Supporting Information

Copper-catalyzed formal [4 + 1] annulation of *N*-propargyl ynamides with diketones

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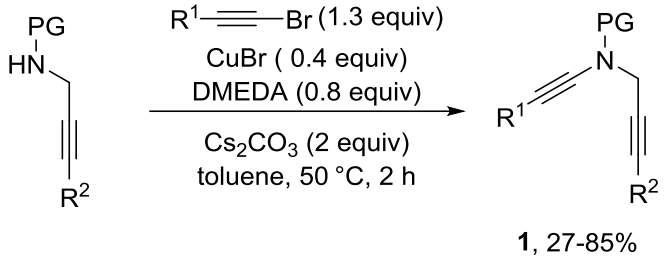
General Information. Acetonitrile (ACS grade), toluene (ACS grade), ethyl acetate (ACS grade) and hexanes (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. All reactions were carried out with a Titan HMS-14 digital magnetic stirrer with hot plate. 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 Agilent 6230 ESI-TOF MS using electron spray ionization. X-ray diffraction analysis was recorded on a Rigaku AFC7R X-ray single crystal diffractometer. HPLC analyses were carried out in a chromatograph equipped with a UV diode-array detector using chiral stationary columns from Daicel.

^{1}H NMR spectra and ^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard for ^{1}H NMR spectra and with the internal chloroform signal at 77.0 ppm as a standard for ^{13}C NMR spectra. 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).

2. General Procedures and Transformations

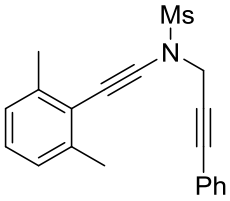
2.1 Representative synthetic procedure for the preparation of ynamides 1 (1a-1y)[1,2]



1, 27-85%

To a solution of the protected propargylamide derivative (1 mmol, 1 equiv) in toluene (0.1 M) was added copper bromide (0.4 mmol, 0.4 equiv), DMEDA (0.8 mmol, 0.8 equiv), Cs_2CO_3 (2 mmol, 2 equiv), acetylene bromide derivative (1.3 mmol, 1.3 equiv). The reaction was stirred at 50 ^oC for about 2 h and the progress of the reaction was monitored by TLC. Upon completion, the solution was then filtered and concentrated under a reduced pressure. The residue was purified by silica gel column chromatography (PE:EA = 15:1). The characterization data of ynamides **1x** and **1z** have been reported in our previous work.[1]

N-((2,6-dimethylphenyl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1a)

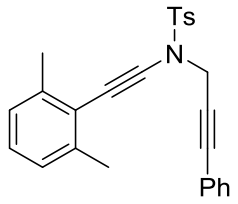


1a

Compound **1a** was prepared in 57% yield (192.3 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a pale yellow solid (mp 64–65 ^oC). ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 2H), 7.40 – 7.28 (m, 3H), 7.13 – 7.07 (m, 1H), 7.06 – 7.01 (m, 2H), 4.64 (s, 2H), 3.27 (s, 3H), 2.44 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 131.8, 129.1, 128.5, 127.6, 126.7, 122.0, 121.7, 89.4, 86.9, 81.5, 69.3, 43.1, 38.4, 21.1; IR (neat): 3020, 2927, 2232, 1490,

1363, 1321, 1167, 1040, 788, 758 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{19}NNaO_2S$ 360.1029; Found 360.1031.

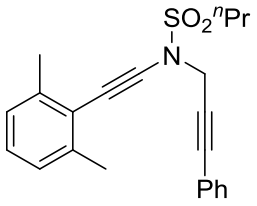
***N*-((2,6-dimethylphenyl)ethynyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1b)**



1b

Compound **1b** was prepared in 69% yield (285.3 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 121–123 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.29 – 7.20 (m, 5H), 7.15 – 7.10 (m, 2H), 7.09 – 7.03 (m, 1H), 7.02 – 6.96 (m, 2H), 4.60 (s, 2H), 2.37 (s, 6H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 139.9, 134.3, 131.6, 129.6, 128.6, 128.2, 128.1, 127.3, 126.5, 122.3, 121.9, 90.0, 86.3, 81.2, 68.9, 43.0, 21.5, 21.0; IR (neat): 3055, 2921, 2230, 1490, 1367, 1168, 1119, 1089, 757, 708 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{26}H_{23}NNaO_2S$ 436.1342; Found 436.1342.

***N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)propane-1-sulfonamide (1c)**

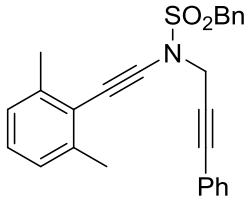


1c

Compound **1c** was prepared in 68% yield (248.5 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a brown solid (mp 68–70 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.37 (m, 2H), 7.36 – 7.25 (m, 3H), 7.10 – 7.03 (m, 1H), 7.03 – 6.96 (m, 2H), 4.60 (s, 2H), 3.39 (t, *J* = 7.6 Hz, 2H), 2.43 (s, 6H), 2.10 – 1.95 (m, 2H), 1.05 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 139.5, 131.6, 128.8, 128.3, 127.2, 126.5, 122.1, 121.7, 89.7, 86.4, 81.9, 68.9, 53.9, 42.5, 20.9, 16.9, 12.8; IR (neat): 3056, 2972, 2232, 1490, 1365, 1158, 1123, 1078, 757, 691 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{23}NNaO_2S$ 388.1342; Found 388.1340.

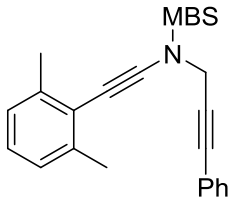
***N*-((2,6-dimethylphenyl)ethynyl)-1-phenyl-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1d)**



1d

Compound **1d** was prepared in 73% yield (301.9 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a pale yellow solid (mp 90–92 °C). ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 2H), 7.44 – 7.39 (m, 2H), 7.38 – 7.26 (m, 6H), 7.10 – 7.05 (m, 1H), 7.04 – 6.99 (m, 2H), 4.61 (s, 2H), 4.34 (s, 2H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 131.7, 130.9, 129.1, 128.8, 128.3, 127.3, 127.2, 126.6, 122.2, 121.8, 89.4, 86.5, 81.8, 69.8, 57.6, 43.2, 21.1; IR (neat): 3058, 2920, 2232, 1491, 1366, 1164, 1122, 1045, 757, 693 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{26}H_{23}NNaO_2S$ 436.1342; Found 436.1342.

***N*-((2,6-dimethylphenyl)ethynyl)-4-methoxy-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1e)**

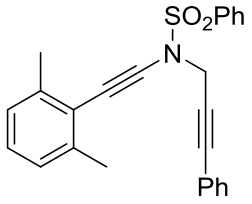


1e

Compound **1e** was prepared in 53% yield (227.7 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 18:1) as a white solid (mp 122–124 °C). ^1H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.8 Hz, 2H),

7.32 – 7.20 (m, 3H), 7.18 – 7.13 (m, 2H), 7.10 – 7.03 (m, 1H), 7.03 – 6.97 (m, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 4.60 (s, 2H), 3.75 (s, 3H), 2.38 (s, 6H); ^{13}C NMR (100 MHz, CDCl3) δ 163.8, 139.9, 131.6, 130.4, 128.8, 128.6, 128.1, 127.2, 126.5, 122.4, 122.0, 114.1, 90.1, 86.3, 81.4, 68.9, 55.5, 43.0, 21.1; IR (neat):3057, 2944, 2229, 1595, 1497, 1366, 1264, 1163, 757, 730 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{26}H_{23}NNaO_3S$ 452.1291; Found 452.1288.

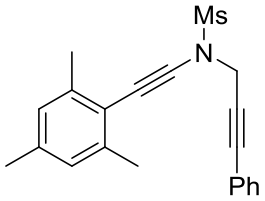
_N_-((2,6-dimethylphenyl)ethynyl)-_N_-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1f)



1f

Compound **1f** was prepared in 65% yield (259.7 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 106–108 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.0 Hz, 2H), 7.62 – 7.45 (m, 3H), 7.30 – 7.12 (m, 5H), 7.10 – 7.03 (m, 1H), 7.03 – 6.96 (m, 2H), 4.63 (s, 2H), 2.36 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 137.3, 133.7, 131.6, 129.0, 128.6, 128.1, 127.4, 126.5, 122.2, 121.8, 89.6, 86.5, 81.1, 69.0, 43.1, 21.0; IR (neat): 3059, 2919, 2231, 1490, 1368, 1172, 1122, 1089, 756, 733 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{25}H_{21}NNaO_2S$ 422.1185; Found 452.1278.

_N_-(mesitylethynyl)-_N_-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1g)

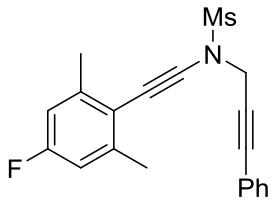


1g

Compound **1g** was prepared in 48% yield (168.7 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 10:1) as a white solid (mp 80–82 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.28 (m, 5H), 6.86 (s,

2H), 4.62 (s, 2H), 3.26 (s, 3H), 2.40 (s, 6H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.00, 137.7, 131.8, 129.0, 128.4, 127.6, 121.7, 118.9, 88.5, 86.9, 81.6, 69.2, 43.1, 38.3, 21.3, 21.0; IR (neat): 3053, 2921, 2238, 1491, 1363, 1265, 1168, 1038, 738, 706 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{21}NNaO_2S$ 374.1185; Found 374.1185.

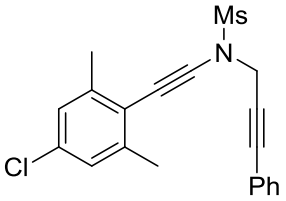
_N_-((4-fluoro-2,6-dimethylphenyl)ethynyl)-_N_-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1h)



1h

Compound **1h** was prepared in 78% yield (277.2 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 2H), 7.39 – 7.29 (m, 3H), 6.74 (d, J = 9.2 Hz, 2H), 4.62 (s, 2H), 3.26 (s, 3H), 2.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.7 (d, J = 247.0 Hz), 142.6 (d, J = 9.0 Hz), 131.7, 129.1, 128.4, 121.6, 117.9 (d, J = 3.0 Hz), 113.7 (d, J = 21.0 Hz), 88.8 (d, J = 1.0 Hz), 86.9, 81.5, 68.2, 43.0, 38.4, 21.1 (d, J = 1.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.7; IR (neat): 3021, 2928, 2242, 1490, 1364, 1168, 1135, 1039, 775, 758 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}FNNaO_2S$ 378.0934; Found 378.0935

_N_-((4-chloro-2,6-dimethylphenyl)ethynyl)-_N_-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1i)

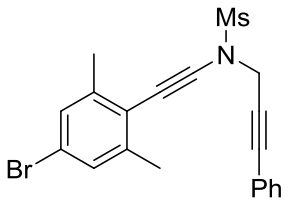


1i

Compound **1i** was prepared in 66% yield (245.4 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as

a pale red solid (mp 52–54 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 2H), 7.39 – 7.29 (m, 3H), 7.03 (s, 2H), 4.63 (s, 2H), 3.27 (s, 3H), 2.40 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 133.1, 131.8, 129.1, 128.5, 126.7, 121.6, 120.6, 90.0, 87.0, 81.4, 68.5, 43.0, 38.5, 20.9; IR (neat): 3055, 2927, 2235, 1491, 1364, 1167, 1121, 1038, 757, 703 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}ClNNaO_2S$ 394.0639; Found 394.0654.

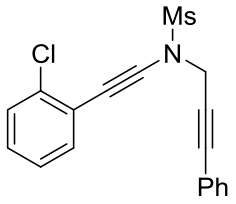
_N_-((4-bromo-2,6-dimethylphenyl)ethynyl)-_N_-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1j)



1j

Compound **1j** was prepared in 60% yield (249.8 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.40 (m, 2H), 7.39 – 7.29 (m, 3H), 7.18 (s, 2H), 4.63 (s, 2H), 3.27 (s, 3H), 2.40 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 131.7, 129.6, 129.1, 128.5, 121.5, 121.4, 121.1, 90.2, 87.0, 81.3, 68.6, 42.9, 38.5, 20.8; IR (neat): 3056, 2928, 2236, 1490, 1365, 1167, 1117, 1038, 773, 758 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}BrNNaO_2S$ 438.0133; Found 438.0139.

_N_-((2-chlorophenyl)ethynyl)-_N_-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1k)

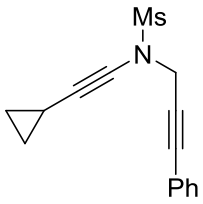


1k

Compound **1k** was prepared in 69% yield (237.2 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.42 (m, 3H), 7.41 – 7.28 (m, 4H),

7.26 – 7.16 (m, 2H), 4.62 (s, 2H), 3.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 132.9, 131.8, 129.1(4), 129.1(0), 129.0, 128.4, 126.4, 122.3, 121.7, 87.1, 86.3, 81.3, 68.7, 43.0, 38.8; IR (neat): 3020, 2928, 2237, 1490, 1364, 1167, 1122, 1037, 780, 755 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{14}ClNNaO_2S$ 366.0326; Found 366.0338.

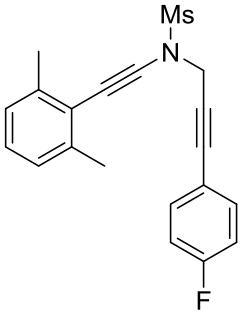
***N*-(cyclopropylethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1l)**



1l

Compound **1l** was prepared in 27% yield (73.8 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 2H), 7.39 – 7.30 (m, 3H), 4.45 (s, 2H), 3.17 (s, 3H), 1.41 – 1.31 (m, 1H), 0.89 – 0.79 (m, 2H), 0.78 – 0.67 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.7, 128.9, 128.4, 121.8, 86.5, 81.7, 75.5, 67.8, 42.8, 38.0, 8.9, -0.9; IR (neat): 3014, 2929, 2247, 1490, 1360, 1165, 1095, 1043, 758, 692 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{15}NNaO_2S$ 296.0716; Found 296.0726.

***N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)methanesulfonamide (1m)**

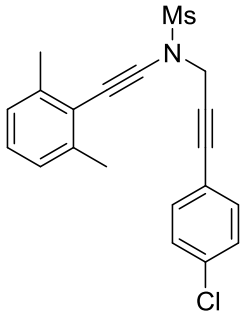


1m

Compound **1m** was prepared in 72% yield (255.9 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 12:1) as a white solid (mp 58–60 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 2H), 7.12 –

7.06 (m, 1H), 7.06 – 6.97 (m, 4H), 4.61 (s, 2H), 3.26 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 250.0 Hz), 139.8, 133.7 (d, *J* = 9.0 Hz), 127.5, 126.6, 121.9, 117.7 (d, *J* = 4.0 Hz), 115.8 (d, *J* = 22.0 Hz), 89.3, 85.8, 81.3, 69.3, 42.9, 38.3, 21.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.4; IR (neat): 2920, 2232, 1507, 1364, 1322, 1231, 1167, 1040, 788, 765 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}FNNaO_2S$ 378.0934; Found 378.0939.

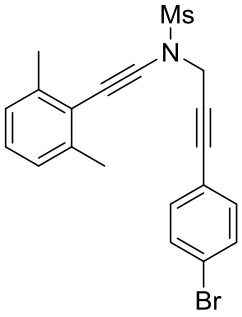
_N_-(3-(4-chlorophenyl)prop-2-yn-1-yl)-_N_-((2,6-dimethylphenyl)ethynyl)methanesulfonamide (1n)



1n

Compound **1n** was prepared in 50% yield (185.9 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a pale red solid (mp 90–92 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.06 (m, 1H), 7.06 – 6.99 (m, 2H), 4.61 (s, 2H), 3.25 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 135.1, 133.0, 128.8, 127.6, 126.6, 121.9, 120.1, 89.2, 85.7, 82.6, 69.4, 42.8, 38.3, 21.0; IR (neat): 3020, 2930, 2232, 1489, 1364, 1167, 1091, 1039, 788, 765 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}ClNNaO_2S$ 394.0639; Found 394.0651.

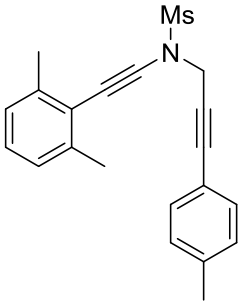
_N_-(3-(4-bromophenyl)prop-2-yn-1-yl)-_N_-((2,6-dimethylphenyl)ethynyl)methanesulfonamide (1o)



1o

Compound **1o** was prepared in 54% yield (224.8 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a yellow solid (mp 92–94 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.07 (m, 1H), 7.06 – 7.00 (m, 2H), 4.62 (s, 2H), 3.25 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 133.2, 131.8, 127.6, 126.7, 123.4, 121.9, 120.6, 89.2, 85.8, 82.7, 69.4, 42.9, 38.4, 21.1; IR (neat): 2927, 2232, 1485, 1364, 1275, 1166, 1071, 1040, 764, 750 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}BrNNaO_2S$ 438.0133; Found 438.0127.

***N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)methanesulfonamide (1p)**

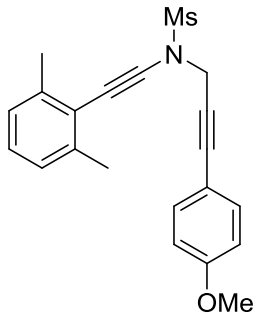


1p

Compound **1p** was prepared in 58% yield (203.8 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a red solid (mp 73–75 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.10 – 6.99 (m, 3H), 4.61 (s, 2H), 3.26 (s, 3H), 2.44 (s, 6H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 139.3, 131.7, 129.2, 127.5, 126.6, 122.0, 118.6, 89.5, 87.1, 80.8, 69.2, 43.1, 38.3, 21.4, 21.0; IR (neat): 2921, 2232, 1509, 1364,

1322, 1166, 1077, 1039, 787, 765 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{21}NNaO_2S$ 374.1185; Found 374.1187.

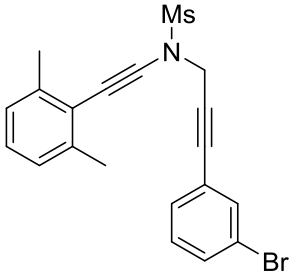
_N_-((2,6-dimethylphenyl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1q)



1q

Compound **1q** was prepared in 52% yield (191.1 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 53–55 ^oC). ^1H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.8 Hz, 2H), 7.12 – 7.05 (m, 1H), 7.05 – 6.97 (m, 2H), 6.83 (d, J = 8.8 Hz, 2H), 4.60 (s, 2H), 3.79 (s, 3H), 3.25 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 139.8, 133.2, 127.4, 126.6, 122.0, 114.0, 113.6, 89.5, 86.9, 80.1, 69.1, 55.2, 43.1, 38.3, 21.0; IR (neat): 2932, 2232, 1606, 1509, 1363, 1249, 1166, 1035, 787, 765 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{21}NNaO_3S$ 390.1134; Found 390.1135.

_N_-(3-(3-bromophenyl)prop-2-yn-1-yl)-_N_-((2,6-dimethylphenyl)ethynyl)methanesulfonamide (1r)

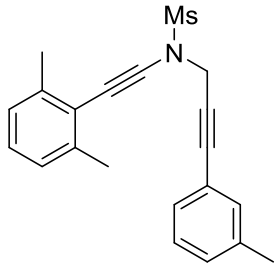


1r

Compound **1r** was prepared in 30% yield (124.9 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as

a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.24 – 7.15 (m, 1H), 7.12 – 6.99 (m, 3H), 4.61 (s, 2H), 3.25 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 134.4, 132.2, 130.3, 129.9, 127.5, 126.6, 123.5, 122.1, 121.8, 89.1, 85.2, 82.9, 69.4, 42.7, 38.3, 21.0; IR (neat): 3019, 2929, 2232, 1473, 1364, 1167, 1077, 1041, 786, 770 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}BrNNaO_2S$ 438.0133; Found 438.0127.

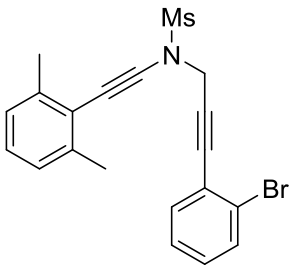
_N_-((2,6-dimethylphenyl)ethynyl)-_N_-(3-(_m_-tolyl)prop-2-yn-1-yl)methanesulfonamide (1s)



1s

Compound **1s** was prepared in 79% yield (277.7 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a yellow solid (mp 47–49 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.21 (m, 2H), 7.20 – 7.12 (m, 2H), 7.11 – 7.05 (m, 1H), 7.04 – 6.98 (m, 2H), 4.59 (s, 2H), 3.24 (s, 3H), 2.44 (s, 6H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 138.1, 132.2, 129.9, 128.8, 128.3, 127.4, 126.6, 121.9, 121.4, 89.4, 87.0, 81.1, 69.2, 42.9, 38.2, 21.0, 20.9; IR (neat): 3021, 2921, 2231, 1468, 1363, 1167, 1078, 1042, 787, 766 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{21}NNaO_2S$ 374.1185; Found 374.1189.

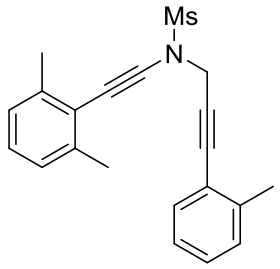
_N_-(3-(2-bromophenyl)prop-2-yn-1-yl)-_N_-((2,6-dimethylphenyl)ethynyl)methanesulfonamide (1t)



1t

Compound **1t** was prepared in 50% yield (208.2 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.46 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.29 – 7.22 (m, 1H), 7.21 – 7.15 (m, 1H), 7.11 – 7.05 (m, 1H), 7.04 – 6.97 (m, 2H), 4.67 (s, 2H), 3.31 (s, 3H), 2.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 133.7, 132.4, 130.2, 127.4, 127.1, 126.5, 125.3, 123.8, 121.9, 89.2, 86.0, 85.1, 69.3, 42.9, 38.5, 21.0; IR (neat): 3019, 2928, 2232, 1470, 1364, 1167, 1078, 1039, 789, 764 ; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}BrNNaO_2S$ 438.0133; Found 438.0134.

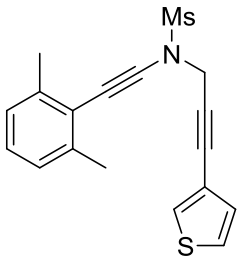
***N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-(*o*-tolyl)prop-2-yn-1-yl)methanesulfonamide (1u)**



1u

Compound **1u** was prepared in 61% yield (214.4 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 71–73 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.6 Hz, 1H), 7.24 – 7.05 (m, 4H), 7.04 – 6.97 (m, 2H), 4.66 (s, 2H), 3.25 (s, 3H), 2.42 (s, 6H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 139.7, 132.1, 129.5, 129.0, 127.4, 126.6, 125.6, 121.9, 121.4, 89.4, 85.7, 85.2, 69.2, 43.0, 38.4, 21.0, 20.6; IR (neat): 3021, 2921, 2232, 1485, 1364, 1167, 1077, 1037, 788, 762 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{21}NNaO_2S$ 374.1185; Found 374.1190.

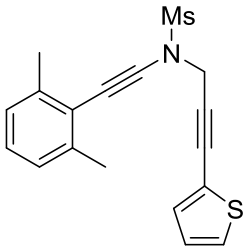
***N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-(thiophen-3-yl)prop-2-yn-1-yl)methanesulfonamide (1v)**



1v

Compound **1v** was prepared in 85% yield (291.9 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 65–67 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 2.8 Hz, 1H), 7.24 (dd, *J* = 4.8, 2.8 Hz, 1H), 7.12 – 7.04 (m, 2H), 7.04 – 6.98 (m, 2H), 4.57 (s, 2H), 3.22 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 129.8, 129.5, 127.4, 126.5, 125.6, 121.8, 120.5, 89.3, 82.0, 81.1, 69.1, 42.8, 38.1, 20.9; IR (neat): 3019, 2927, 2231, 1467, 1361, 1166, 1077, 1039, 786, 765 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{17}NNaO_2S_2$ 366.0593; Found 366.0597.

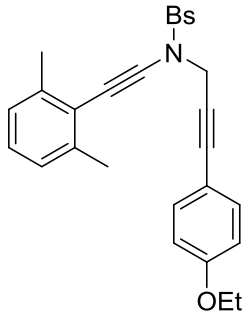
***N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-(thiophen-2-yl)prop-2-yn-1-yl)methanesulfonamide (1w)**



1w

Compound **1w** was prepared in 64% yield (219.8 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a brown solid (mp 65–67 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.30 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.19 – 7.13 (m, 1H), 7.13 – 7.07 (m, 2H), 7.04 (dd, *J* = 5.2, 3.6 Hz, 1H), 4.69 (s, 2H), 3.31 (s, 3H), 2.51 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 133.0, 128.0, 127.5, 127.0, 126.6, 121.8, 121.3, 89.2, 85.5, 80.3, 69.3, 43.1, 38.2, 21.0; IR (neat): 3019, 2929, 2231, 1467, 1363, 1167, 1077, 1034, 788, 765 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{17}NNaO_2S_2$ 366.0593; Found 366.0591.

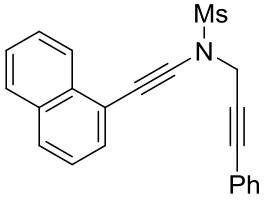
4-bromo-*N*-((2,6-dimethylphenyl)ethynyl)-*N*-(3-(4-ethoxyphenyl)prop-2-yn-1-yl)benzenesulfonamide (1y)



1y

Compound **1y** was prepared in 34% yield (177.6 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a pale yellow solid (mp 106–108 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.10 – 6.95 (m, 5H), 6.76 (d, *J* = 8.8 Hz, 2H), 4.58 (s, 2H), 3.98 (q, *J* = 6.8 Hz, 2H), 2.36 (s, 6H), 1.38 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 140.0, 136.3, 133.0, 132.1, 129.6, 129.0, 127.4, 126.5, 122.0, 114.4, 113.4, 89.5, 86.8, 79.4, 69.0, 63.4, 43.3, 21.0, 14.6; IR (neat): 2980, 2926, 2231, 1605, 1508, 1371, 1172, 1043, 784, 747 cm^{-1}; HRMS (ESI) m/z: $[M + K]^+$ Calcd for $C_{27}H_{24}BrNNaO_3S$ 560.0292; Found 560.0284.

***N*-(naphthalen-1-ylethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1aa)**

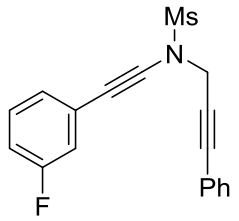


1aa

Compound **1aa** was prepared in 39% yield (140.2 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.85 – 7.73 (m, 2H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.51 – 7.28 (m, 8H), 4.68 (s, 2H), 3.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.2, 133.1, 131.8, 130.2, 129.1, 128.6, 128.4, 128.2, 126.8, 126.3,

126.0, 125.1, 121.6, 119.8, 87.2, 85.8, 81.6, 69.7, 43.0, 38.6; IR (neat): 3057, 2925, 2230, 1489, 1360, 1321, 1189, 1165, 800, 756 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NNaO_2S$ 382.0878; Found 382.0881.

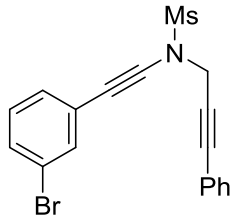
***N*-((3-fluorophenyl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1ab)**



1ab

Compound **1ab** was prepared in 57% yield (186.6 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.42 (m, 2H), 7.38 – 7.28 (m, 3H), 7.28 – 7.20 (m, 2H), 7.13 (d, *J* = 9.2 Hz, 1H), 7.03 – 6.93 (m, 1H), 4.59 (s, 2H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, *J* = 245.0 Hz), 131.7, 129.8 (d, *J* = 9.0 Hz), 129.0, 128.4, 127.2 (d, *J* = 3.0 Hz), 124.0 (d, *J* = 10.0 Hz), 121.5, 118.1 (d, *J* = 23.0 Hz), 115.3 (d, *J* = 21.0 Hz), 87.0, 82.2, 81.2, 70.2 (d, *J* = 4.0 Hz), 42.7, 38.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.8; IR (neat): 3020, 2930, 2241, 1489, 1363, 1324, 1166, 1038, 869, 757 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{14}FNNaO_2S$ 350.0627; Found 350.0630.

***N*-((3-bromophenyl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1ac)**

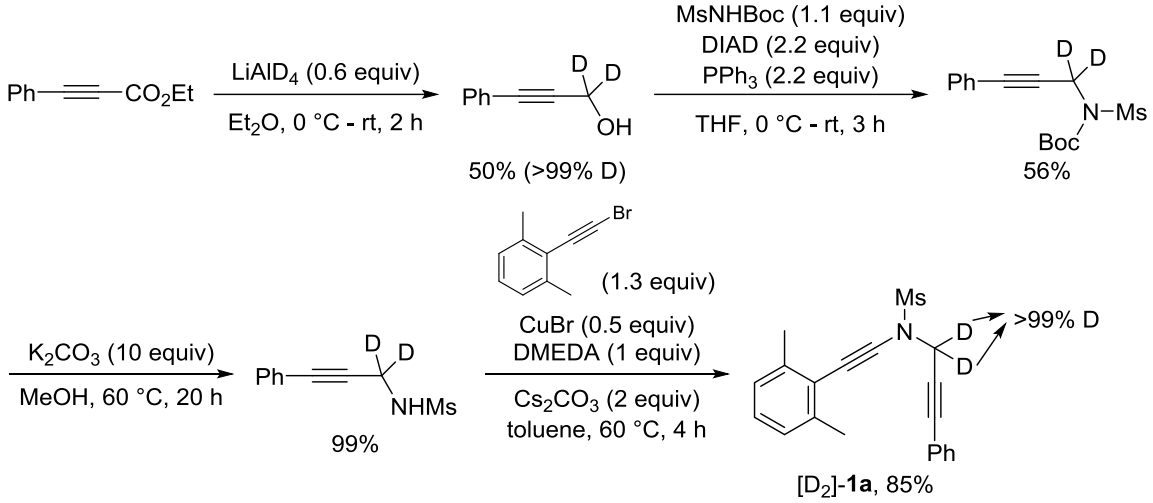


1ac

Compound **1ac** was prepared in 64% yield (248.5 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.56 (m, 1H), 7.48 – 7.43 (m, 2H),

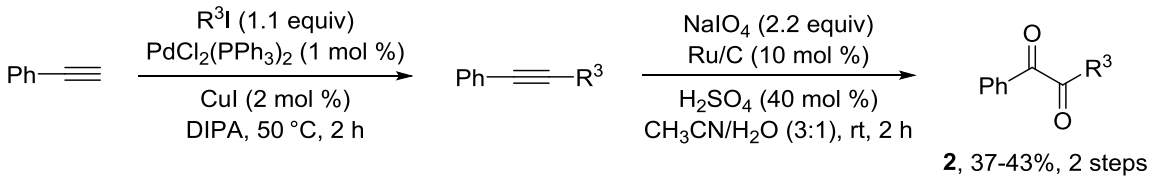
7.43 – 7.38 (m, 1H), 7.38 – 7.29 (m, 4H), 7.18 – 7.11 (m, 1H), 4.59 (s, 2H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.0, 131.7, 131.1, 129.9, 129.7, 129.0, 128.4, 124.2, 121.9, 121.4, 87.1, 82.5, 81.2, 70.0, 42.8, 38.8; IR (neat): 3020, 2929, 2237, 1490, 1364, 1323, 1167, 1039, 789, 758 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{18}H_{14}BrNNaO_2S$ 409.9826; Found 409.9825.

[D_2]-**1a** (>99% D)



Compound [D_2]-**1a** was prepared in 85% yield (288.5 mg) according to the above general procedure.[2] The substrate was isolated through silica gel column chromatography (PE:EA = 15:1) as a red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 2H), 7.37 – 7.27 (m, 3H), 7.11 – 7.05 (m, 1H), 7.05 – 6.98 (m, 2H), 3.24 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 131.7, 129.0, 128.4, 127.5, 126.6, 121.9, 121.6, 89.3, 86.8, 81.4, 69.2, 38.2, 21.0; IR (neat): 3020, 2918, 2240, 1489, 1363, 1321, 1169, 1105, 961, 757 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{20}H_{17}D_2NNaO_2S$ 362.1160; Found 362.1158.

