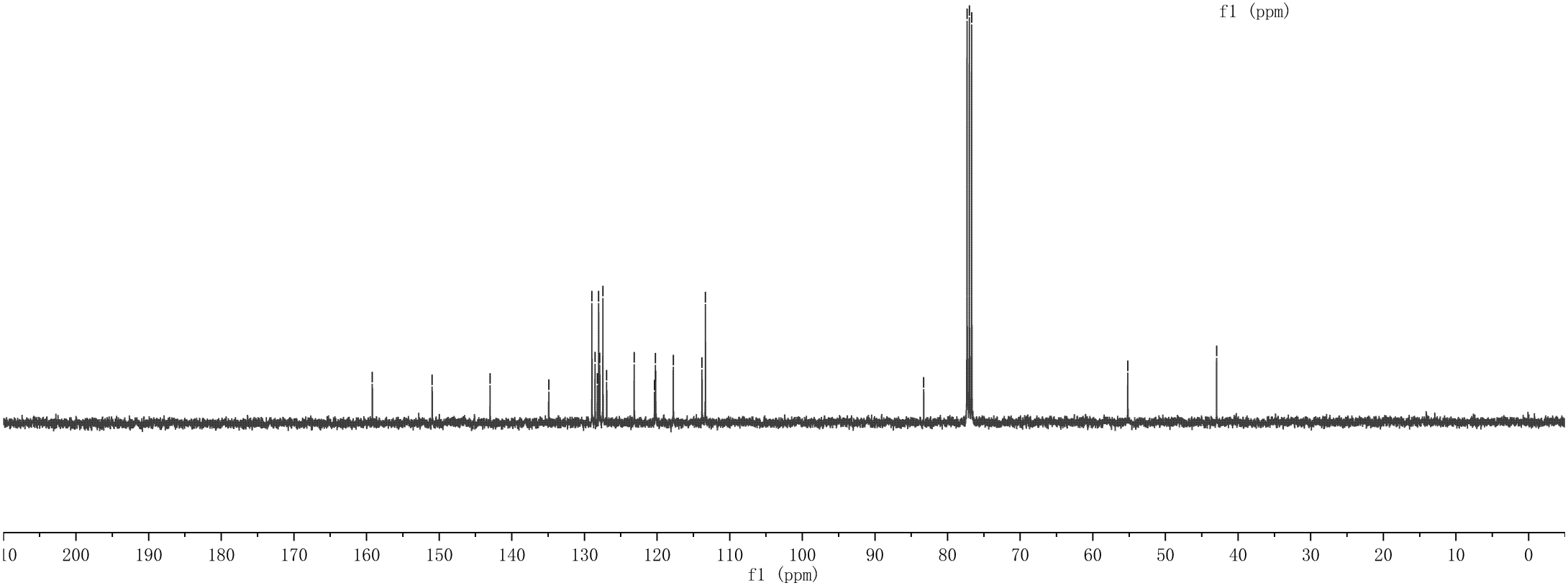
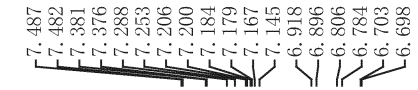
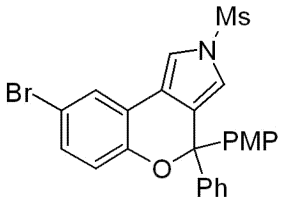






Parameter	Value
1 Title	ZJJ-13-206-4-Br-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-03T17:02:16
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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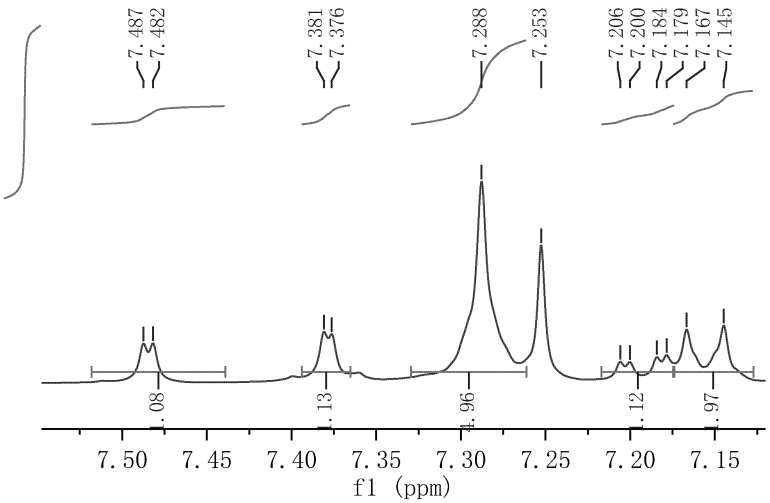

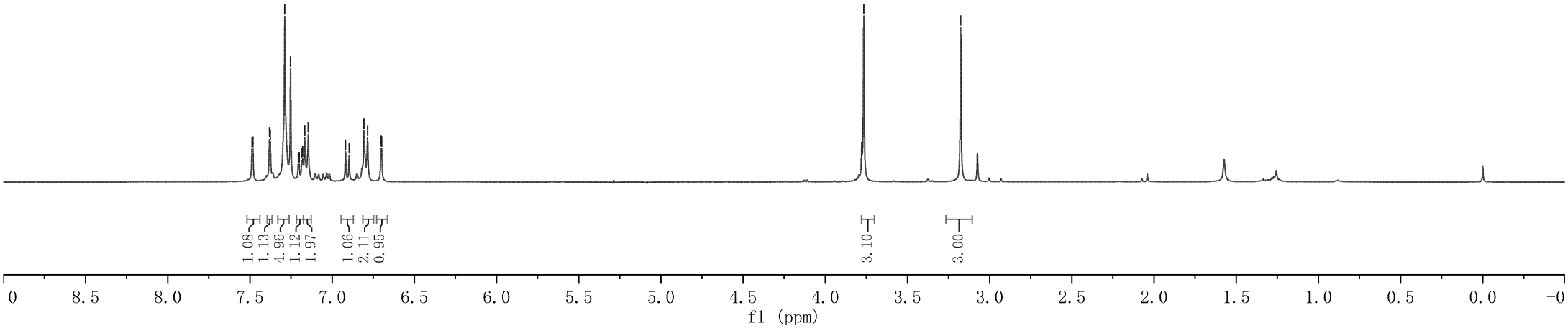

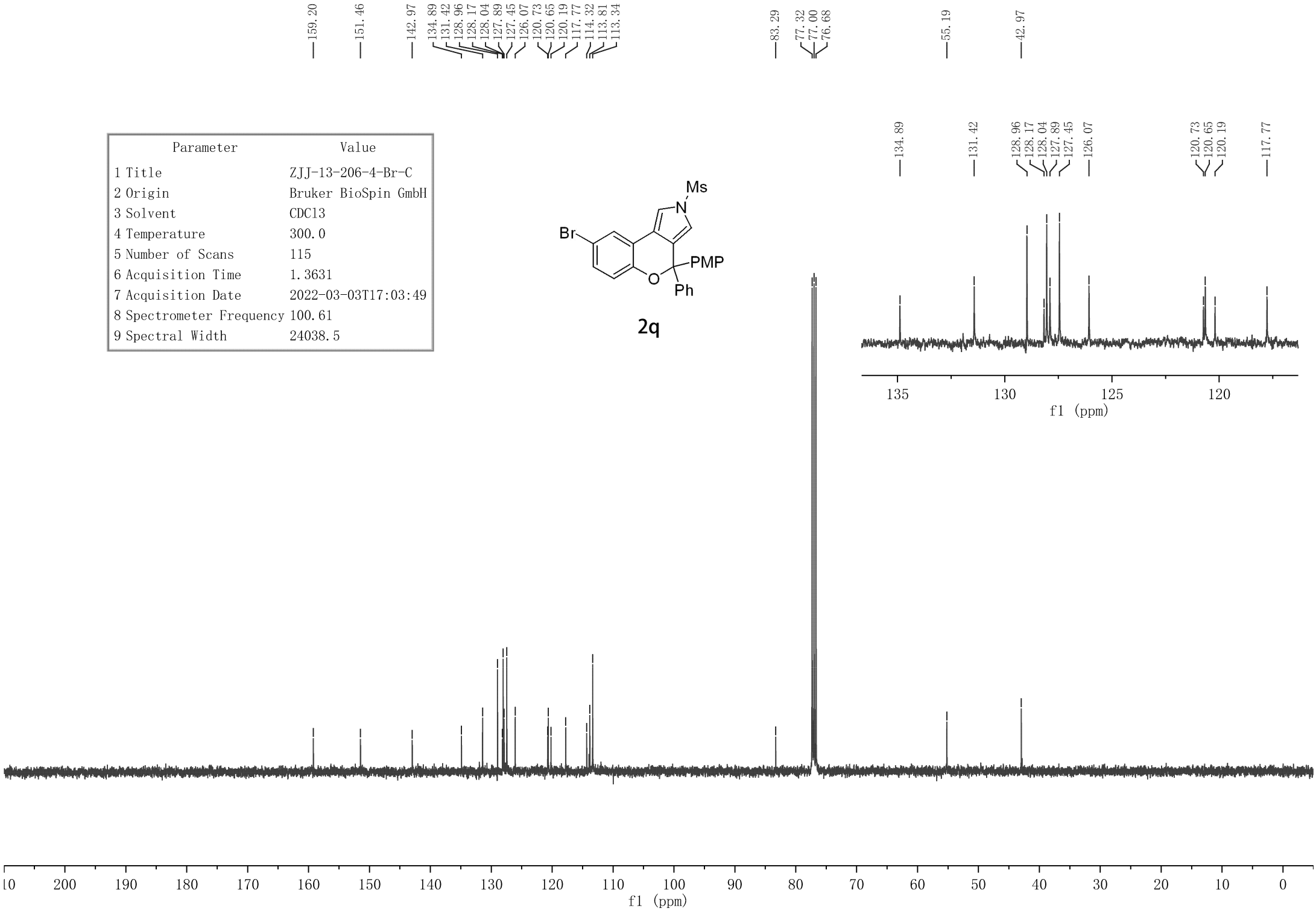
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134.89
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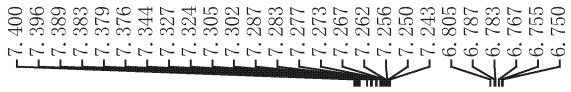
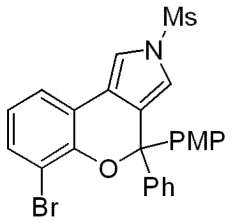
128.96
128.17
128.04
127.89
127.45
126.07
120.73
120.65
120.19
117.77
114.32
113.81
113.34
83.29
77.32
77.00
76.68
55.19
42.97
Parameter Value
1 Title ZJJ-13-206-4-Br-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 115
6 Acquisition Time 1.3631
7 Acquisition Date 2022-03-03T17:03:49
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Br
PMP
O
Ph
2q
f1 (ppm)
f1 (ppm)



Parameter	Value
1 Title	zjj-14-4-6-Br-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	13
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-05T09:35:09
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7



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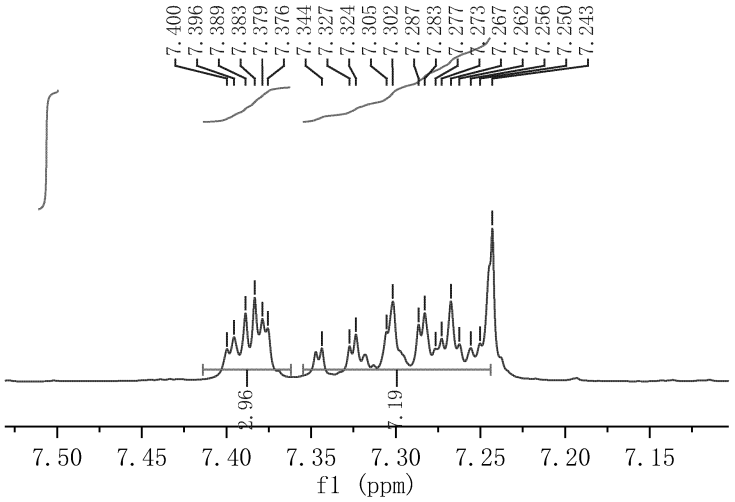

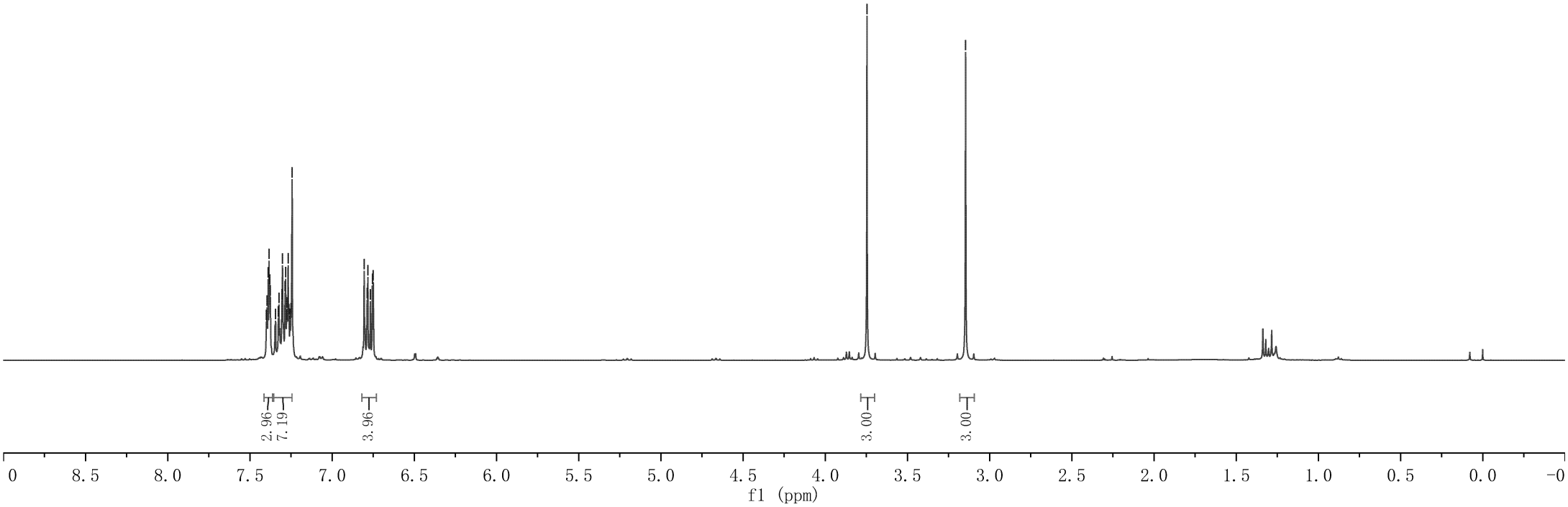

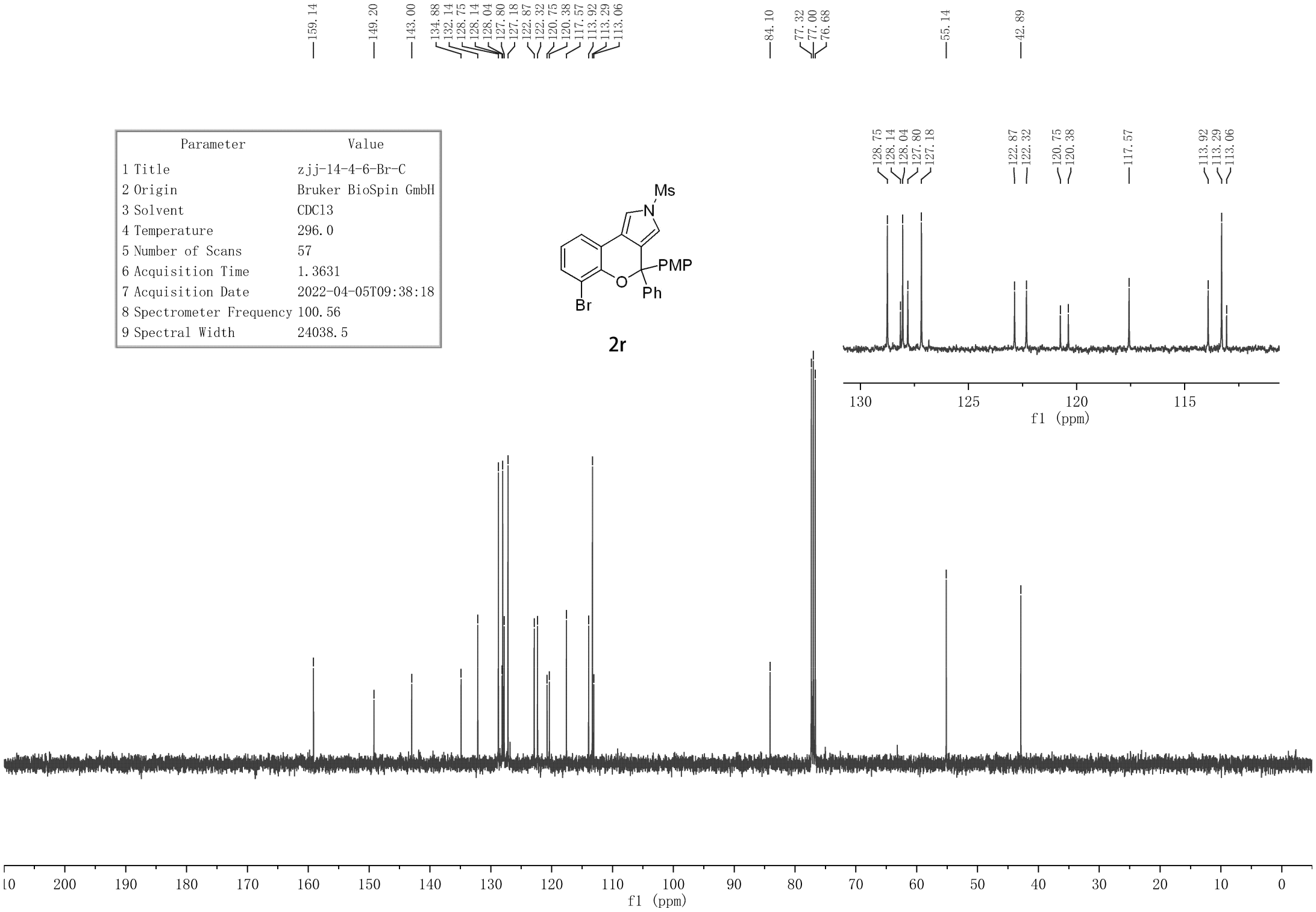
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128.04
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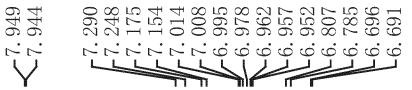
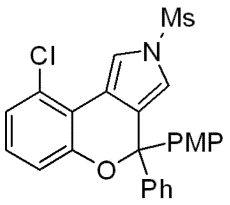
127.18
122.87
122.32
120.75
120.38
117.57
113.92
113.29
113.06
84.10
77.32
77.00
76.68
55.14
42.89
Parameter Value
1 Title zjj-14-4-6-Br-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.0
5 Number of Scans 57
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-05T09:38:18
8 Spectrometer Frequency 100.56
9 Spectral Width 24038.5
Ms
N
PMP
O
Ph
Br
2r
f1 (ppm)
f1 (ppm)



Parameter	Value
1 Title	LFS-2-125-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-04T14:14:31
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



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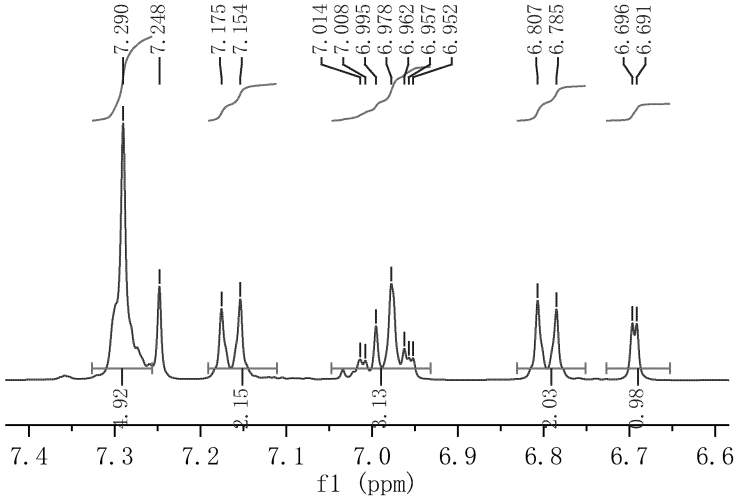