2.2 General procedure for the synthesis of diketones 2 (2b-2c) [3,4]

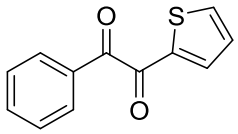


To a solution of styrene (2.0 mmol) in DIPA (0.2 M) was added copper iodide (0.04

mmol, 7.6 mg), $Pd(PPh_3)_2Cl_2$ (0.01 mmol, 7.0 mg), aryl iodide (2.2 mmol, 1.1 equiv). The reaction was stirred at 50 ^oC for about 2 h and the progress of the reaction was monitored by TLC. Upon completion, the solution was then filtered and concentrated under a reduced pressure. The residue was purified by silica gel column chromatography (PE).

The above product was added to a stirred solution of Ru/C (0.2 mmol, 20 mg), H_2SO_4 (0.8 mmol) in CH_3CN (7.5 mL) and H_2O (2.5 mL), The resulting mixture was then stirred at room temperature for about 2 h and the progress of the reaction was monitored by TLC. Upon completion, the solution was then filtered and concentrated under a reduced pressure. The residue was purified by silica gel column chromatography (PE).

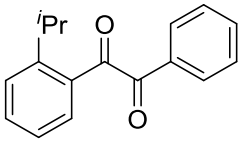
1-phenyl-2-(thiophen-2-yl)ethane-1,2-dione (2b)



2b

Compound **2b** was prepared in 37% yield (160.0 mg) according to the general procedure. The substrate was isolated through silica gel column chromatography (PE) as a yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.2 Hz, 2H), 7.82 (d, *J* = 4.8 Hz, 1H), 7.79 (d, *J* = 3.6 Hz, 1H), 7.68 – 7.58 (m, 1H), 7.55 – 7.40 (m, 2H), 7.22 – 7.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 185.5, 139.7, 136.8, 136.6, 134.8, 132.5, 130.1, 128.8, 128.7; IR (neat): 3103, 2924, 1676, 1652, 1595, 1410, 1213, 1178, 742, 717 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{12}H_8NaO_2S$ 239.0137; Found 239.0129.

1-(2-isopropylphenyl)-2-phenylethane-1,2-dione (2c)

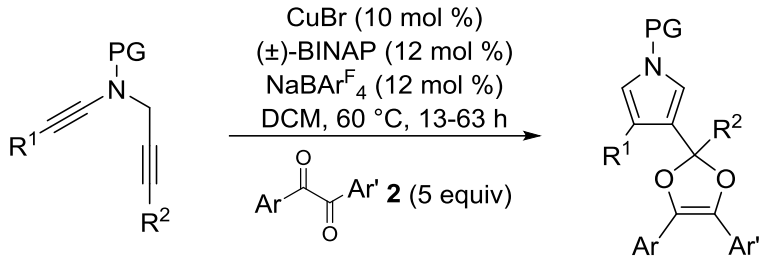


2c

Compound **2c** was prepared in 43% yield (236.6 mg) according to the general procedure.

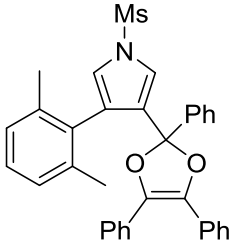
The substrate was isolated through silica gel column chromatography (PE) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.6 Hz, 2H), 7.55 – 7.33 (m, 6H), 7.14 – 7.06 (m, 1H), 3.90 – 3.71 (m, 1H), 1.19 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 194.2, 151.6, 134.6, 133.7, 133.0, 132.4, 131.7, 129.8, 128.9, 127.0, 125.6, 29.2, 23.7; IR (neat): 2967, 2870, 1676, 1597, 1449, 1210, 1198, 1178, 759, 724 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{16}NaO_2$ 275.1043; Found 275.1041.

2.3 General procedure for the synthesis of pyrrole-substituted dioxoles 3



The powdered CuBr (0.01 mmol, 1.4 mg), (±)-BINAP (0.012 mmol, 7.5 mg), NaBAr$^F_4$ (0.012 mmol, 10.6 mg) were introduced into the Schlenk tubes. After DCM (2.5 mL) was added to the Schlenk tubes, the solution was stirred at 60 ºC for 0.5 h. Subsequently, the *N*-propargyl ynamide **1** (0.1 mmol) and diketone **2** (0.5 mmol) in DCM (2.5 mL) were introduced into the system. The resulting mixture was stirred at 60 ℃ and the progress of the reaction was monitored by TLC. Upon completion, the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired pyrrole-substituted dioxole **3**.

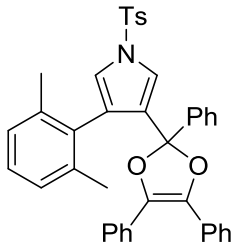
3-(2,6-dimethylphenyl)-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3a)



3a

Compound **3a** was prepared in 89% yield (48.7 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 64–65 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.45 (m, 2H), 7.33 – 7.19 (m, 13H), 7.07 (d, *J* = 2.4 Hz, 1H), 7.02 – 6.97 (m, 1H), 6.90 (d, *J* = 2.4 Hz, 1H), 6.85 (d, *J* = 7.6 Hz, 2H), 3.16 (s, 3H), 1.95 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 138.2, 133.1, 132.4, 129.2, 129.1, 128.6, 128.0, 127.8, 127.7, 127.4, 127.0, 126.6, 126.2, 125.7, 120.8, 119.0, 108.4, 42.8, 20.8; IR (neat): 3026, 2927, 1370, 1260, 1175, 1107, 1080, 983, 759, 693 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{29}NNaO_4S$ 570.1710; Found 570.1701.

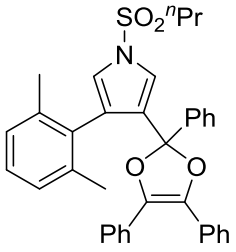
3-(2,6-dimethylphenyl)-1-tosyl-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3b)



3b

Compound **3b** was prepared in 71% yield (44.3 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 169–171 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 6.8 Hz, 2H), 7.33 – 7.15 (m, 15H), 7.10 (d, *J* = 2.4 Hz, 1H), 7.00 – 6.94 (m, 1H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.81 (d, *J* = 7.6 Hz, 2H), 2.47 – 2.35 (s, 3H), 1.82 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 141.0, 138.1, 136.0, 133.1, 132.5, 129.9, 129.2, 129.1, 128.5, 128.0, 127.7, 127.6, 127.3, 127.2, 126.7, 126.5, 126.2, 125.7, 121.3, 119.7, 108.5, 21.6, 20.7; IR (neat): 3059, 2922, 1374, 1261, 1188, 1174, 1106, 1079, 759, 693 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{40}H_{33}NNaO_4S$ 646.2023; Found 646.2018.

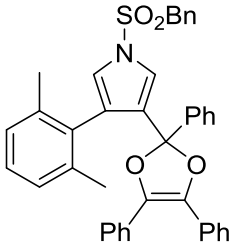
3-(2,6-dimethylphenyl)-1-(propylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3c)



3c

Compound **3c** was prepared in 72% yield (41.4 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 147–149 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 6.8 Hz, 2H), 7.34 – 7.16 (m, 13H), 7.07 – 6.96 (m, 2H), 6.90 – 6.82 (m, 3H), 3.22 (t, *J* = 8.0, 2H), 1.95 (s, 6H), 1.78 – 1.66 (m, 2H), 1.00 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 138.2, 133.1, 132.5, 129.1, 128.9, 128.6, 128.0, 127.8, 127.7, 127.3, 126.6, 126.2, 125.7, 121.0, 119.5, 108.5, 57.2, 20.8, 17.1, 12.6; IR (neat): 3060, 2922, 1372, 1261, 1168, 1106, 1079, 1024, 759, 695 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{36}H_{33}NNaO_4S$ 598.2023; Found 598.2031.

1-(benzylsulfonyl)-3-(2,6-dimethylphenyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3d)

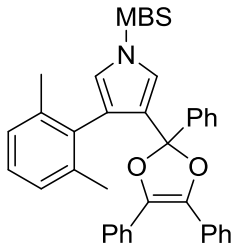


3d

Compound **3d** was prepared in 66% yield (41.2 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 149–151 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.28 (m, 5H), 7.28 – 7.20 (m, 13H), 7.13 (d, *J* = 7.2 Hz, 2H), 7.01 – 6.95 (m, 1H), 6.83 (d, *J* = 7.6 Hz, 2H), 6.67 (d, *J* = 2.4 Hz, 1H), 6.59 (d, *J* = 2.4 Hz, 1H), 4.47 (s, 2H), 1.93 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 138.2, 133.0, 132.4, 130.4, 129.4, 129.1, 129.0, 128.5, 128.0, 127.7, 127.6, 127.3, 126.9, 126.6, 126.5, 126.2, 125.7, 121.8, 119.2, 108.4, 61.4, 21.0; IR

(neat): 3060, 2923, 1373, 1261, 1168, 1106, 1080, 1024, 759, 695 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{40}H_{33}NNaO_4S$ 646.2023; Found 646.2018.

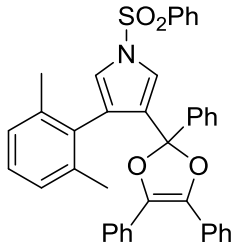
3-(2,6-dimethylphenyl)-1-((4-methoxyphenyl)sulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3e)



3e

Compound **3e** was prepared in 80% yield (51.2 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 25:1) as a white solid (mp 159–161 °C). ^1H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.8 Hz, 2H), 7.42 (d, *J* = 6.8 Hz, 2H), 7.30 – 7.17 (m, 13H), 7.09 (s, 1H), 7.01 – 6.87 (m, 4H), 6.81 (d, *J* = 7.6 Hz, 2H), 3.86 (s, 3H), 1.82 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 141.0, 138.2, 133.1, 132.6, 130.3, 129.1, 129.0, 128.5, 128.0, 127.7, 127.6, 127.3, 127.1, 126.5, 126.2, 125.7, 121.2, 119.5, 114.5, 108.5, 55.7, 20.7; IR (neat): 3059, 2924, 1595, 1498, 1374, 1263, 1167, 1079, 760, 680 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{40}H_{33}NNaO_5S$ 662.1972; Found 662.1969.

3-(2,6-dimethylphenyl)-1-(phenylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3f)

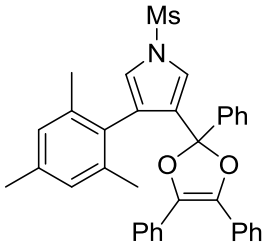


3f

Compound **3f** was prepared in 66% yield (40.2 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 25:1) as a

white solid (mp 150–152 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 2H), 7.63 – 7.56 (m, 1H), 7.53 – 7.46 (m, 2H), 7.41 (d, *J* = 6.8 Hz, 2H), 7.32 – 7.17 (m, 13H), 7.12 (d, *J* = 2.0 Hz, 1H), 7.01 – 6.89 (m, 2H), 6.81 (d, *J* = 7.6 Hz, 2H), 1.80 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 138.8, 138.1, 133.9, 133.1, 132.4, 129.5, 129.3, 129.0, 128.5, 128.0, 127.8, 127.7, 127.5, 127.3, 126.6, 126.5, 126.2, 125.7, 121.4, 119.7, 108.4, 20.6; IR (neat): 3060, 2922, 1448, 1376, 1260, 1184, 1176, 1079, 760, 727 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{39}H_{31}NNaO_4S$ 632.1866; Found 632.1871.

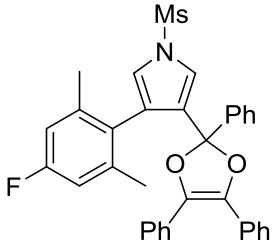
3-mesityl-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3g)



3g

Compound **3g** was prepared in 64% yield (35.9 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 6.8 Hz, 2H), 7.31 – 7.20 (m, 13H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.66 (s, 2H), 3.17 (s, 3H), 2.17 (s, 3H), 1.92 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 137.9, 136.8, 133.1, 129.4, 129.1, 128.6, 128.0, 127.7, 127.4, 127.1, 126.2, 125.7, 120.7, 119.1, 108.5, 42.8, 21.0, 20.7; IR (neat): 3026, 2926, 1448, 1370, 1261, 1173, 1084, 1024, 760, 694 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{35}H_{31}NNaO_4S$ 584.1866; Found 584.1868.

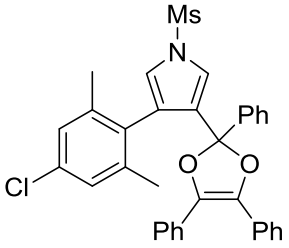
3-(4-fluoro-2,6-dimethylphenyl)-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3h)



3h

Compound **3h** was prepared in 88% yield (49.8 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 195–197 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 6.4 Hz, 2H), 7.34 – 7.20 (m, 13H), 7.07 (d, *J* = 2.4 Hz, 1H), 6.89 (d, *J* = 2.4 Hz, 1H), 6.55 (d, *J* = 9.6 Hz, 2H), 3.17 (s, 3H), 1.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, *J* = 244.0 Hz), 140.9, 140.6, 140.5, 133.1, 129.3, 129.0, 128.7, 128.1, 127.8 (d, *J* = 9.0 Hz), 126.1, 125.6, 120.8, 119.4, 113.1 (d, *J* = 21.0 Hz), 108.3, 42.9, 21.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.6; IR (neat): 3058, 2927, 1371, 1261, 1173, 1130, 1085, 1024, 760, 694 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}FNNaO_4S$ 588.1615; Found 588.1613.

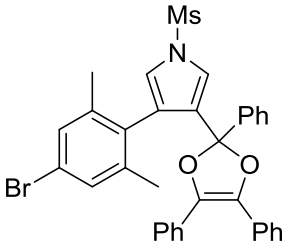
3-(4-chloro-2,6-dimethylphenyl)-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3i)



3i

Compound **3i** was prepared in 89% yield (51.8 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 196–198 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.53 (m, 2H), 7.37 – 7.26 (m, 13H), 7.09 (d, *J* = 2.4 Hz, 1H), 6.94 (d, *J* = 2.4 Hz, 1H), 6.87 (s, 2H), 3.23 (s, 3H), 1.98 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 140.1, 133.1, 132.8, 131.0, 129.2, 128.9, 128.7, 128.1, 127.9, 127.8, 126.4, 126.1, 125.9, 125.6, 121.0, 119.1, 108.3, 42.9, 20.8; IR (neat): 3026, 2927, 1371, 1260, 1175, 1122, 1084, 1024, 751, 694 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}ClNNaO_4S$ 604.1320; Found 604.1335.

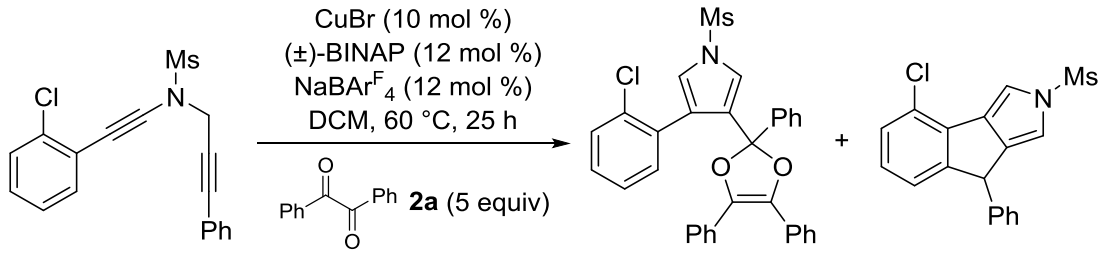
3-(4-bromo-2,6-dimethylphenyl)-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3j)



3j

Compound **3j** was prepared in 85% yield (53.3 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 188–190 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.49 (m, 2H), 7.33 – 7.21 (m, 13H), 7.03 (d, *J* = 2.4 Hz, 1H), 6.97 (s, 2H), 6.89 (d, *J* = 2.4 Hz, 1H), 3.17 (s, 3H), 1.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 140.5, 133.2, 131.7, 129.4, 129.2, 129.0, 128.8, 128.2, 128.0, 127.9, 126.2, 126.0, 125.7, 121.3, 121.1, 119.1, 108.4, 43.0, 20.8; IR (neat): 3056, 2927, 1371, 1264, 1175, 1120, 1083, 1024, 751, 739 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}BrNNaO_4S$ 648.0815; Found 648.0822.

3-(2-chlorophenyl)-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3k)

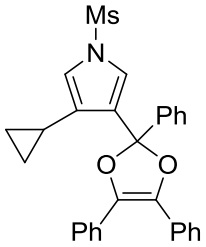


1k **3k**, 54% **3k'**, 29%

Compound **3k** was prepared in 54% yield (29.9 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 88–90 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.50 (m, 2H), 7.36 – 7.20 (m, 15H), 7.12 (d, *J* = 2.4 Hz, 1H), 7.10 – 7.04 (m, 1H), 7.01 (d, *J* = 2.4 Hz, 1H), 7.01 – 6.96 (m, 1H), 3.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 134.4, 133.2, 132.9, 132.2, 129.3, 129.1, 128.8, 128.7, 128.6, 128.1, 127.9, 127.8, 126.3, 125.8, 125.6, 120.8, 120.4, 108.6, 43.0; IR (neat): 3056, 2927, 1371, 1264, 1175, 1097, 1063, 1023, 755, 738 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{32}H_{24}ClNNaO_4S$ 576.1007;

Found 576.0996.

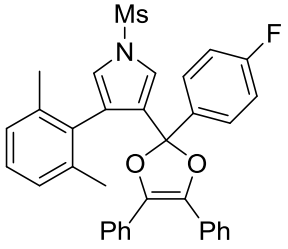
3-cyclopropyl-1-(methylsulfonyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3l)



3l

Compound **3l** was prepared in 77% yield (37.2 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 71–73 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.68 (m, 2H), 7.59 – 7.53 (m, 4H), 7.43 – 7.36 (m, 3H), 7.32 – 7.24 (m, 6H), 6.89 (d, *J* = 2.4 Hz, 1H), 6.74 (d, *J* = 1.6 Hz, 1H), 3.09 (s, 3H), 1.81 – 1.72 (m, 1H), 0.72 – 0.66 (m, 2H), 0.50 – 0.44 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 133.6, 131.1, 129.6, 129.3, 128.9, 128.3, 128.1, 128.0, 126.3, 126.2, 120.8, 117.1, 109.2, 42.8, 7.3, 6.7; IR (neat): 3057, 2929, 1369, 1263, 1172, 1087, 1061, 1025, 753, 696 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{29}H_{25}NNaO_4S$ 506.1397; Found 506.1392.

3-(2,6-dimethylphenyl)-4-(2-(4-fluorophenyl)-4,5-diphenyl-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3m)

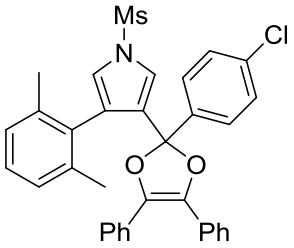


3m

Compound **3m** was prepared in 88% yield (49.8 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 152–154 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 8.8, 5.6 Hz, 2H), 7.32 – 7.19 (m, 10H), 7.13 (d, *J* = 2.4 Hz, 1H), 7.04 – 6.97 (m, 1H), 6.97 – 6.83 (m,

5H), 3.19 (s, 3H), 1.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 246.0 Hz), 138.1, 136.9 (d, *J* = 3.0 Hz), 133.1, 132.2, 128.9(2), 128.9(0), 128.1, 127.9, 127.6 (d, *J* = 9.0 Hz), 127.5, 126.9, 126.6, 126.2, 120.5, 119.1, 114.6 (d, *J* = 21.0 Hz), 108.1, 42.9, 20.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.4; IR (neat): 3056, 2926, 1371, 1264, 1222, 1175, 1107, 1079, 760, 738 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}FNNaO_4S$ 588.1615; Found588.1612.

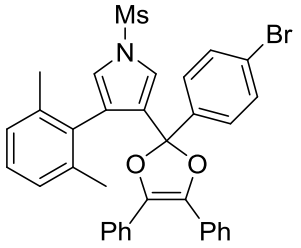
3-(2-(4-chlorophenyl)-4,5-diphenyl-1,3-dioxol-2-yl)-4-(2,6-dimethylphenyl)-1-(methylsulfonyl)-1*H*-pyrrole (3n)



3n

Compound **3n** was prepared in 79% yield (46.0 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.4 Hz, 2H), 7.30 – 7.20 (m, 12H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.04 – 6.98 (m, 1H), 6.92 (d, *J* = 2.4 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.19 (s, 3H), 1.95 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 138.1, 134.5, 133.2, 132.2, 128.8, 128.6, 128.1, 128.0, 127.9, 127.5, 127.2, 126.9, 126.7, 126.2, 120.6, 119.1, 108.0, 42.9, 20.8; IR (neat): 3056, 2927, 1371, 1263, 1214, 1175, 1107, 1080, cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}ClNNaO_4S$ 604.1320; Found 604.1325.

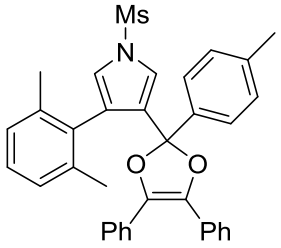
3-(2-(4-bromophenyl)-4,5-diphenyl-1,3-dioxol-2-yl)-4-(2,6-dimethylphenyl)-1-(methylsulfonyl)-1*H*-pyrrole (3o)



3o

Compound **3o** was prepared in 77% yield (48.2 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 179–181 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.6 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H), 7.30 – 7.20 (m, 10H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.04 – 6.98 (m, 1H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.19 (s, 3H), 1.95 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 138.1, 133.2, 132.2, 130.9, 128.8, 128.5, 128.1, 128.0, 127.5, 127.4, 126.8, 126.7, 126.2, 122.8, 120.6, 119.1, 108.0, 42.9, 20.8; IR (neat): 3056, 2926, 1371, 1263, 1214, 1175, 1107, 1080, 770, 738 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}BrNNaO_4S$ 648.0815; Found 648.0801.

3-(2,6-dimethylphenyl)-4-(4,5-diphenyl-2-(*p*-tolyl)-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3p)

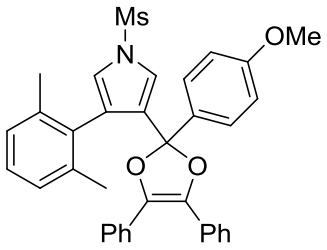


3p

Compound **3p** was prepared in 85% yield (47.7 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 176–178 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.2 Hz, 2H), 7.28 – 7.18 (m, 10H), 7.09 (d, *J* = 7.2 Hz, 2H), 7.03 – 6.95 (m, 2H), 6.93 – 6.82 (m, 3H), 3.17 (s, 3H), 2.34 (s, 3H), 1.99 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 138.2, 138.1, 133.1, 132.5, 129.4, 129.1, 128.4, 127.9, 127.7, 127.3, 127.2, 126.6, 126.2, 125.6, 121.0, 118.9, 108.5, 42.8, 21.2, 20.9; IR (neat): 3056, 2925, 1371, 1263, 1219, 1176,

1107, 1079, 769, 693 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{35}H_{31}NNaO_4S$ 584.1866; Found 584.1871.

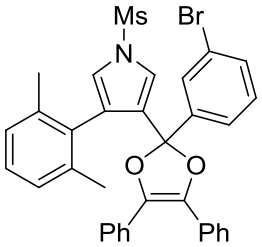
3-(2,6-dimethylphenyl)-4-(2-(4-methoxyphenyl)-4,5-diphenyl-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3q)



3q

Compound **3q** was prepared in 66% yield (38.1 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 150–152 ^oC). ^1H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.8 Hz, 2H), 7.30 – 7.19 (m, 10H), 7.05 (d, *J* = 2.4 Hz, 1H), 7.02 – 6.96 (m, 1H), 6.90 (d, *J* = 2.4 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 3.17 (s, 3H), 1.97 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 138.1, 133.3, 133.1, 132.5, 129.5, 129.2, 128.0, 127.7, 127.3, 127.1, 127.0, 126.6, 126.2, 120.8, 119.0, 113.1, 108.5, 55.3, 42.8, 20.9; IR (neat): 3055, 2927, 1370, 1264, 1216, 1173, 1106, 1079, 759, 739 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{35}H_{31}NNaO_5S$ 600.1815; Found 600.1814.

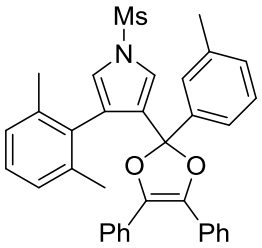
3-(2-(3-bromophenyl)-4,5-diphenyl-1,3-dioxol-2-yl)-4-(2,6-dimethylphenyl)-1-(methylsulfonyl)-1*H*-pyrrole (3r)



3r

Compound **3r** was prepared in 54% yield (33.8 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.49 (m, 1H), 7.44 – 7.36 (m, 2H), 7.34 – 7.28 (m, 4H), 7.26 – 7.21 (m, 6H), 7.16 (d, *J* = 2.4 Hz, 1H), 7.14 – 7.09 (m, 1H), 7.06 – 7.00 (m, 1H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 2H), 3.19 (s, 3H), 1.93 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 138.1, 133.2, 132.0, 131.7, 129.4, 128.8, 128.7, 128.5, 128.1, 128.0, 127.6, 126.8, 126.7, 126.3, 124.4, 122.0, 120.5, 119.2, 107.6, 42.9, 20.8; IR (neat): 3055, 2927, 1371, 1264, 1216, 1173, 1106, 1079, 769, 738 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}BrNNaO_4S$ 648.0815; Found 648.0822.

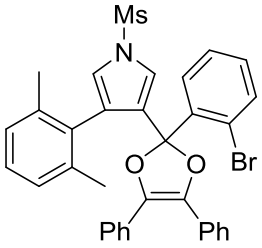
3-(2,6-dimethylphenyl)-4-(4,5-diphenyl-2-(*m*-tolyl)-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3s)



3s

Compound **3s** was prepared in 83% yield (46.6 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 167–169 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 5H), 7.24 – 7.18 (m, 7H), 7.18 – 7.13 (m, 1H), 7.12 – 7.07 (m, 2H), 7.03 – 6.97 (m, 1H), 6.89 (d, *J* = 2.4 Hz, 1H), 6.86 (d, *J* = 7.2 Hz, 2H), 3.17 (s, 3H), 2.28 (s, 3H), 1.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 138.2, 137.3, 133.2, 132.4, 129.4, 129.3, 129.2, 128.0, 127.8, 127.6, 127.4, 127.0, 126.6, 126.3, 126.2, 122.9, 120.7, 119.0, 108.5, 42.8, 21.5, 20.8; IR (neat): 3056, 2925, 1371, 1264, 1175, 1107, 1080, 1024, 769, 738 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{35}H_{31}NNaO_4S$ 584.1866; Found 584.1870.

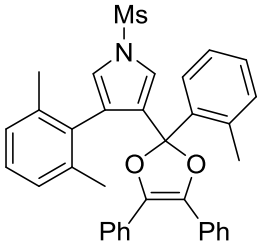
3-(2-(2-bromophenyl)-4,5-diphenyl-1,3-dioxol-2-yl)-4-(2,6-dimethylphenyl)-1-(methylsulfonyl)-1*H*-pyrrole (3t)



3t

Compound **3t** was prepared in 46% yield (28.8 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 199–201 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.47 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.37 – 7.30 (m, 4H), 7.27 – 7.21 (m, 6H), 7.19 – 7.09 (m, 3H), 6.97 – 6.91 (m, 2H), 6.79 (d, *J* = 7.6 Hz, 2H), 3.18 (s, 3H), 2.03 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 138.2, 134.7, 133.2, 132.1, 130.3, 128.8, 128.1, 127.9, 127.8, 127.3, 127.2, 126.8, 126.7, 126.6, 126.3, 122.2, 121.3, 119.0, 108.0, 42.9, 20.9; IR (neat): 3055, 2926, 1371, 1265, 1175, 1106, 1081, 1024, 756, 739 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{34}H_{28}BrNNaO_4S$ 648.0815; Found 648.0816.

3-(2,6-dimethylphenyl)-4-(4,5-diphenyl-2-(*o*-tolyl)-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3u)

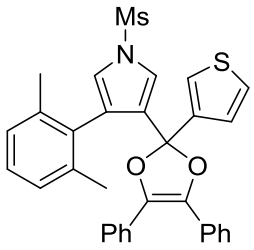


3u

Compound **3u** was prepared in 47% yield (26.4 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 227–229 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.24 (m, 5H), 7.23 – 7.14 (m, 7H), 7.09 – 7.03 (m, 1H), 6.99 – 6.90 (m, 3H), 6.81 (d, *J* = 7.6 Hz, 2H), 3.16 (s, 3H), 2.47 (s, 3H), 2.02 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 138.0, 136.3, 133.0, 132.4, 131.7, 129.1, 128.8, 128.5, 128.0, 127.7, 127.4, 127.3, 126.7, 126.3, 125.7, 125.1, 121.2, 119.2, 108.9, 42.8, 21.1, 20.9; IR (neat): 3056, 2926,

1371, 1264, 1175, 1105, 1077, 1024, 758, 692 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{35}H_{31}NNaO_4S$ 584.1866; Found 584.1869.

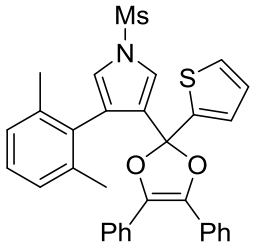
3-(2,6-dimethylphenyl)-4-(4,5-diphenyl-2-(thiophen-3-yl)-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3v)



3v

Compound **3v** was prepared in 75% yield (41.5 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 151–153 °C). ^1H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 4H), 7.24 – 7.17 (m, 9H), 7.12 (dd, *J* = 4.4, 2.0 Hz, 1H), 7.03 – 6.97 (m, 1H), 6.92 (d, *J* = 2.4 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.19 (s, 3H), 1.98 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 138.2, 133.1, 132.4, 129.0, 128.6, 128.0, 127.8, 127.4, 126.9, 126.6, 126.3, 126.1, 125.7, 123.0, 120.6, 119.1, 107.2, 42.9, 20.8; IR (neat): 3055, 2926, 1371, 1264, 1175, 1106, 1078, 1024, 762, 738 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{32}H_{27}NNaO_4S_2$ 576.1274; Found 576.1280.

3-(2,6-dimethylphenyl)-4-(4,5-diphenyl-2-(thiophen-2-yl)-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3w)

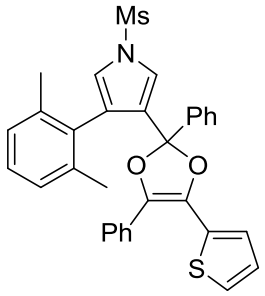


3w

Compound **3w** was prepared in 66% yield (36.5 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a

white solid (mp 168–170 °C). ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.18 (m, 12H), 7.12 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.01 – 6.92 (m, 3H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.19 (s, 3H), 2.03 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 138.1, 133.2, 132.4, 128.8, 128.5, 128.0, 127.9, 127.4, 127.1, 126.7, 126.6, 126.4, 125.7(3), 125.7(1), 121.4, 119.1, 107.0, 42.9, 20.9; IR (neat): 3056, 2923, 1370, 1263, 1175, 1106, 1077, 1023, 770, 759 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{32}H_{27}NNaO_4S_2$ 576.1274; Found 576.1284.

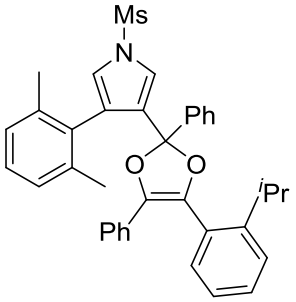
3-(2,6-dimethylphenyl)-4-(2,4-diphenyl-5-(thiophen-2-yl)-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3x)



3x

Compound **3x** was prepared in 64% yield (35.4 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 2H), 7.39 – 7.35 (m, 2H), 7.30 – 7.18 (m, 7H), 7.08 – 6.98 (m, 3H), 6.94 – 6.83 (m, 4H), 3.17 (s, 3H), 1.97 (s, 3H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 138.2, 138.1, 133.2, 132.3, 130.6, 128.9, 128.7, 128.6, 128.5, 128.0, 127.9, 127.8, 127.4, 127.0, 126.9, 126.6, 126.5, 126.1, 125.7, 125.1, 125.0, 120.8, 119.0, 108.8, 42.9, 20.8(3), 20.8(1); IR (neat): 3057, 2925, 1654, 1410, 1265, 1213, 1175, 1076, 772, 739 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{32}H_{27}NNaO_4S_2$ 576.1274; Found 576.1284.