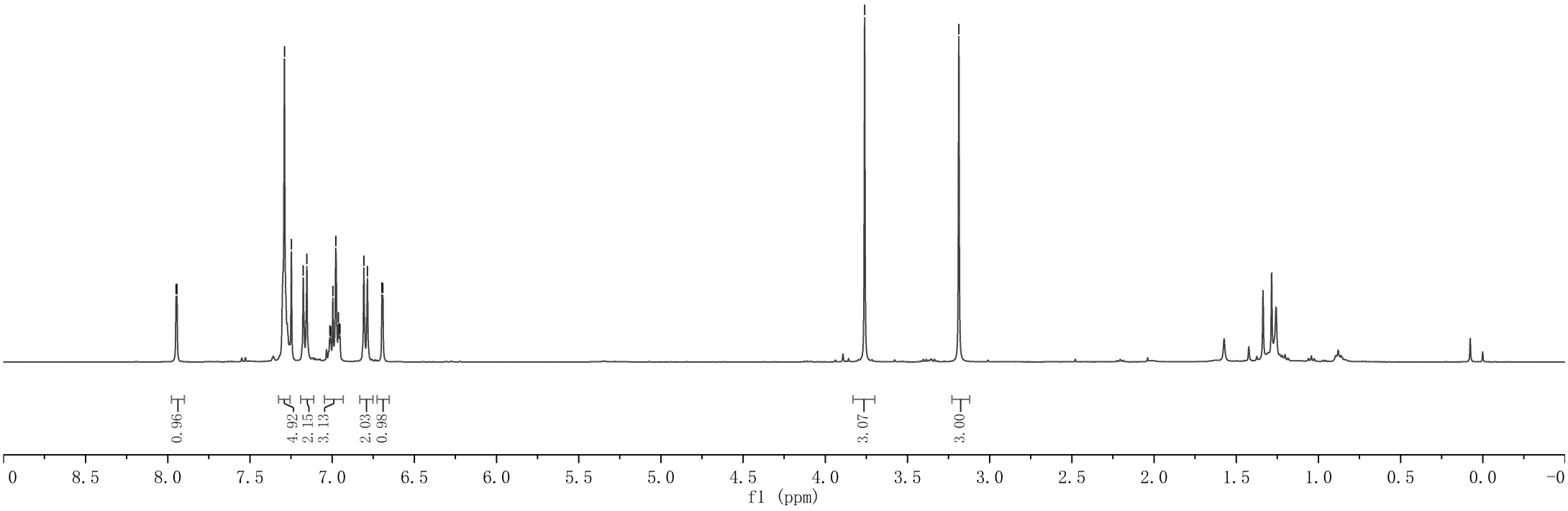

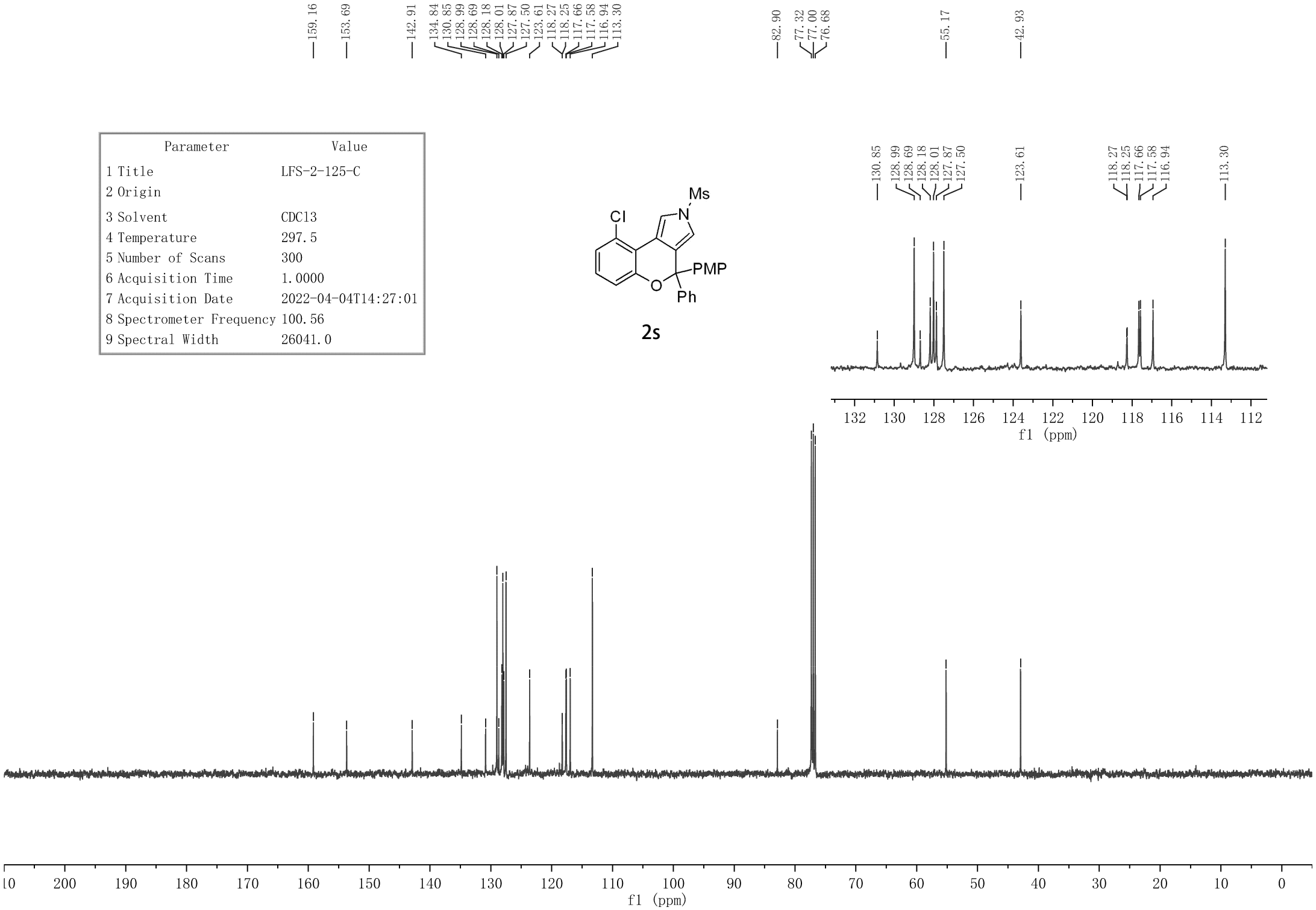
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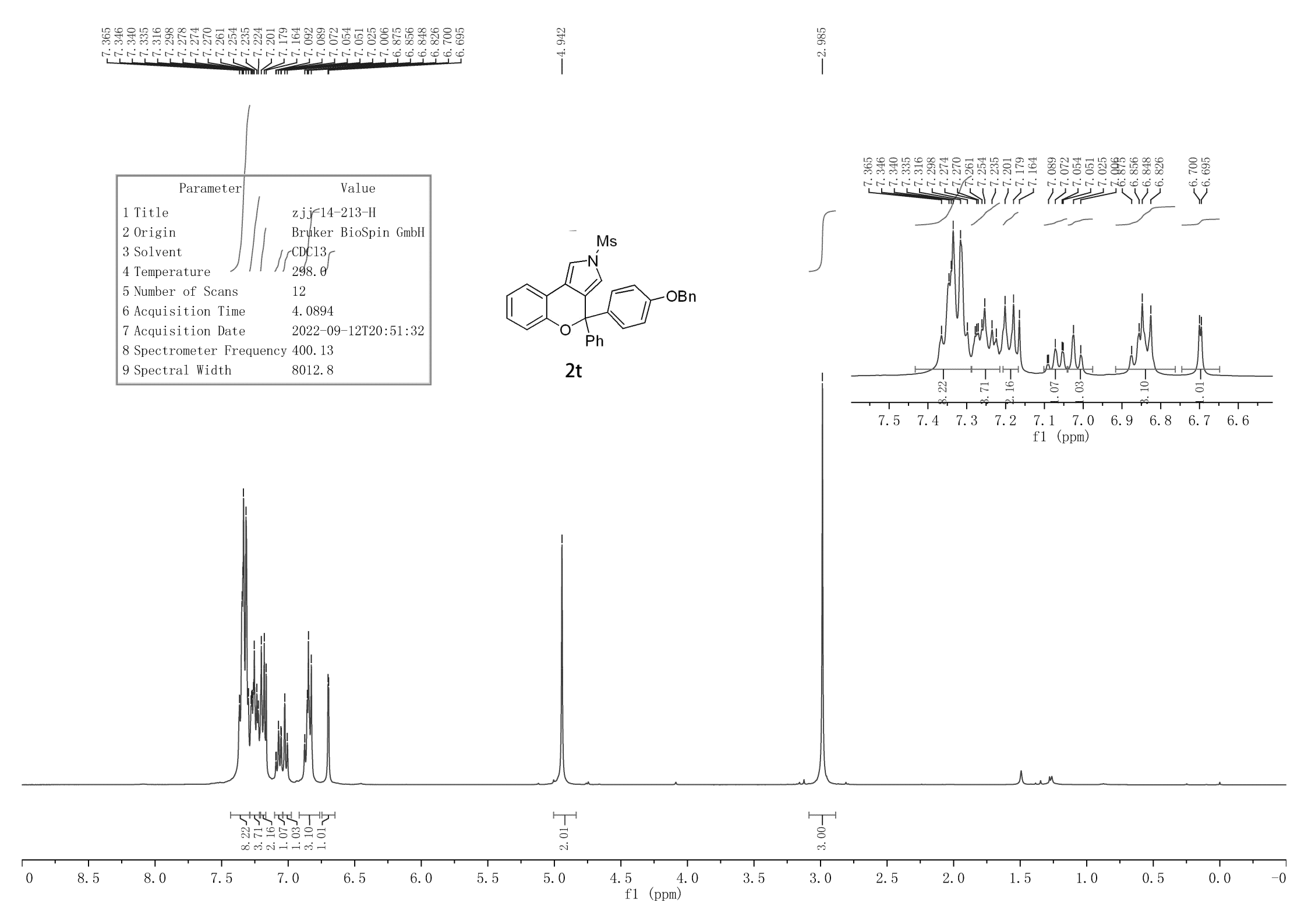
128.99
128.69
128.18
128.01
127.87
127.50
123.61
118.27
118.25
117.66
117.58
116.94
113.30
82.90
77.32
77.00
76.68
55.17
42.93
Parameter Value
1 Title LFS-2-125-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.5
5 Number of Scans 300
6 Acquisition Time 1.0000
7 Acquisition Date 2022-04-04T14:27:01
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Cl
PMP
O
Ph
2s
f1 (ppm)
f1 (ppm)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7.235
7.224
7.201
7.179
7.164
7.092
7.089
7.072
7.054
7.051
7.025
7.006
6.875
6.856
6.848
6.826
6.700
6.695
4.942
2.985
Parameter Value
1 Title zjj-14-213-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 12
6 Acquisition Time 4.0894
7 Acquisition Date 2022-09-12T20:51:32
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
OBn
O
Ph
2t
8.22
3.71
2.16
1.07
1.03
3.10
1.01
2.01
3.00
f1 (ppm)

158.28
152.30
143.28
136.72
135.54
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128.74
128.46
128.31
127.91
127.89
127.65
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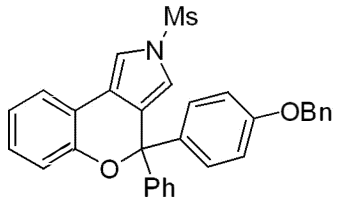
127.40
123.31
122.00
121.10
118.78
118.61
117.52
114.07
113.30
82.85
77.32
77.00
76.68
69.87
42.55

Parameter	Value
1 Title	zjj-14-213-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	18
6 Acquisition Time	1.3631
7 Acquisition Date	2022-09-12T20:54:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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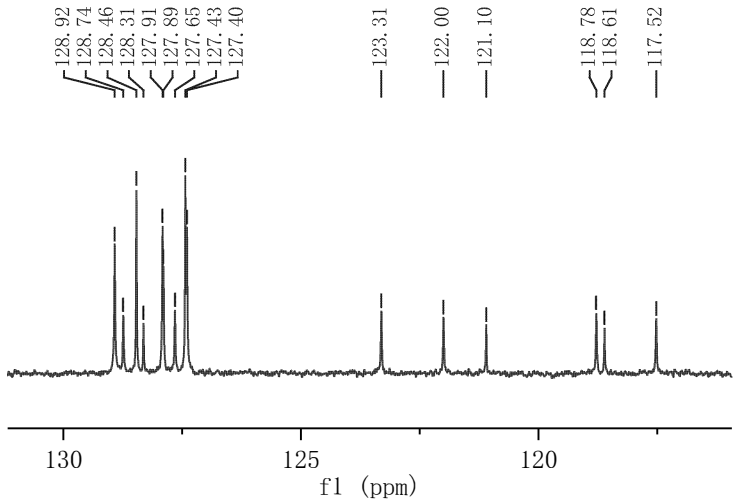
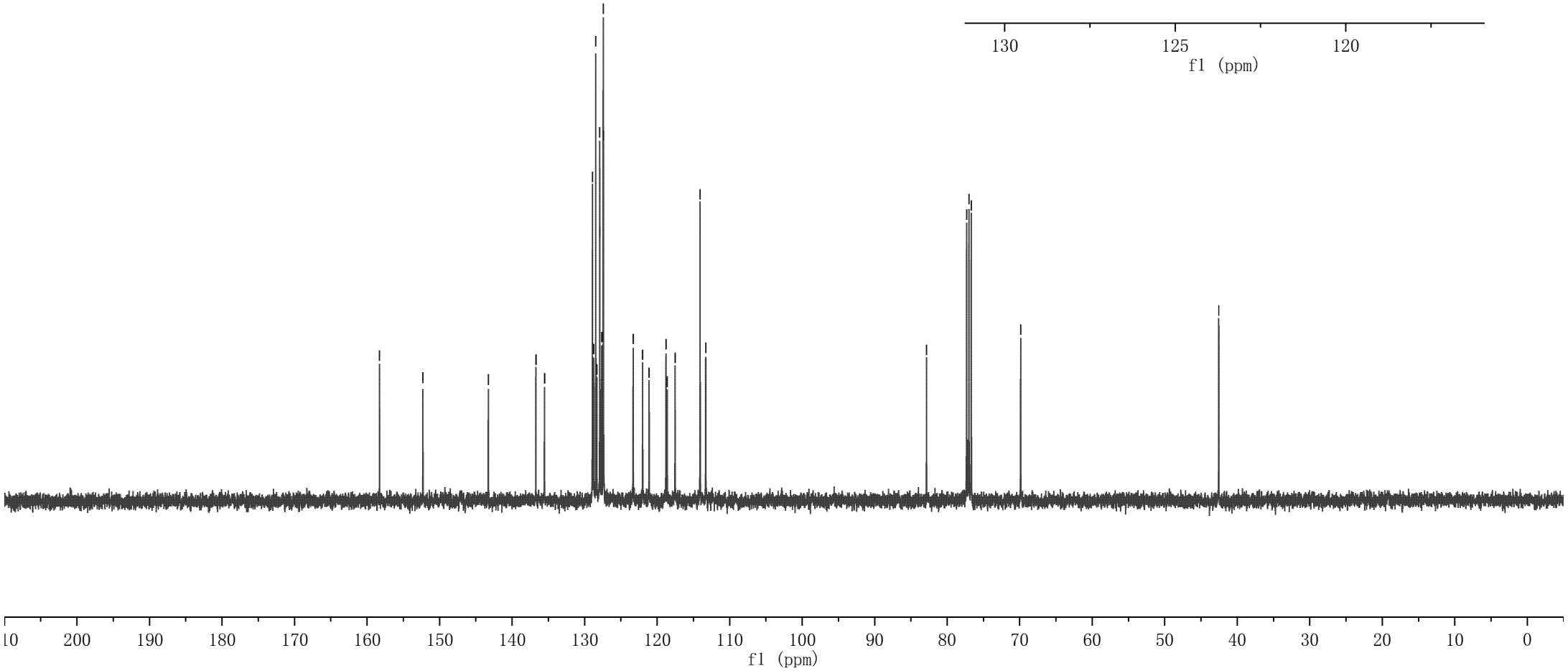
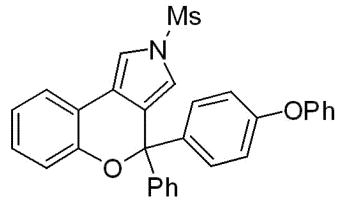
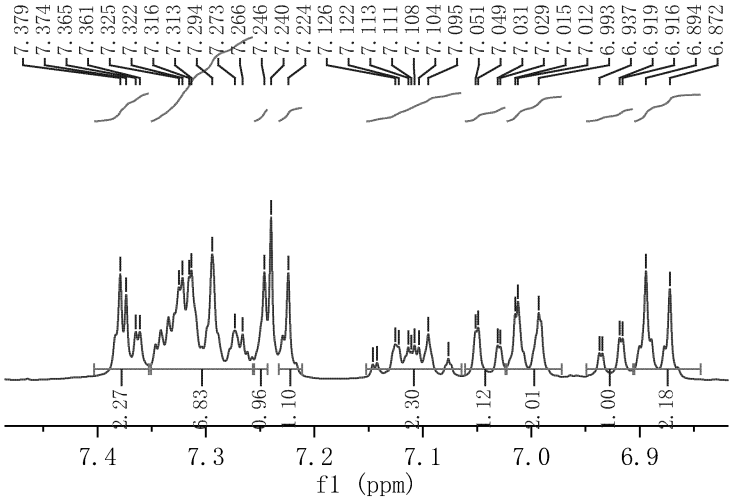


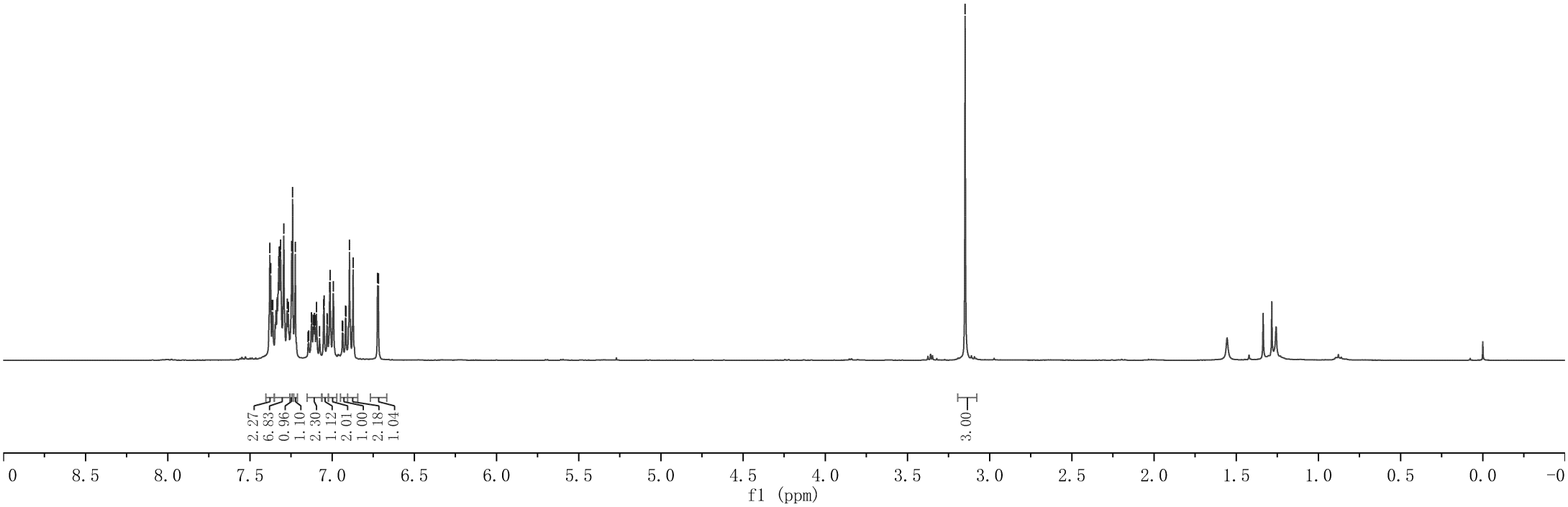


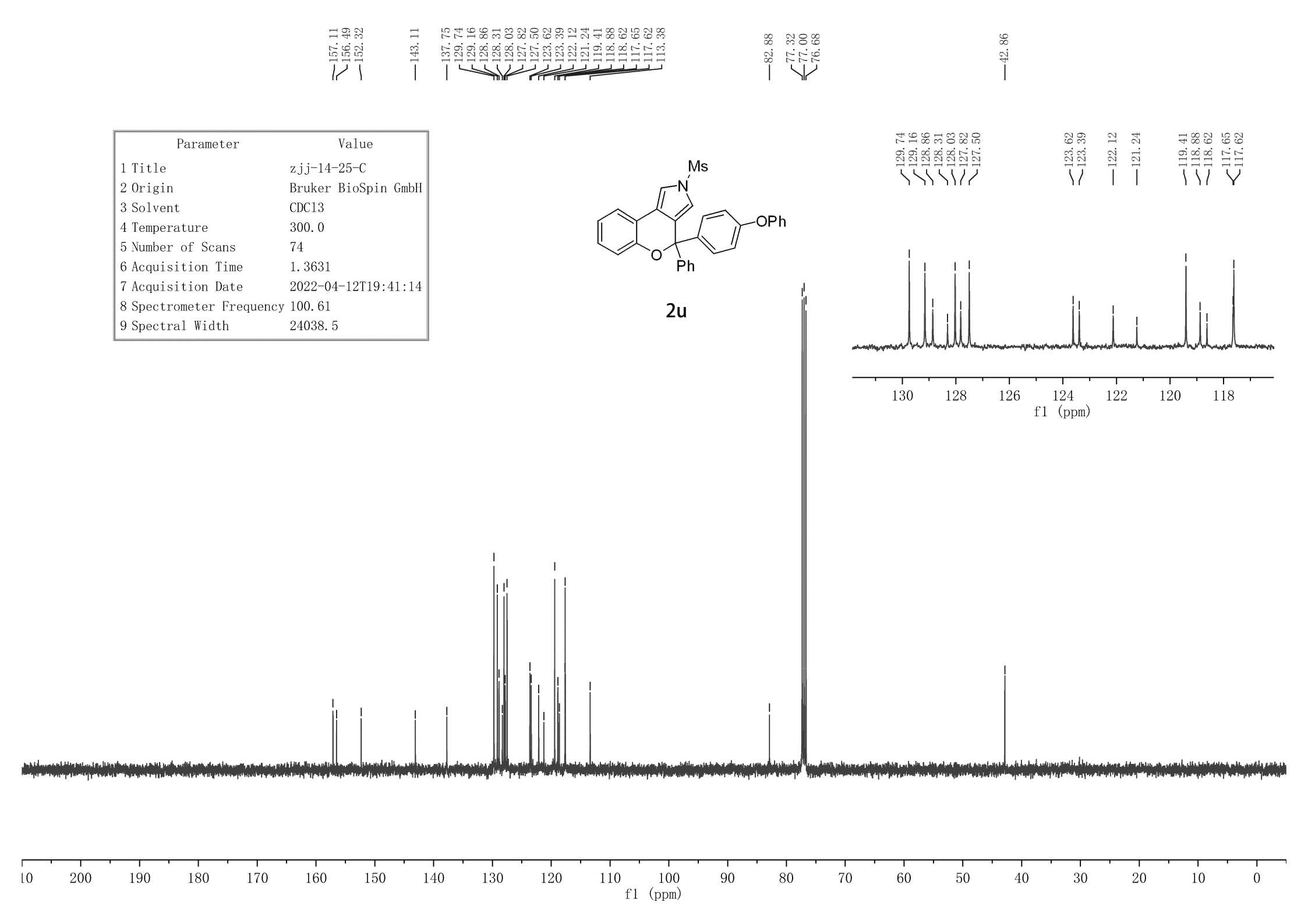
Parameter	Value
1 Title	zjj-14-25-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-12T19:39:18
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2u



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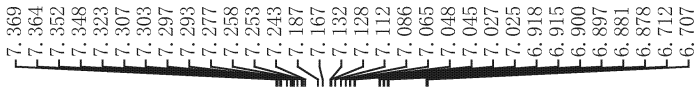
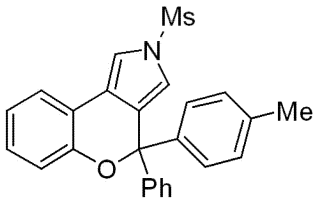
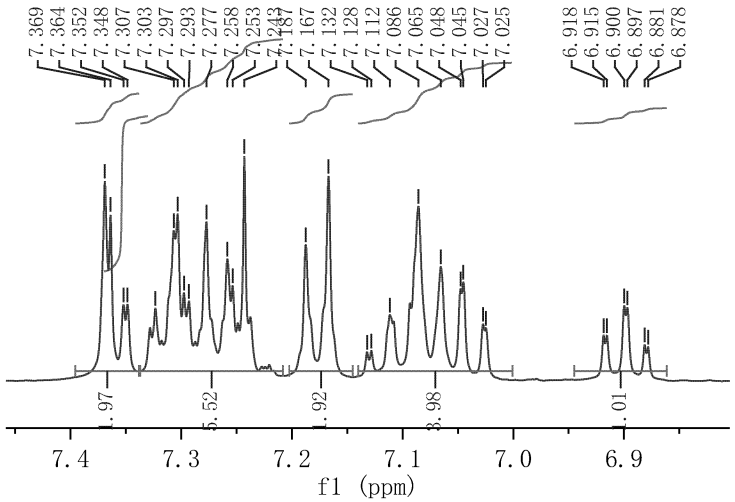
127.82
127.50
123.62
123.39
122.12
121.24
119.41
118.88
118.62
117.65
117.62
113.38
82.88
77.32
77.00
76.68
42.86
Parameter Value
1 Title zjj-14-25-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 74
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-12T19:41:14
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
OPh
O
Ph
2u
f1 (ppm)
f1 (ppm)

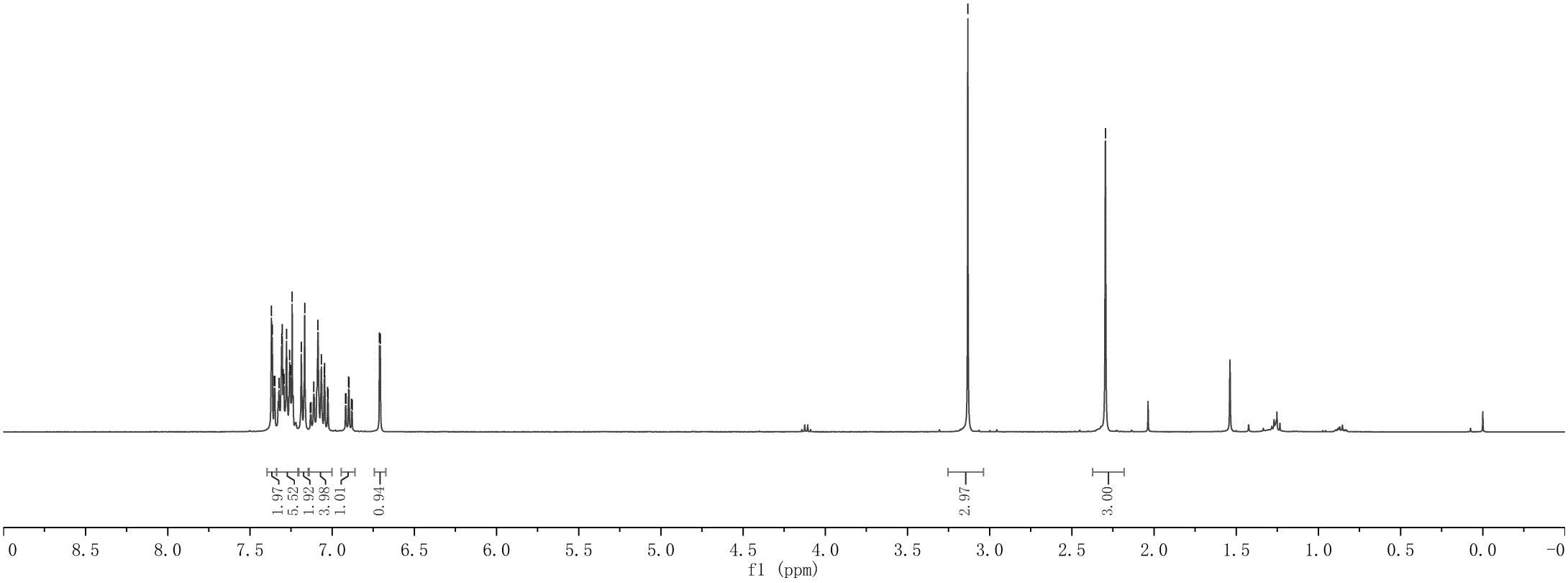


Parameter	Value
1 Title	zjj-14-24-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-12T19:29:46
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



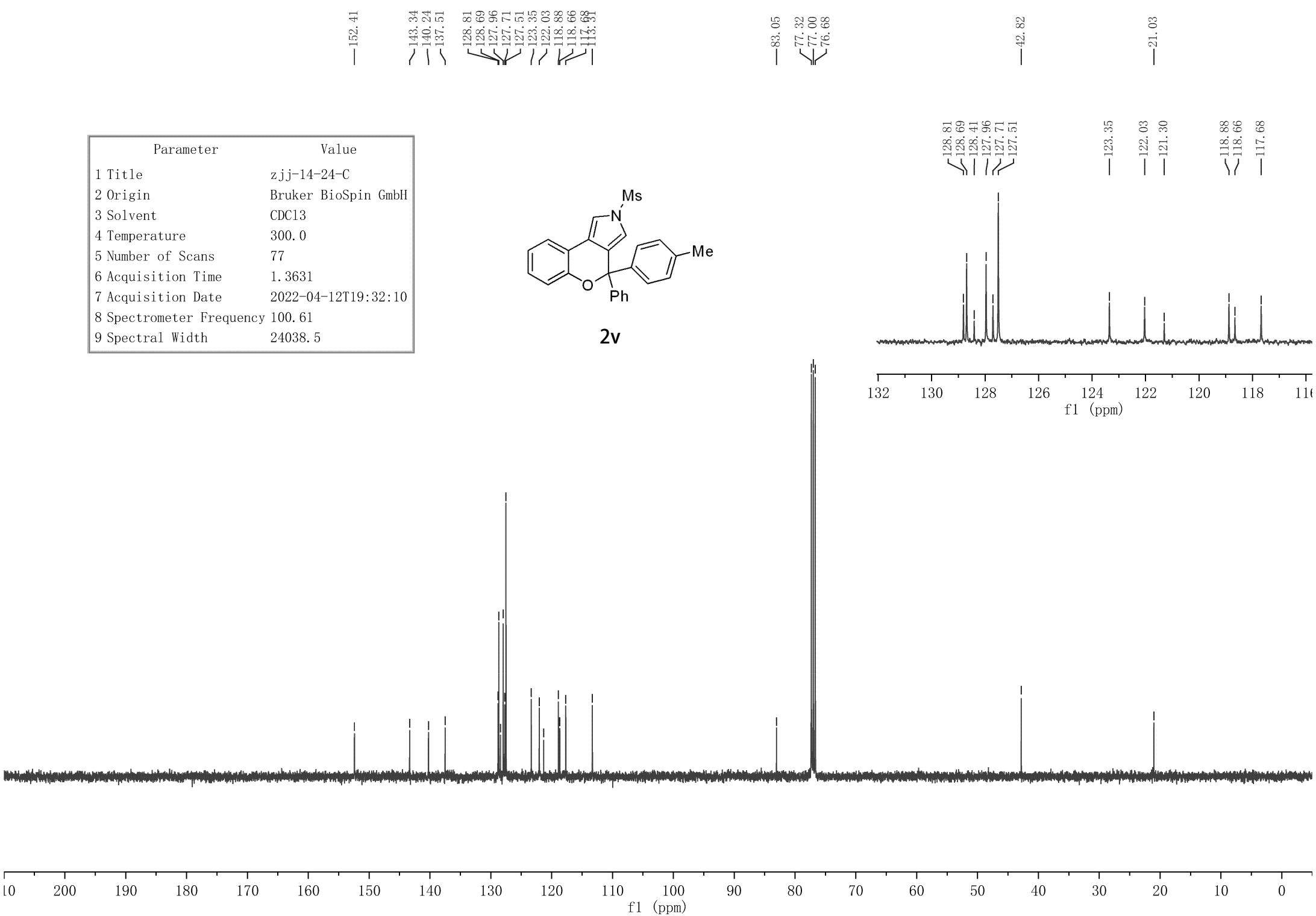
2v

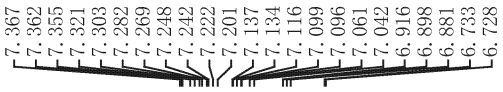




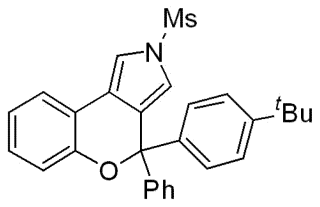
Parameter	Value
1 Title	zjj-14-24-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	77
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-12T19:32:10
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

2v

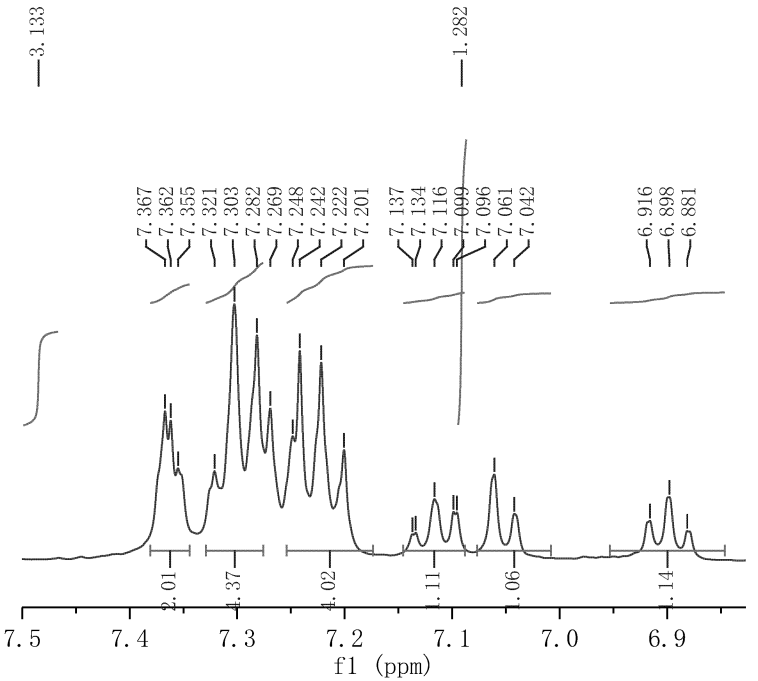


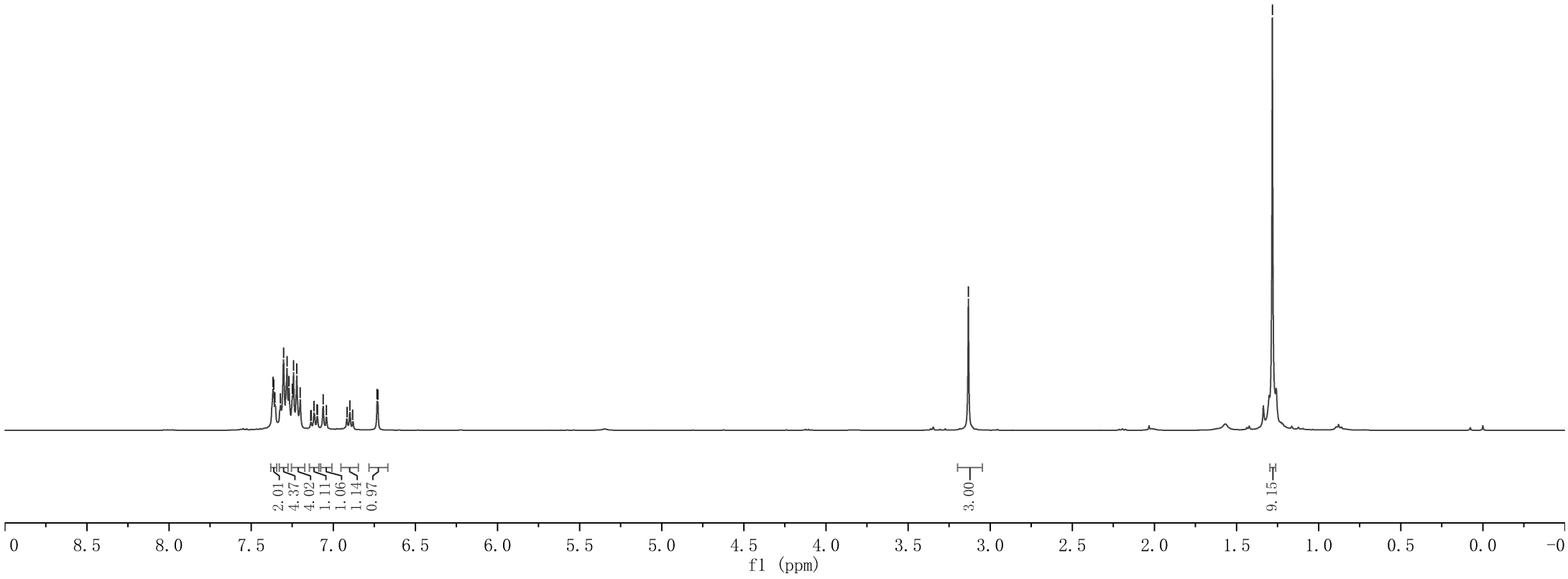


Parameter	Value
1 Title	LFS-2-181-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	18
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-25T09:36:20
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



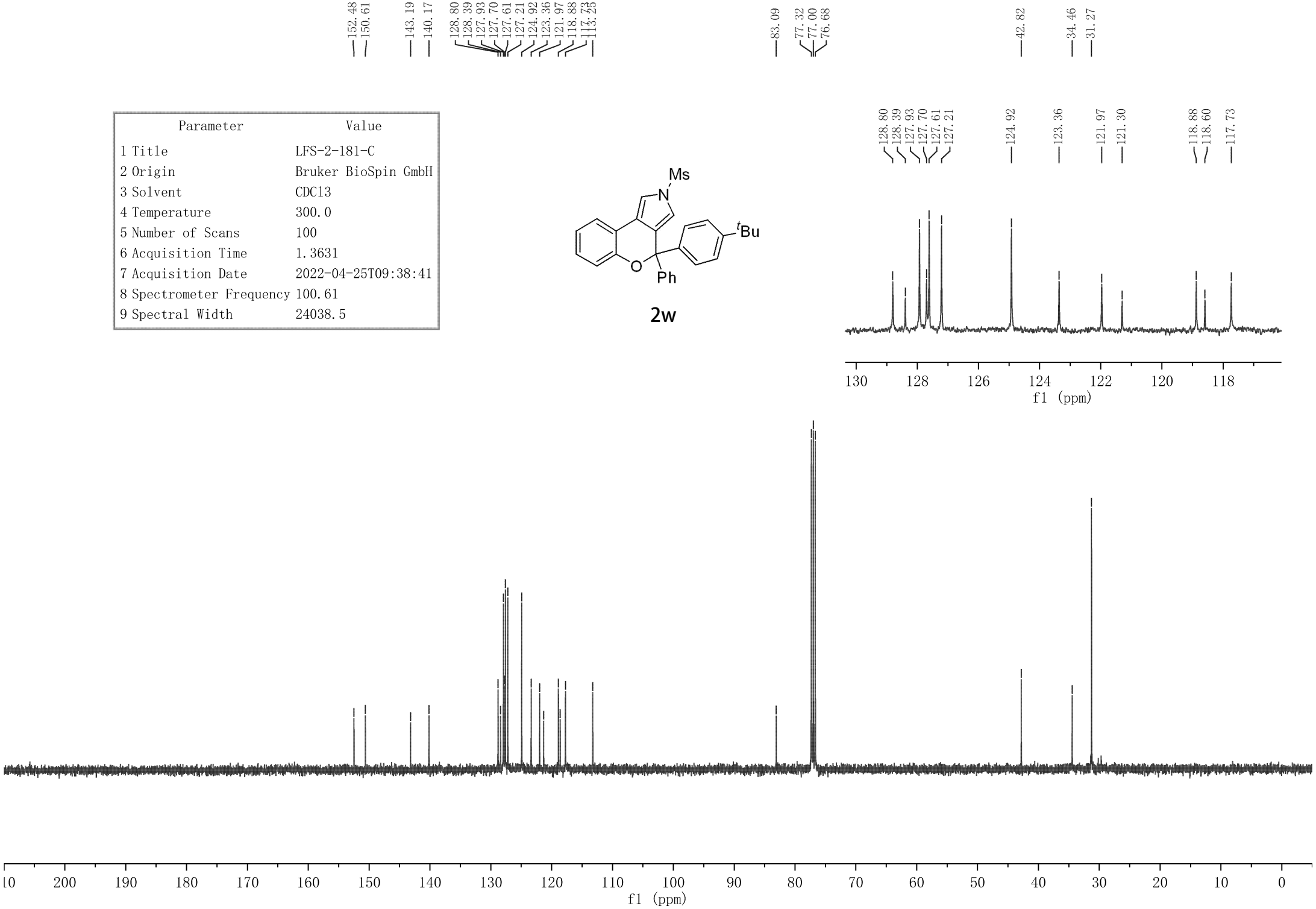
2w

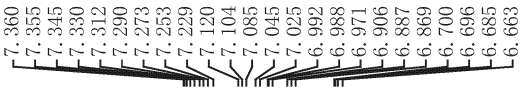




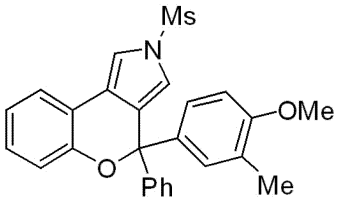
Parameter	Value
1 Title	LFS-2-181-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	100
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-25T09:38:41
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

2w





Parameter	Value
1 Title	LFS-2-211-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	22
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-02T19:29:05
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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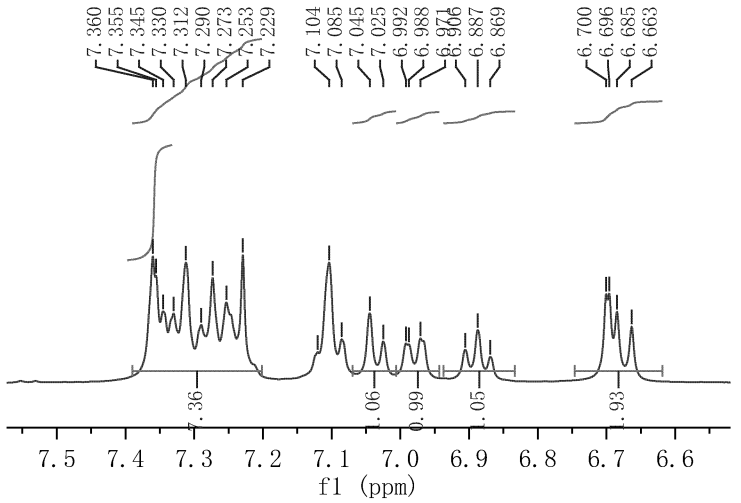

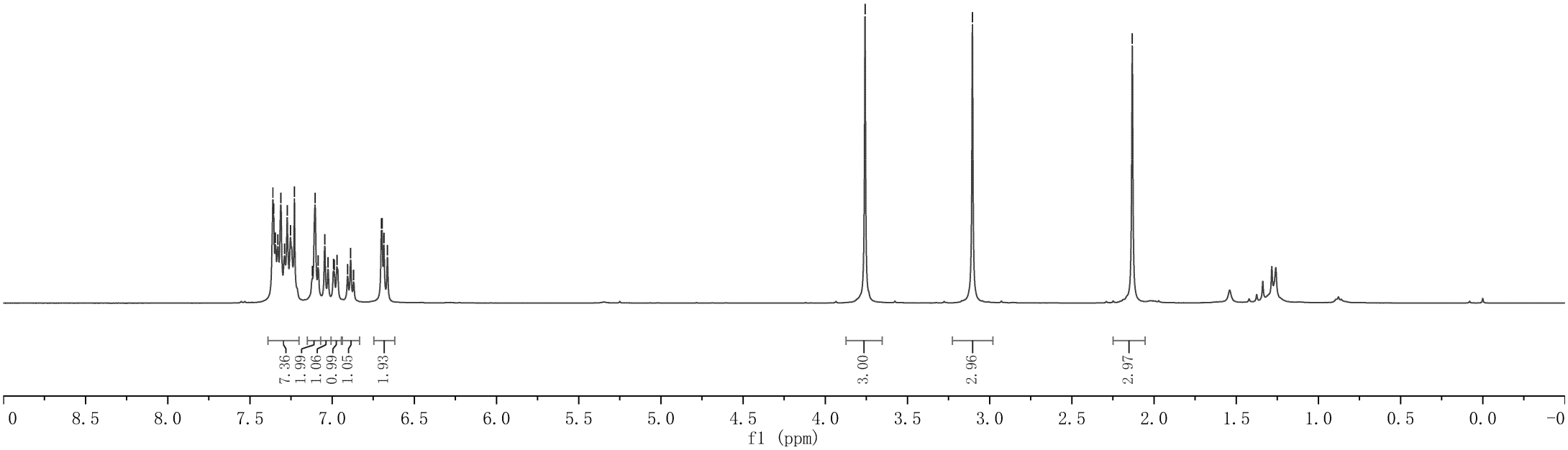

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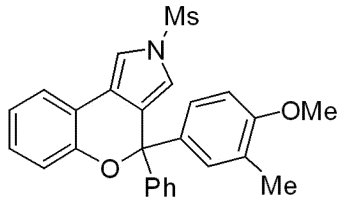
108.94
83.00
77.32
77.00
76.68
55.19
42.75
16.40

Parameter	Value
1 Title	LFS-2-211-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDC13
4 Temperature	300.0
5 Number of Scans	82
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-02T19:31:52
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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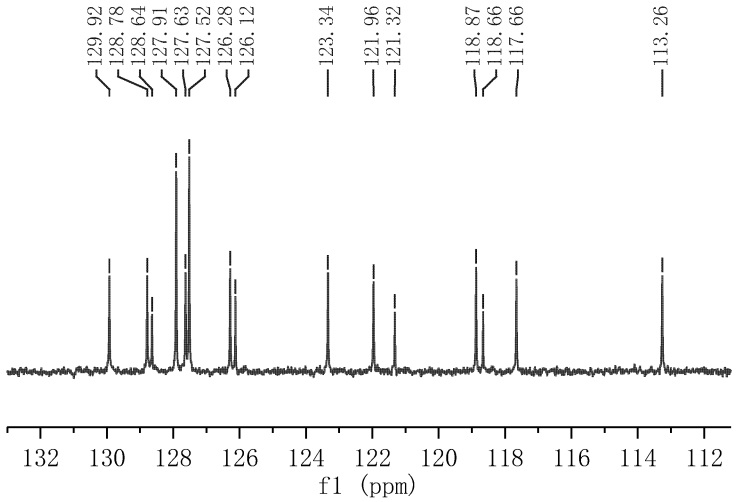
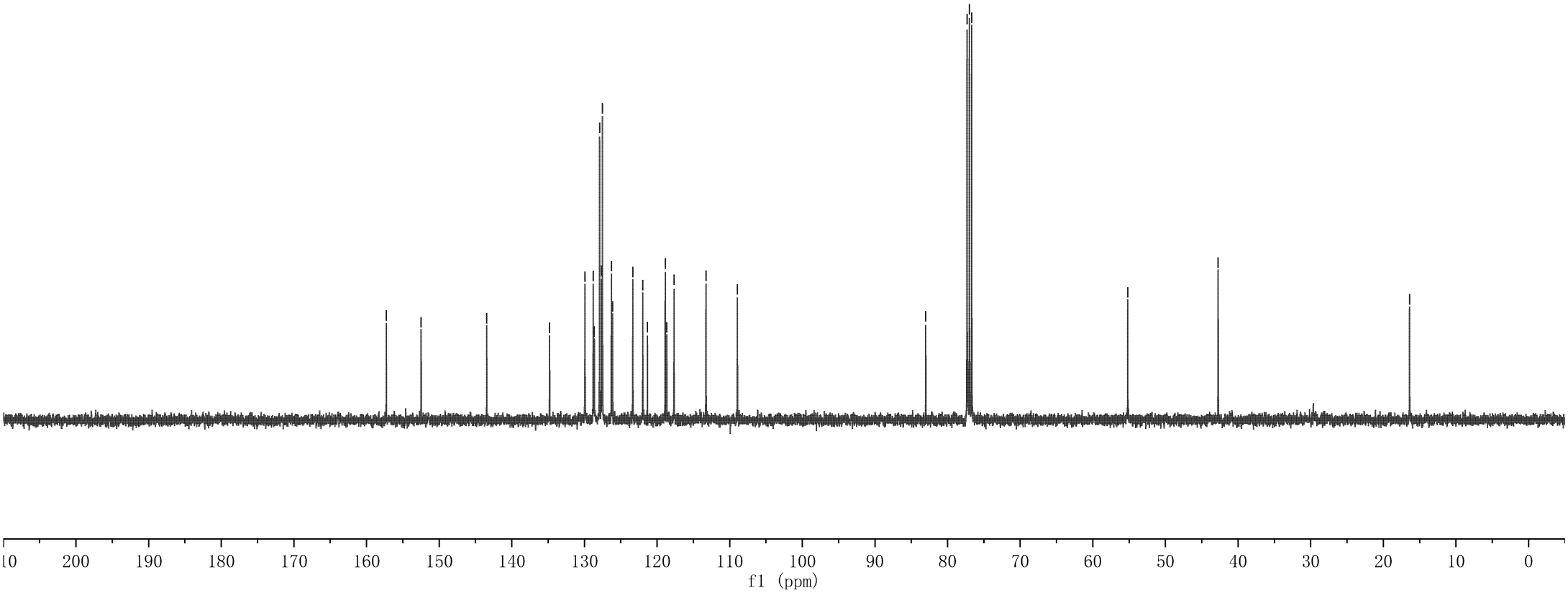
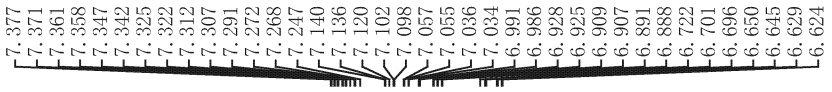
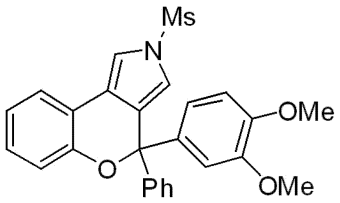