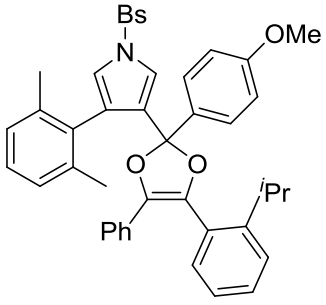
3-(2,6-dimethylphenyl)-4-(4-(2-isopropylphenyl)-2,5-diphenyl-1,3-dioxol-2-yl)-1-(methylsulfonyl)-1*H*-pyrrole (3y)



3y

Compound **3y** was prepared in 68% yield (40.1 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 79–81 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.41 (m, 2H), 7.39 – 7.33 (m, 1H), 7.32 – 7.23 (m, 4H), 7.17 – 6.97 (m, 9H), 6.93 – 6.83 (m, 3H), 3.18 (s, 3H), 2.76 – 2.64 (m, 1H), 2.03 (s, 3H), 1.88 (s, 3H), 0.95 (d, *J* = 6.8 Hz, 3H), 0.83 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 141.0, 138.4, 138.3, 133.6, 133.1, 132.5, 131.3, 130.0, 129.0, 128.9, 128.5, 127.9, 127.5, 127.4, 127.2, 127.0, 126.7, 126.6, 126.5, 125.9, 125.8, 125.7, 123.9, 120.8, 119.1, 109.0, 42.8, 29.8, 23.9, 23.6, 21.0, 20.6; IR (neat): 2962, 2927, 1371, 1264, 1176, 1107, 1078, 1024, 760, 741 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{37}H_{35}NNaO_4S$ 612.2179; Found 612.2186.

1-((4-bromophenyl)sulfonyl)-3-(2,6-dimethylphenyl)-4-(4-(2-isopropylphenyl)-2-(4-methoxyphenyl)-5-phenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3z)

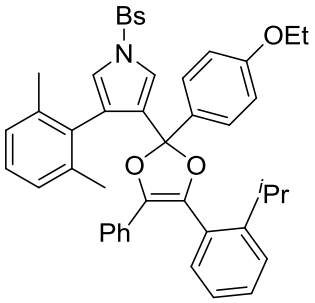


3z

Compound **3z** was prepared in 63% yield (47.9 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 30:1) as a white solid (mp 86–88 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.59 (m, 4H), 7.43 – 7.25 (m, 4H), 7.18 – 6.72 (m, 14H), 3.79 (s, 3H), 2.78 – 2.65 (m, 1H), 1.90 (s, 3H), 1.75

(s, 3H), 0.96 (d, *J* = 6.4 Hz, 3H), 0.85 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 149.7, 138.3, 138.1, 138.0, 133.5, 133.1, 133.0, 132.7, 132.4, 131.3, 130.2, 129.9, 129.2, 128.9, 128.1, 127.9, 127.8, 127.4, 127.3, 127.1, 126.6, 126.5, 126.4, 125.9, 125.7, 123.8, 121.2, 119.8, 112.9, 109.0, 55.3, 29.9, 23.9, 23.6, 20.9, 20.5; IR (neat): 2961, 2926, 1391, 1379, 1252, 1185, 1176, 1076, 760, 744 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{43}H_{38}BrNNaO_5S$ 782.1546; Found 782.1550.

1-((4-bromophenyl)sulfonyl)-3-(2,6-dimethylphenyl)-4-(2-(4-ethoxyphenyl)-4-(2-isopropylphenyl)-5-phenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (3aa)

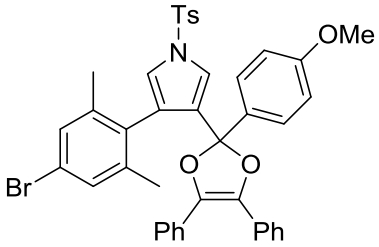


3aa

Compound **3aa** was prepared in 54% yield (41.8 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 30:1) as a white solid (mp 78–80 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.61 (m, 4H), 7.38 – 7.24 (m, 4H), 7.16 (d, *J* = 2.4 Hz, 1H), 7.13 – 6.94 (m, 8H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.87 – 6.79 (m, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 2.80 – 2.65 (m, 1H), 1.90 (s, 3H), 1.74 (s, 3H), 1.41 (t, *J* = 7.2 Hz, 3H), 0.95 (d, *J* = 6.8 Hz, 3H), 0.85 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 149.7, 138.3, 138.1, 138.0, 133.5, 133.0, 132.9, 132.7, 132.4, 131.3, 130.2, 129.9, 129.2, 129.0, 128.1, 127.9, 127.8, 127.4, 127.3, 127.1, 126.6, 126.5, 126.4, 125.9, 125.7, 123.8, 121.2, 119.7, 113.5, 109.1, 63.5, 29.8, 23.9, 23.6, 20.9, 20.5, 14.8; IR (neat): 2961, 2925, 1391, 1251, 1185, 1175, 1090, 1076, 759, 744 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{44}H_{40}BrNNaO_5S$ 796.1703; Found 796.1701.

3-(4-bromo-2,6-dimethylphenyl)-4-(2-(4-methoxyphenyl)-4,5-diphenyl-1,3-dioxol-2-

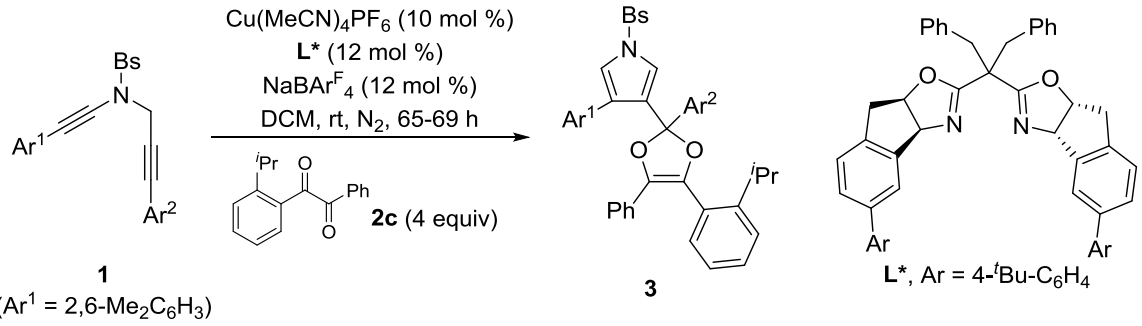
yl)-1-tosyl-1*H*-pyrrole (3ab)



3ab

Compound **3ab** was prepared in 60% yield (44.0 mg) according to the general procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1) as a white solid (mp 212–214 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.15 (m, 10H), 7.05 (d, *J* = 2.4 Hz, 1H), 6.92 (s, 2H), 6.90 (d, *J* = 2.4 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 2H), 3.80 (s, 3H), 2.42 (s, 3H), 1.82 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 145.2, 140.3, 135.9, 133.1, 133.0, 131.8, 130.0, 129.4, 129.2, 129.0, 128.1, 127.8, 127.0, 126.7, 126.2, 126.1, 121.6, 121.1, 119.6, 113.1, 108.4, 55.3, 21.6, 20.6; IR (neat): 3054, 2925, 1376, 1264, 1188, 1173, 1079, 1024, 739, 704 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{41}H_{34}BrNNaO_5S$ 754.1233; Found 754.1231.

2.4 General procedure for the synthesis of chiral pyrrole-substituted dioxoles 3



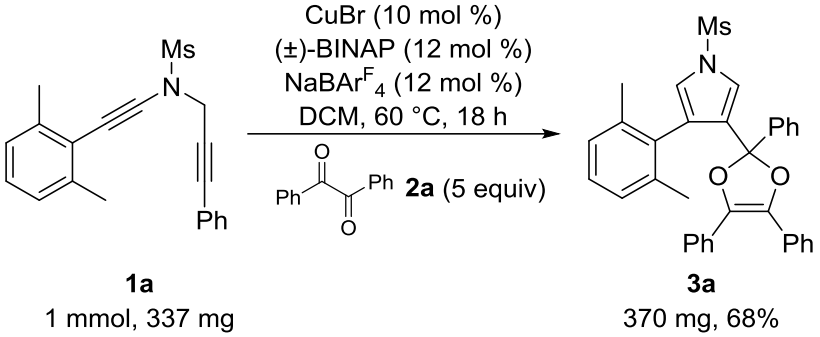
The powdered $Cu(MeCN)_4PF_6$ (0.01 mmol, 3.7 mg), **L*** (0.012 mmol, 9.3 mg), $NaBAr^F_4$ (0.012 mmol, 10.6 mg) were introduced into an oven-dried Schlenk tube under argon atmosphere. After DCM (1 mL) was injected to the Schlenk tube, the solution was stirred at room temperature under argon atmosphere for 2 h. Subsequently, the *N*-propargyl ynamide **1** (0.1 mmol) and diketone **2c** (0.5 mmol) in DCM (1 mL) were introduced into the system. The resulting mixture was stirred at room temperature and the progress of the

reaction was monitored by TLC. Upon completion, the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired chiral pyrrole-substituted dioxole **3**.

Compound (+)-**3z** was prepared in 30% yield (22.8 mg) according to the above procedure. The product was isolated through silica gel column chromatography (PE:EA = 30:1) as a white solid. $[\alpha]_D^{20}$ = +15.86 º(c = 1.0, $CHCl_3$). 30% ee (determined by HPLC (IB, *n*-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, I = 254 nm) tR = 6.80 min (minor), 7.58 min (major)).

Compound (+)-**3aa** was prepared in 36% yield (27.8 mg) according to the above procedure. The product was isolated through silica gel column chromatography (PE:EA = 30:1) as a white solid $[\alpha]_D^{20}$ = +15.00 º(c = 1.0, $CHCl_3$). 29% ee (determined by HPLC (IB, *n*-hexane/2-propanol = 98/2, flow rate = 1.0 mL/min, I = 254 nm) tR = 7.27 min (minor), 8.19 min (major)).

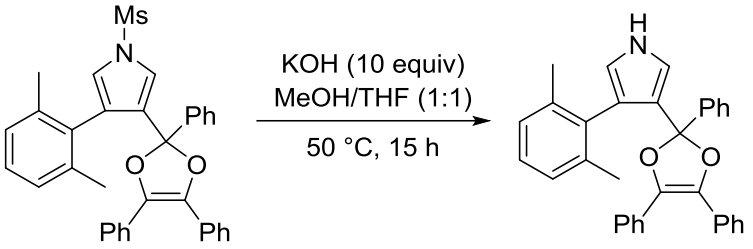
2.5 Preparative-scale synthesis of 3a



The powdered CuBr (0.1 mmol, 14.1 mg), (±)-BINAP (0.12 mmol, 74.7 mg), $NaBAr^F_4$ (0.12 mmol, 106.3 mg) were introduced into the Schlenk tubes. After DCM (25 mL) was added to the Schlenk tubes, the solution was stirred at 60 ℃ for 0.5 h. Subsequently, the *N*-propargyl ynamide **1a** (1.0 mmol, 337 mg) and diketone **2a** (5.0 mmol) in DCE (25 mL) were introduced into the system. The resulting mixture was stirred at 60 ℃ and the progress of the reaction was monitored by TLC. Upon completion, the mixture was concentrated and the residue was purified by flash chromatography on silica gel (PE:EA = 15:1) to afford the desired product **3a** (370 mg, 68% yield).

2.6 Transformations

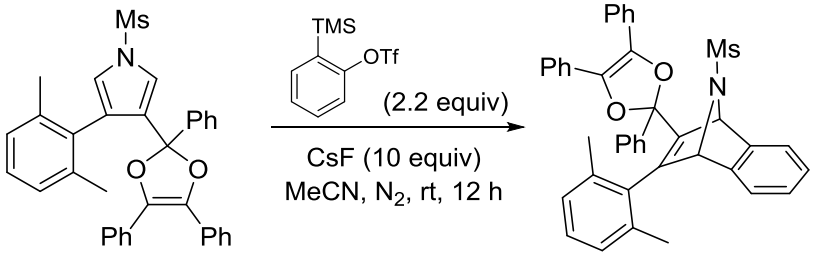
3-(2,6-dimethylphenyl)-4-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1*H*-pyrrole (4a)



3a **4a**, 85%

Compound **4a** was prepared in 85% yield (39.9 mg) according to the above known procedure (0.1 mmol scale).[5] The product was isolated through silica gel column chromatography (PE:EA = 10:1) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.61 – 7.52 (m, 2H), 7.33 – 7.23 (m, 7H), 7.22 – 7.13 (m, 6H), 6.99 – 6.91 (m, 1H), 6.85 (d, *J* = 7.6 Hz, 2H), 6.61 – 6.56 (m, 1H), 6.53 – 6.46 (m, 1H), 2.01 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 138.7, 135.2, 133.1, 129.7, 128.0, 127.9, 127.4, 127.3, 126.5, 126.3(2), 126.3(1), 125.8, 123.4, 122.2, 119.1, 116.9, 109.8, 21.0; IR (neat): 3432, 3057, 2922, 1447, 1264, 1101, 1072, 1024, 758, 749 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{33}H_{27}NNaO_2$ 492.1934; Found 492.1943.

(±)-2-(2,6-dimethylphenyl)-9-(methylsulfonyl)-3-(2,4,5-triphenyl-1,3-dioxol-2-yl)-1,4-dihydro-1,4-epiminonaphthalene (4b)



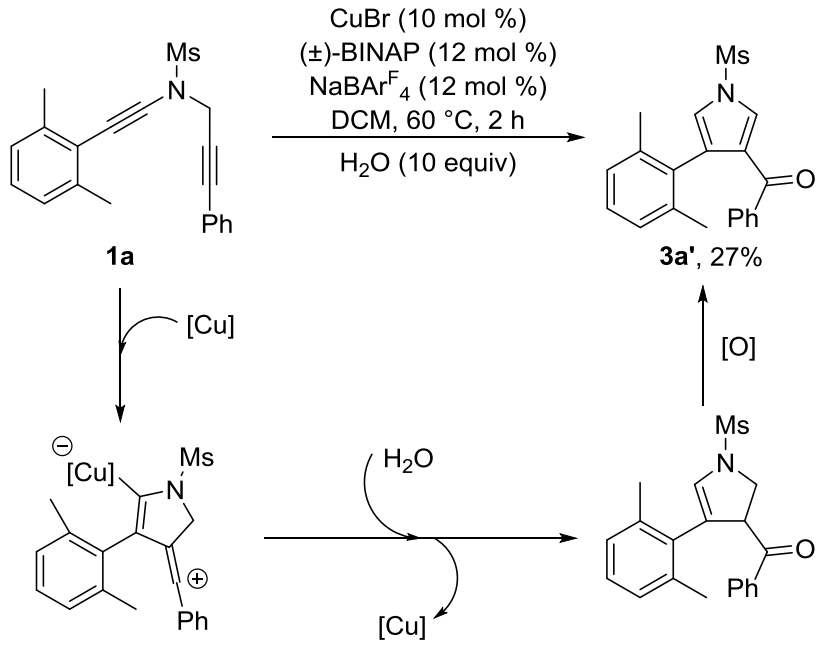
3a **4b**, 69%

Compound **4b** was prepared in 69% yield (43.0 mg) according to the above known procedure (0.1 mmol scale).[6] The product was isolated through silica gel column chromatography (PE:EA = 5:1) as pale yellow solid (mp 200–202 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.37 – 7.23 (m, 9H), 7.18 (s, 5H), 7.05 – 6.96 (m,

3H), 6.90 – 6.85 (m, 1H), 6.80 (d, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 5.66 (d, *J* = 1.6 Hz, 1H), 5.25 (d, *J* = 1.6 Hz, 1H), 2.29 (s, 3H), 2.08 (s, 3H), 1.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 147.7, 147.6, 146.6, 138.4, 136.5, 135.0, 133.5, 133.4, 132.9, 129.1, 128.8, 128.5, 128.2, 128.0(8), 128.0(3), 128.0(0), 127.9, 127.6, 127.0, 126.9, 126.4, 126.2, 126.0, 125.5, 122.1, 121.9, 109.3, 72.8, 68.9, 38.0, 20.6, 20.1; IR (neat): 3057, 2925, 1449, 1341, 1264, 1154, 1069, 1025, 760, 740 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{40}H_{33}NNaO_4S$ 646.2023; Found 646.2038.

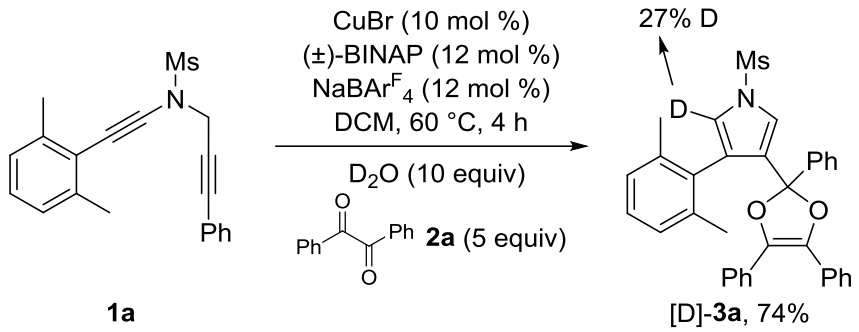
2.7 Control experiments

(4-(2,6-dimethylphenyl)-1-(methylsulfonyl)-1*H*-pyrrol-3-yl)(phenyl)methanone (3a')



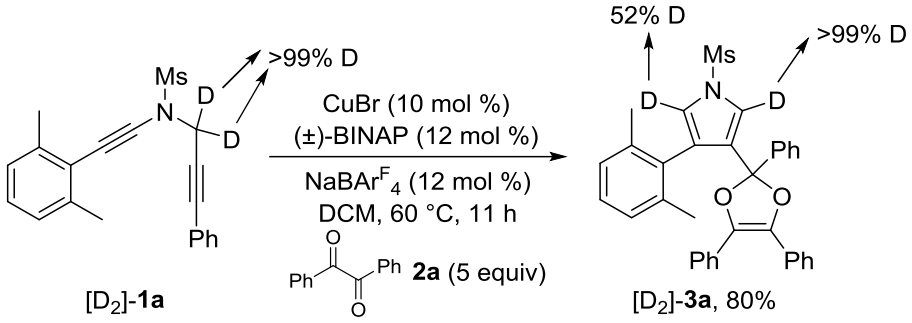
Compound **3a'** was prepared in 27% yield (9.5 mg) according to the general procedure (0.1 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.2 Hz, 2H), 7.60 (d, *J* = 2.0 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.45 – 7.37 (m, 2H), 7.15 – 7.10 (m, 1H), 7.08 – 7.01 (m, 3H), 3.27 (s, 3H), 2.11 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 138.3, 137.0, 132.5, 132.2, 129.1, 128.4, 128.1, 127.6, 127.1, 127.0, 126.2, 119.4, 43.1, 20.9. IR (neat): 2924, 2852, 1652, 1508, 1369, 1275, 1174, 1069, 802, 766 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{19}NNaO_3S$ 376.0983; Found 376.0986.

[D]-**3a** (27% D)



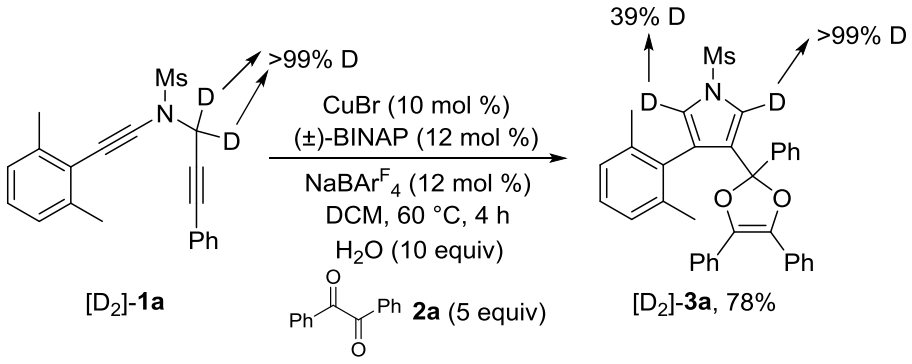
Compound [D]-**3a** was prepared in 74% yield (40.6 mg) according to the above general procedure (0.1 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 2H), 7.31 – 7.19 (m, 13H), 7.07 (d, *J* = 2.8 Hz, 1H), 7.02 – 6.97 (m, 1H), 6.90 (d, *J* = 2.8 Hz, 0.73H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.17 (s, 3H), 1.95 (s, 6H).

[D_2]-**3a** (52% D)



Compound [D_2]-**3a** was prepared in 80% yield (43.9 mg) according to the above general procedure (0.1 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.32 – 7.19 (m, 13H), 7.03 – 6.97 (m, 1H), 6.90 (s, 0.48H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.17 (s, 3H), 1.95 (s, 6H).

[D_2]-**3a** (39% D)



Compound [D_2]-**3a** was prepared in 78% yield (42.7 mg) according to the general procedure (0.1 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.45 (m, 2H), 7.32 – 7.19 (m, 13H), 7.02 – 6.97 (m, 1H), 6.90 (s, 0.61H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.17 (s, 3H), 1.95 (s, 6H).

3. Reference

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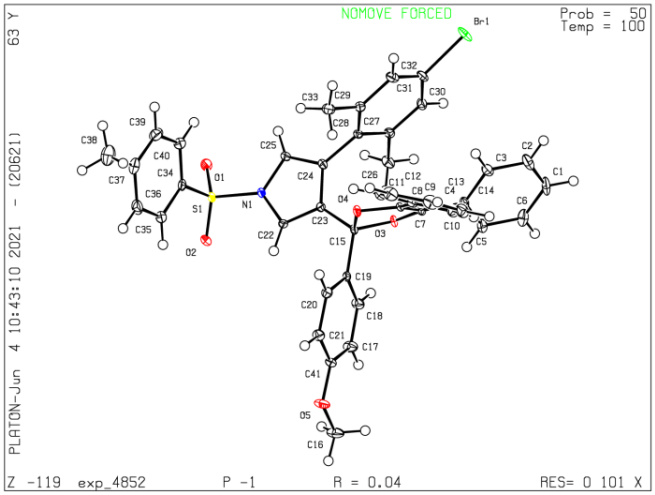
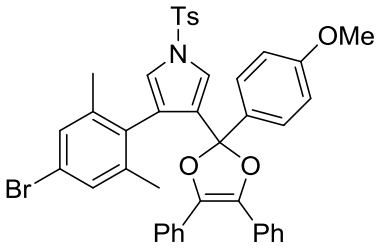
Crystal data and structure refinement for 3ab. CCDC Number = 2203937

ORTEP drawing of **3ab** (thermal ellipsoids set at 50% probability). Recrystallization from *n*-hexane/DCM afforded single crystals suitable for X-ray diffraction analysis.





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alpha=73.868(1) beta=88.437(1) gamma=78.631(1)
Temperature: 100 K

	Calculated	Reported
Volume	1723.41(4)	1723.41(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C41 H34 Br N O5 S	C41 H34 Br N O5 S
Sum formula	C41 H34 Br N O5 S	C41 H34 Br N O5 S
Mr	732.65	732.66
Dx,g cm-3	1.412	1.412
Z	2	2
Mu (mm-1)	2.573	2.573
F000	756.0	756.0
F000'	757.27	
h,k,lmax	12,16,18	12,16,18
Nref	7105	6843
Tmin,Tmax	0.975,0.975	0.609,1.000
Tmin'	0.975	

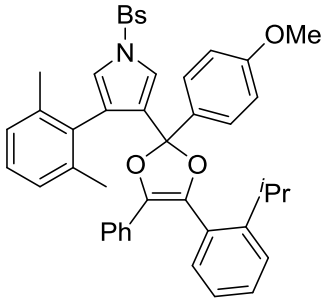
Correction method= # Reported T Limits: Tmin=0.609 Tmax=1.000
AbsCorr = MULTI-SCAN

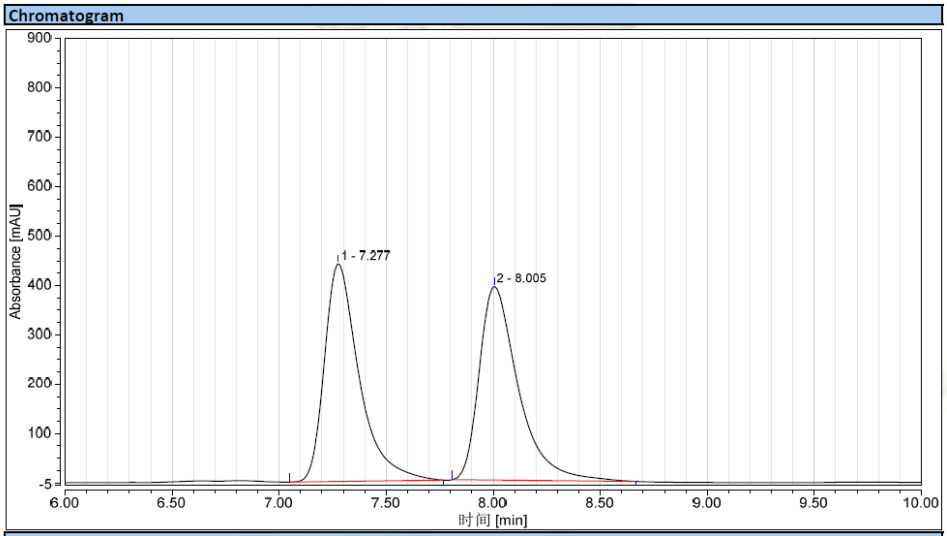
Data completeness= 0.963 Theta(max)= 74.943

R(reflections)= 0.0409(6634) wR2(reflections)= 0.1083(6843)

S = 1.133 Npar= 446

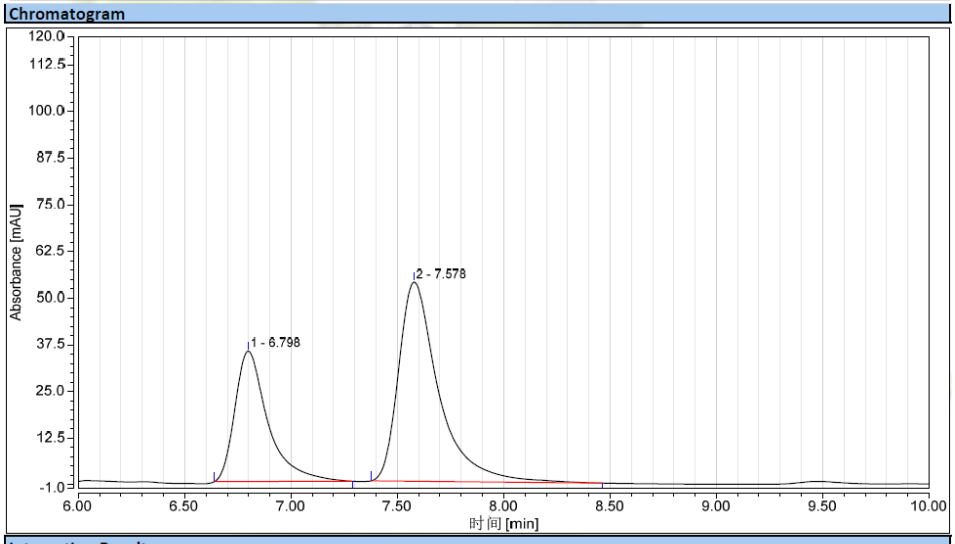
(+)-3z/L*: HPLC (IE, *n*-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, I = 254 nm)





Integration Results

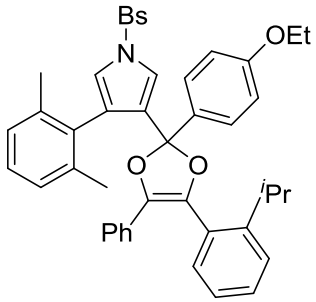
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.277	82.877	440.572	49.99	52.92	n.a.
2		8.005	82.908	391.907	50.01	47.08	n.a.
Total:			**165.786**	**832.479**	**100.00**	**100.00**	



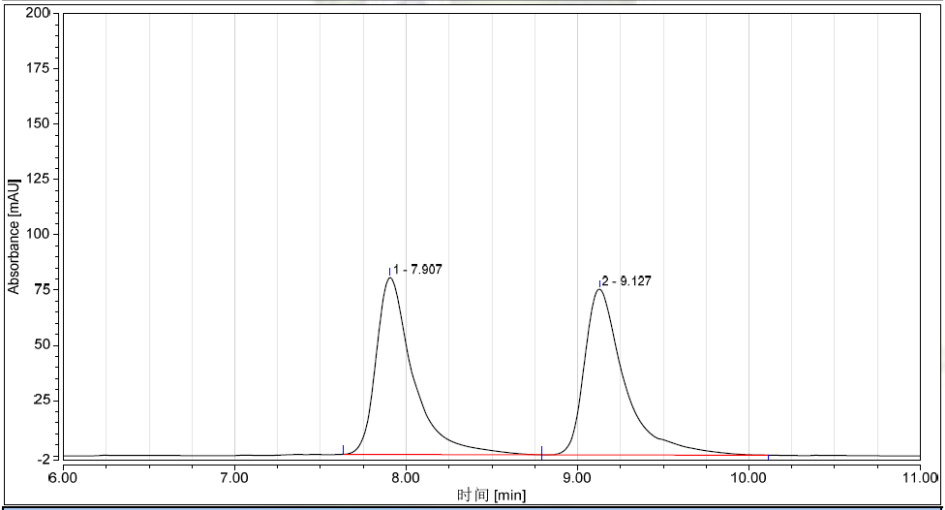
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.798	6.297	34.991	35.00	39.58	n.a.
2		7.578	11.694	53.424	65.00	60.42	n.a.
Total:			**17.991**	**88.415**	**100.00**	**100.00**	

(+)-3aa/L*: HPLC (IE, *n*-hexane/2-propanol = 98/2, flow rate = 1.0 mL/min, I = 254 nm)



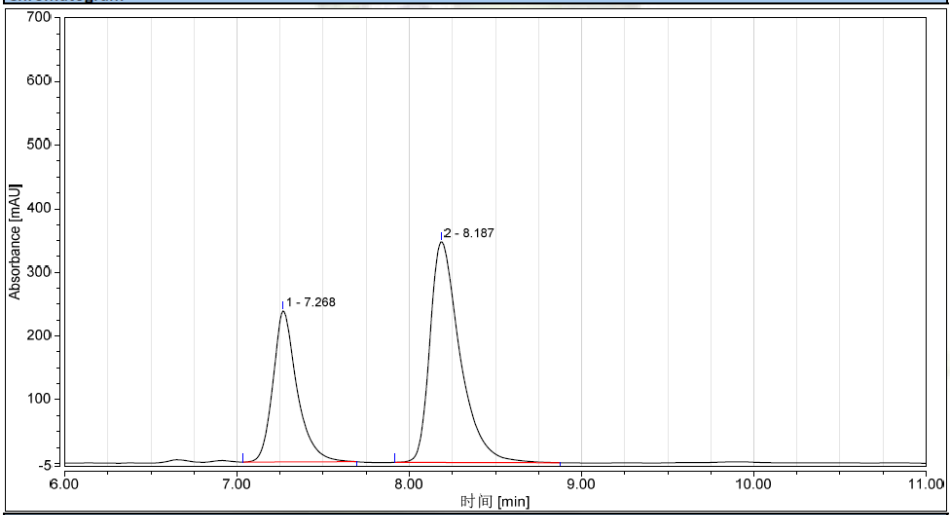
Chromatogram



Integration Results

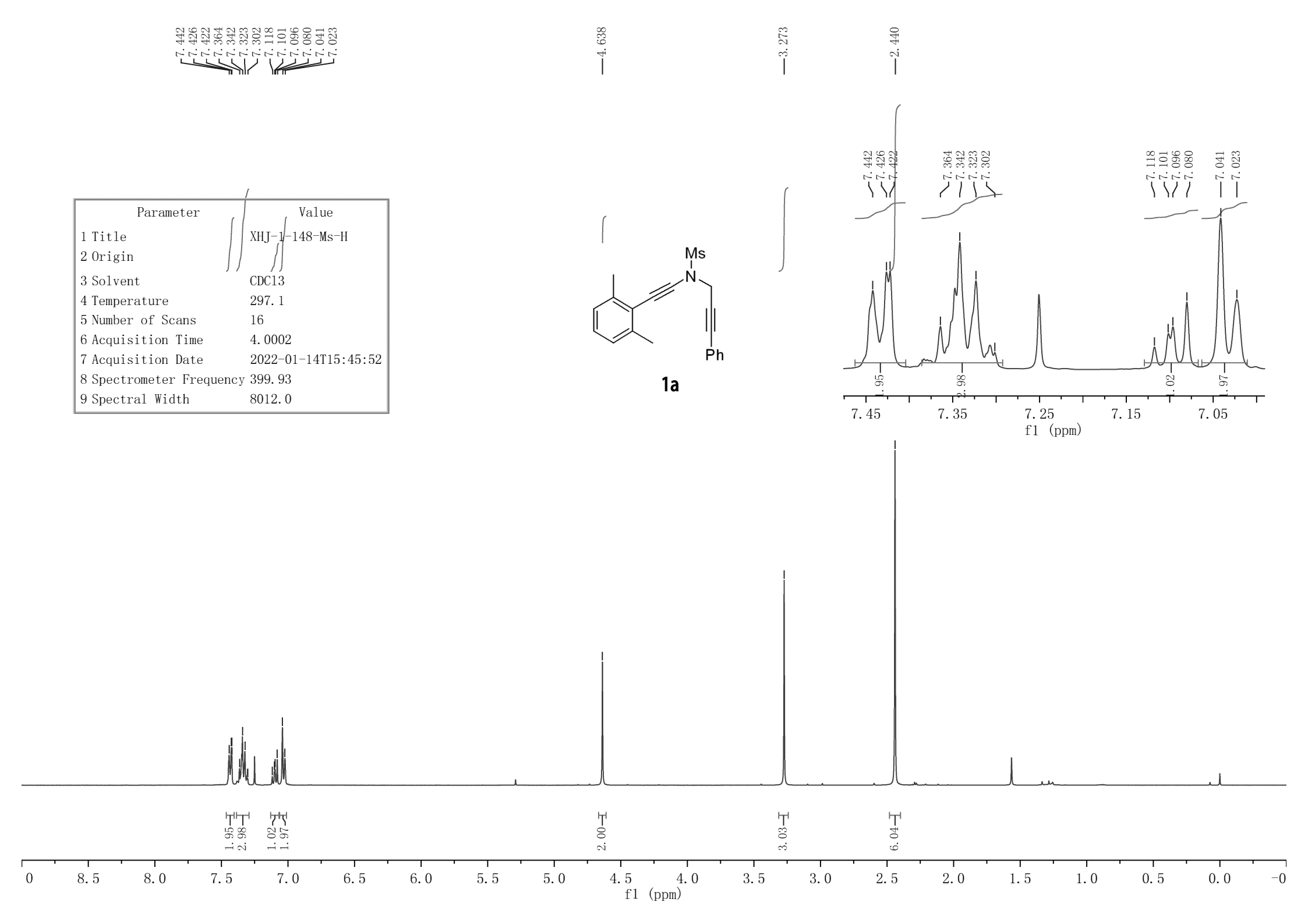
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.907	20.089	80.036	49.73	51.64	n.a.
2		9.127	20.309	74.938	50.27	48.36	n.a.
Total:			**40.398**	**154.974**	**100.00**	**100.00**	