Parameter	Value
1 Title	LFS-2-177-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	14
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-22T15:08:22
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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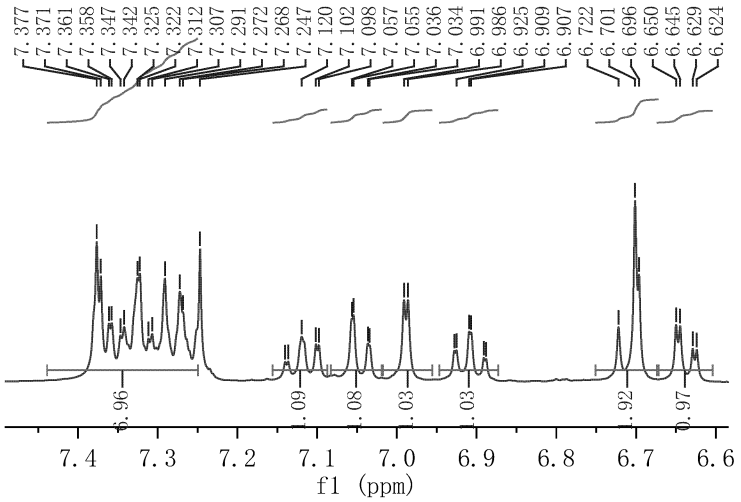
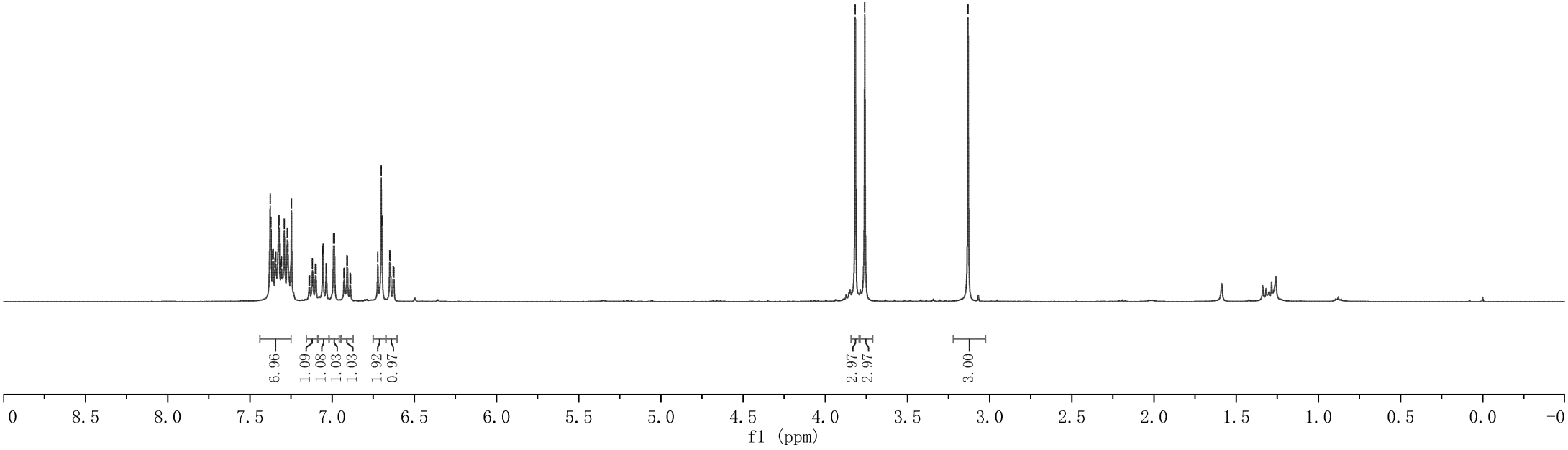
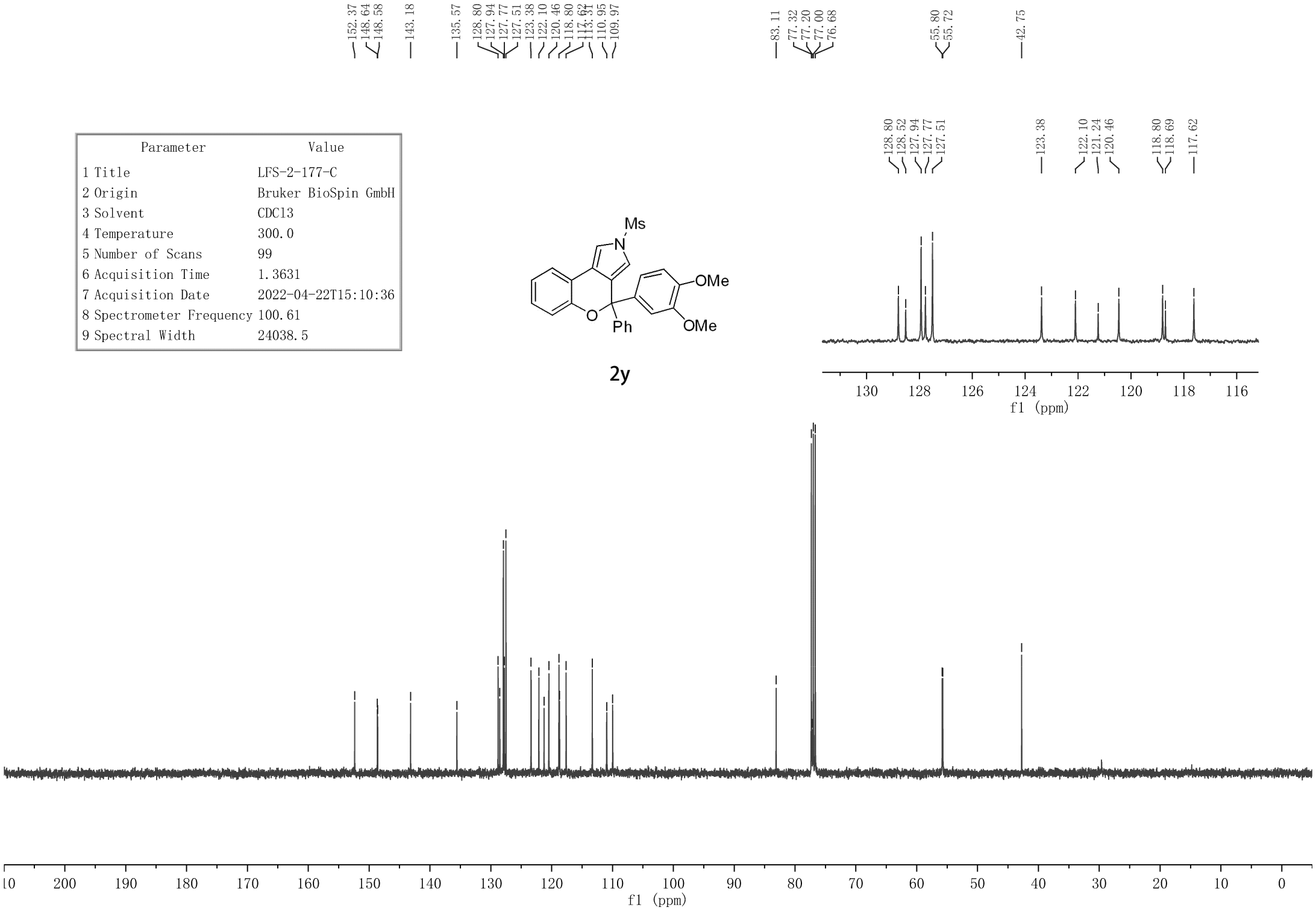


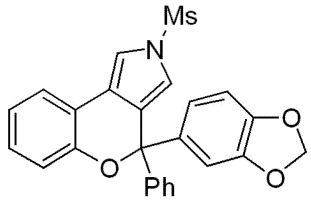


Parameter	Value
1 Title	LFS-2-177-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	99
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-22T15:10:36
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

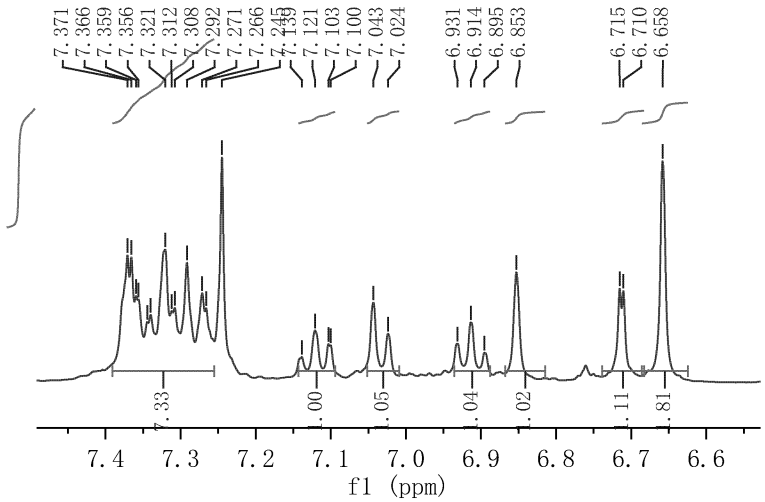
2y

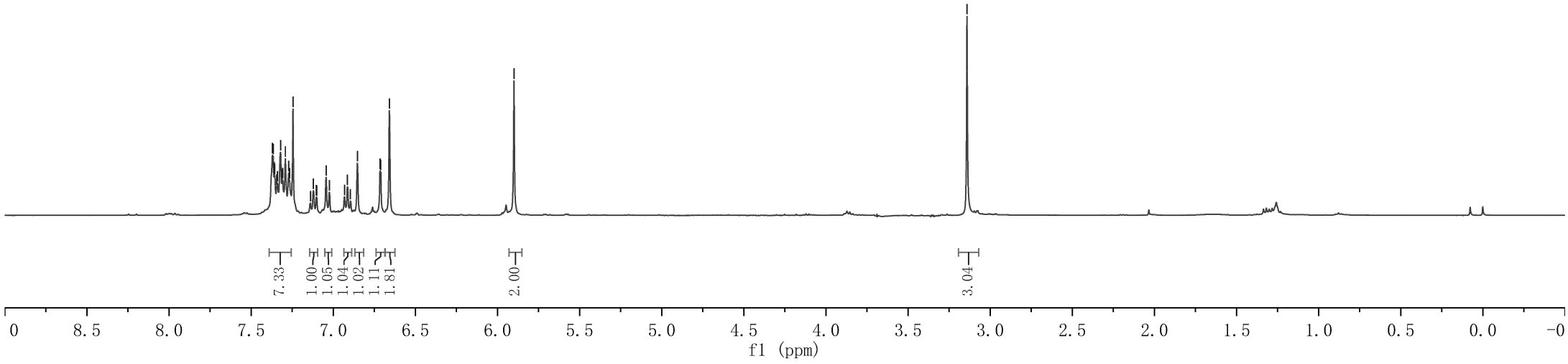


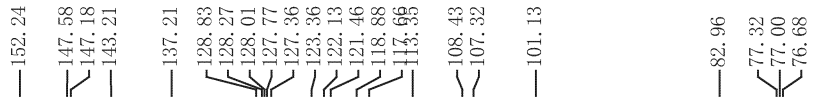
Parameter	Value
1 Title	zjj-14-34-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-16T21:07:37
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



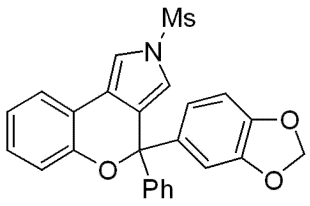
2z







Parameter	Value
1 Title	zjj-14-34-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	48
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-16T21:08:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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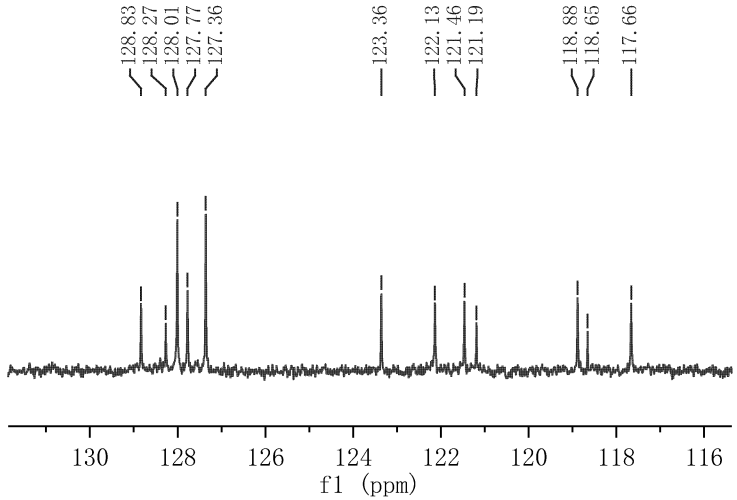
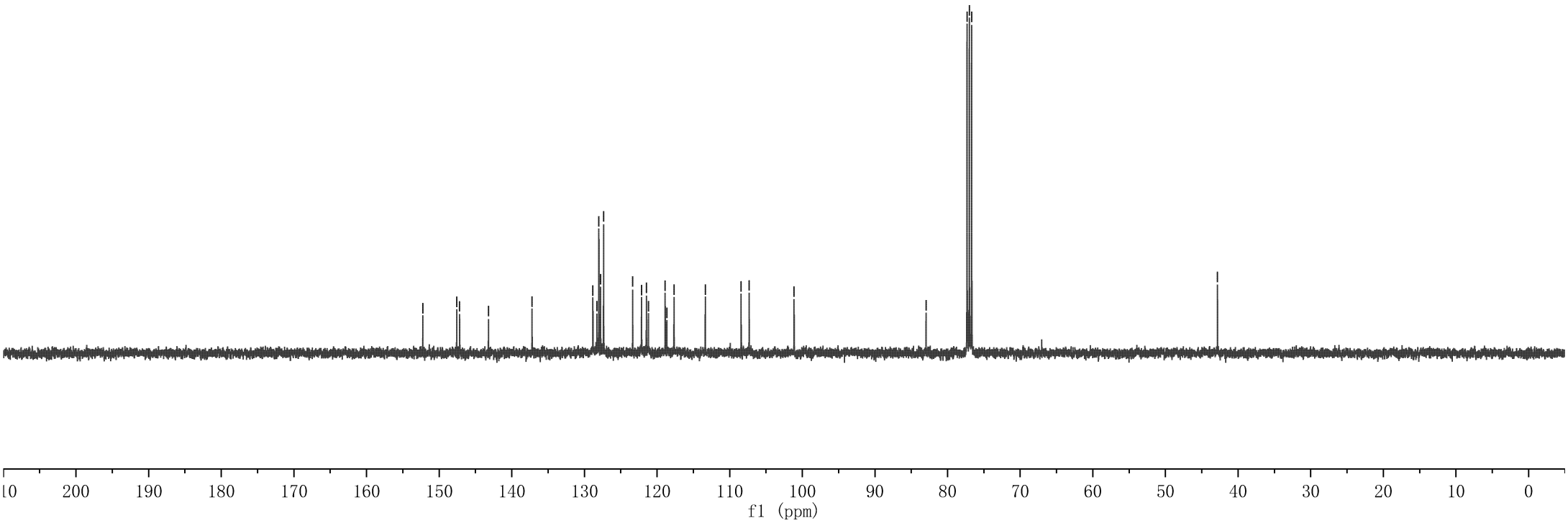
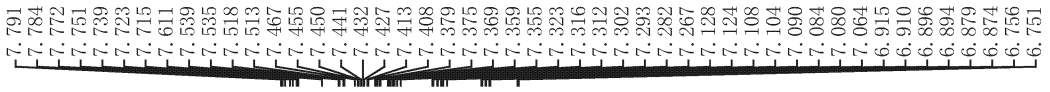
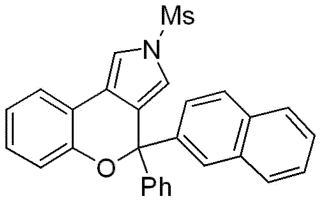






Parameter	Value
1 Title	zjj-14-40-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-22T21:54:05
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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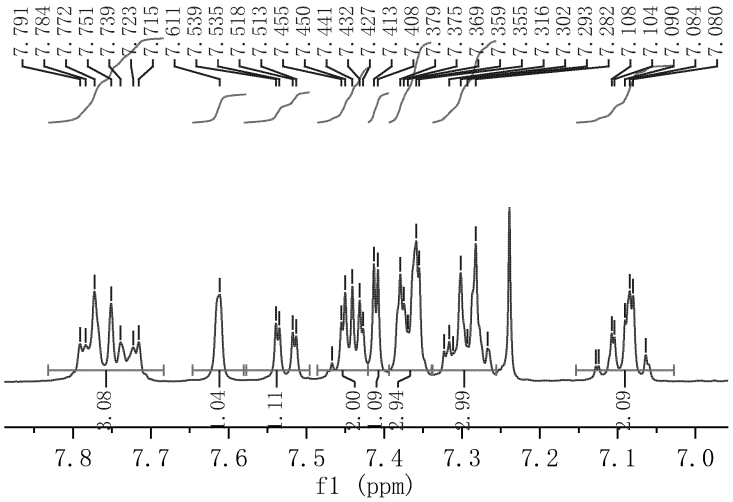
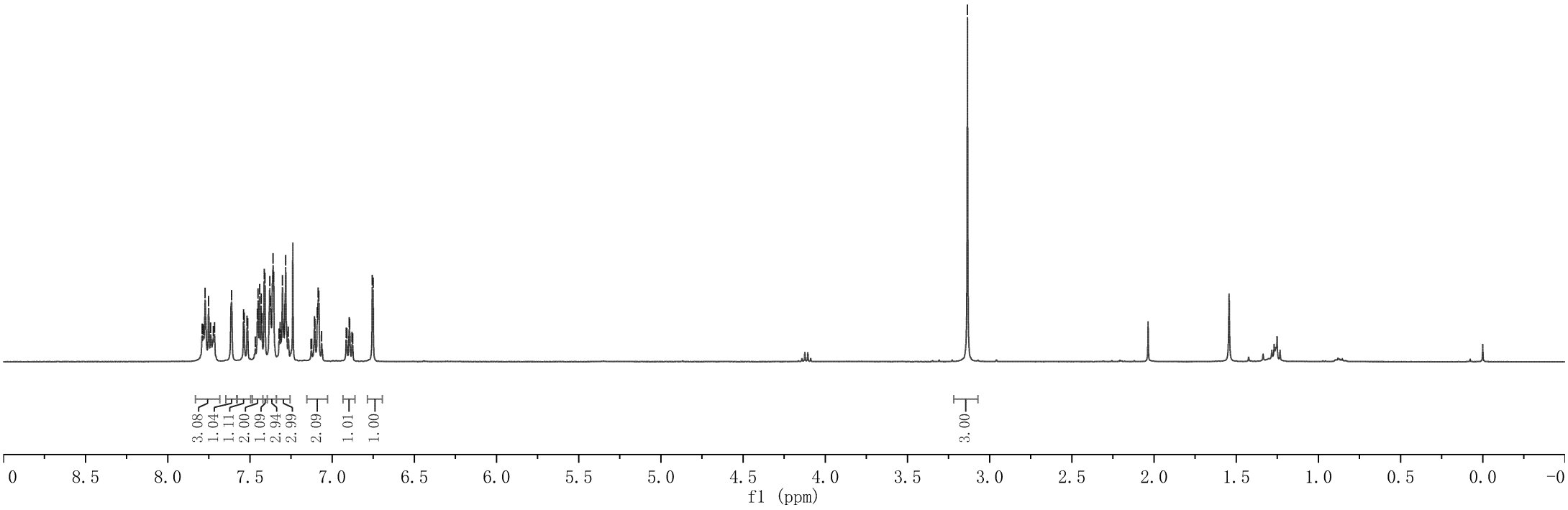
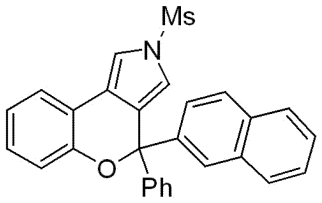
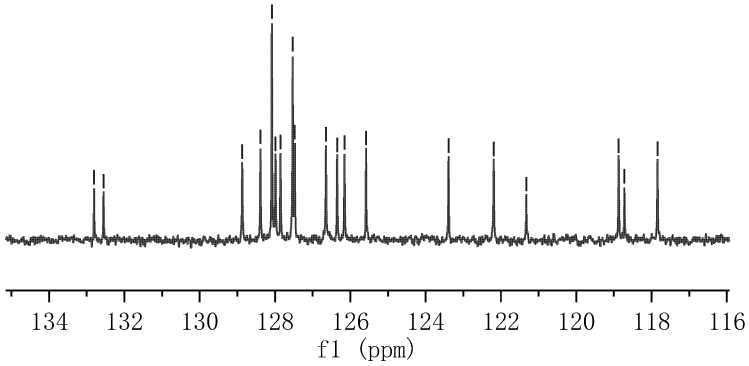