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.268	38.427	237.641	35.46	40.64	n.a.
2		8.187	69.930	347.048	64.54	59.36	n.a.
Total:			**108.357**	**584.689**	**100.00**	**100.00**	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7.023
4.638
3.273
2.440
Parameter
Value
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XHJ-1-148-Ms-H
2 Origin
3 Solvent
CDCl3
4 Temperature
297.1
5 Number of Scans
16
6 Acquisition Time
4.0002
7 Acquisition Date
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Ph
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2.98
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1.97
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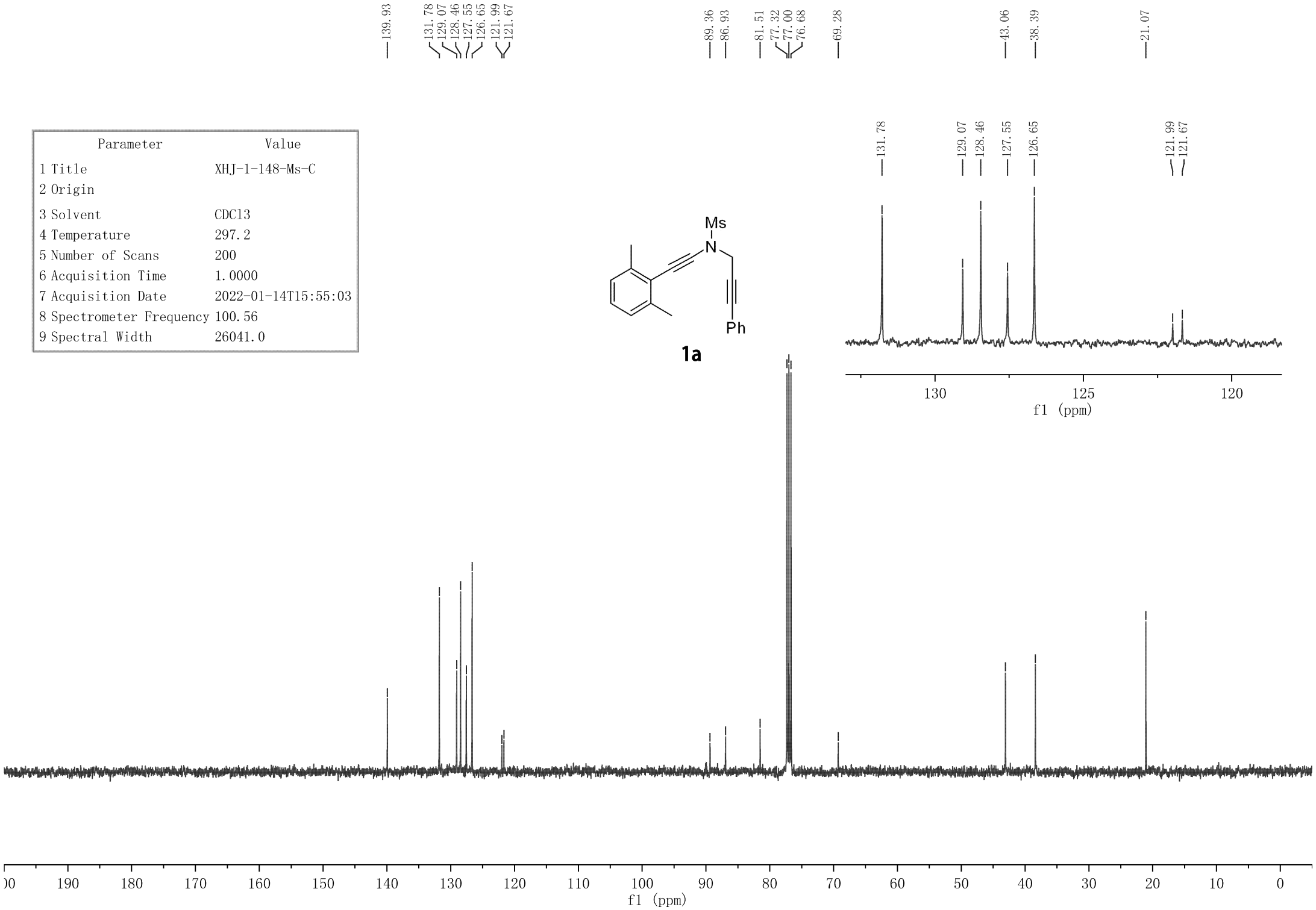
3.03
6.04
f1 (ppm)


139.93
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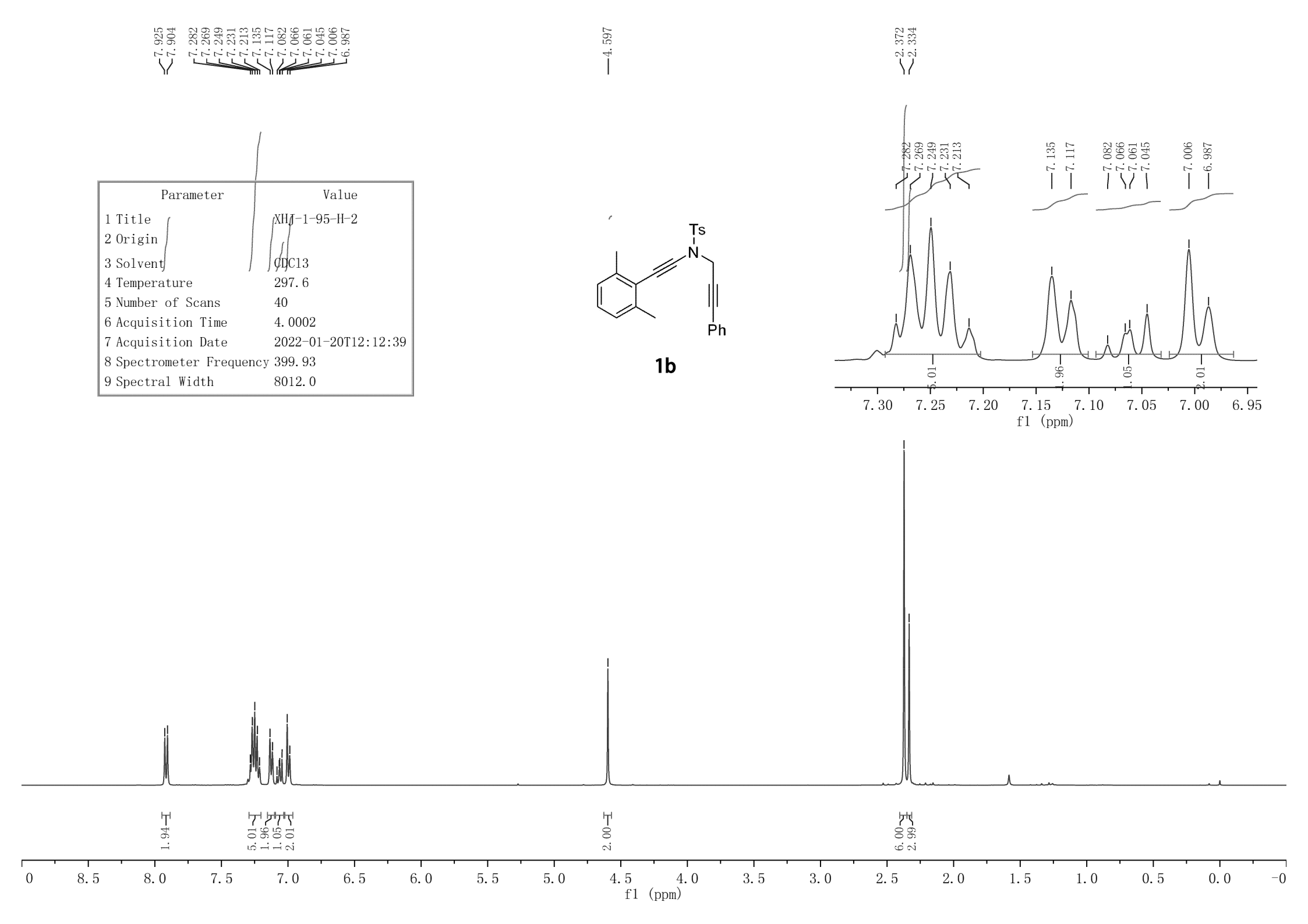
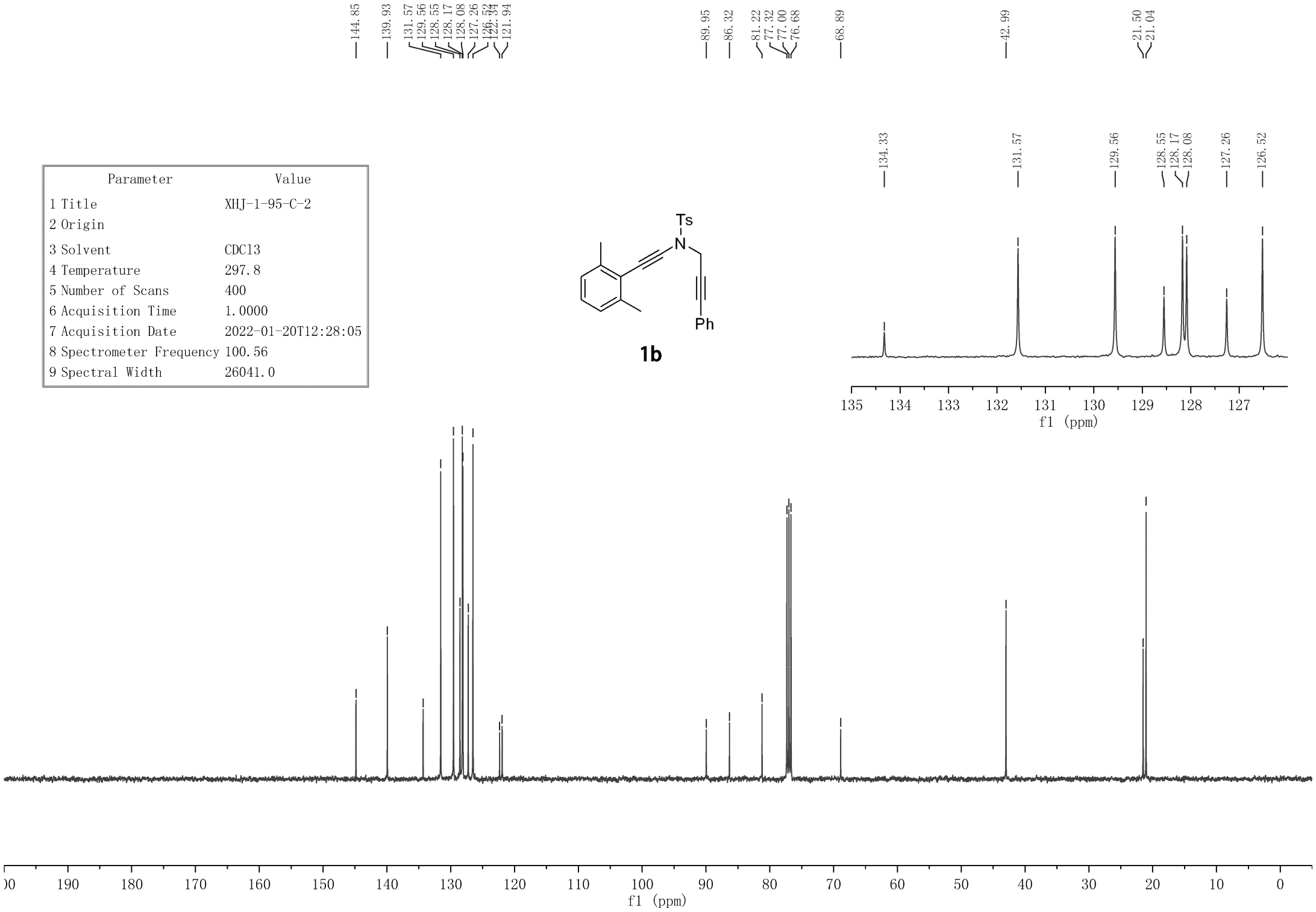
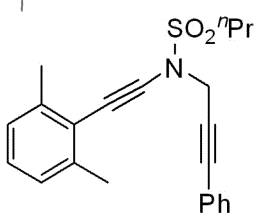
126.65
121.99
121.67
89.36
86.93
81.51
77.32
77.00
76.68
69.28
43.06
38.39
21.07
Parameter Value
1 Title XHJ-1-148-Ms-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.2
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-14T15:55:03
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Ph
1a
f1 (ppm)

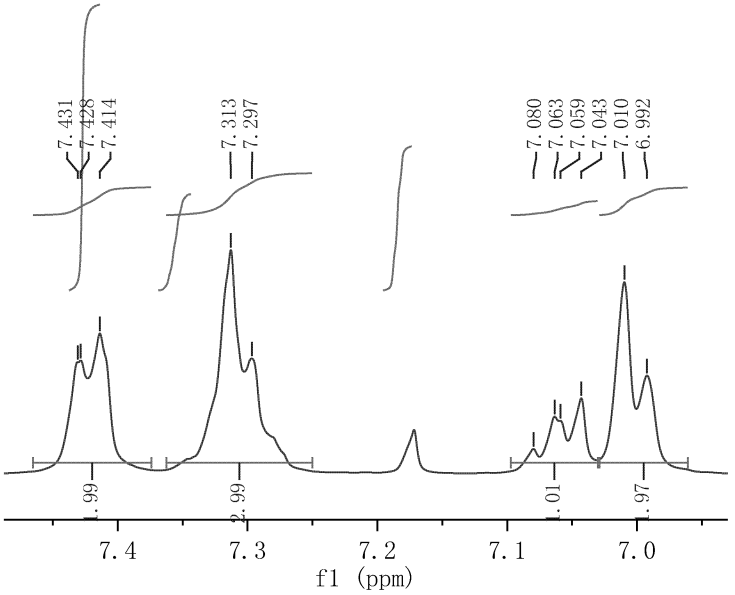

7.925
7.904
7.282
7.269
7.249
7.231
7.213
7.135
7.117
7.082
7.066
7.061
7.045
7.006
6.987
4.597
2.372
2.334
Parameter Value
1 Title XHJ-1-95-H-2
2 Origin
3 Solvent CDCl3
4 Temperature 297.6
5 Number of Scans 40
6 Acquisition Time 4.0002
7 Acquisition Date 2022-01-20T12:12:39
8 Spectrometer Frequency 399.93
9 Spectral Width 8012.0
Ts
N
Ph
1b
5.01
1.96
1.05
2.01
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
f1 (ppm)
1.94
5.01
1.96
1.05
2.01
2.00
6.00
2.99
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

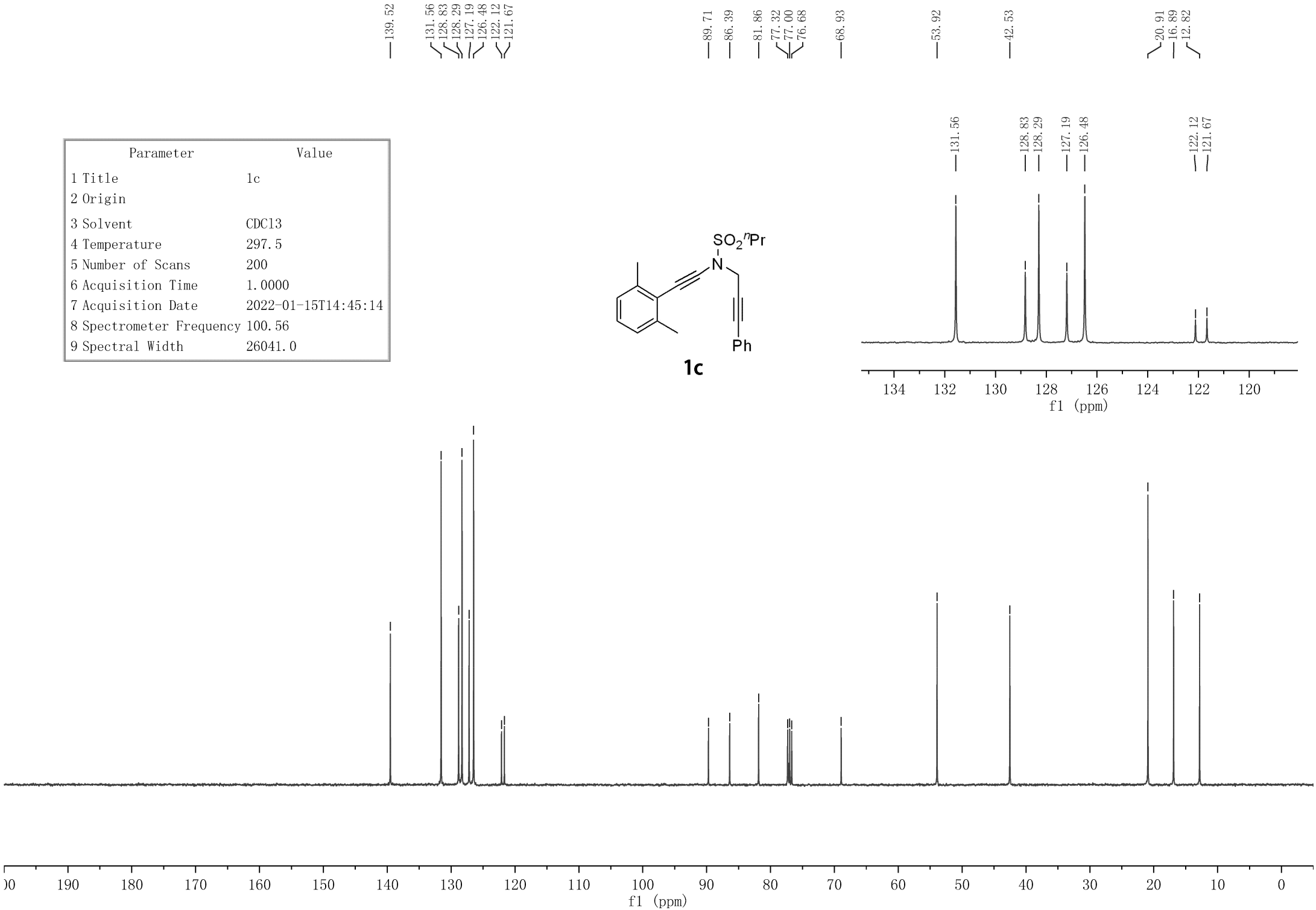

144.85
139.93
131.57
129.56
128.55
128.17
128.08
127.26
126.52
122.34
121.94
89.95
86.32
81.22
77.32
77.00
76.68
68.89
42.99
21.50
21.04
Parameter Value
1 Title XHJ-1-95-C-2
2 Origin
3 Solvent CDCl3
4 Temperature 297.8
5 Number of Scans 400
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-20T12:28:05
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ts
N
Ph
1b
134.33
131.57
129.56
128.55
128.17
128.08
127.26
126.52
135 134 133 132 131 130 129 128 127
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

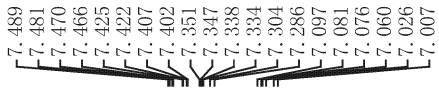
Parameter	Value
1 Title	1c
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-01-15T14:36:25
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



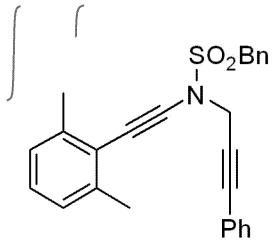
1c



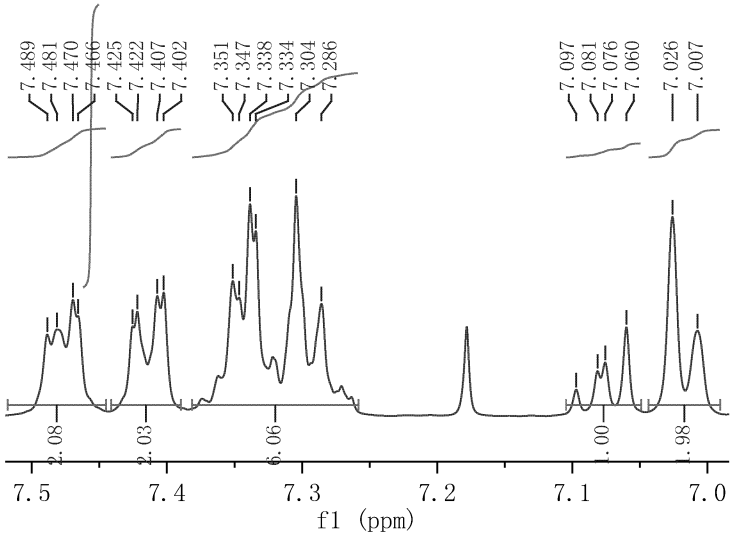

139.52
131.56
128.83
128.29
127.19
126.48
122.12
121.67
89.71
86.39
81.86
77.32
77.00
76.68
68.93
53.92
42.53
20.91
16.89
12.82
Parameter Value
1 Title 1c
2 Origin
3 Solvent CDCl3
4 Temperature 297.5
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-15T14:45:14
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
SO2nPr
N
Ph
1c
f1 (ppm)
f1 (ppm)

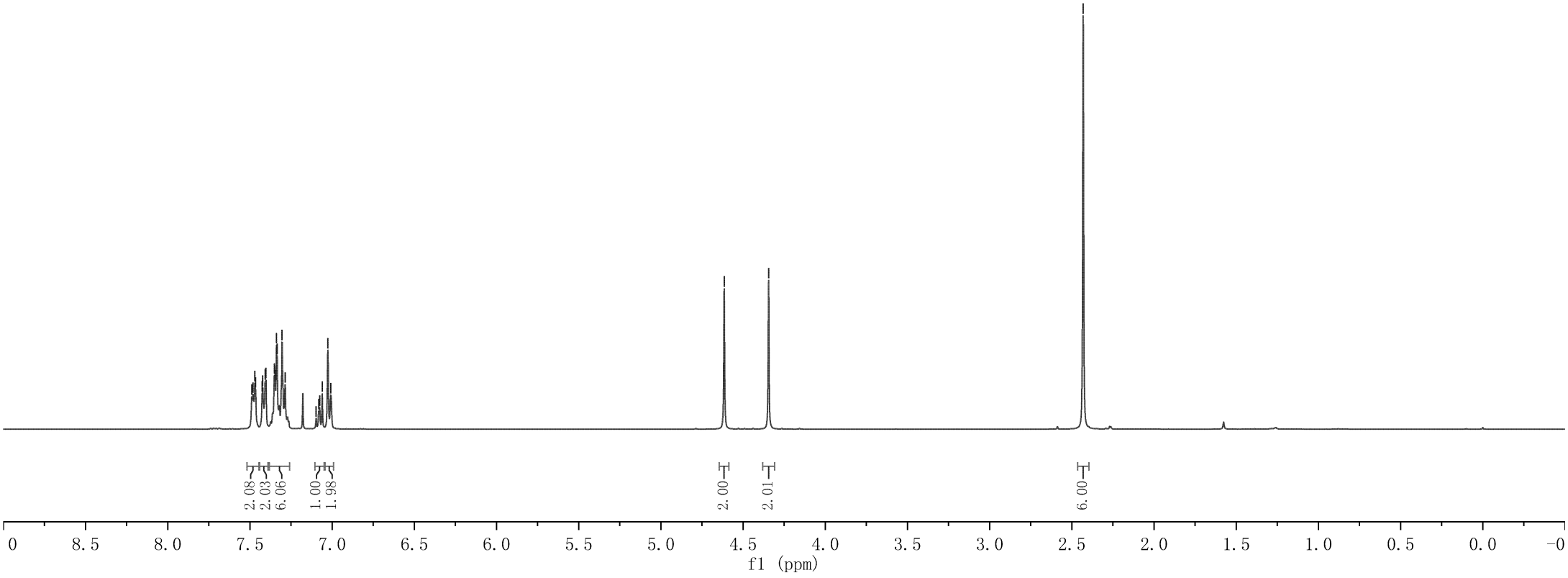


Parameter	Value
1 Title	XHJ-1-160-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.1
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-01-15T23:37:05
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0

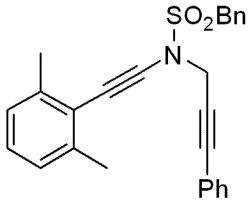


1d

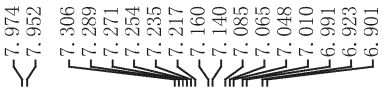




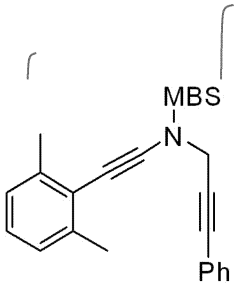
Parameter	Value
1 Title	XHJ-1-160-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.1
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-01-15T23:46:00
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



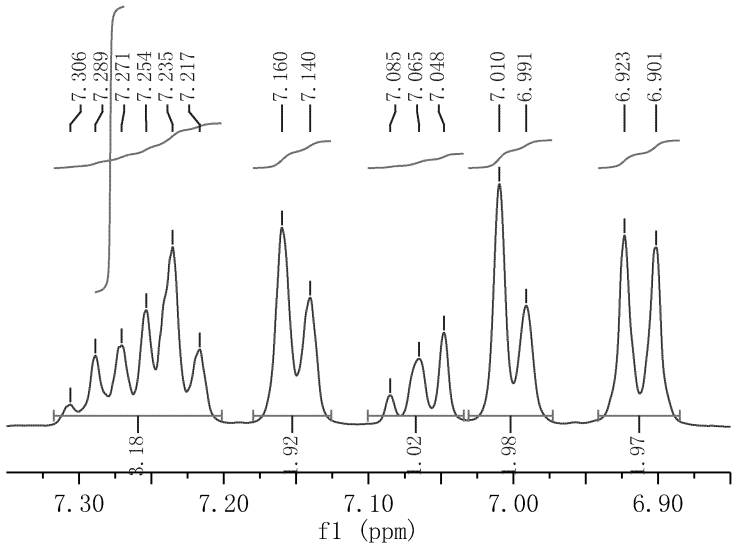
1d

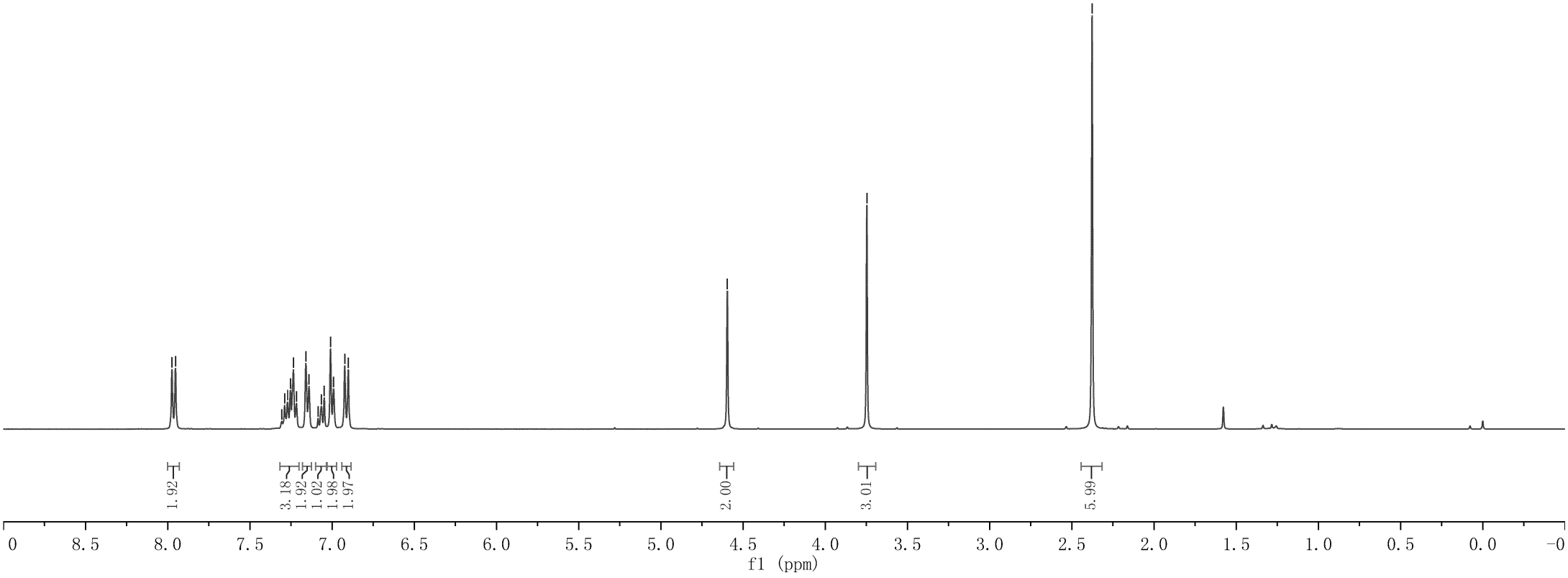


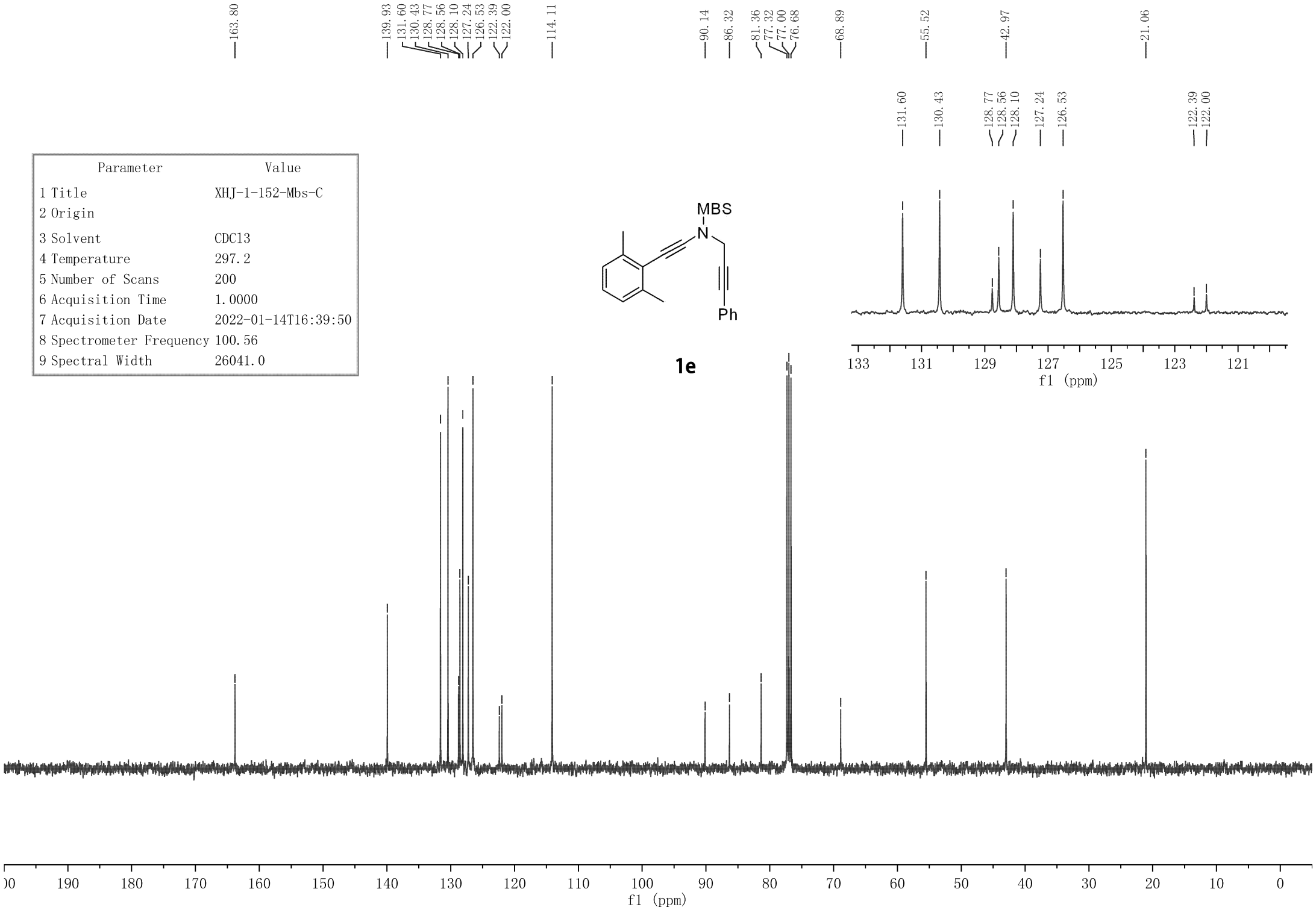
Parameter	Value
1 Title	XHJ-1-152-Mbs-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.1
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-01-14T16:31:04
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