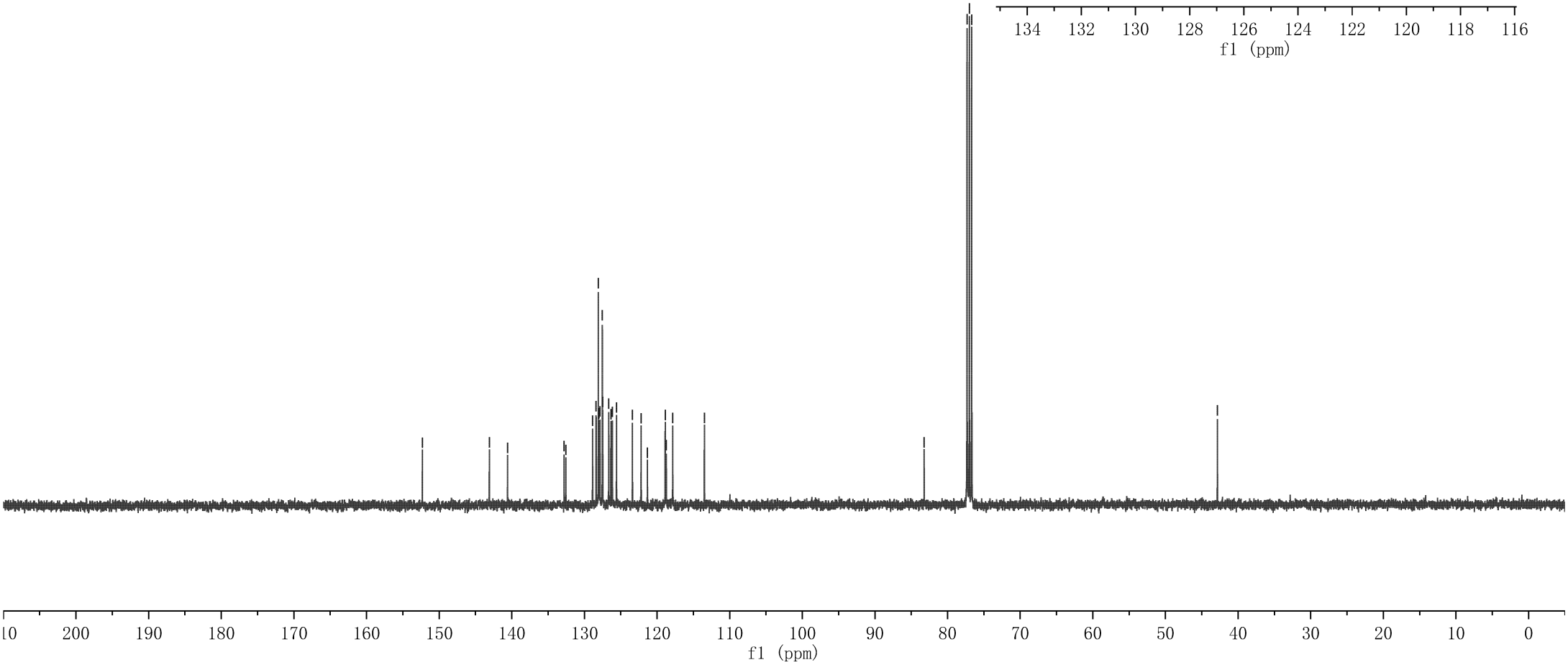


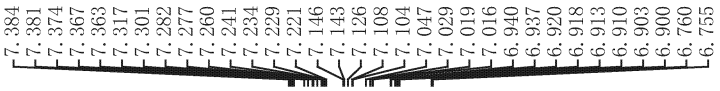
Parameter	Value
1 Title	zjj-14-40-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	117
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-22T21:57:27
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



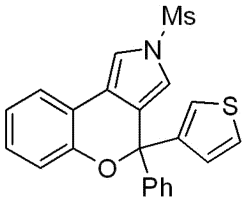
2aa







Parameter	Value
1 Title	LFS-2-179-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	20
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-25T09:25:19
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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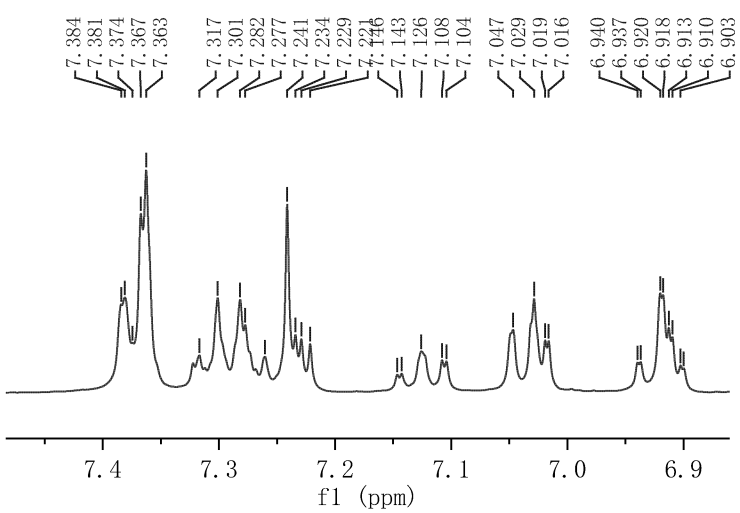

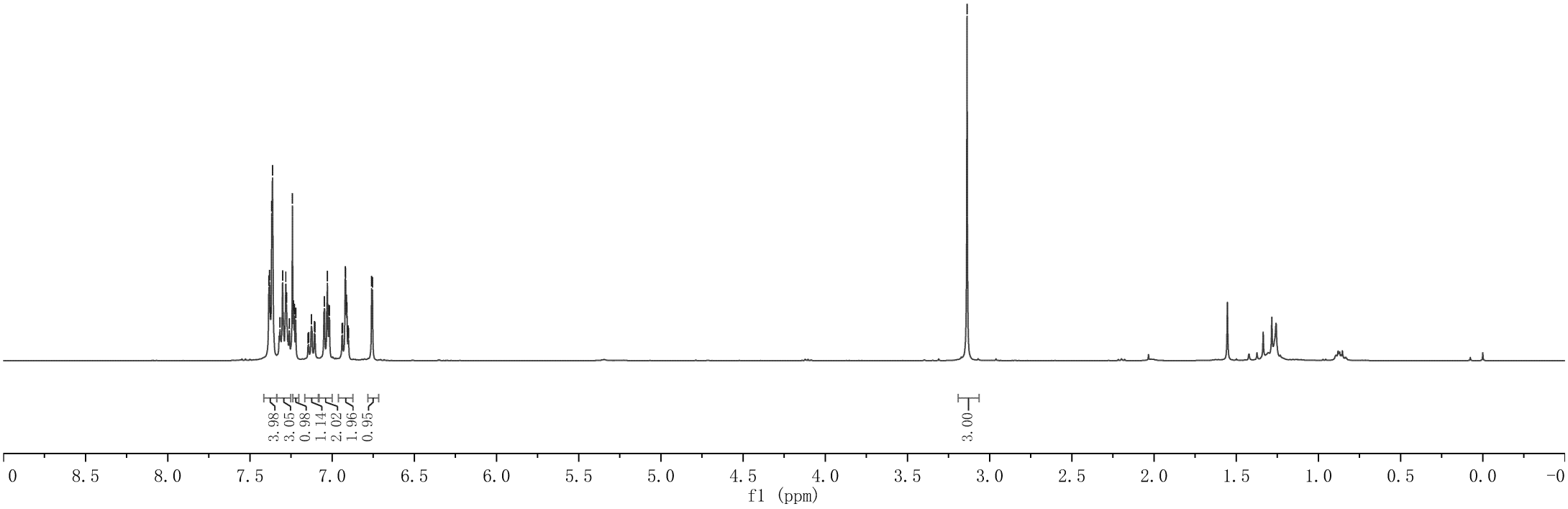

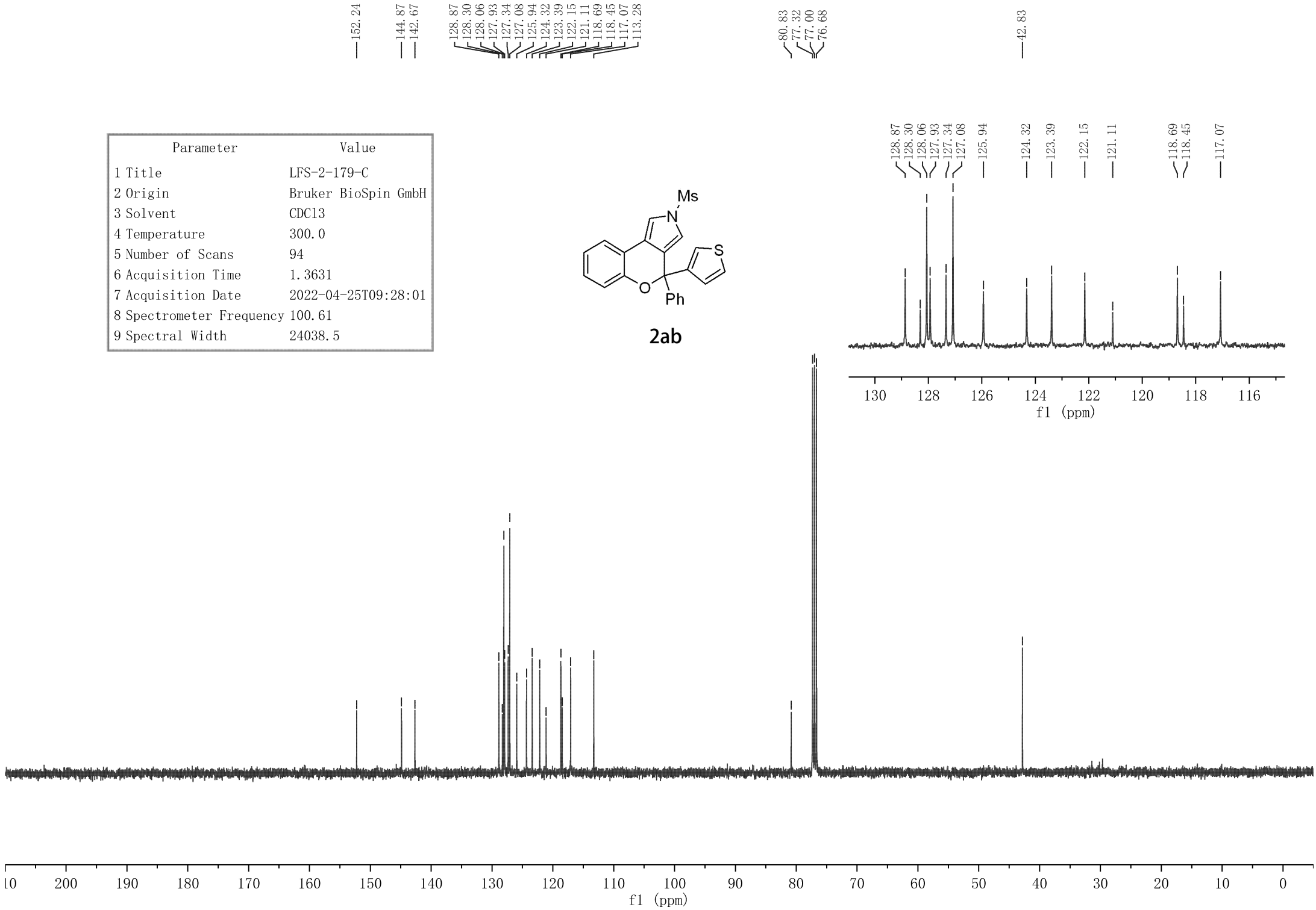
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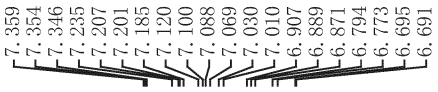
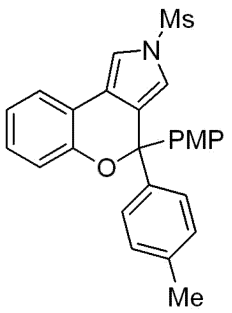
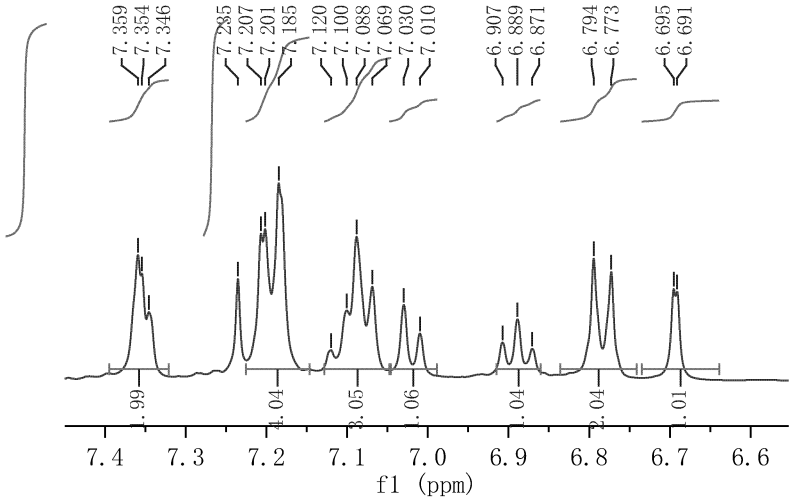
142.67
128.87
128.30
128.06
127.93
127.34
127.08
125.94
124.32
123.39
122.15
121.11
118.69
118.45
117.07
113.28
80.83
77.32
77.00
76.68
42.83
Parameter Value
1 Title LFS-2-179-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 94
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-25T09:28:01
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
S
O
Ph
2ab
f1 (ppm)
f1 (ppm)

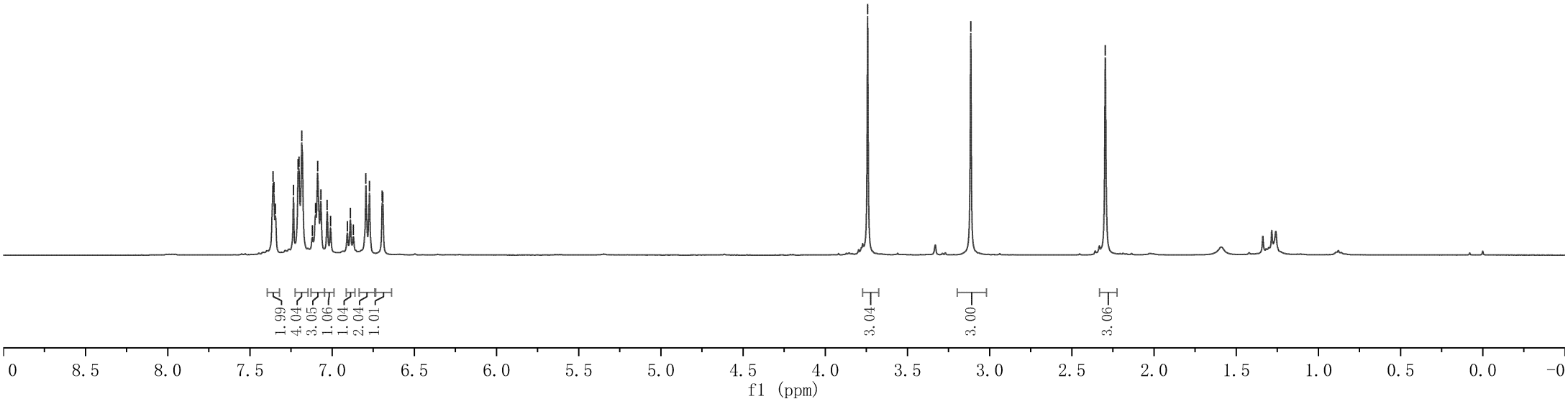


Parameter	Value
1 Title	LFS-2-200-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-29T10:14:24
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



2ac





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140.43
137.41
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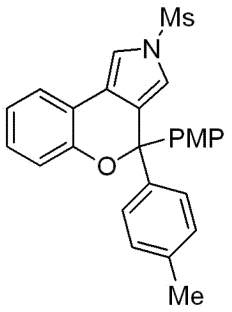
128.93
128.77
128.75
128.65
127.46
123.34
121.96
121.33
118.85
118.67
117.55
113.26
113.23
82.88
77.32
77.00
76.68
55.14
42.76
21.00

Parameter	Value
1 Title	LFS-2-200-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	67
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-29T10:16:38
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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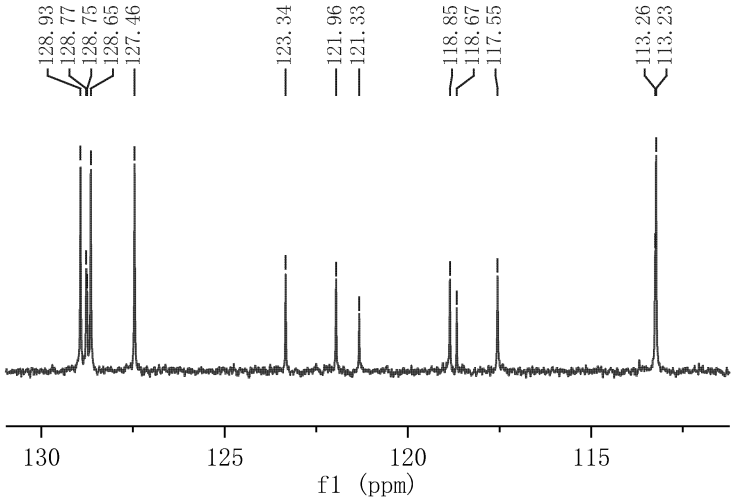
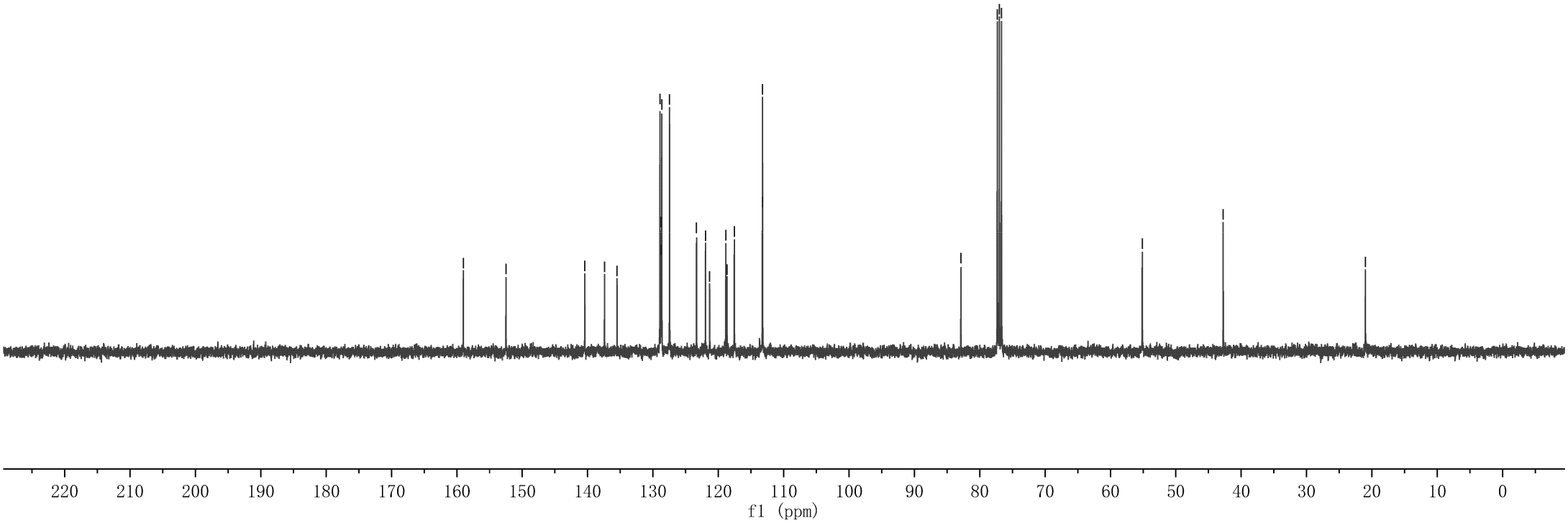
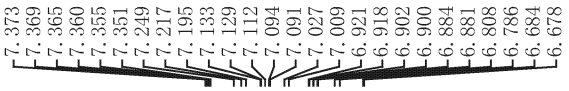
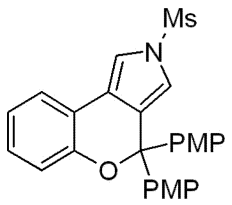






Parameter	Value
1 Title	zjj-13-203-PMP-chanwu-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-28T16:50:07
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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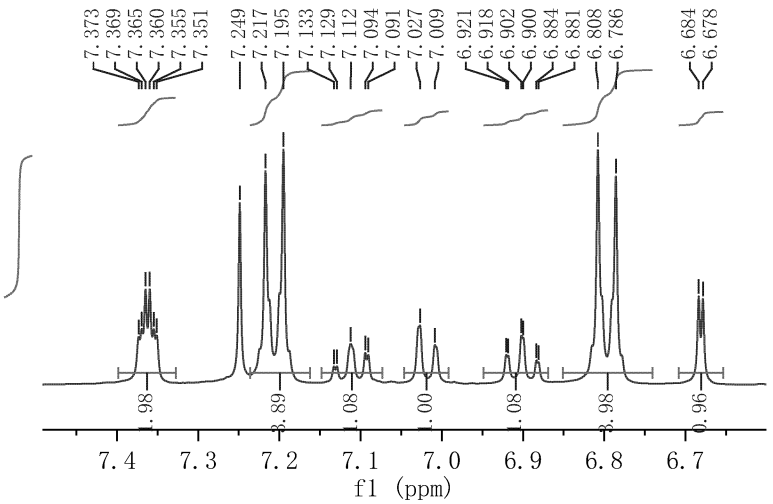