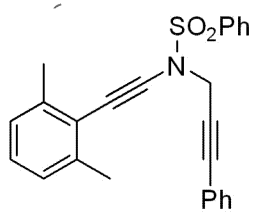
1e



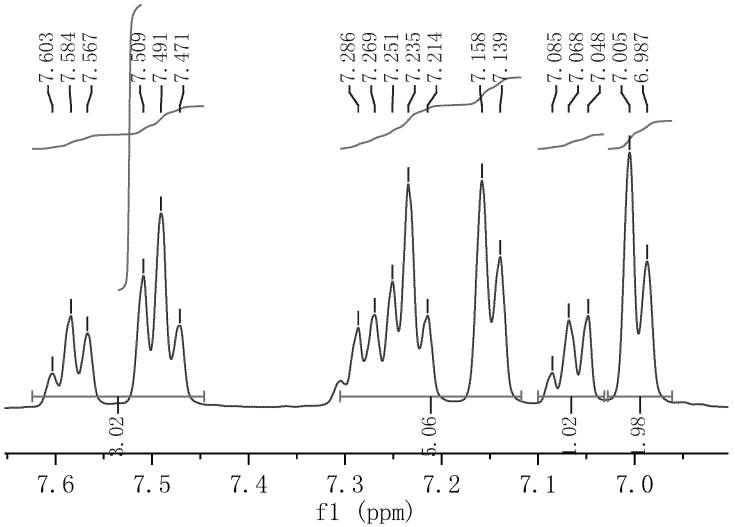


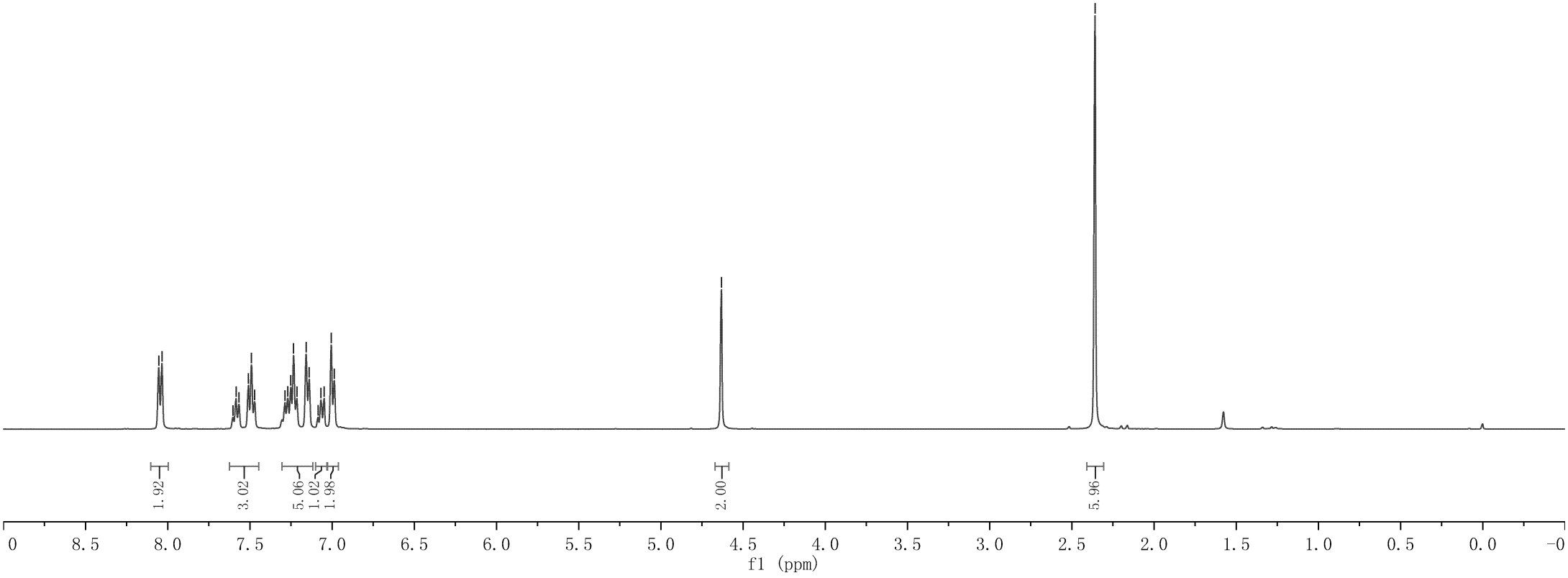

163.80
139.93
131.60
130.43
128.77
128.56
128.10
127.24
126.53
122.39
122.00
114.11
90.14
86.32
81.36
77.32
77.00
76.68
68.89
55.52
42.97
21.06
Parameter Value
1 Title XHJ-1-152-Mbs-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.2
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-14T16:39:50
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
MBS
N
Ph
1e
f1 (ppm)

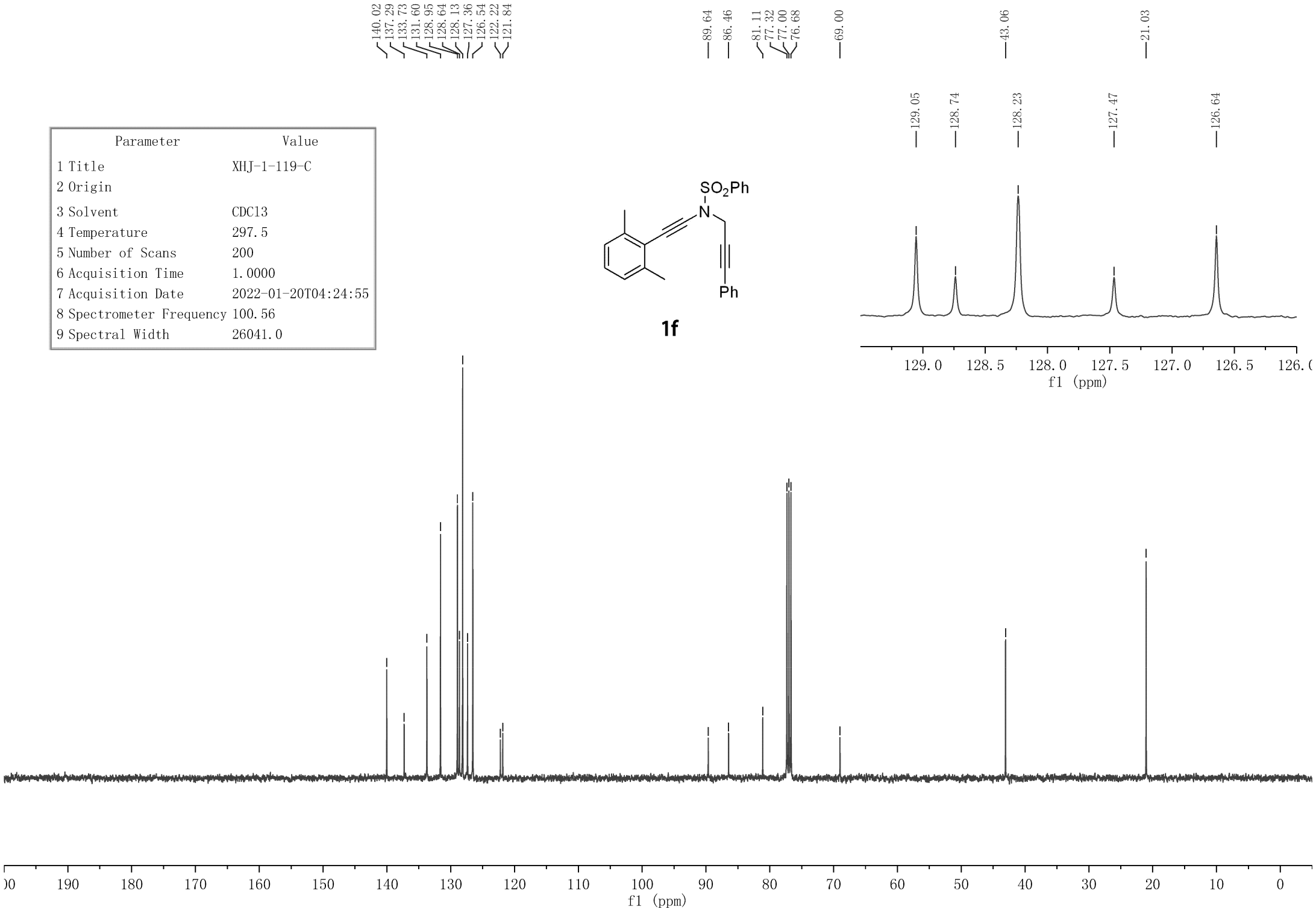
Parameter	Value
1 Title	XHJ-1-119-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.4
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-01-20T04:15:52
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



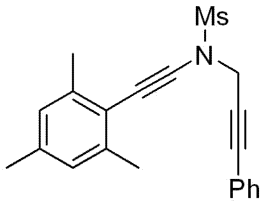
1f



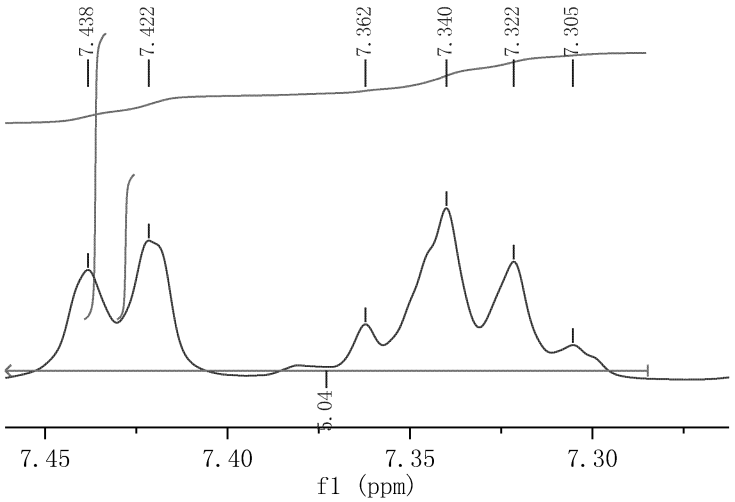


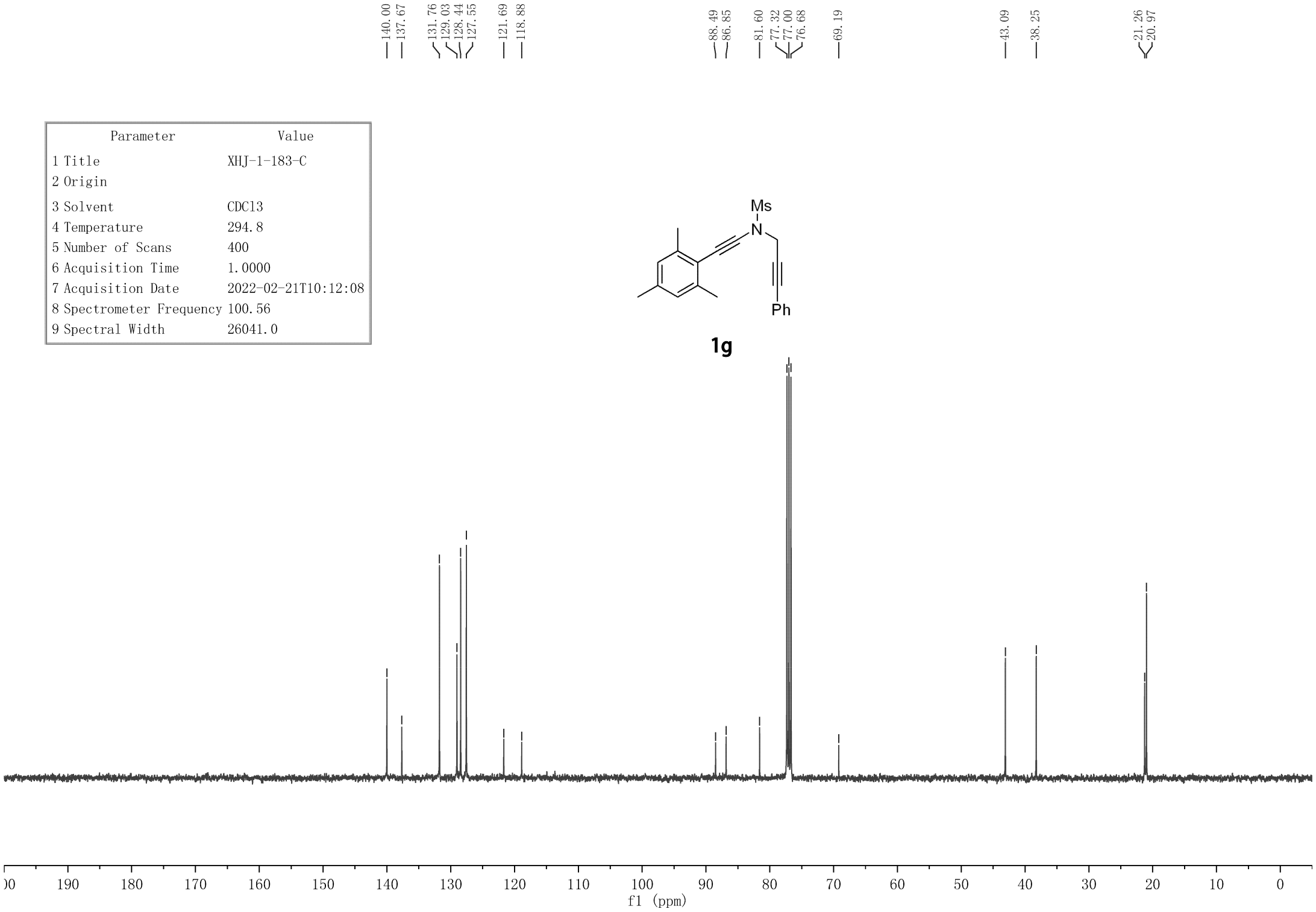

140.02
137.29
133.73
131.60
128.95
128.64
128.13
127.36
126.54
122.22
121.84
89.64
86.46
81.11
77.32
77.00
76.68
69.00
43.06
21.03
129.05
128.74
128.23
127.47
126.64
Parameter Value
1 Title XHJ-1-119-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.5
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-20T04:24:55
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
SO2Ph
N
Ph
1f
129.0
128.5
128.0
127.5
127.0
126.5
f1 (ppm)
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	XHJ-1-183-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	294.5
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-02-21T09:56:19
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0

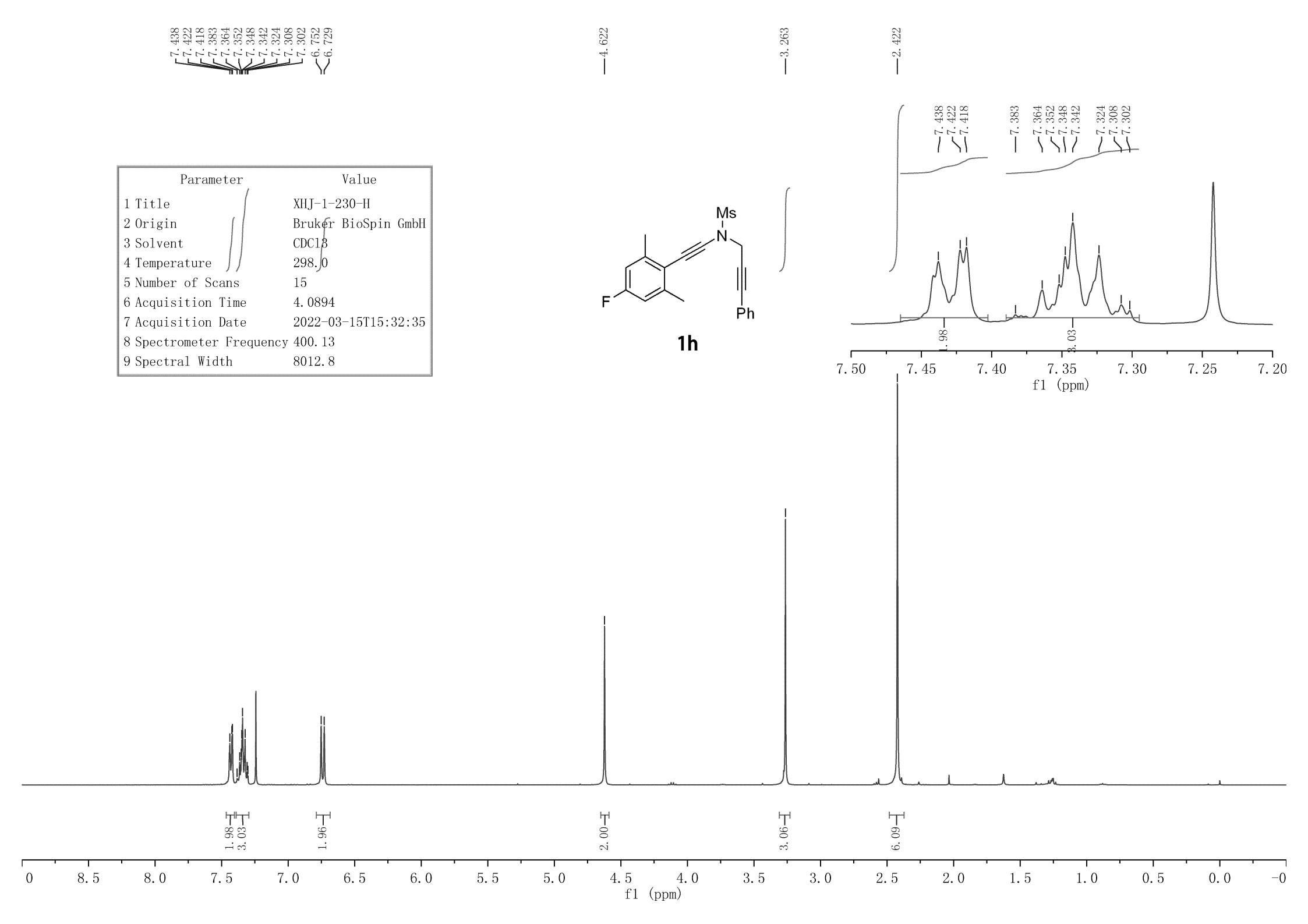


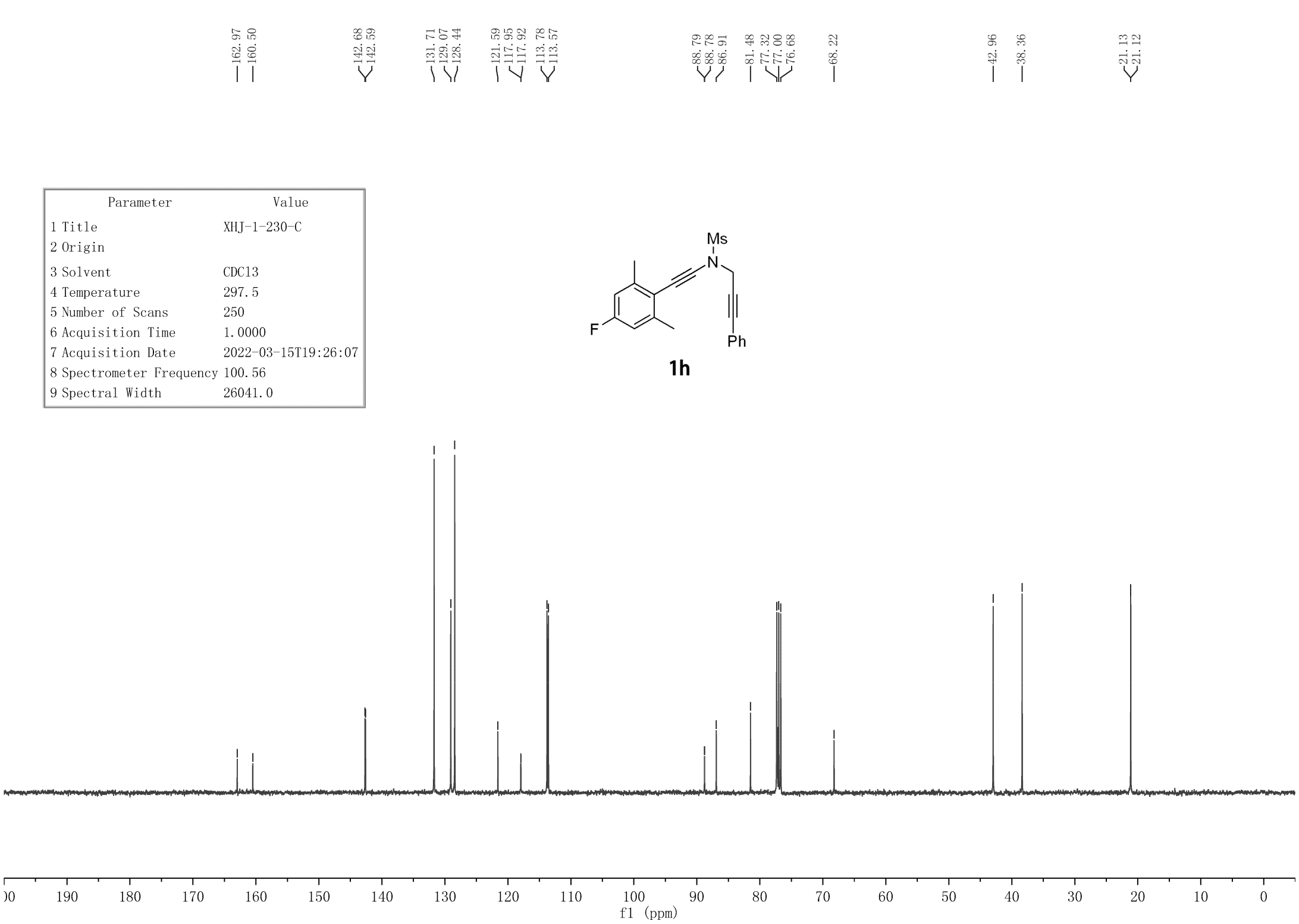
1g



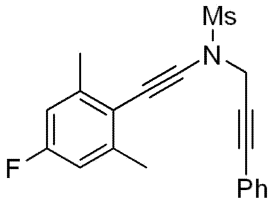


Parameter	Value
1 Title	XHJ-1-183-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	294.8
5 Number of Scans	400
6 Acquisition Time	1.0000
7 Acquisition Date	2022-02-21T10:12:08
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0


7.438
7.422
7.418
7.383
7.364
7.352
7.348
7.342
7.324
7.308
7.302
6.752
6.729
4.622
3.263
2.422
Parameter
Value
1 Title
XHJ-1-230-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
2022-03-15T15:32:35
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
Ms
N
F
Ph
1h
1.98
3.03
1.96
2.00
3.06
6.09
f1 (ppm)

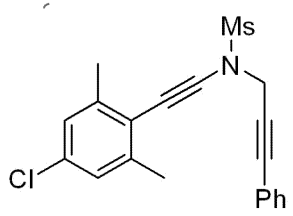

162.97
160.50
142.68
142.59
131.71
129.07
128.44
121.59
117.95
117.92
113.78
113.57
88.79
88.78
86.91
81.48
77.32
77.00
76.68
68.22
42.96
38.36
21.13
21.12
Parameter Value
1 Title XHJ-1-230-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.5
5 Number of Scans 250
6 Acquisition Time 1.0000
7 Acquisition Date 2022-03-15T19:26:07
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
F
Ph
1h
f1 (ppm)

Parameter	Value
1 Title	XHJ-1-230-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.2
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-08-16T20:03:52
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

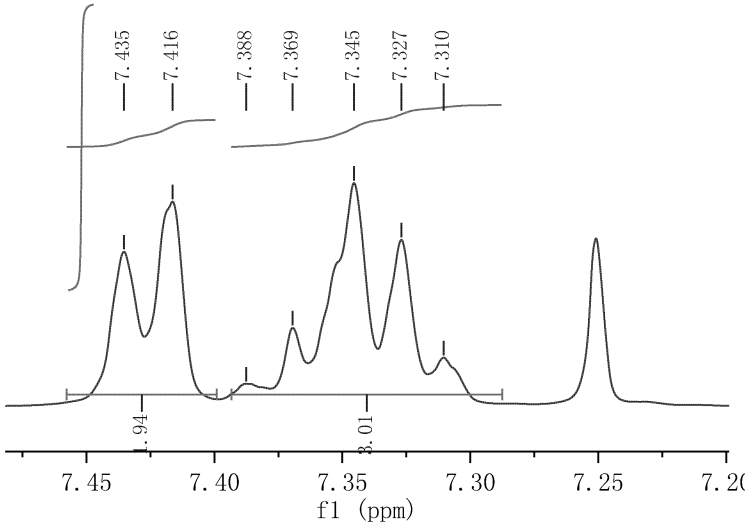


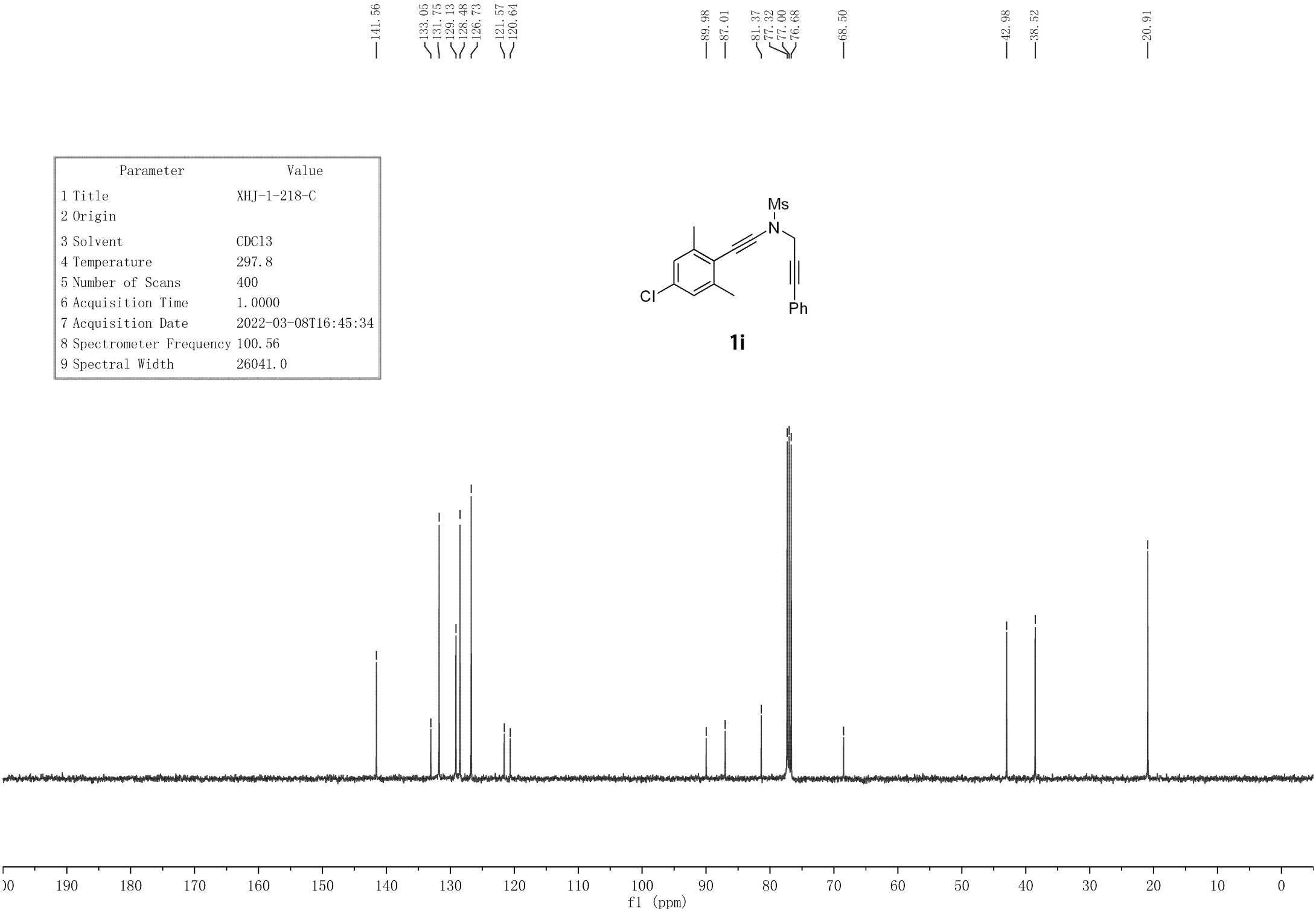
1h

Parameter	Value
1 Title	XHJ-1-218-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-03-08T16:29:55
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0

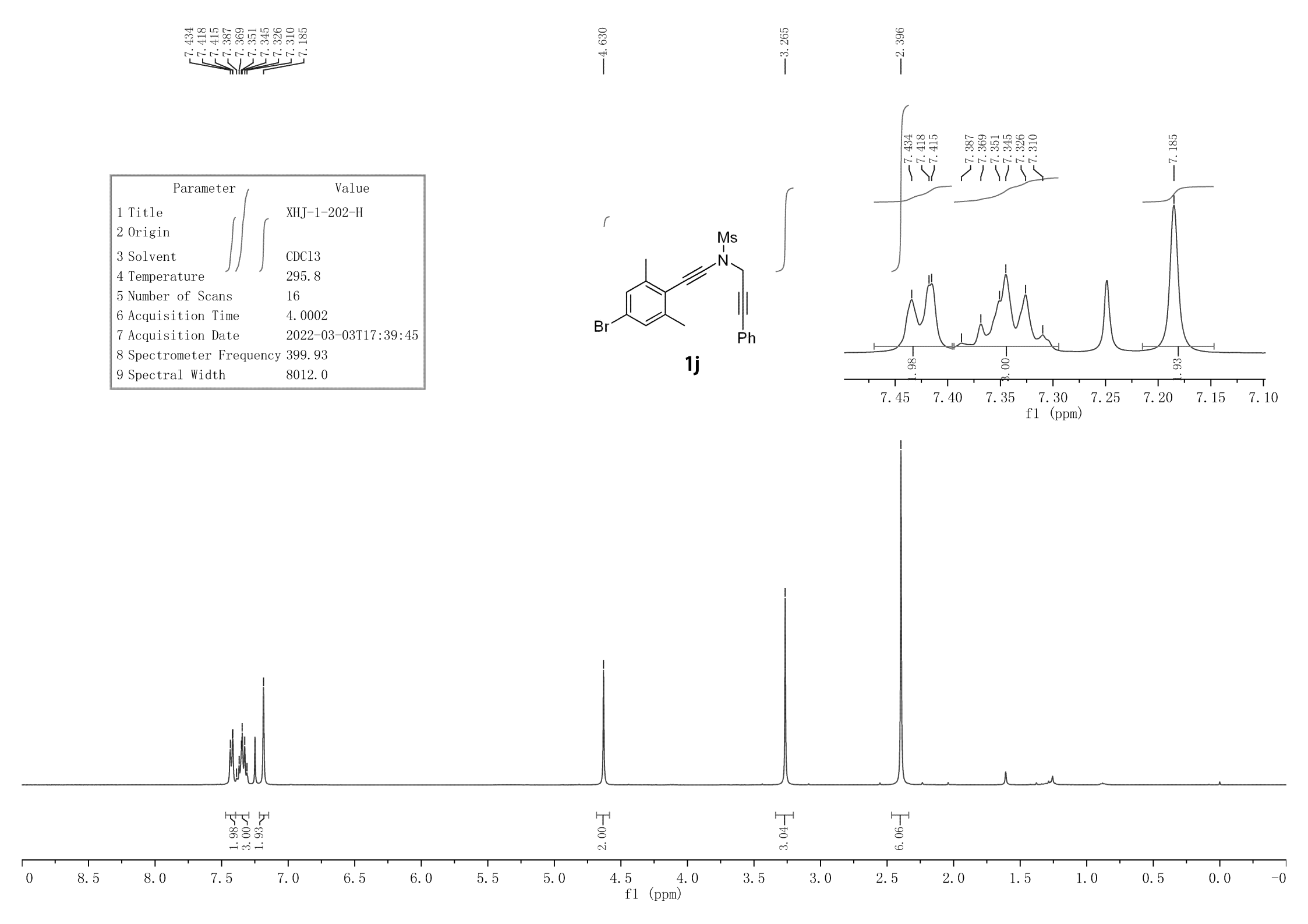


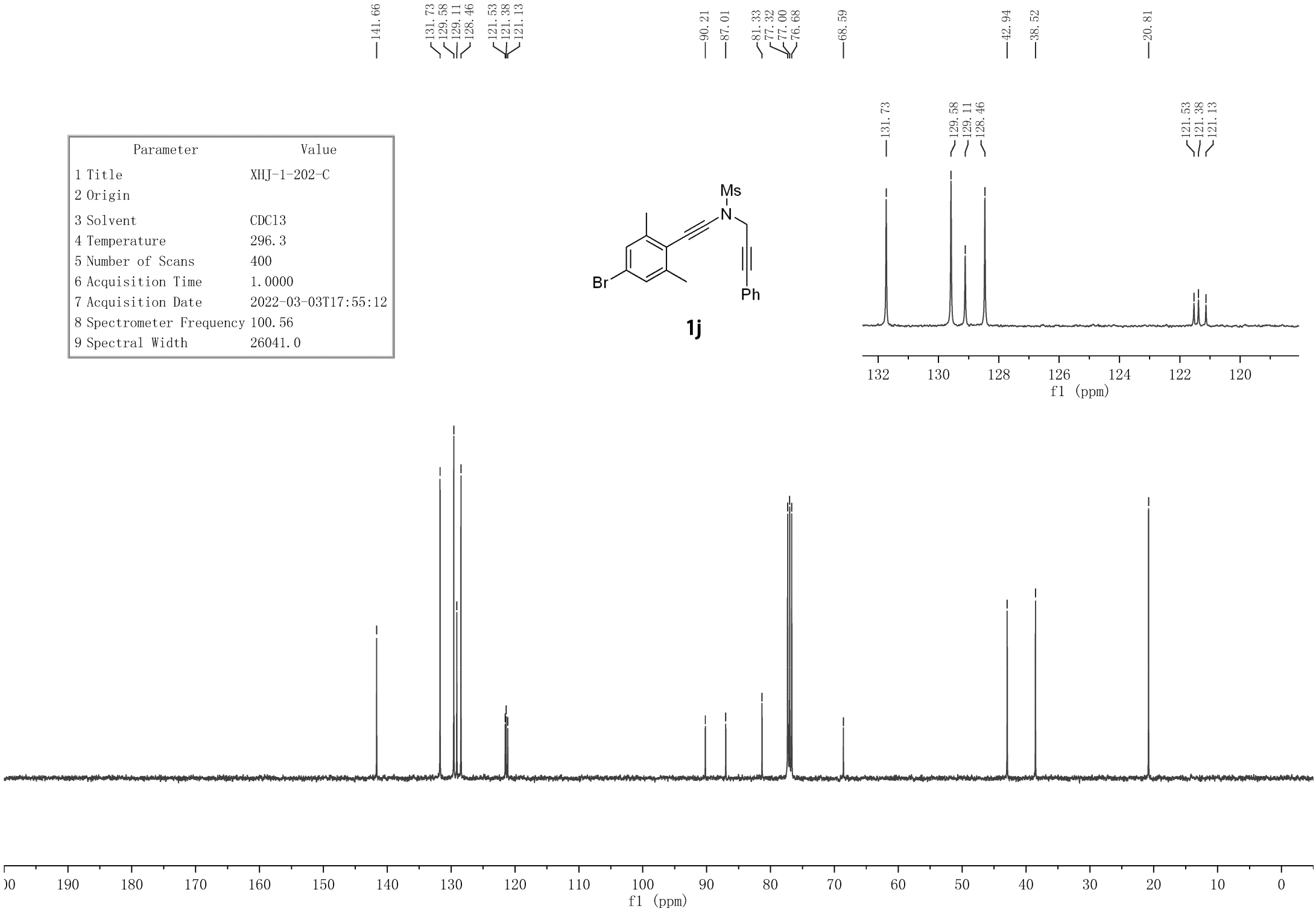
1i

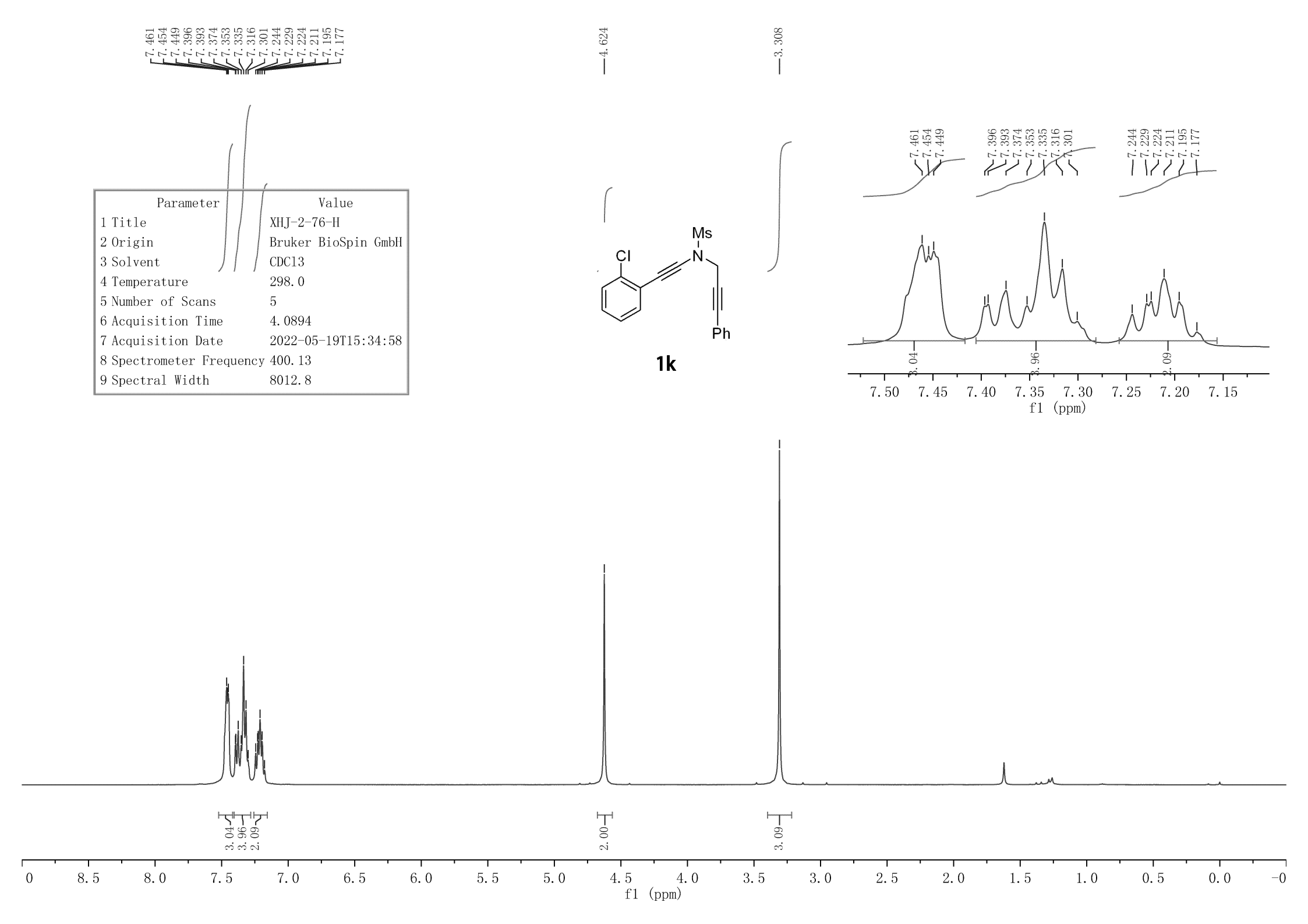


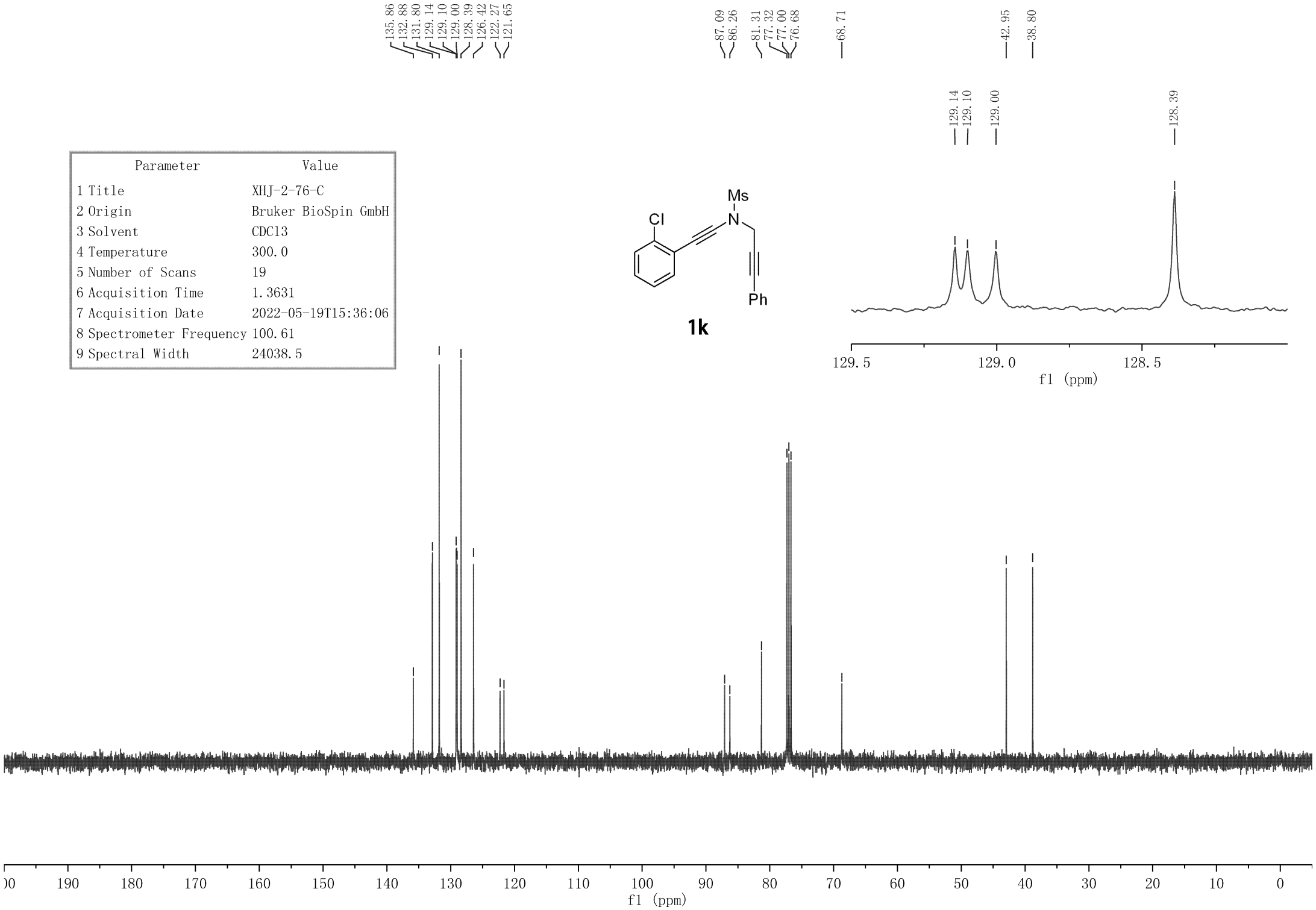


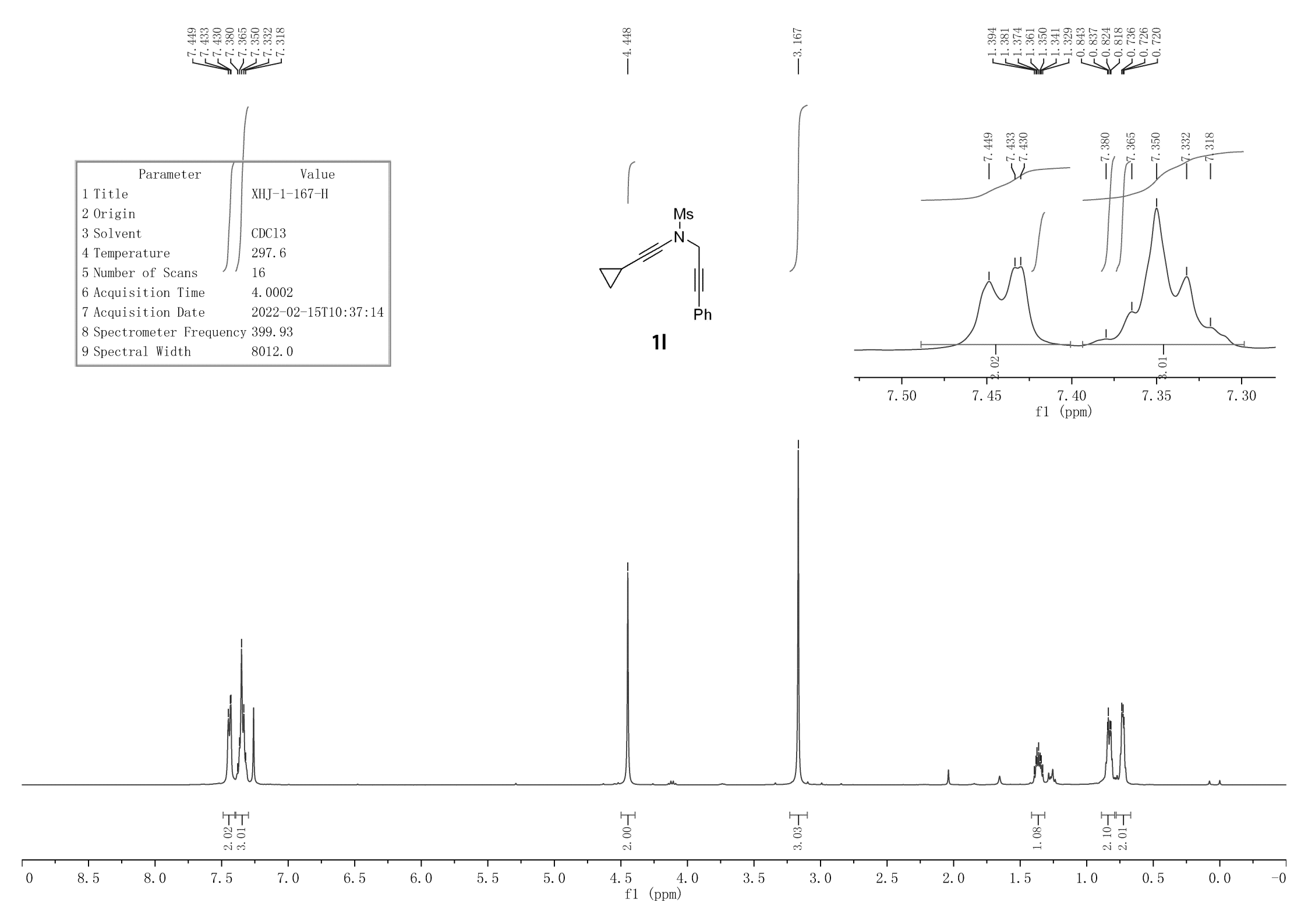
Parameter	Value
1 Title	XHJ-1-218-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.8
5 Number of Scans	400
6 Acquisition Time	1.0000
7 Acquisition Date	2022-03-08T16:45:34
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0


7.434
7.418
7.415
7.387
7.369
7.351
7.345
7.326
7.310
7.185
4.630
3.265
2.396
Parameter Value
1 Title XHJ-1-202-H
2 Origin
3 Solvent CDCl3
4 Temperature 295.8
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-03-03T17:39:45
8 Spectrometer Frequency 399.93
9 Spectral Width 8012.0
Ms
N
Br
Ph
1j
1.98
3.00
1.93
7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10
f1 (ppm)
1.98
3.00
1.93
2.00
3.04
6.06
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


141.66
131.73
129.58
129.11
128.46
121.53
121.38
121.13
90.21
87.01
81.33
77.32
77.00
76.68
68.59
42.94
38.52
20.81
Parameter Value
1 Title XHJ-1-202-C
2 Origin
3 Solvent CDCl3
4 Temperature 296.3
5 Number of Scans 400
6 Acquisition Time 1.0000
7 Acquisition Date 2022-03-03T17:55:12
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Br
Ph
1j
f1 (ppm)
f1 (ppm)

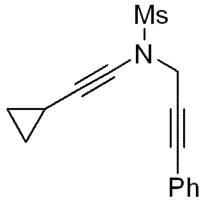

7.461
7.454
7.449
7.396
7.393
7.374
7.353
7.335
7.316
7.301
7.244
7.229
7.224
7.211
7.195
7.177
4.624
3.308
Parameter Value
1 Title XHJ-2-76-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 5
6 Acquisition Time 4.0894
7 Acquisition Date 2022-05-19T15:34:58
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
Cl
Ph
1k
3.04
3.96
2.09
7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15
f1 (ppm)
3.04
3.96
2.09
2.00
3.09
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


135.86
132.88
131.80
129.14
129.10
129.00
128.39
126.42
122.27
121.65
87.09
86.26
81.31
77.32
77.00
76.68
68.71
42.95
38.80
129.14
129.10
129.00
128.39
129.5
129.0
128.5
f1 (ppm)
Parameter Value
1 Title XHJ-2-76-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 19
6 Acquisition Time 1.3631
7 Acquisition Date 2022-05-19T15:36:06
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Cl
Ph
1k
f1 (ppm)

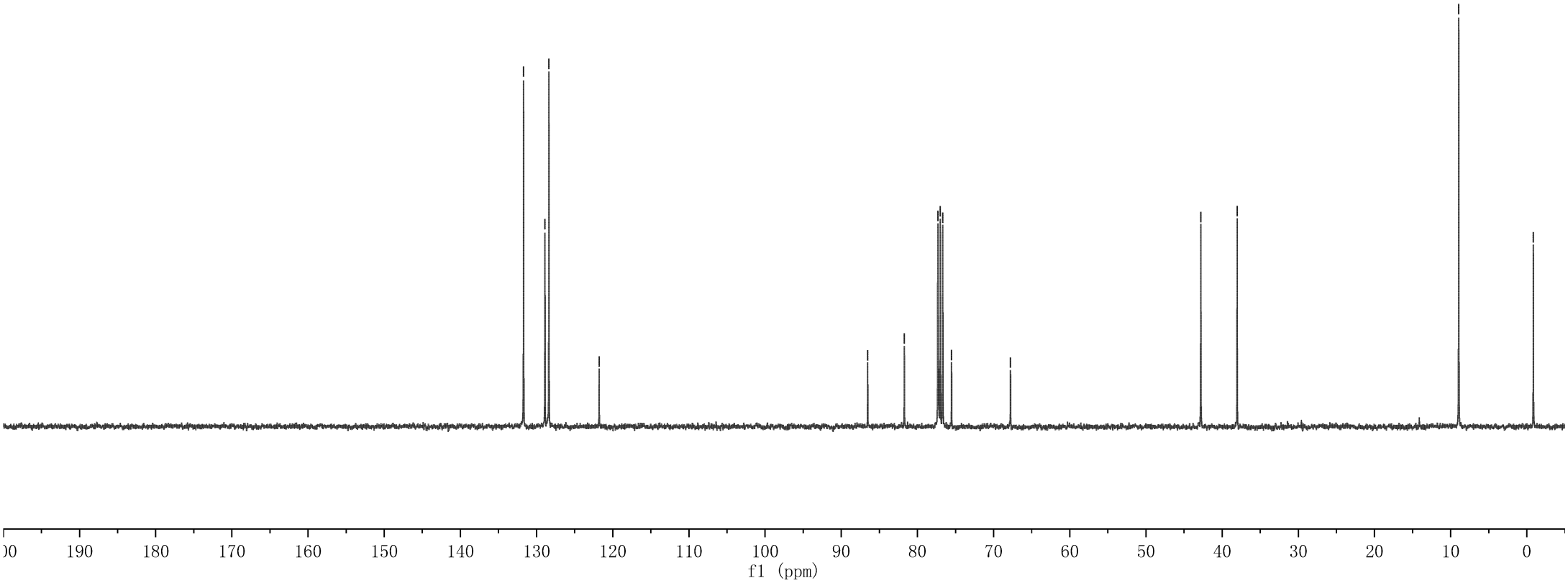

7.449
7.433
7.430
7.380
7.365
7.350
7.332
7.318
4.448
3.167
1.394
1.381
1.374
1.361
1.350
1.341
1.329
0.843
0.837
0.824
0.818
0.736
0.726
0.720
Parameter Value
1 Title XHJ-1-167-H
2 Origin
3 Solvent CDCl3
4 Temperature 297.6
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-02-15T10:37:14
8 Spectrometer Frequency 399.93
9 Spectral Width 8012.0
Ms
N
Ph
1l
2.02
3.01
7.50
7.45
7.40
7.35
7.30
f1 (ppm)
2.02
3.01
2.00
3.03
1.08
2.10
2.01
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

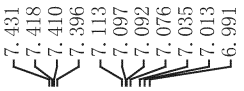
131.70
128.90
128.38
121.78
86.53
81.72
77.32
77.00
76.68
75.52
67.78
42.80
38.03
8.94
-0.85

Parameter	Value
1 Title	XHJ-1-167-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-02-15T10:46:09
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

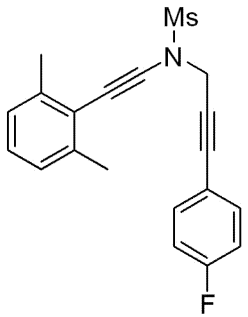


1l

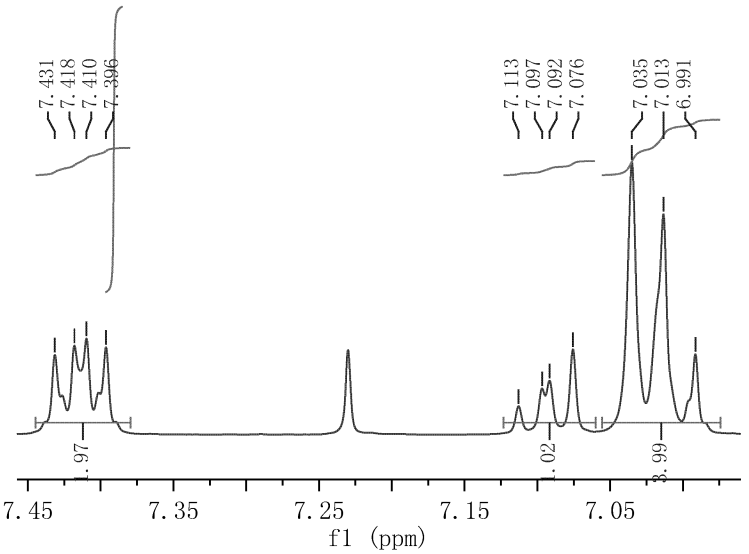


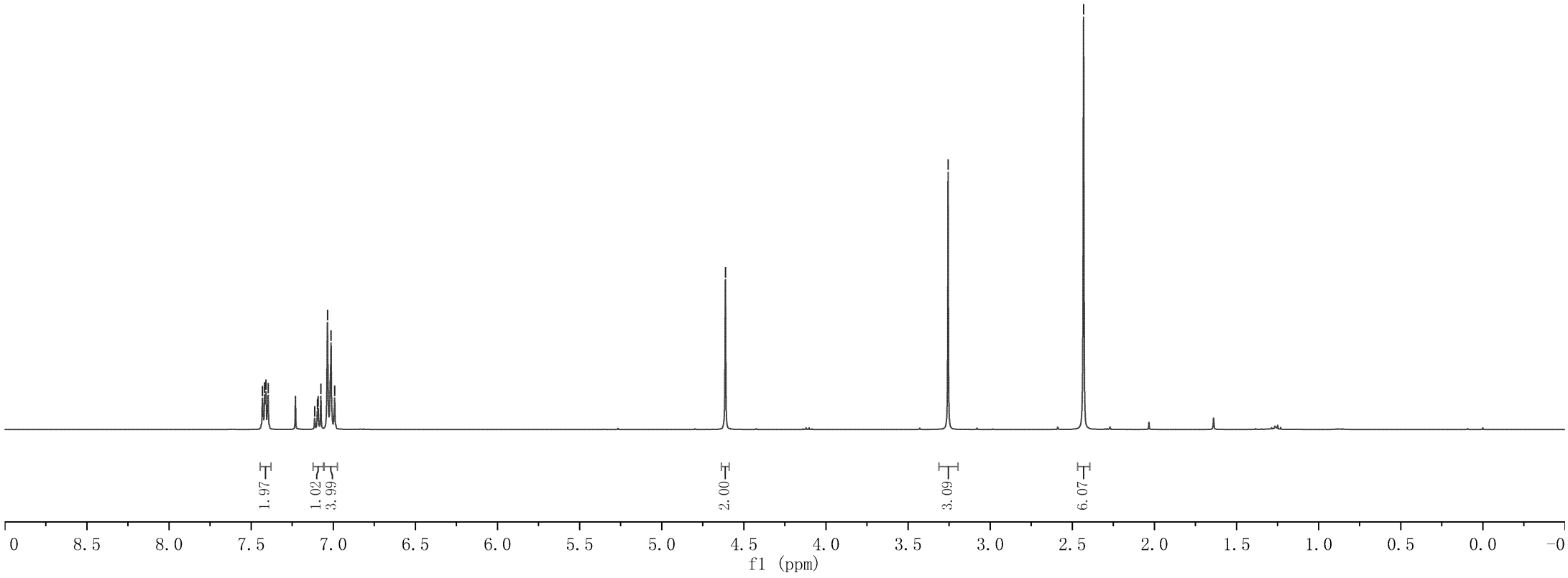


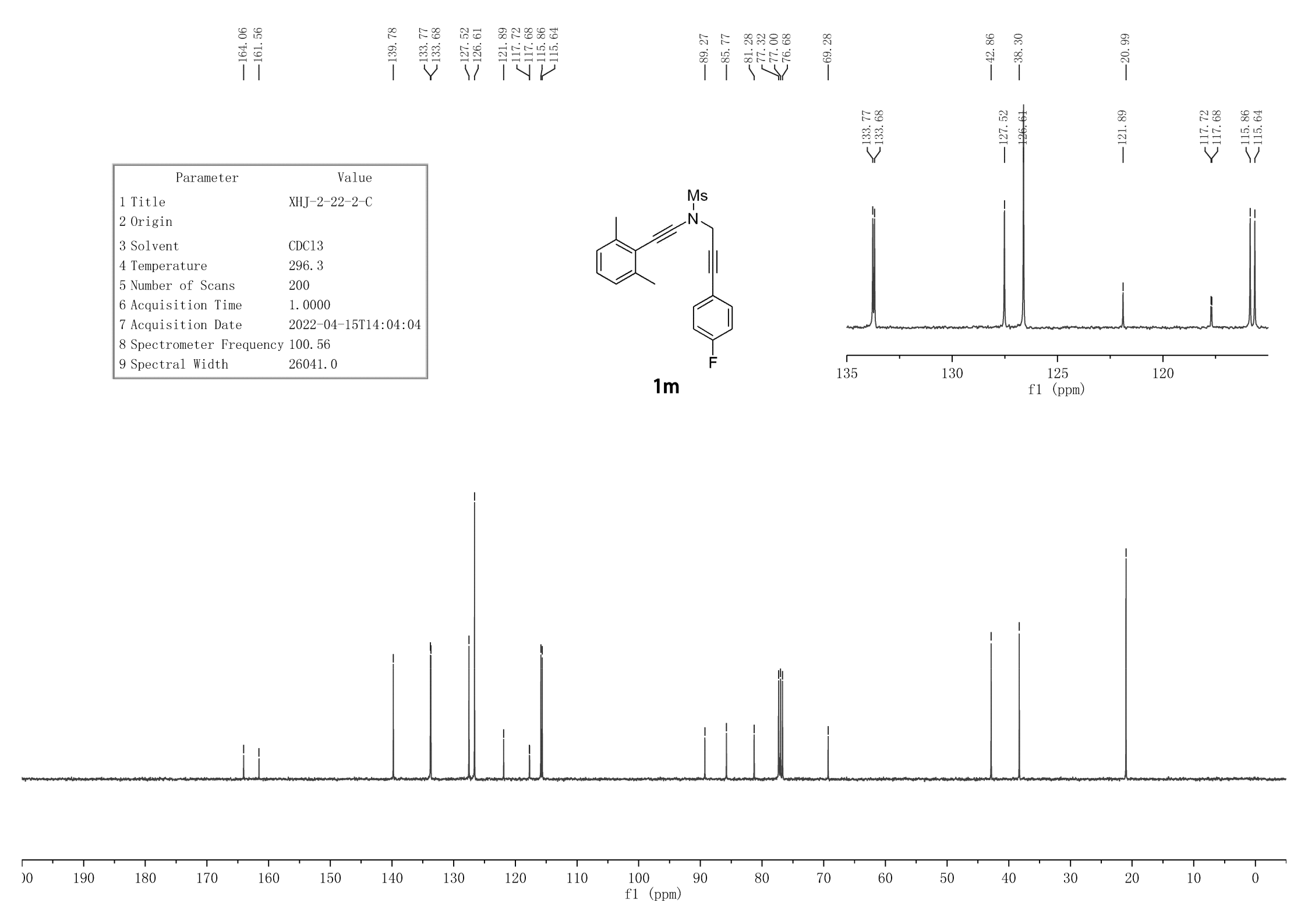
Parameter	Value
1 Title	XHJ-2-22-2-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-15T14:07:33
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



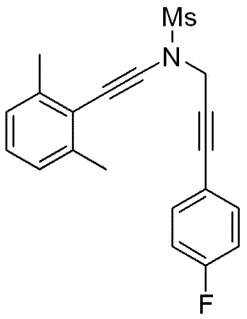
1m





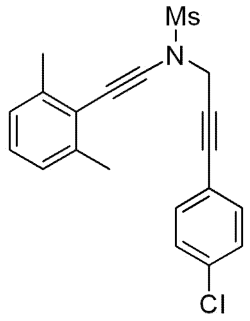

164.06
161.56
139.78
133.77
133.68
127.52
126.61
121.89
117.72
117.68
115.86
115.64
89.27
85.77
81.28
77.32
77.00
76.68
69.28
42.86
38.30
20.99
Parameter Value
1 Title XHJ-2-22-2-C
2 Origin
3 Solvent CDCl3
4 Temperature 296.3
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-04-15T14:04:04
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
F
1m
133.77
133.68
127.52
126.61
121.89
117.72
117.68
115.86
115.64
135
130
125
120
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	XHJ-2-22-F-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.1
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-08-16T20:18:57
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