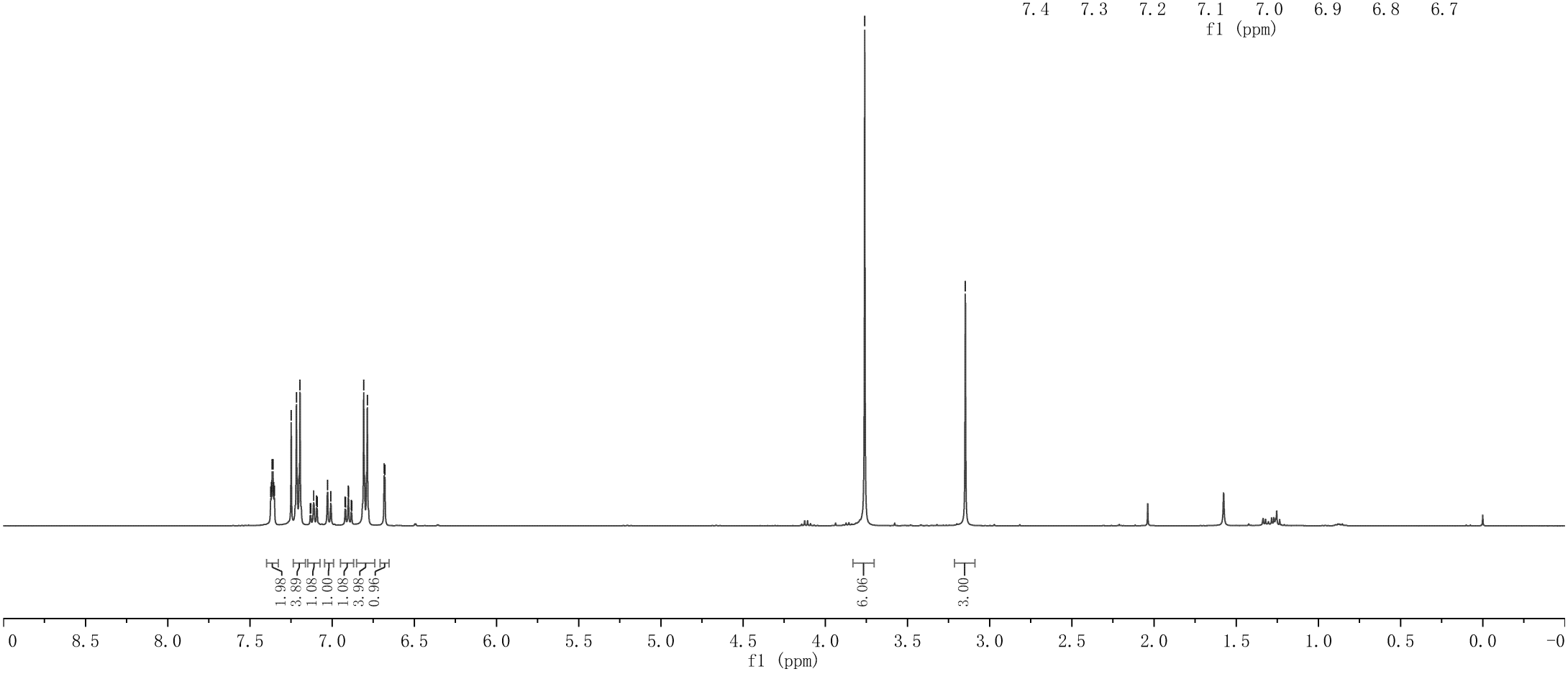

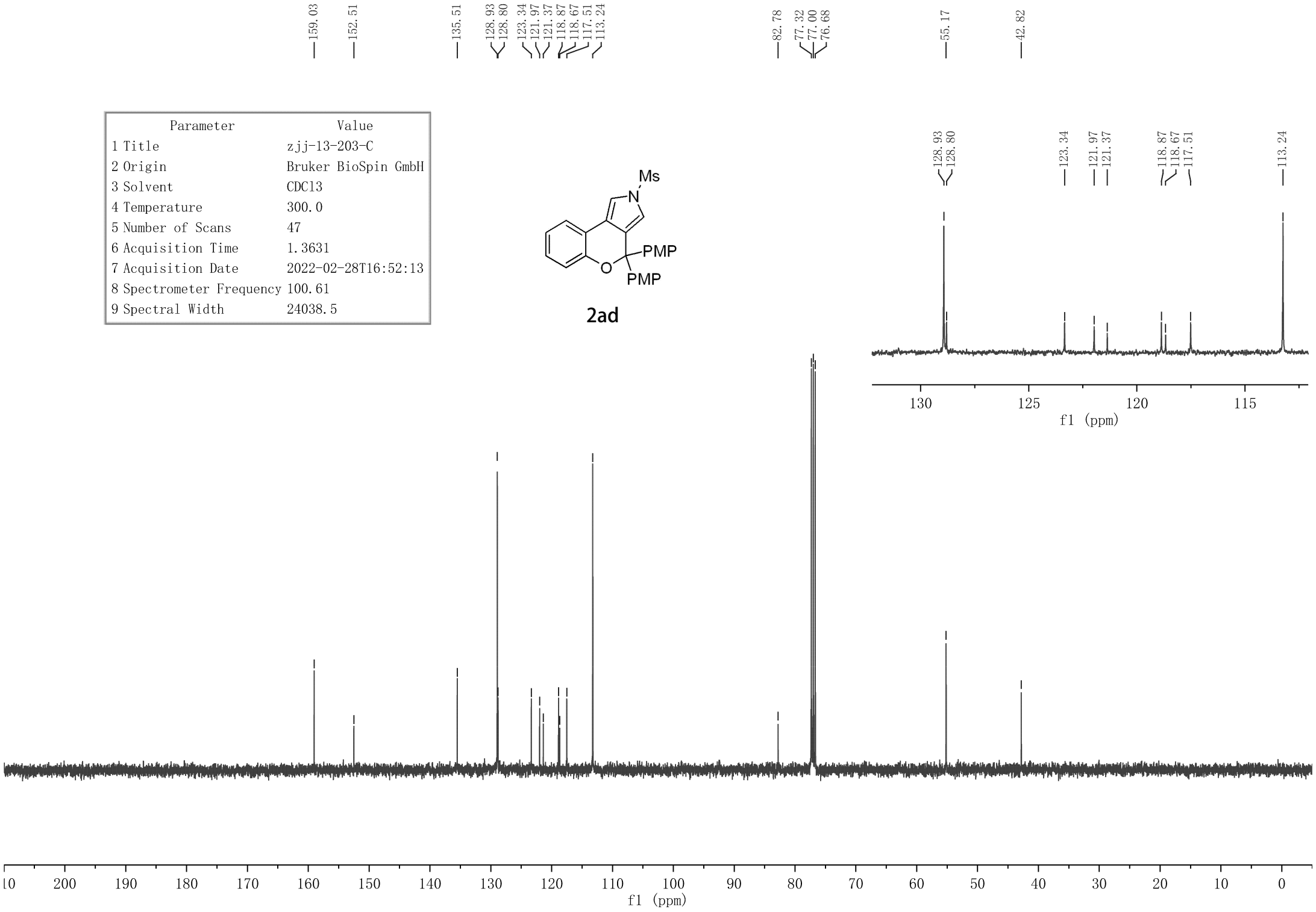
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152.51
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123.34
121.97
121.37
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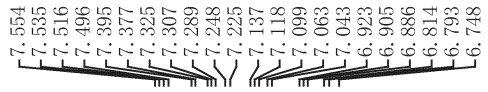
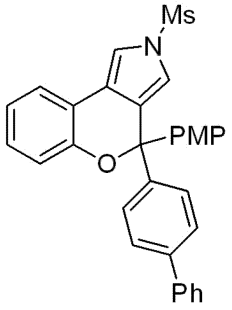
118.67
117.51
113.24
82.78
77.32
77.00
76.68
55.17
42.82
Parameter Value
1 Title zjj-13-203-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 47
6 Acquisition Time 1.3631
7 Acquisition Date 2022-02-28T16:52:13
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
PMP
O
PMP
2ad
f1 (ppm)
f1 (ppm)



Parameter	Value
1 Title	LFS-2-198-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.3
5 Number of Scans	32
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-29T17:19:31
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0



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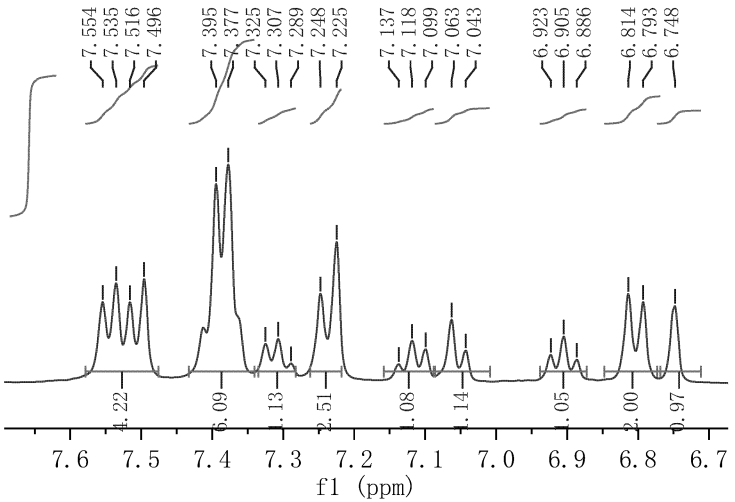
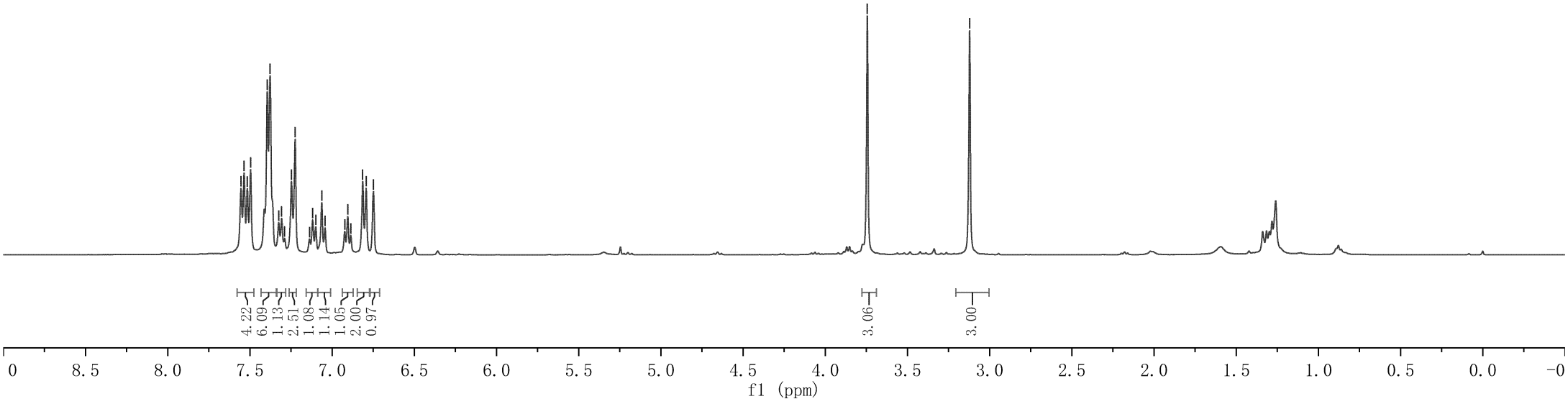
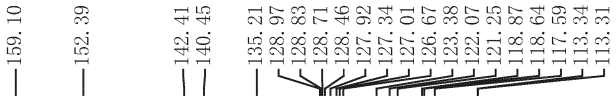
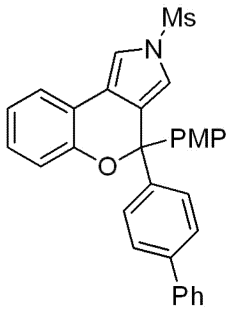






Parameter	Value
1 Title	LFS-2-198-C-4-Ph-Ph
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.2
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-29T17:28:39
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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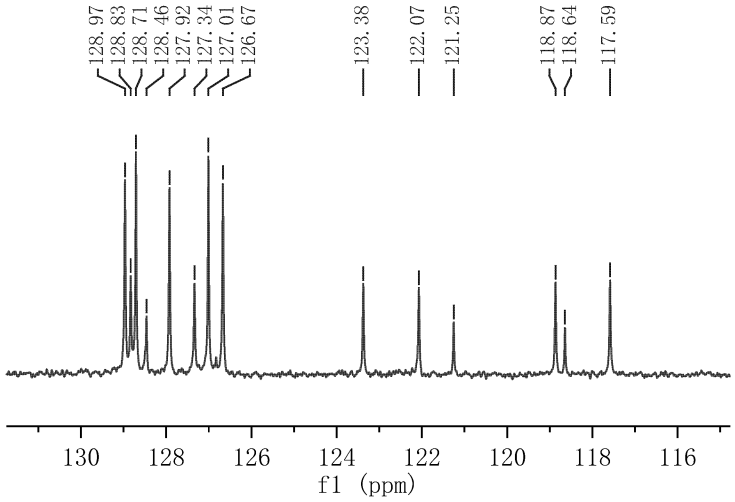
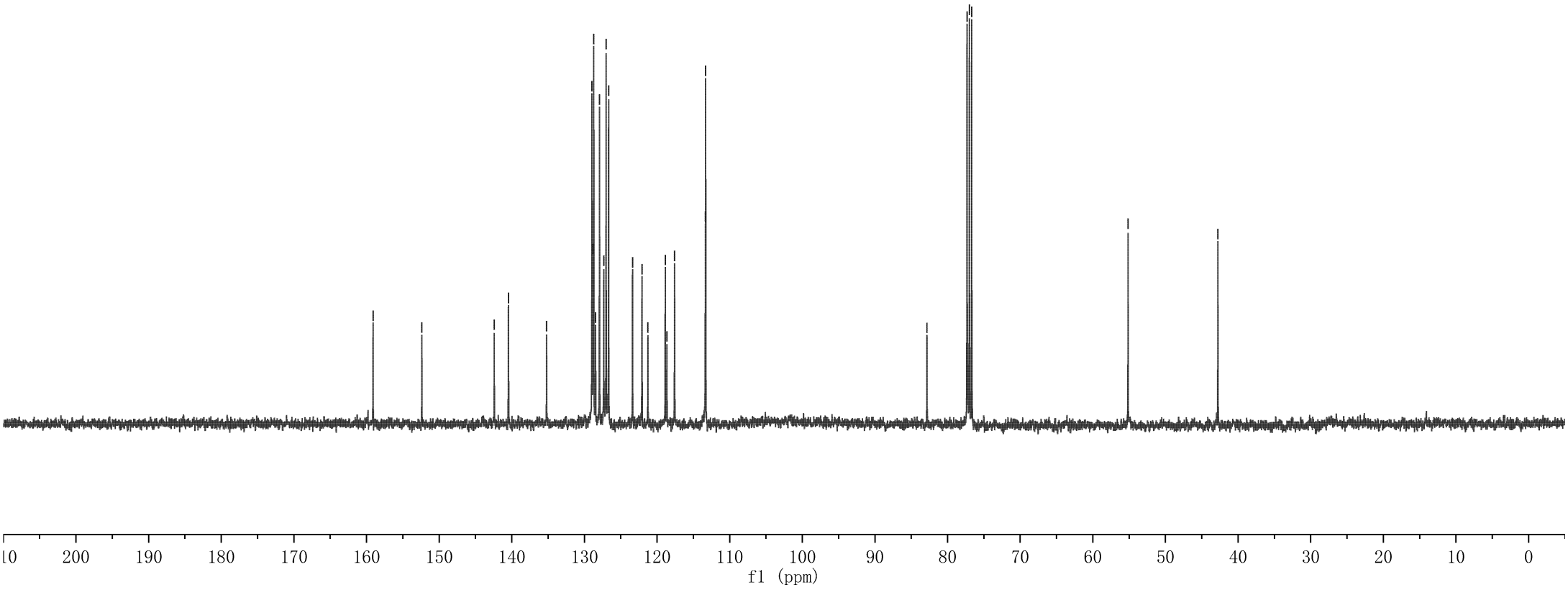
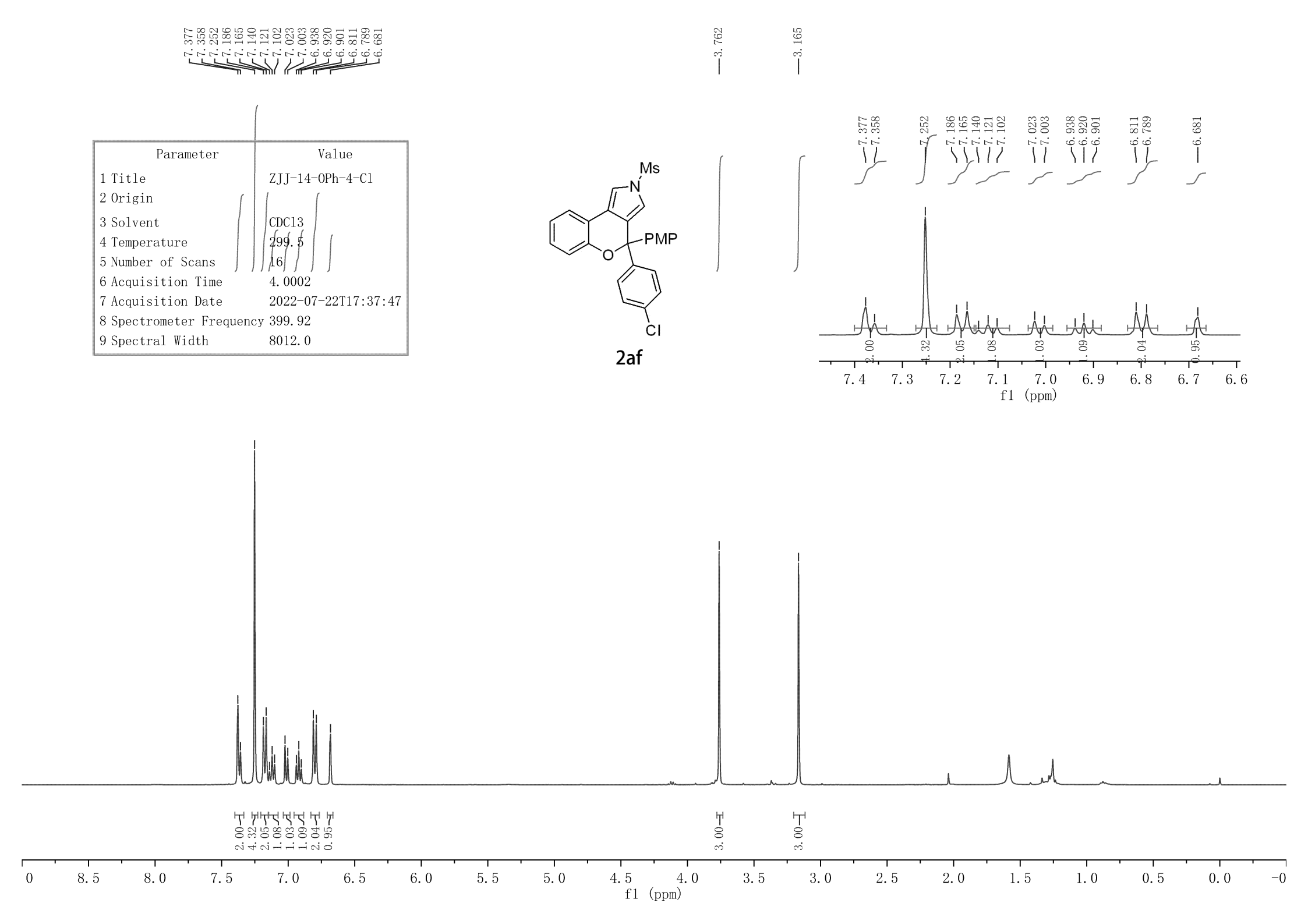
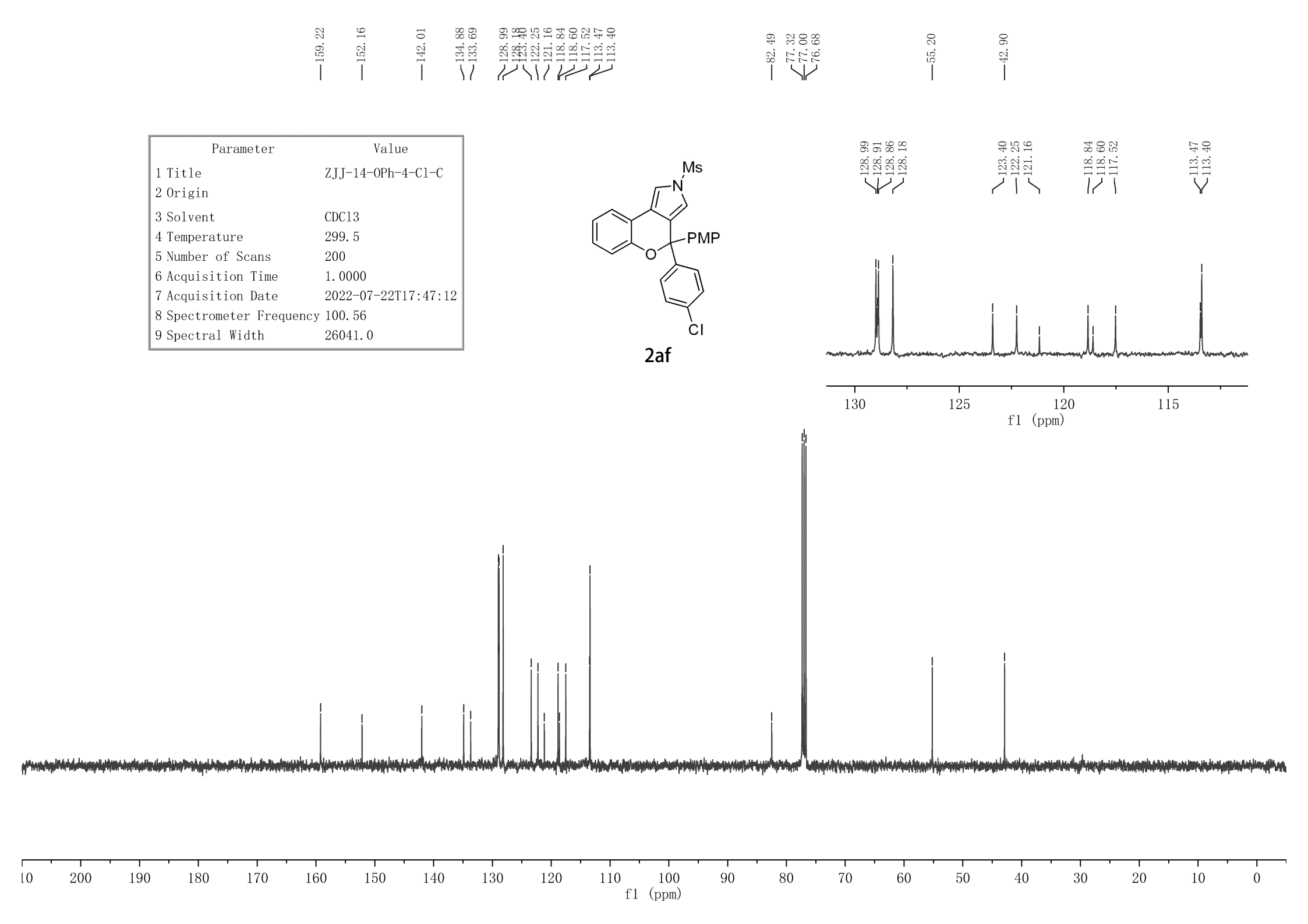
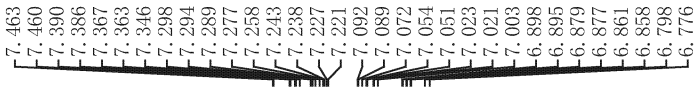


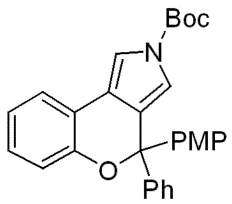



7.377
7.358
7.252
7.186
7.165
7.140
7.121
7.102
7.023
7.003
6.938
6.920
6.901
6.811
6.789
6.681
3.762
3.165
Parameter Value
1 Title ZJJ-14-OPh-4-Cl
2 Origin
3 Solvent CDCl3
4 Temperature 299.5
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-07-22T17:37:47
8 Spectrometer Frequency 399.92
9 Spectral Width 8012.0
Ms
N
PMP
O
Cl
2af
2.00
4.32
2.05
1.08
1.03
1.09
2.04
0.95
3.00
3.00
f1 (ppm)