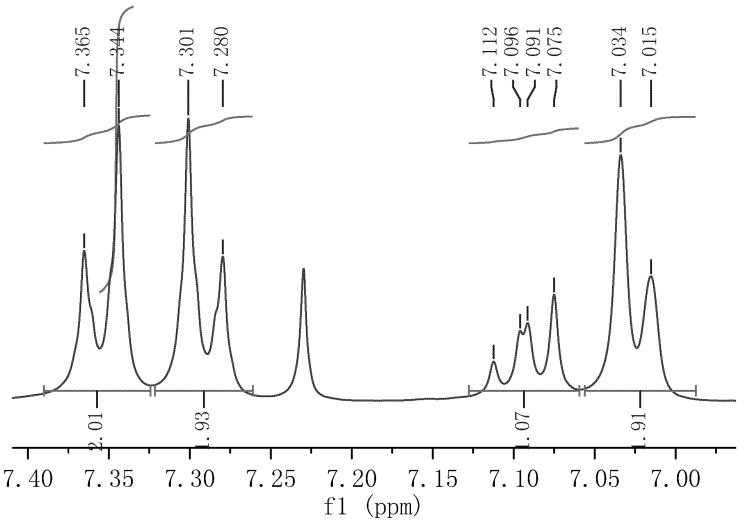


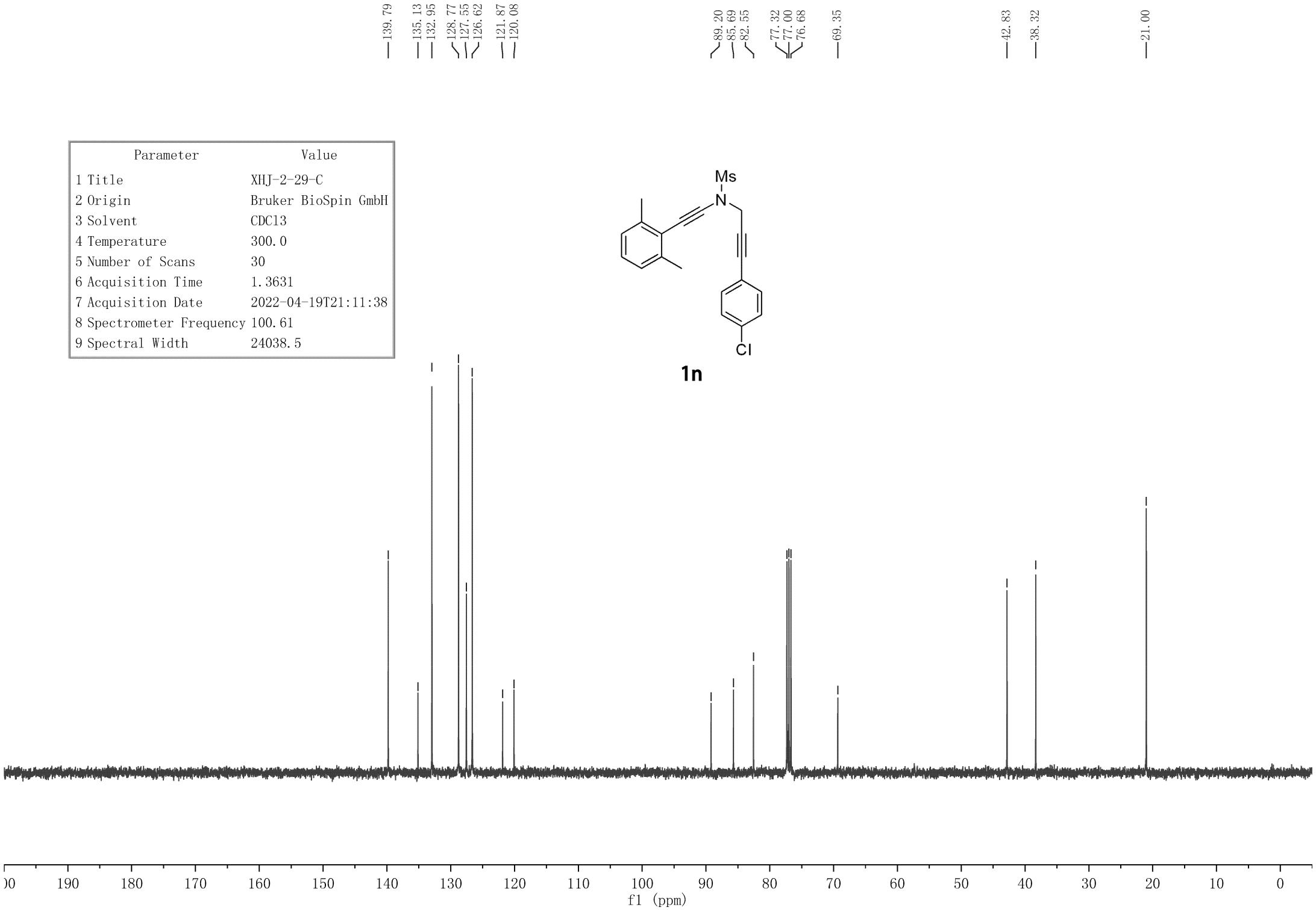
1m

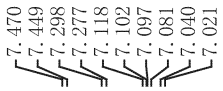
Parameter	Value
1 Title	XHJ-2-29-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-19T21:10:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



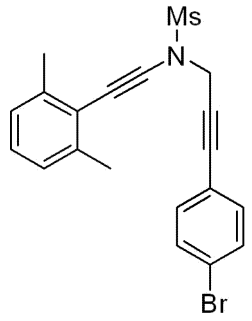
1n



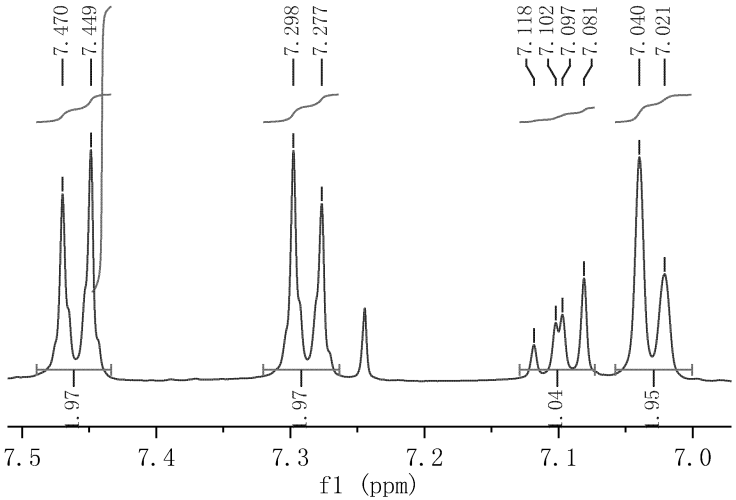

139.79
135.13
132.95
128.77
127.55
126.62
121.87
120.08
89.20
85.69
82.55
77.32
77.00
76.68
69.35
42.83
38.32
21.00
Parameter Value
1 Title XHJ-2-29-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 30
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-19T21:11:38
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Cl
1n
f1 (ppm)

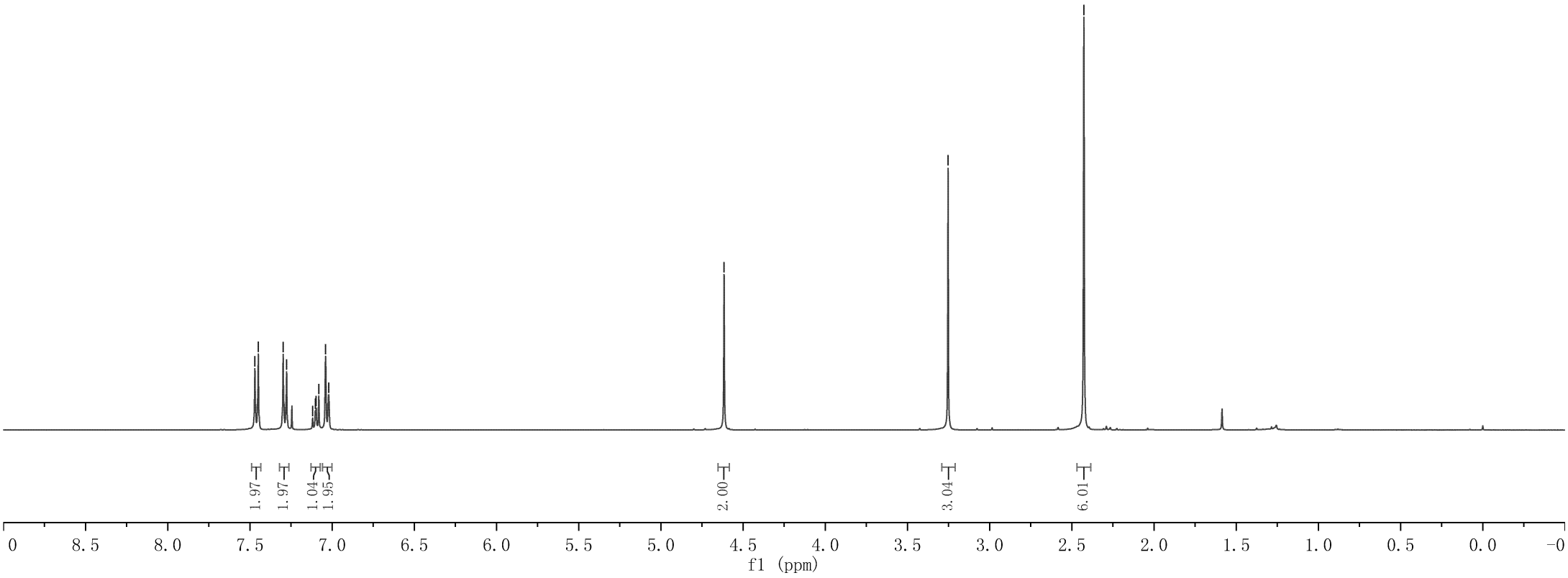


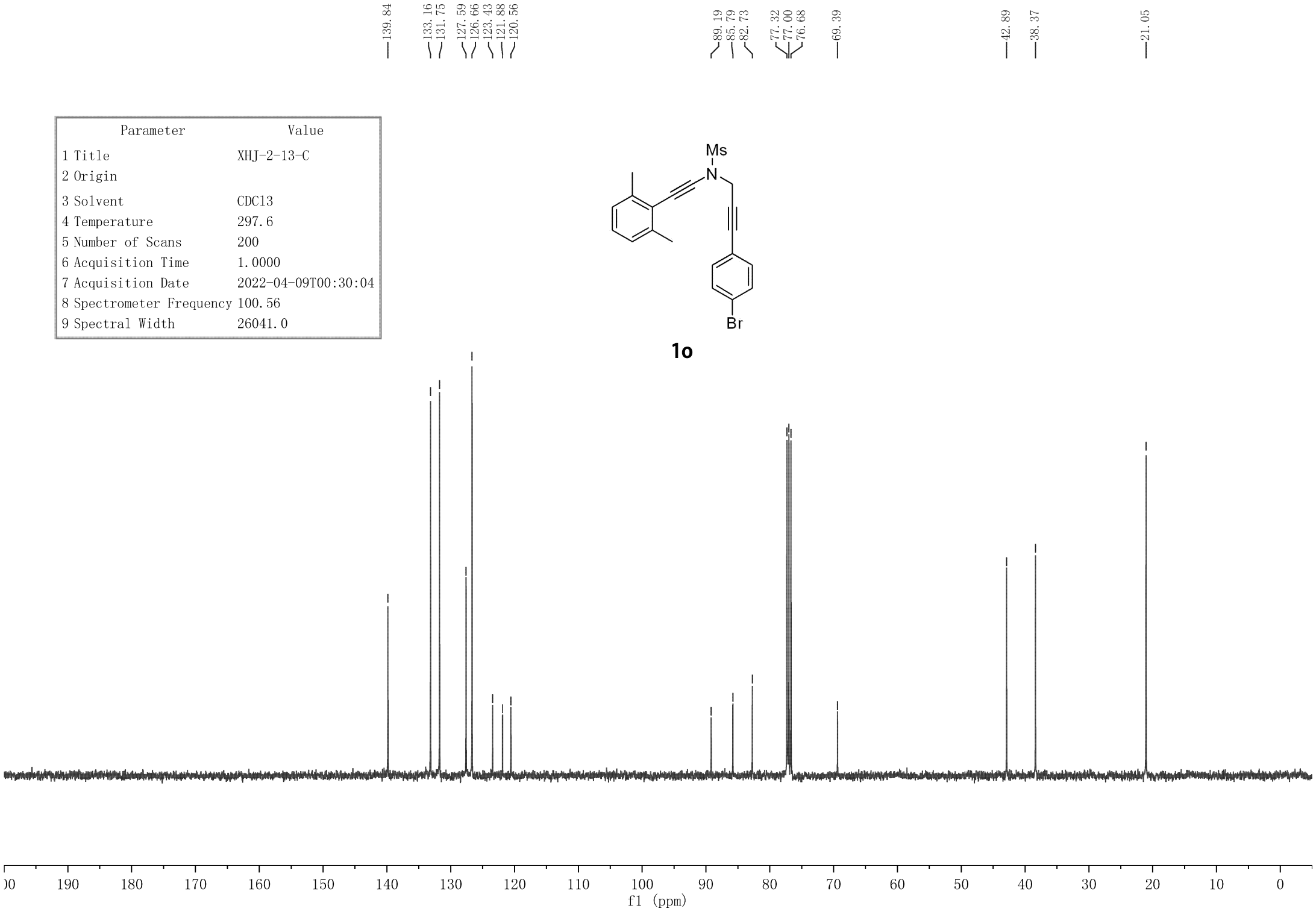
Parameter	Value
1 Title	XHJ-2-13-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	9
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-08T22:16:07
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

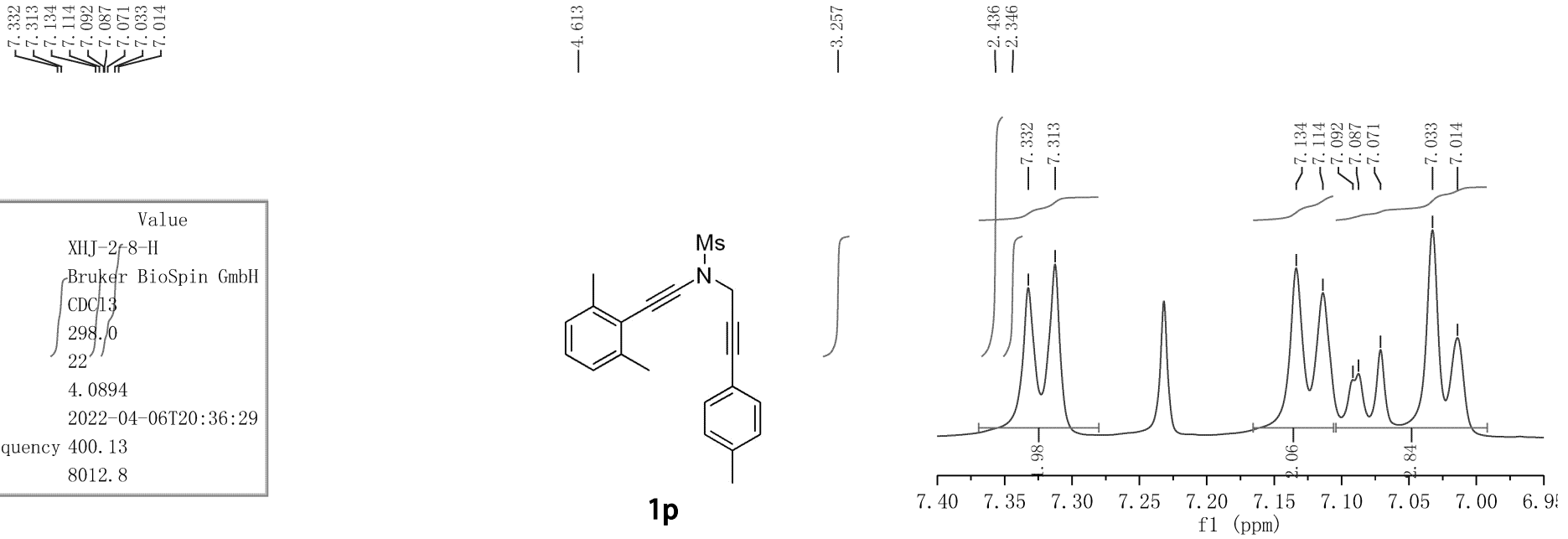


1o

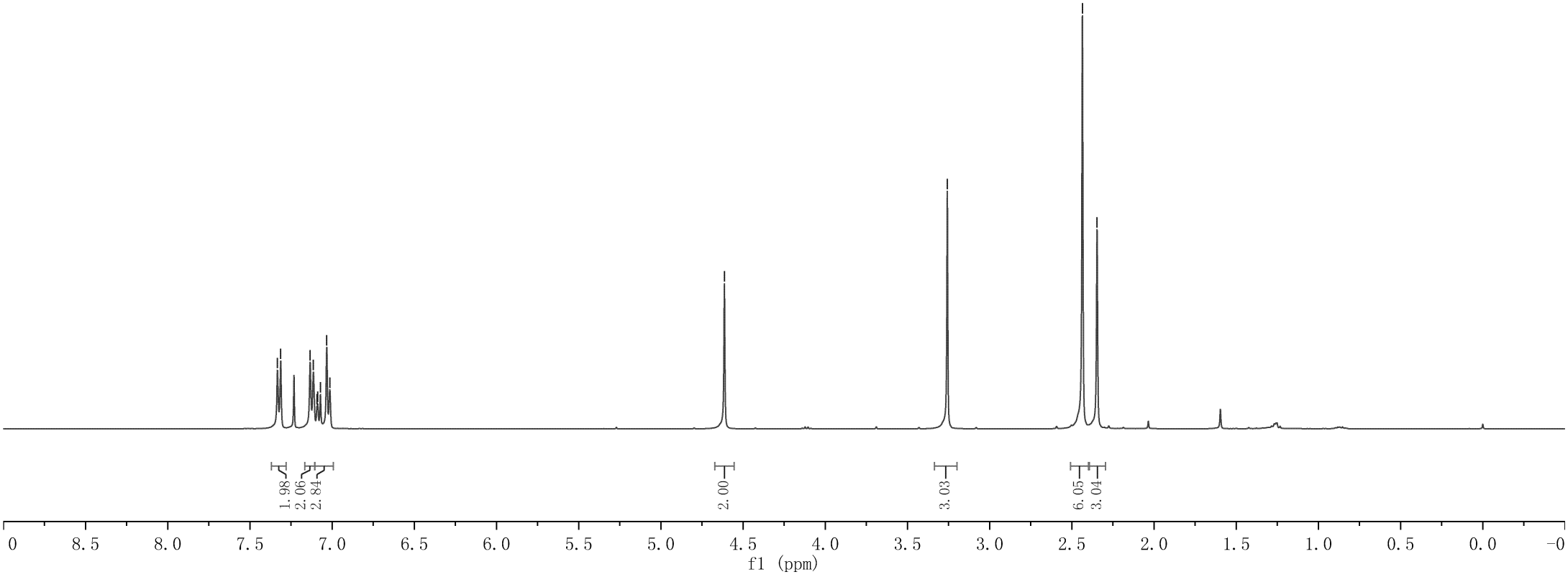


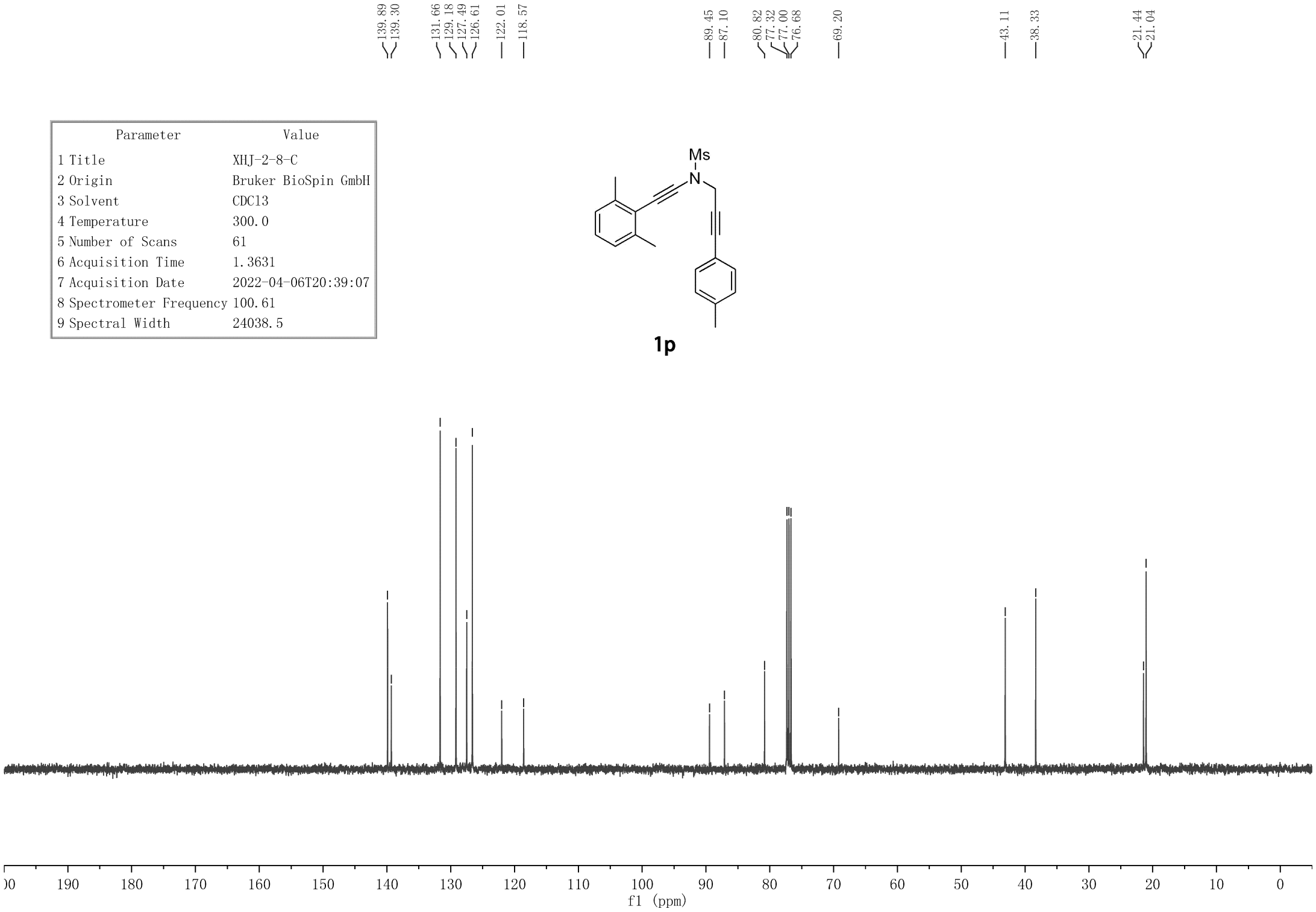



139.84
133.16
131.75
127.59
126.66
123.43
121.88
120.56
89.19
85.79
82.73
77.32
77.00
76.68
69.39
42.89
38.37
21.05
Parameter Value
1 Title XHJ-2-13-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.6
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-04-09T00:30:04
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Br
1o
f1 (ppm)



Parameter	Value
1 Title	XHJ-2-8-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	2022-04-06T20:36:29
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

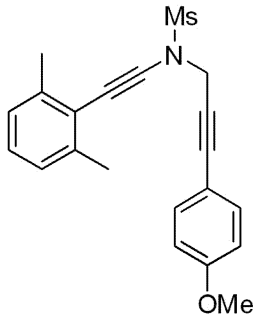




Parameter	Value
1 Title	XHJ-2-8-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	61
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-06T20:39:07
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

1p

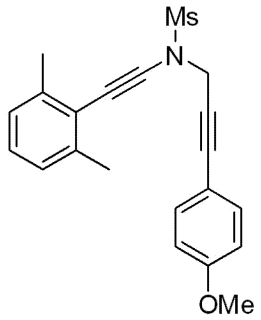
Parameter	Value
1 Title	XHJ-2-30-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-20T11:32:00
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



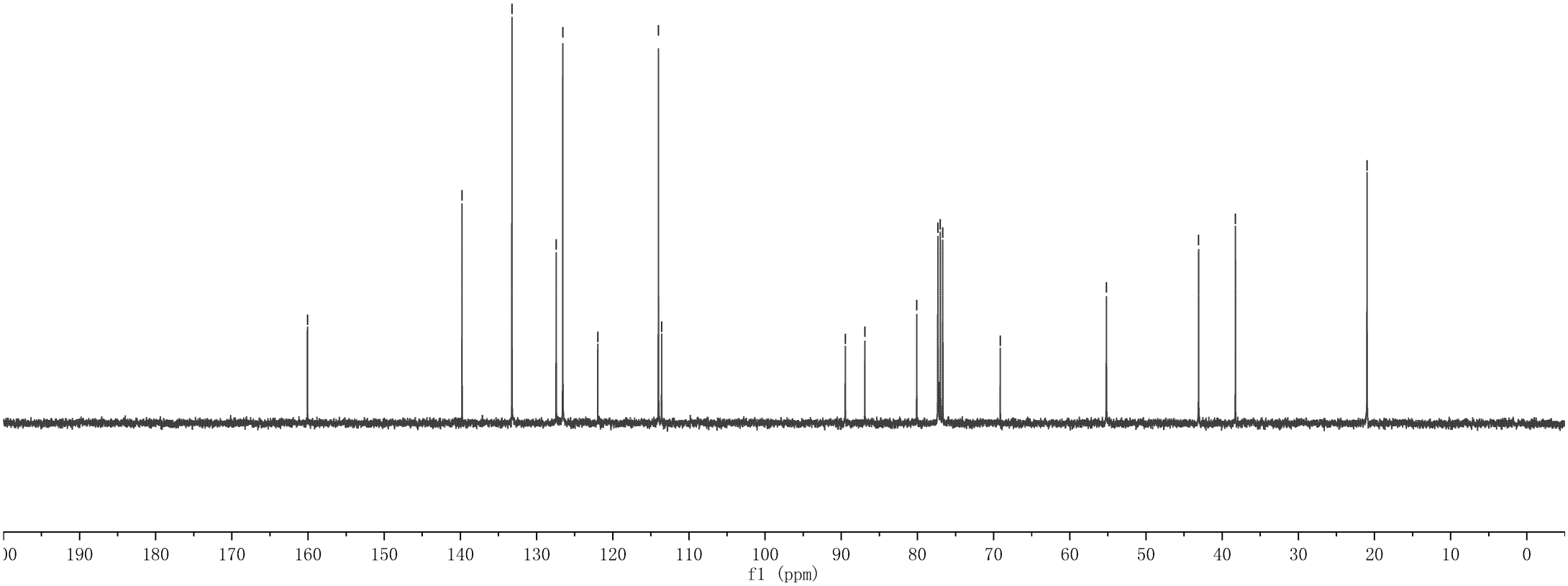
1q

160.08
139.79
133.23
127.43
126.56
121.97
114.00
113.58
89.47
86.91
80.10
77.32
77.00
76.68
69.13
55.19
43.09
38.26
20.98

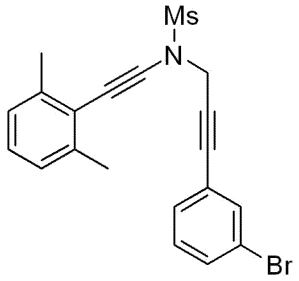
Parameter	Value
1 Title	XHJ-2-30-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-20T11:33:25
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



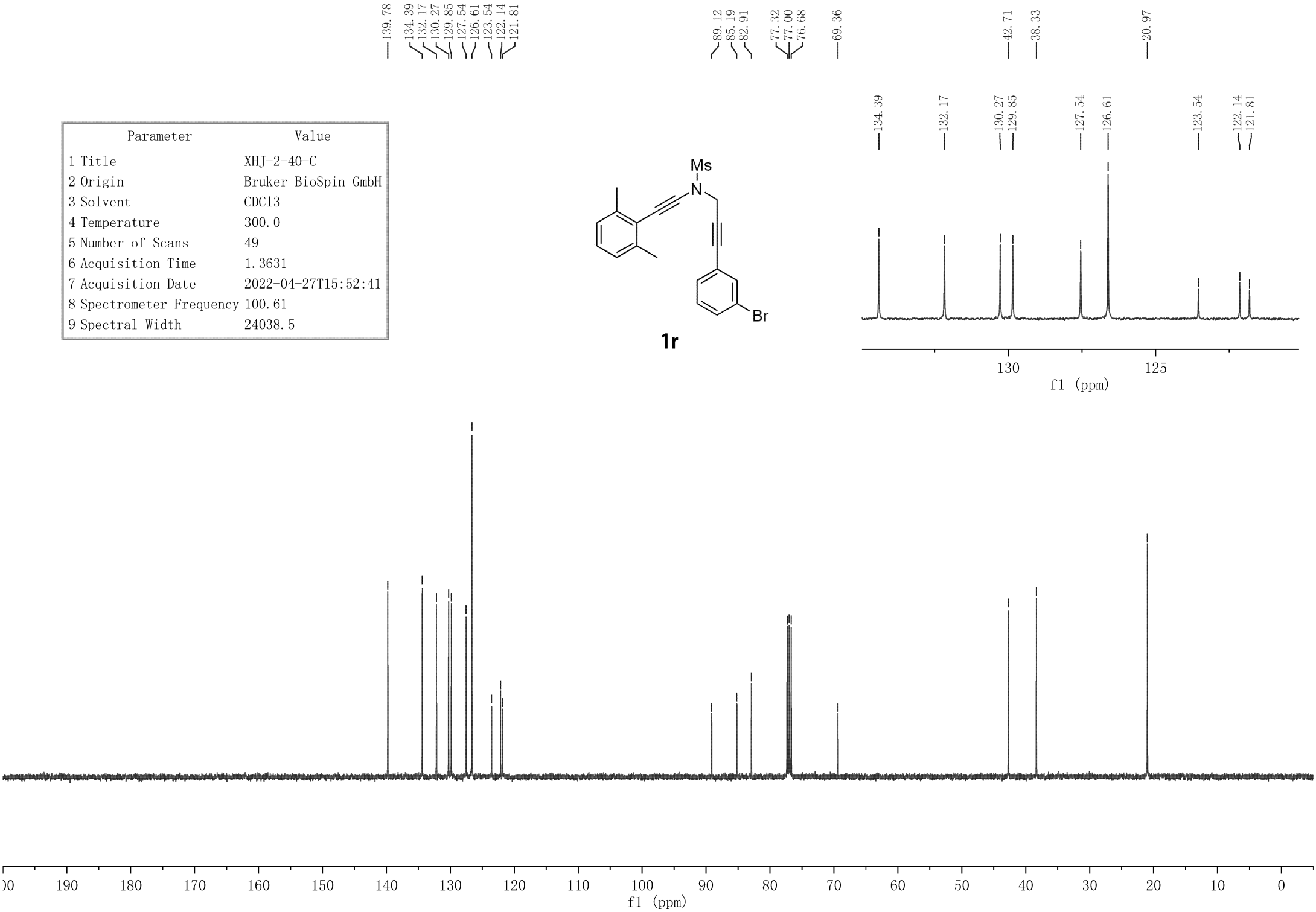
1q

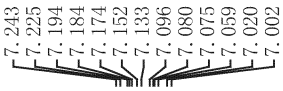


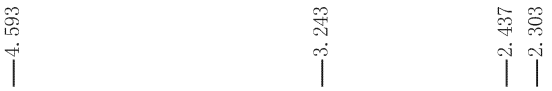
Parameter	Value
1 Title	XHJ-2-40-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-27T15:51:03
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



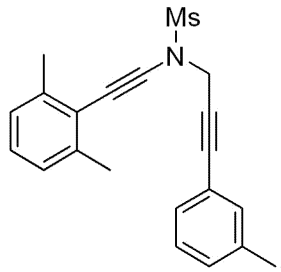
1r


139.78
134.39
132.17
130.27
129.85
127.54
126.61
123.54
122.14
121.81
89.12
85.19
82.91
77.32
77.00
76.68
69.36
42.71
38.33
20.97
Parameter Value
1 Title XHJ-2-40-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 49
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-27T15:52:41
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Br
1r
f1 (ppm)