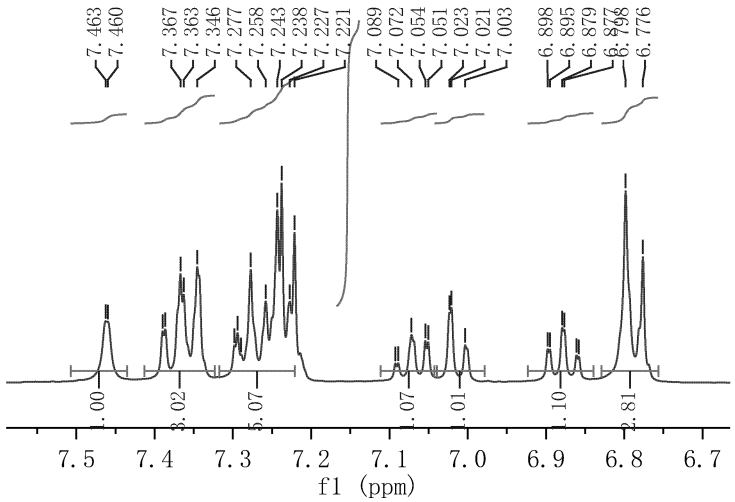

159.22
152.16
142.01
134.88
133.69
128.99
128.91
128.86
128.18
123.40
122.25
121.16
118.84
118.60
117.52
113.47
113.40
82.49
77.32
77.00
76.68
55.20
42.90
Parameter Value
1 Title ZJJ-14-OPh-4-Cl-C
2 Origin
3 Solvent CDCl3
4 Temperature 299.5
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-07-22T17:47:12
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
PMP
O
Cl
2af
f1 (ppm)
f1 (ppm)

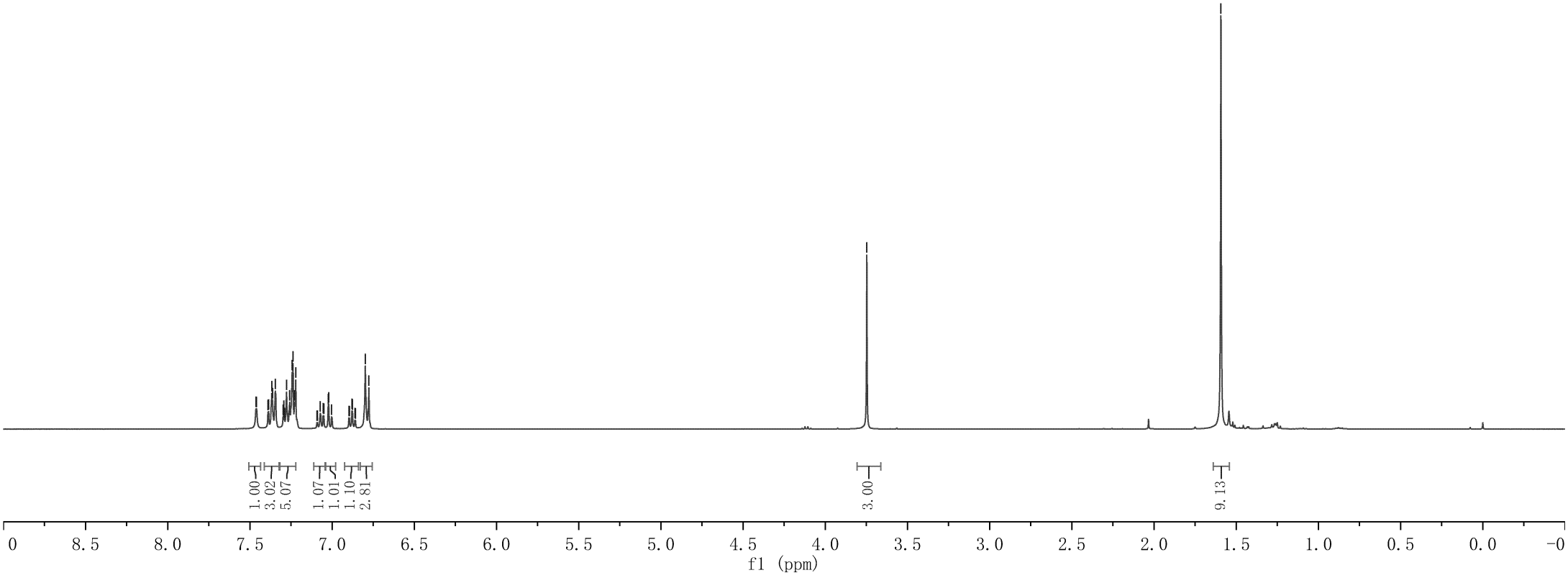


Parameter	Value
1 Title	zjj-14-88-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-21T11:38:13
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



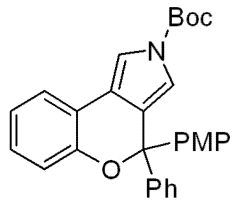
3a



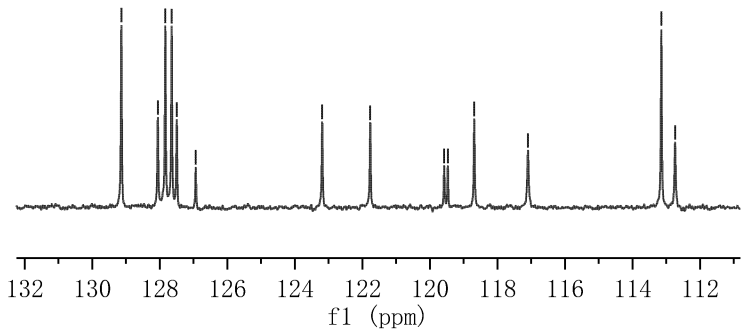


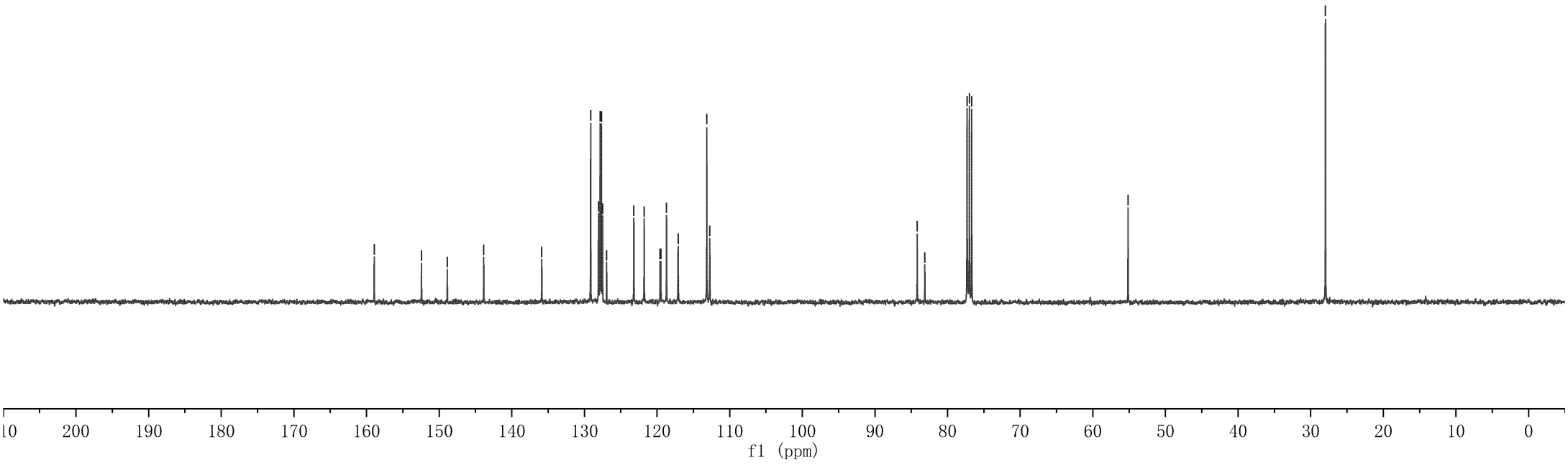
158.94
152.43
148.88
143.86
135.87
129.14
128.06
127.84
127.65
127.50
126.93
123.19
121.77
119.58
119.47
118.69
117.10
113.15
112.74
84.18
83.13
77.32
77.00
76.68
55.15
27.97

Parameter	Value
1 Title	ZJJ-14-88-1
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.4
5 Number of Scans	600
6 Acquisition Time	1.0000
7 Acquisition Date	2022-05-23T11:04:33
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

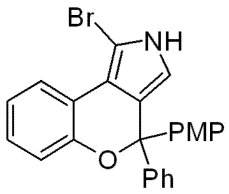


3a

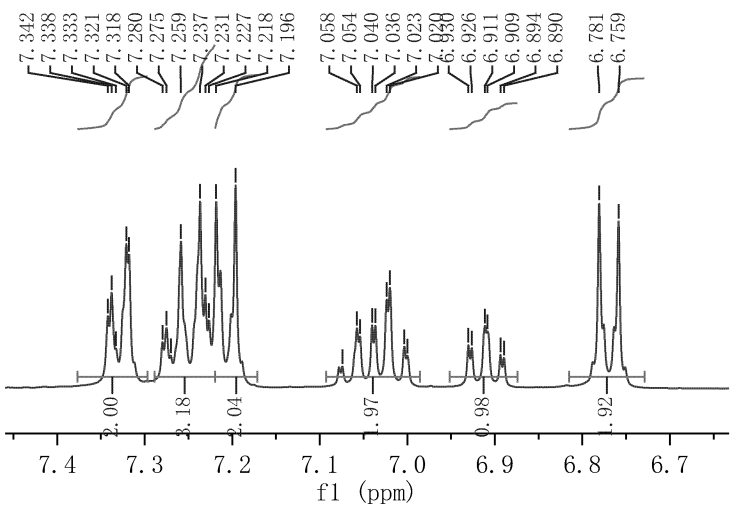


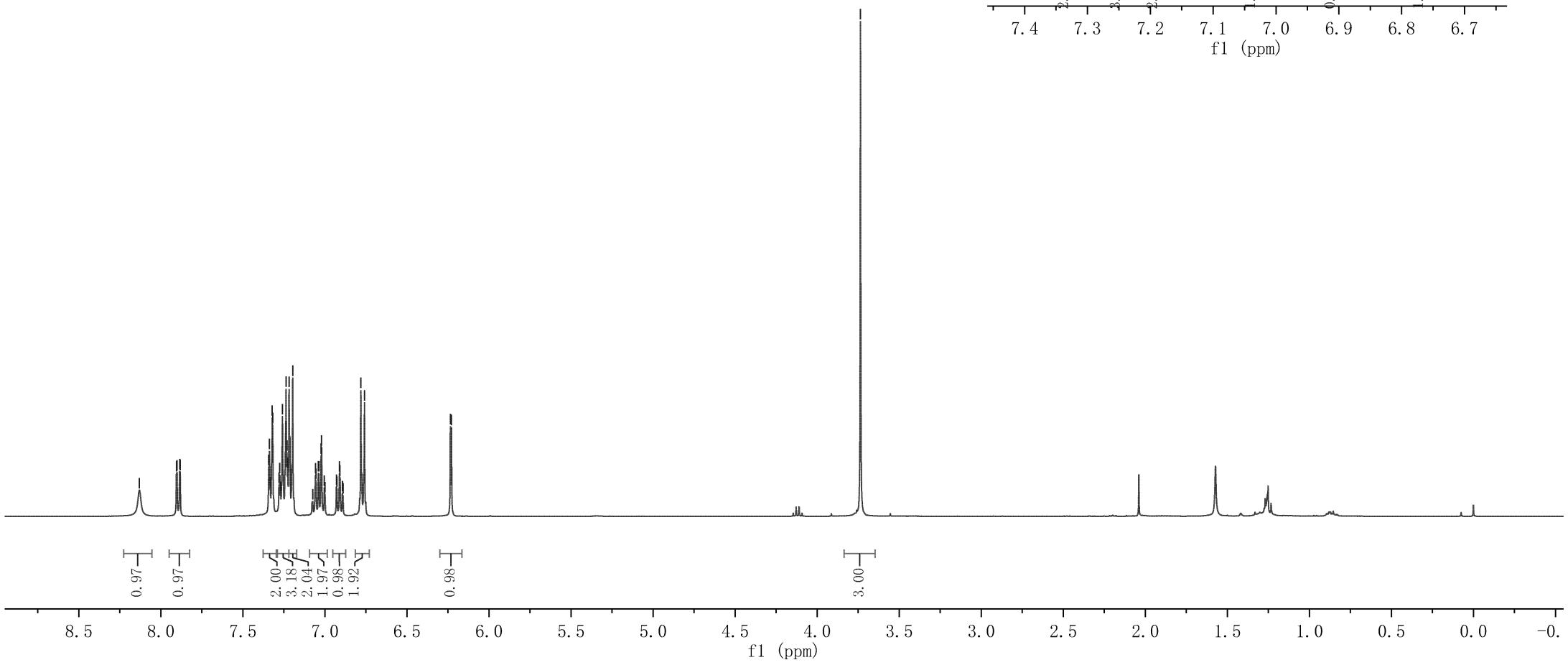


Parameter	Value
1 Title	zjj-14-158-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	17
6 Acquisition Time	4.0894
7 Acquisition Date	2022-07-30T13:56:14
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



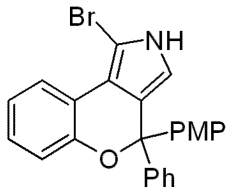
4a



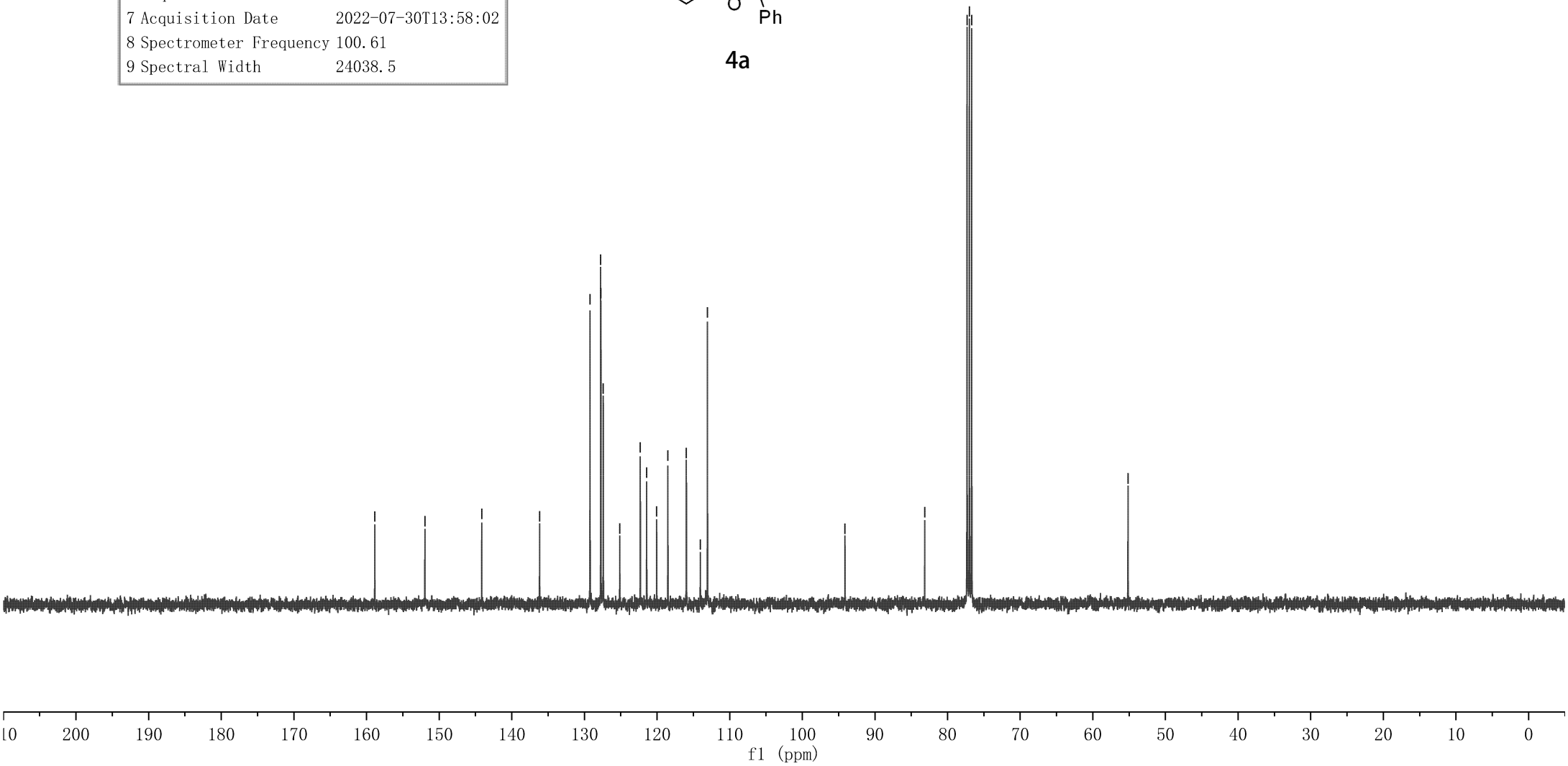


158.86
151.96
144.14
136.17
129.23
127.75
127.72
127.40
125.13
122.31
121.43
120.05
118.51
115.96
114.04
113.06
94.12
83.15
77.32
77.00
76.68
55.16

Parameter	Value
1 Title	zjj-14-158-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	114
6 Acquisition Time	1.3631
7 Acquisition Date	2022-07-30T13:58:02
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

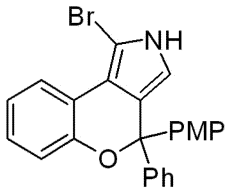


4a

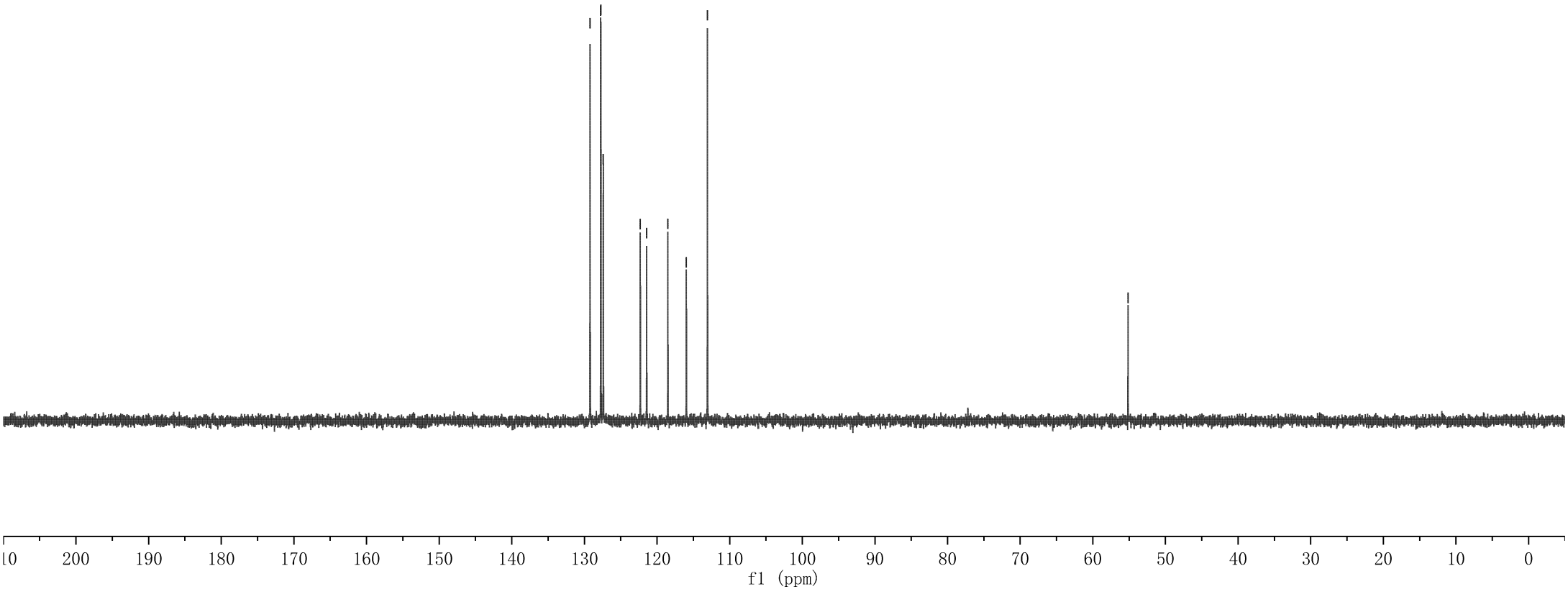


129.23
127.76
127.73
127.40
122.31
121.43
118.51
115.96
113.06
55.16

Parameter	Value
1 Title	zjj-14-158-C-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	52
6 Acquisition Time	1.3631
7 Acquisition Date	2022-07-30T14:05:18
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

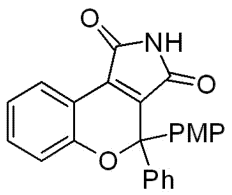


4a

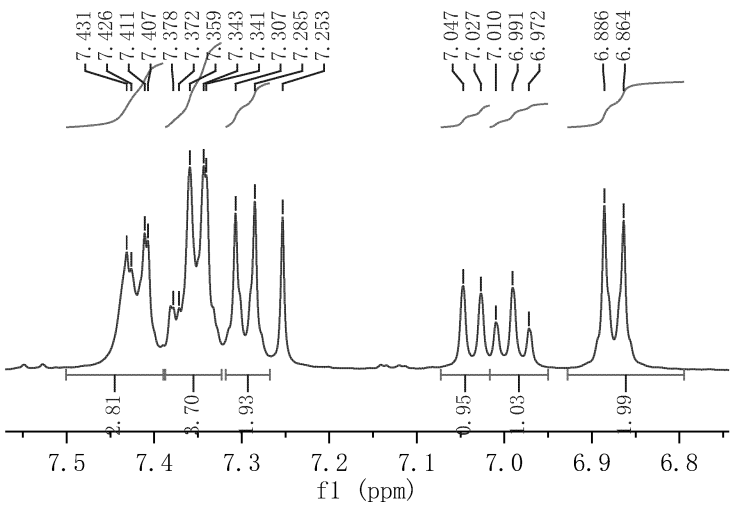


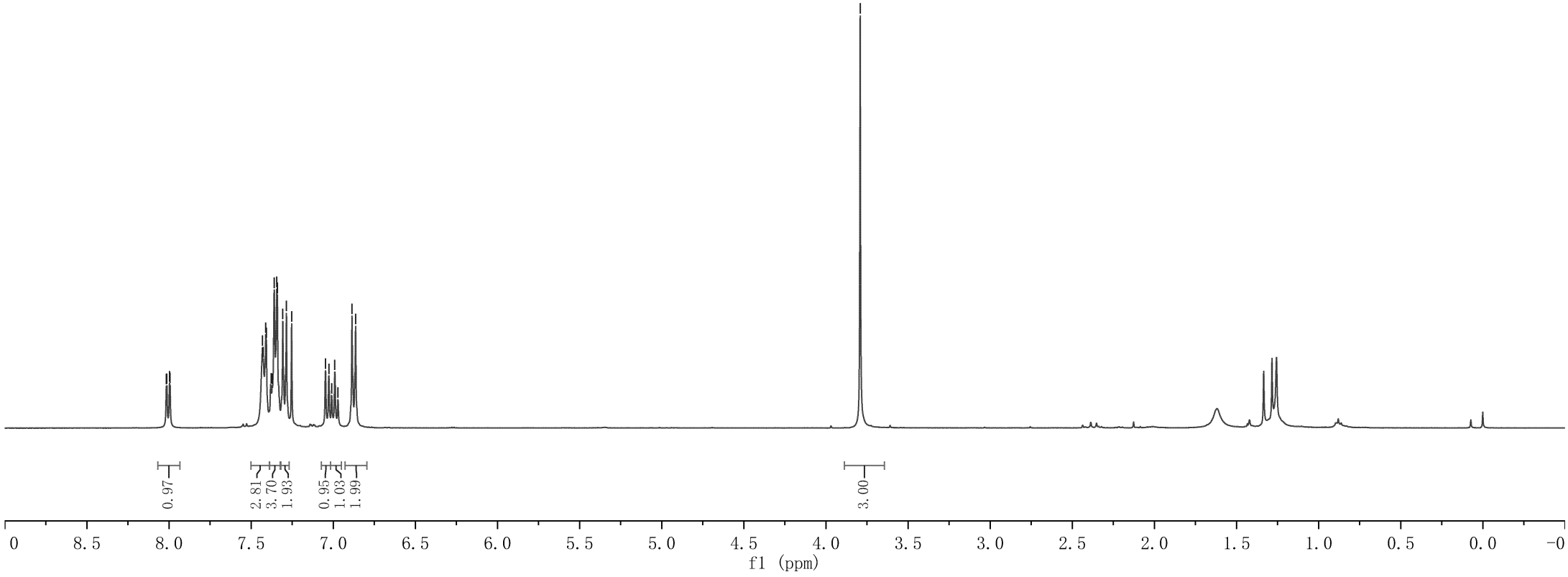
8.016
8.013
7.997
7.994
7.359
7.343
7.341
7.307
7.285
7.253
7.047
7.027
7.010
6.991
6.972
6.886
6.864
3.791

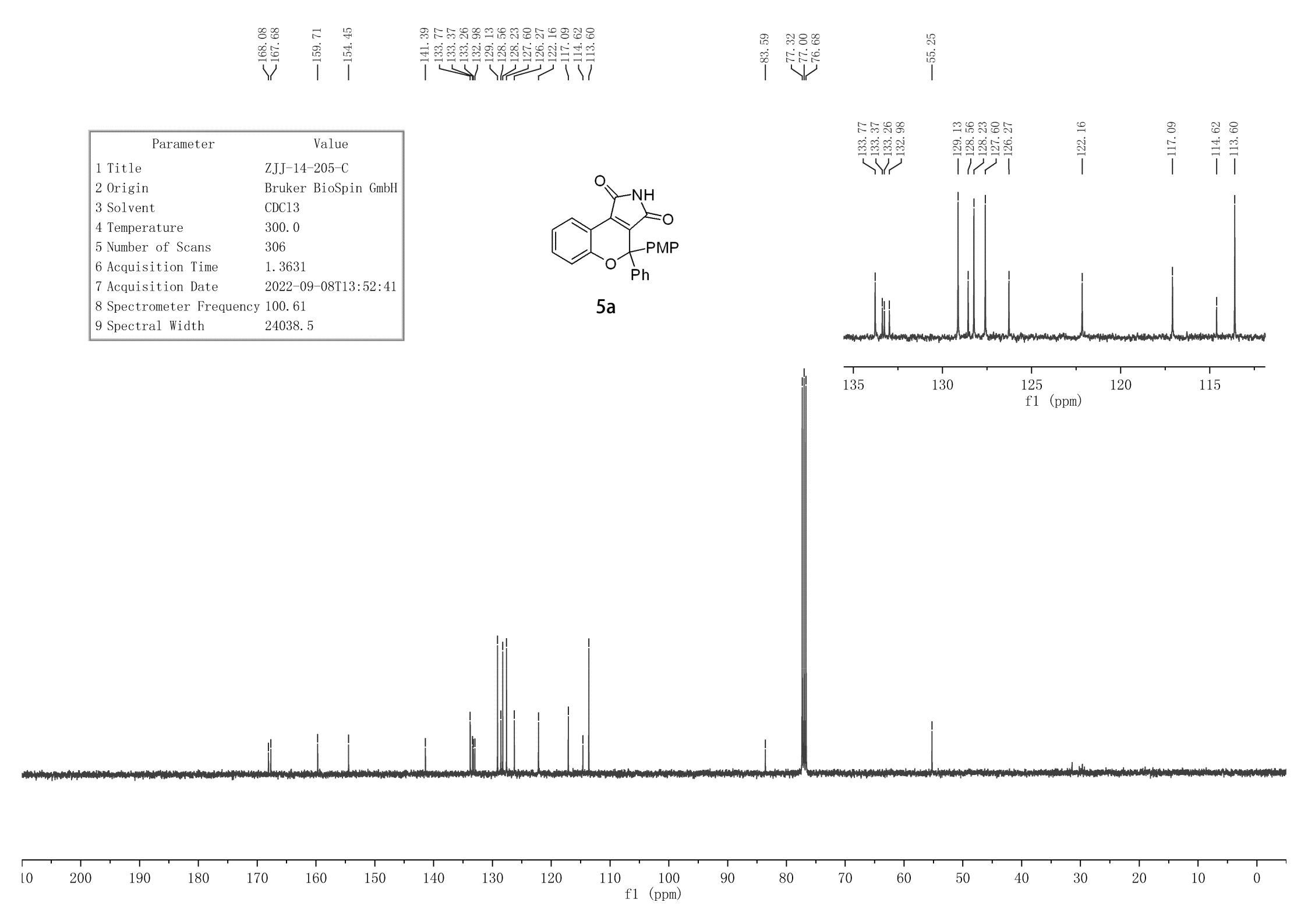
Parameter	Value
1 Title	ZJJ-14-205-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-09-08T13:50:00
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



5a

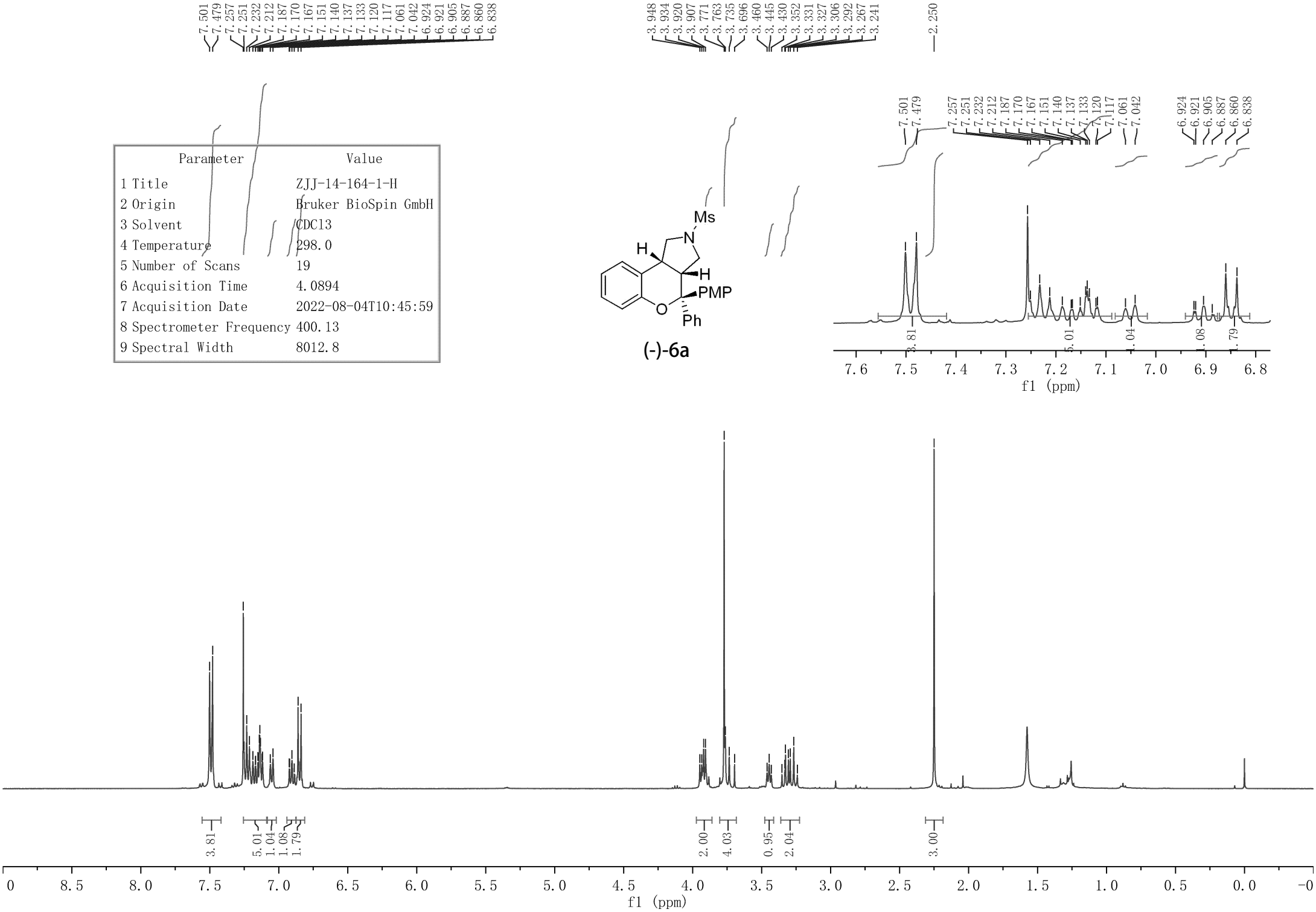


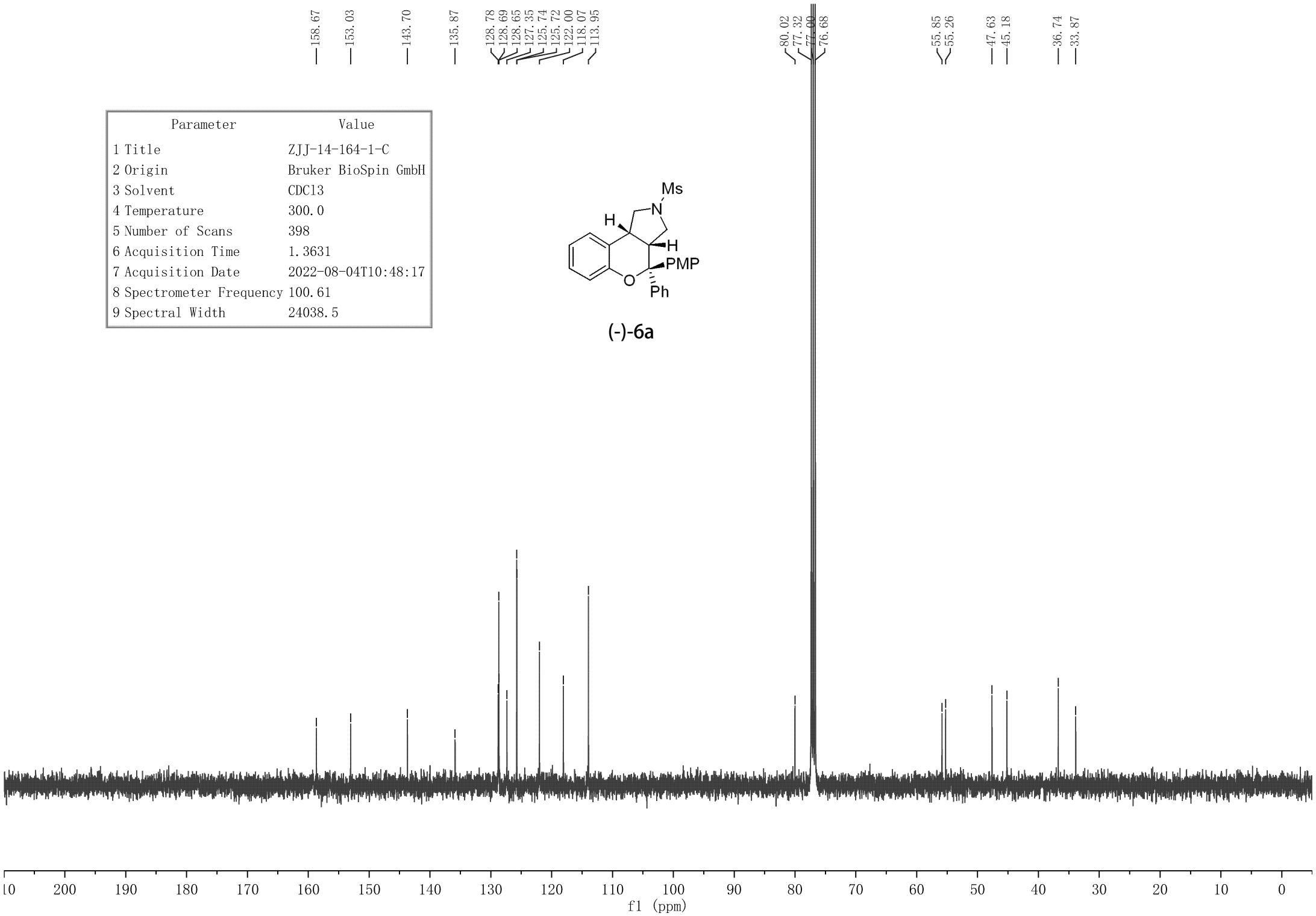



168.08
167.68
159.71
154.45
141.39
133.77
133.37
133.26
132.98
129.13
128.56
128.23
127.60
126.27
122.16
117.09
114.62
113.60
83.59
77.32
77.00
76.68
55.25
Parameter Value
1 Title ZJJ-14-205-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 306
6 Acquisition Time 1.3631
7 Acquisition Date 2022-09-08T13:52:41
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
NH
O
O
PMP
O
Ph
5a
f1 (ppm)
f1 (ppm)

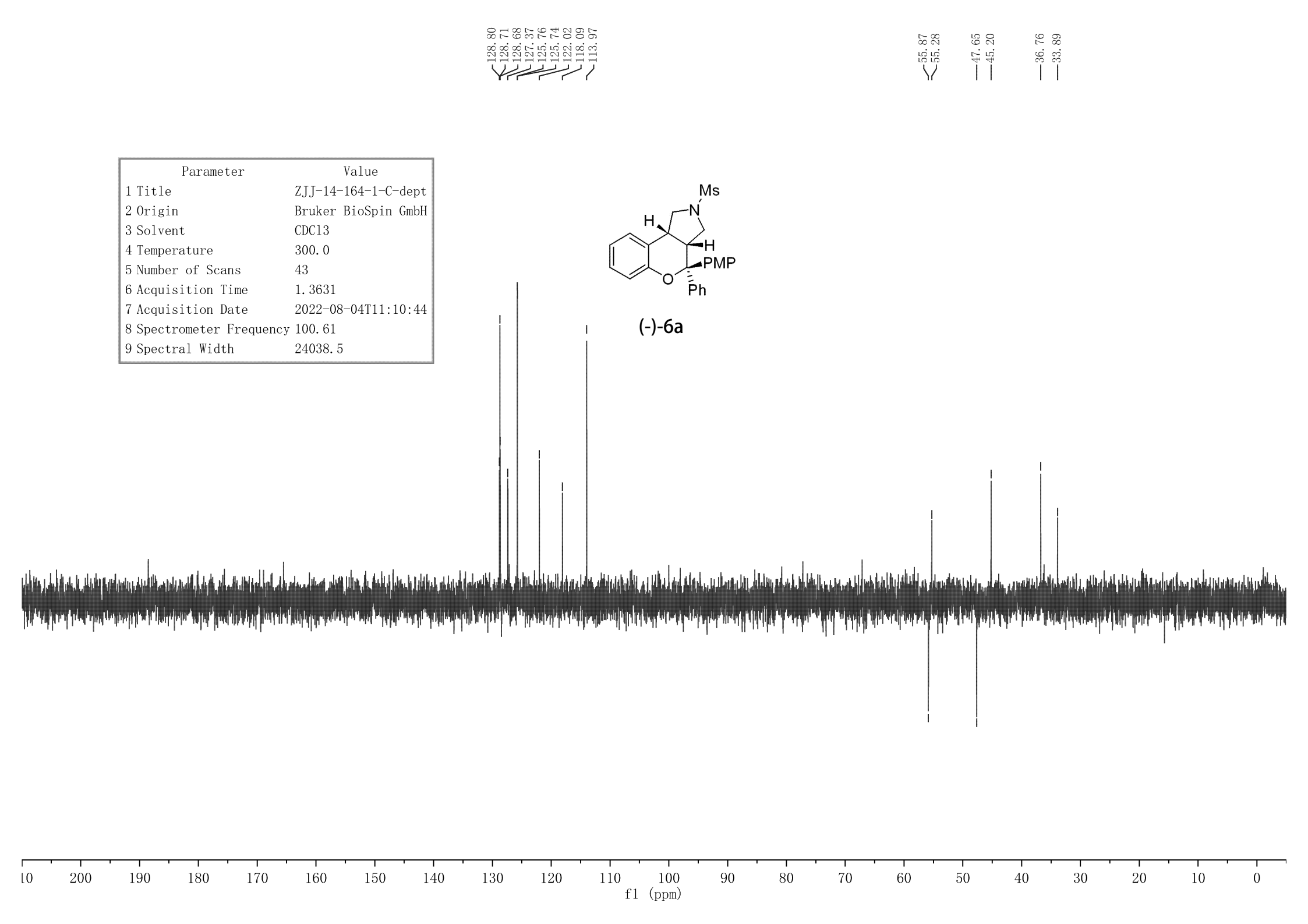
Parameter	Value
1 Title	ZJJ-14-164-1-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	19
6 Acquisition Time	4.0894
7 Acquisition Date	2022-08-04T10:45:59
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

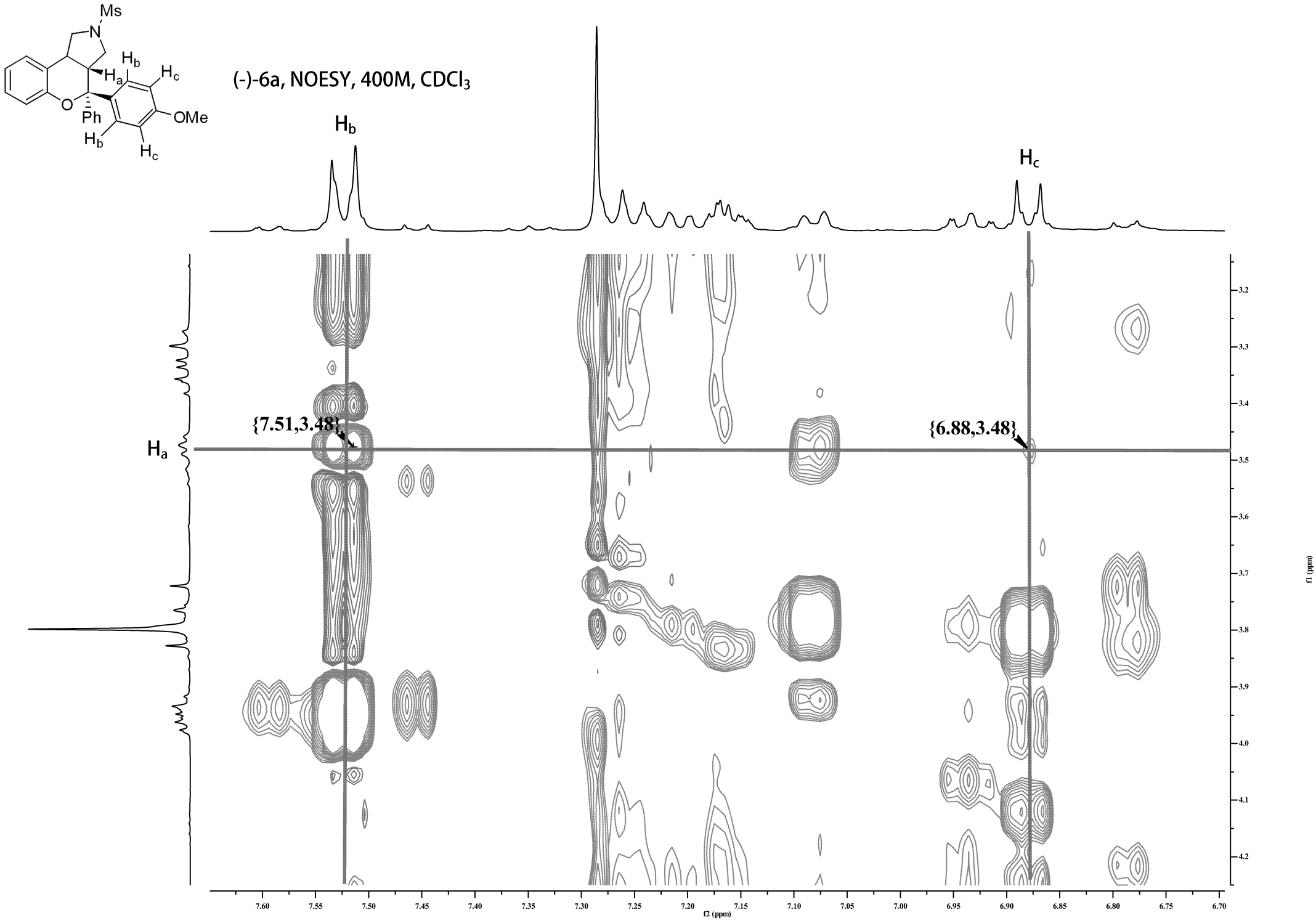
(-)-6a





Parameter	Value
1 Title	ZJJ-14-164-1-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	398
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-04T10:48:17
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5


128.80
128.71
128.68
127.37
125.76
125.74
122.02
118.09
113.97
55.87
55.28
47.65
45.20
36.76
33.89
Parameter Value
1 Title ZJJ-14-164-1-C-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 43
6 Acquisition Time 1.3631
7 Acquisition Date 2022-08-04T11:10:44
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
H
H
PMP
O
Ph
(-)-6a
f1 (ppm)


Ms
N
Hb
Ha
Hc
O
Ph
OMe
Hb
Hc
(-)-6a, NOESY, 400M, CDCl3
Hb
Hc
Ha
{7.51,3.48}
{6.88,3.48}
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
f2 (ppm)
3.2
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4.0
4.1
4.2
f1 (ppm)