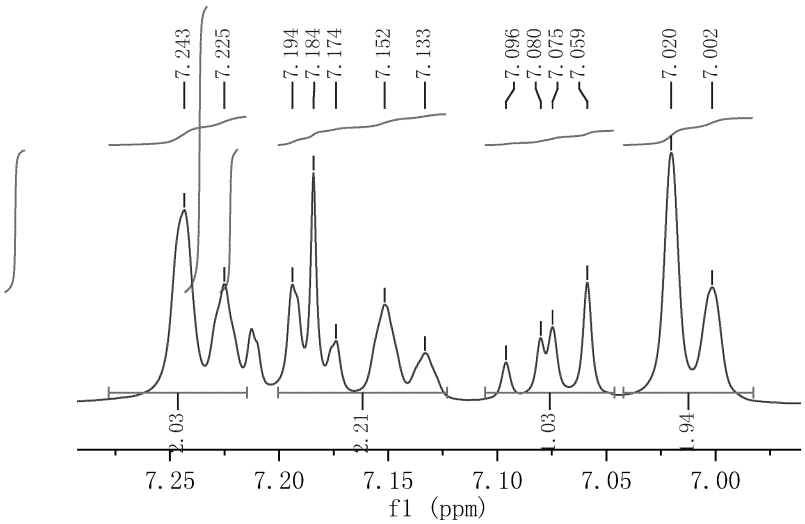


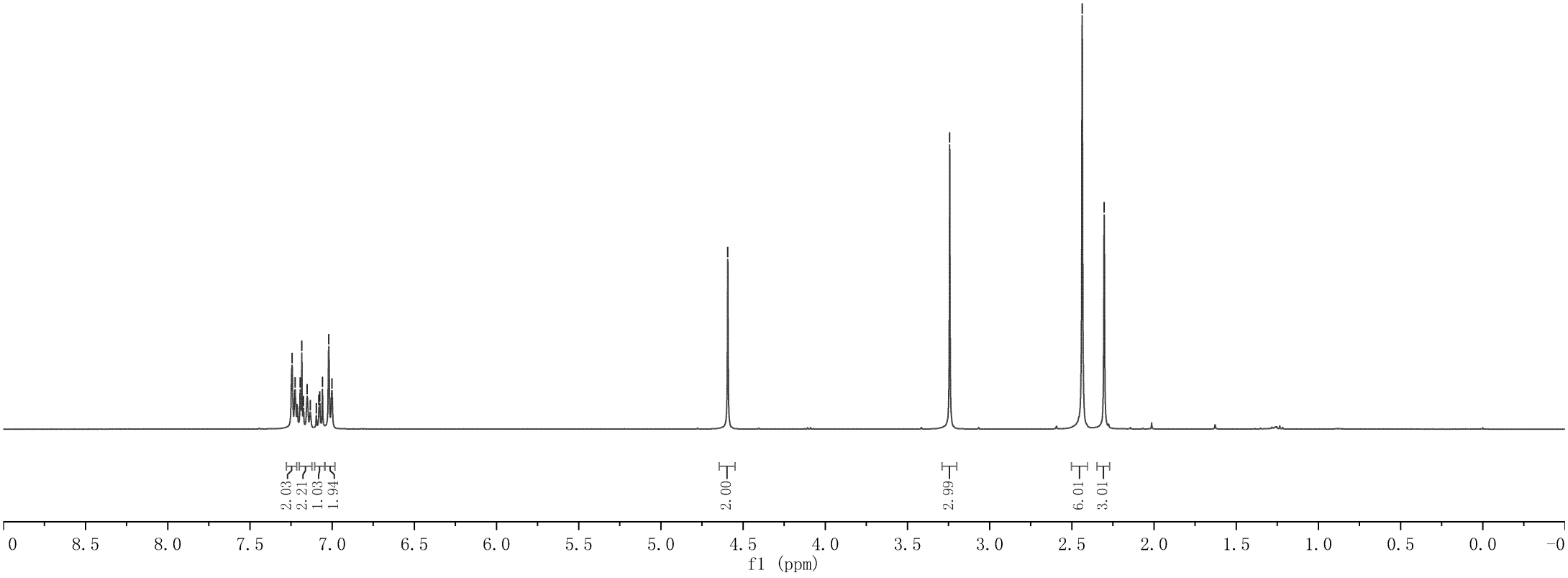


Parameter	Value
1 Title	XHJ-2-54-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-03T15:43:38
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

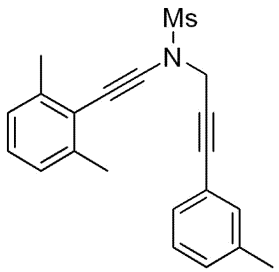


1s

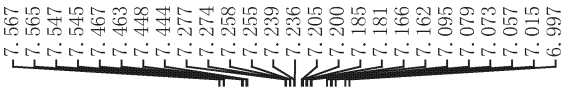




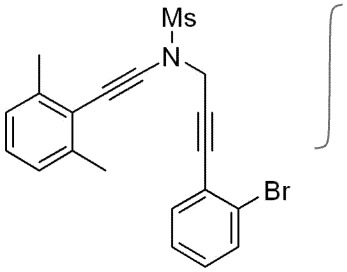
Parameter	Value
1 Title	XHJ-2-54-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	14
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-03T16:03:44
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



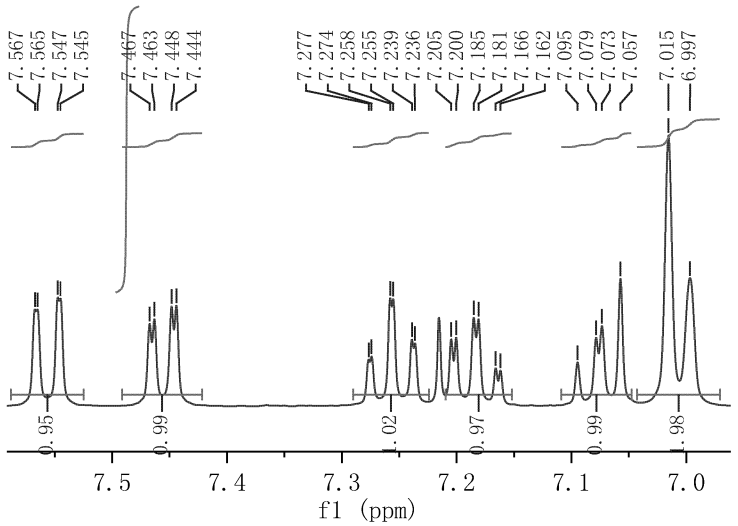
1s

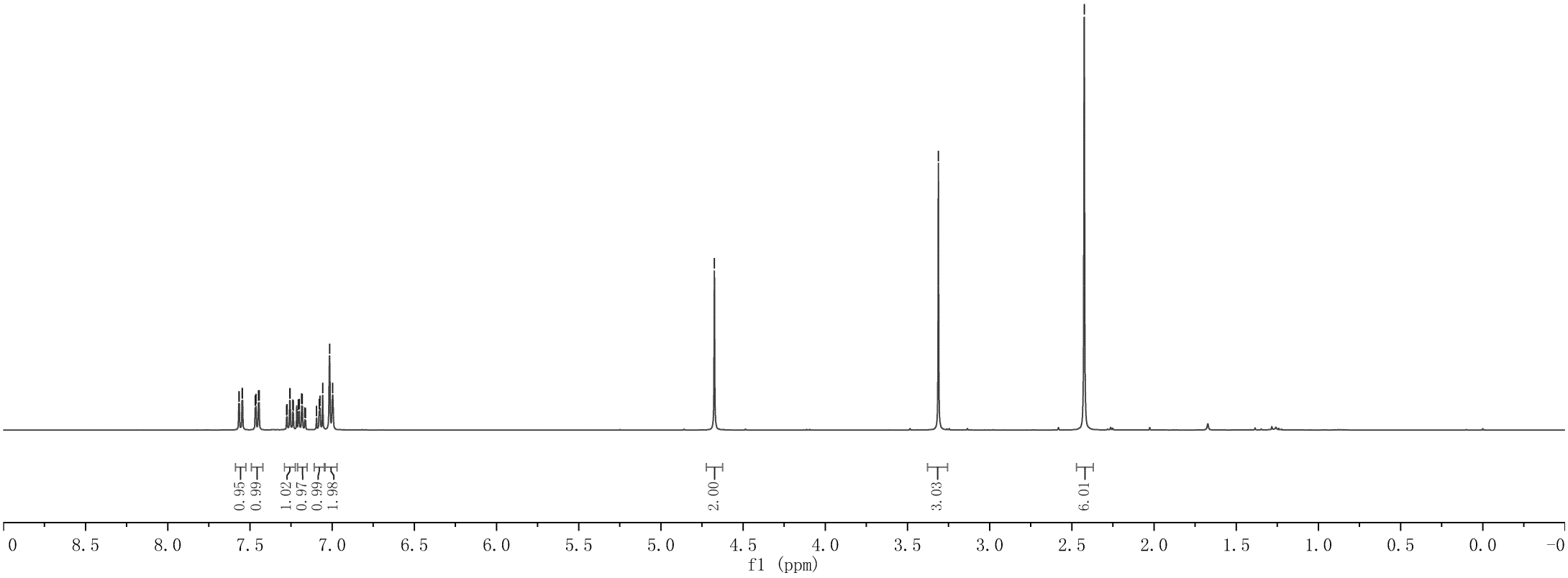


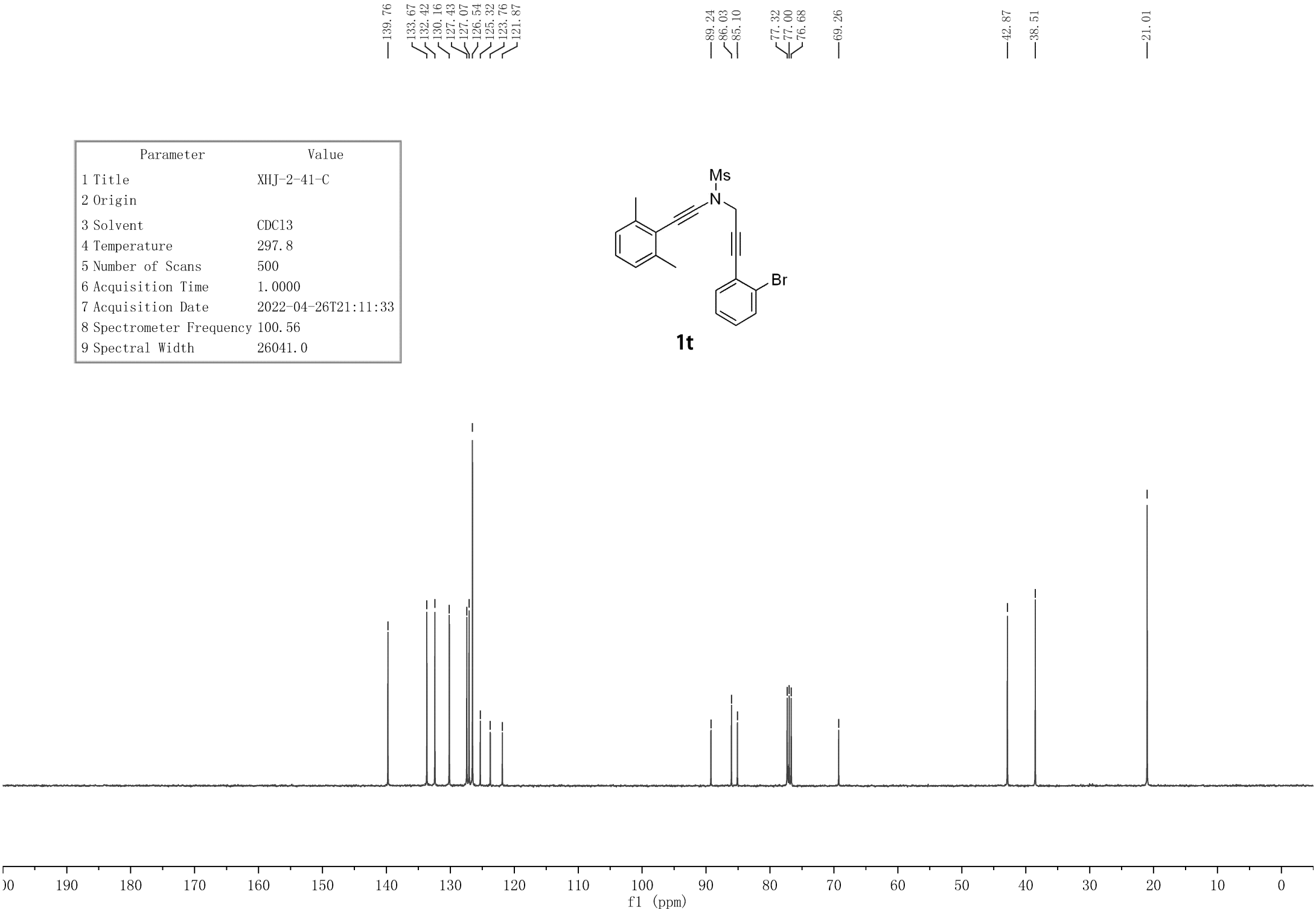
Parameter	Value
1 Title	XHJ-2-41-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-04-26T20:52:32
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0

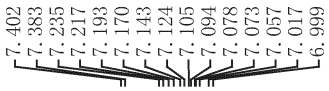


1t

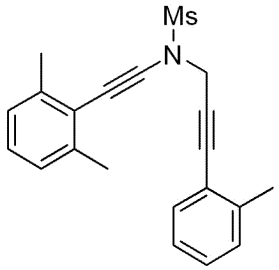





139.76
133.67
132.42
130.16
127.43
127.07
126.54
125.32
123.76
121.87
89.24
86.03
85.10
77.32
77.00
76.68
69.26
42.87
38.51
21.01
Parameter Value
1 Title XHJ-2-41-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.8
5 Number of Scans 500
6 Acquisition Time 1.0000
7 Acquisition Date 2022-04-26T21:11:33
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Br
1t
f1 (ppm)



Parameter	Value
1 Title	XHJ-2-53-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-05-03T11:54:04
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0



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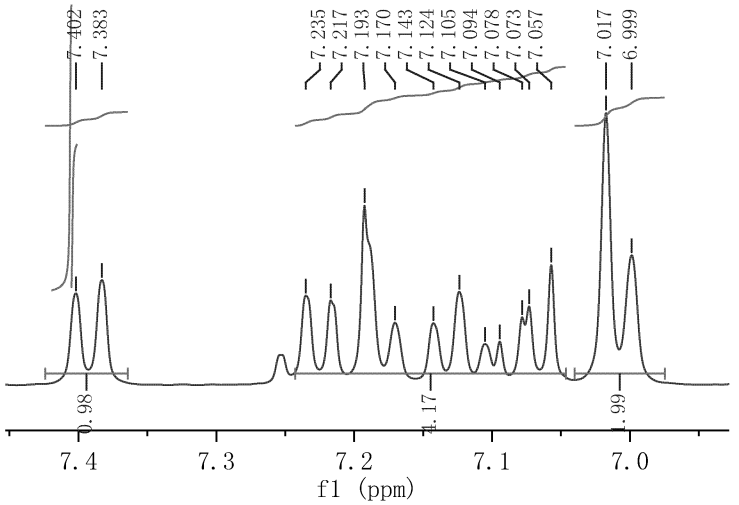

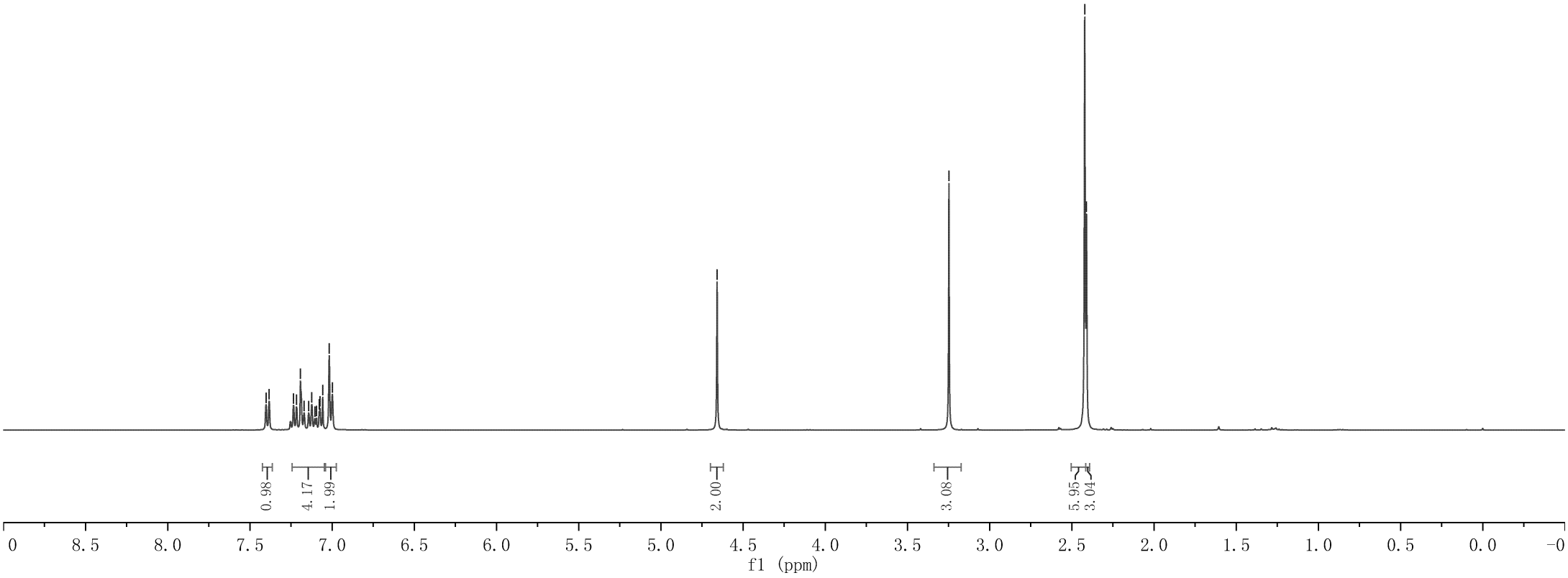

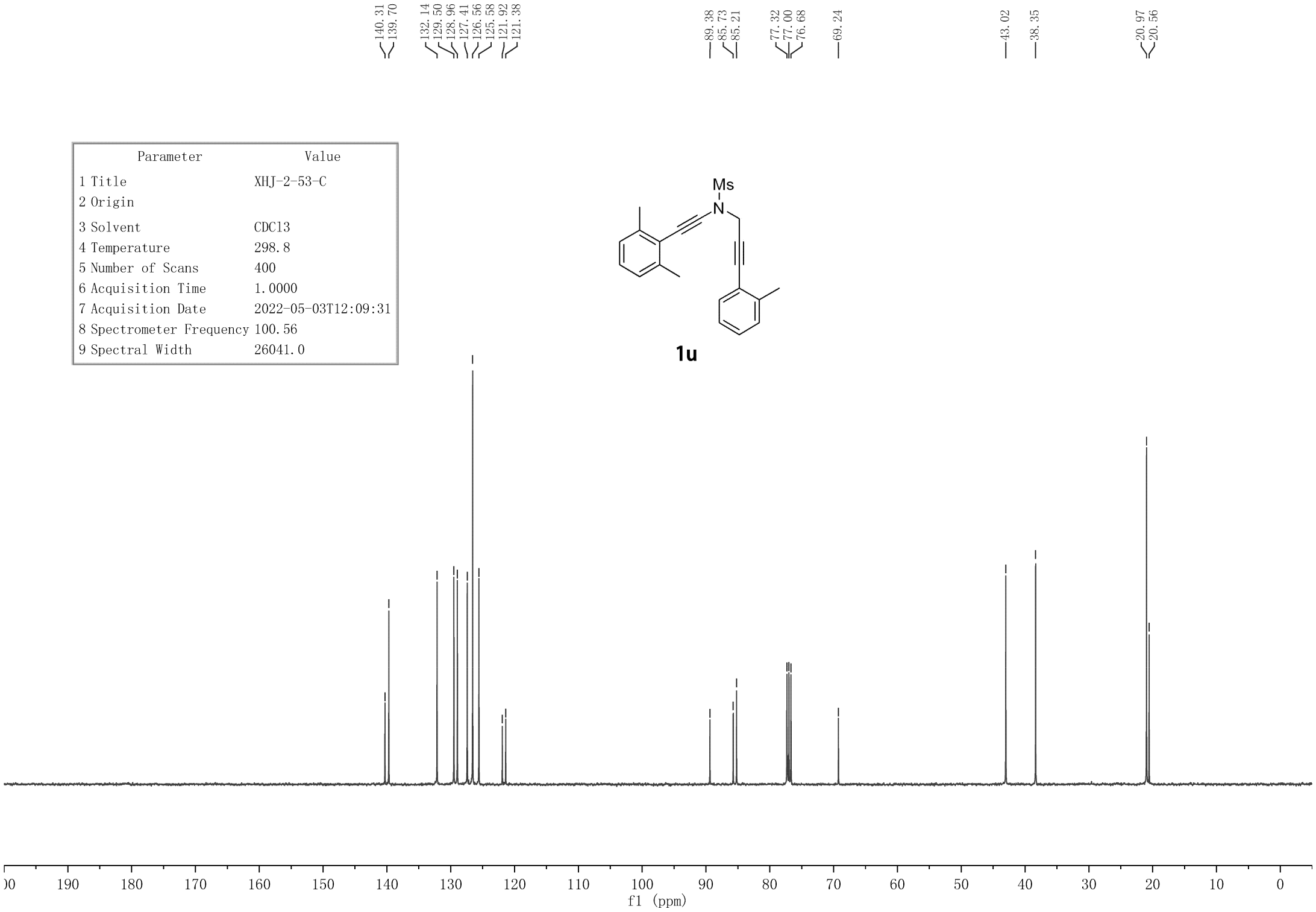
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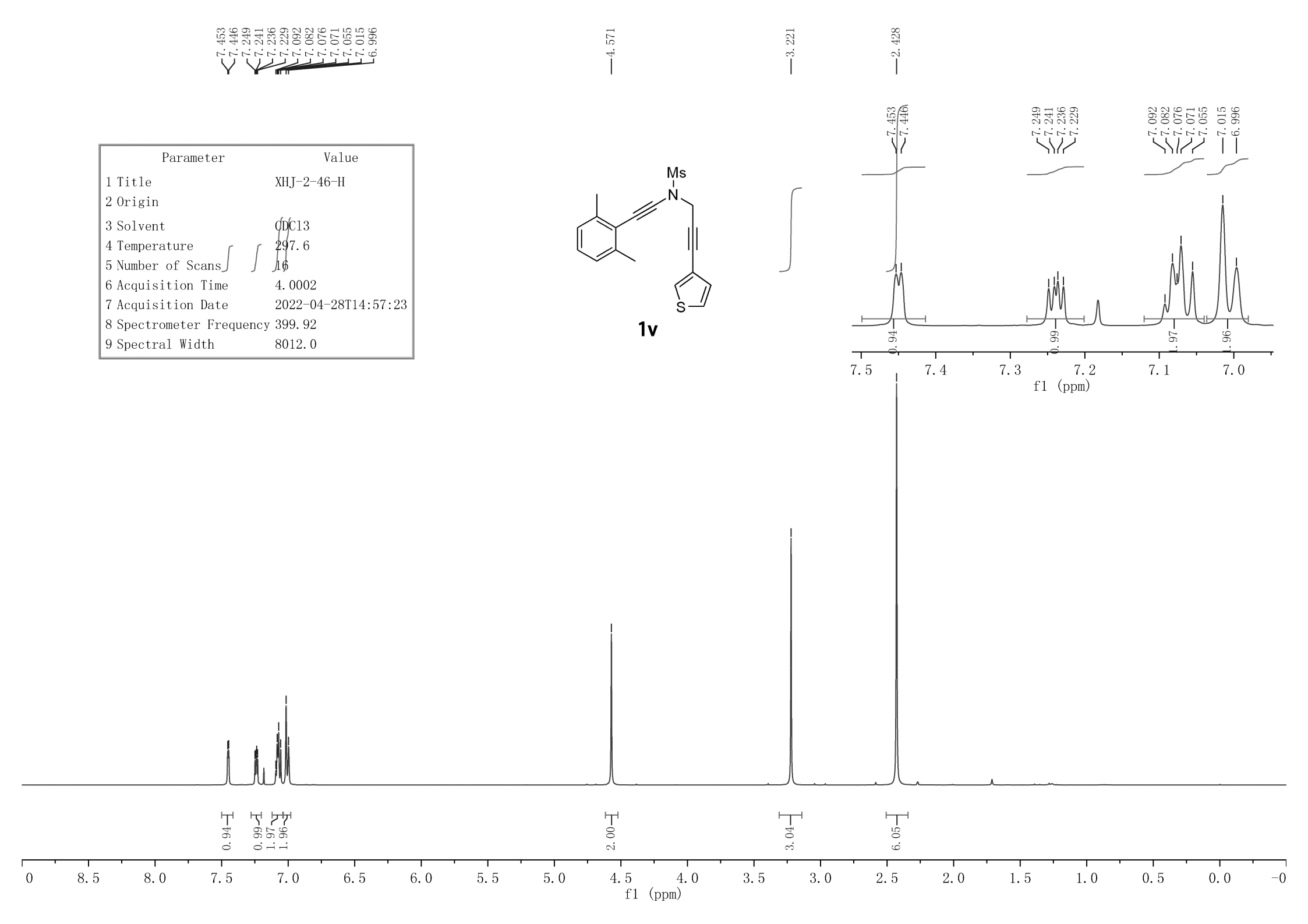
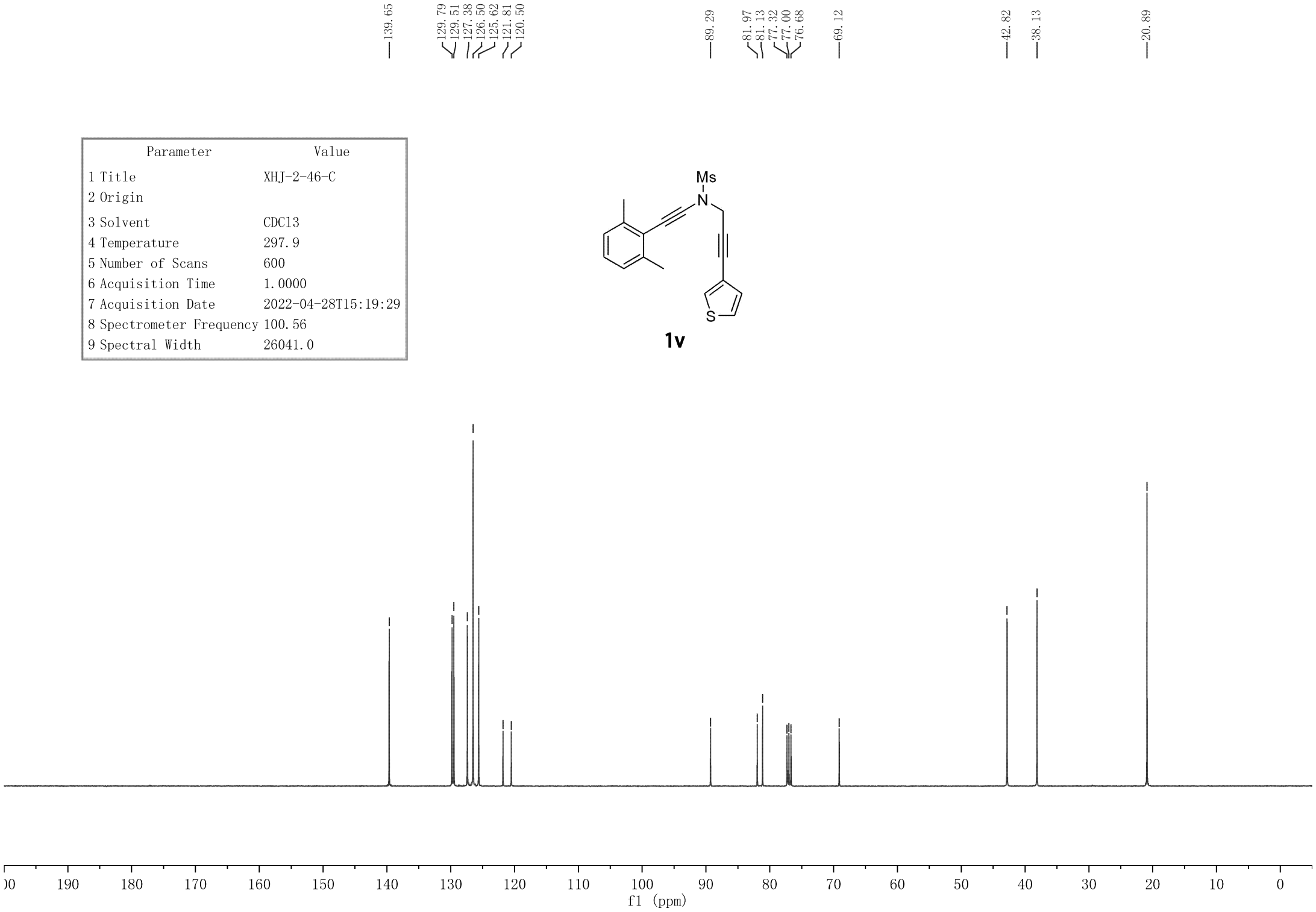
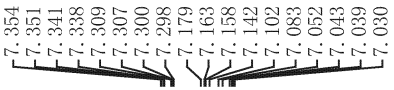
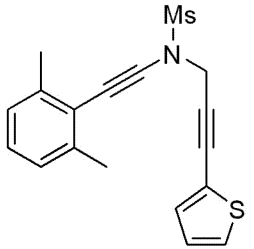
139.70
132.14
129.50
128.96
127.41
126.56
125.58
121.92
121.38
89.38
85.73
85.21
77.32
77.00
76.68
69.24
43.02
38.35
20.97
20.56
Parameter Value
1 Title XHJ-2-53-C
2 Origin
3 Solvent CDCl3
4 Temperature 298.8
5 Number of Scans 400
6 Acquisition Time 1.0000
7 Acquisition Date 2022-05-03T12:09:31
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
1u
f1 (ppm)


7.453
7.446
7.249
7.241
7.236
7.229
7.092
7.082
7.076
7.071
7.055
7.015
6.996
4.571
3.221
2.428
Parameter Value
1 Title XHJ-2-46-H
2 Origin
3 Solvent CDCl3
4 Temperature 297.6
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-04-28T14:57:23
8 Spectrometer Frequency 399.92
9 Spectral Width 8012.0
Ms
N
S
1v
0.94
0.99
1.97
1.96
2.00
3.04
6.05
f1 (ppm)


139.65
129.79
129.51
127.38
126.50
125.62
121.81
120.50
89.29
81.97
81.13
77.32
77.00
76.68
69.12
42.82
38.13
20.89
Parameter Value
1 Title XHJ-2-46-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.9
5 Number of Scans 600
6 Acquisition Time 1.0000
7 Acquisition Date 2022-04-28T15:19:29
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
S
1v
f1 (ppm)



Parameter	Value
1 Title	XHJ-2-62-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	3
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-10T20:59:33
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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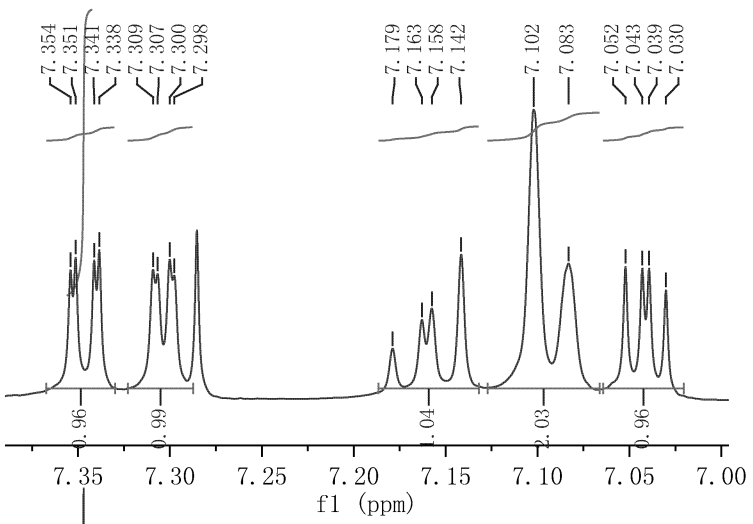
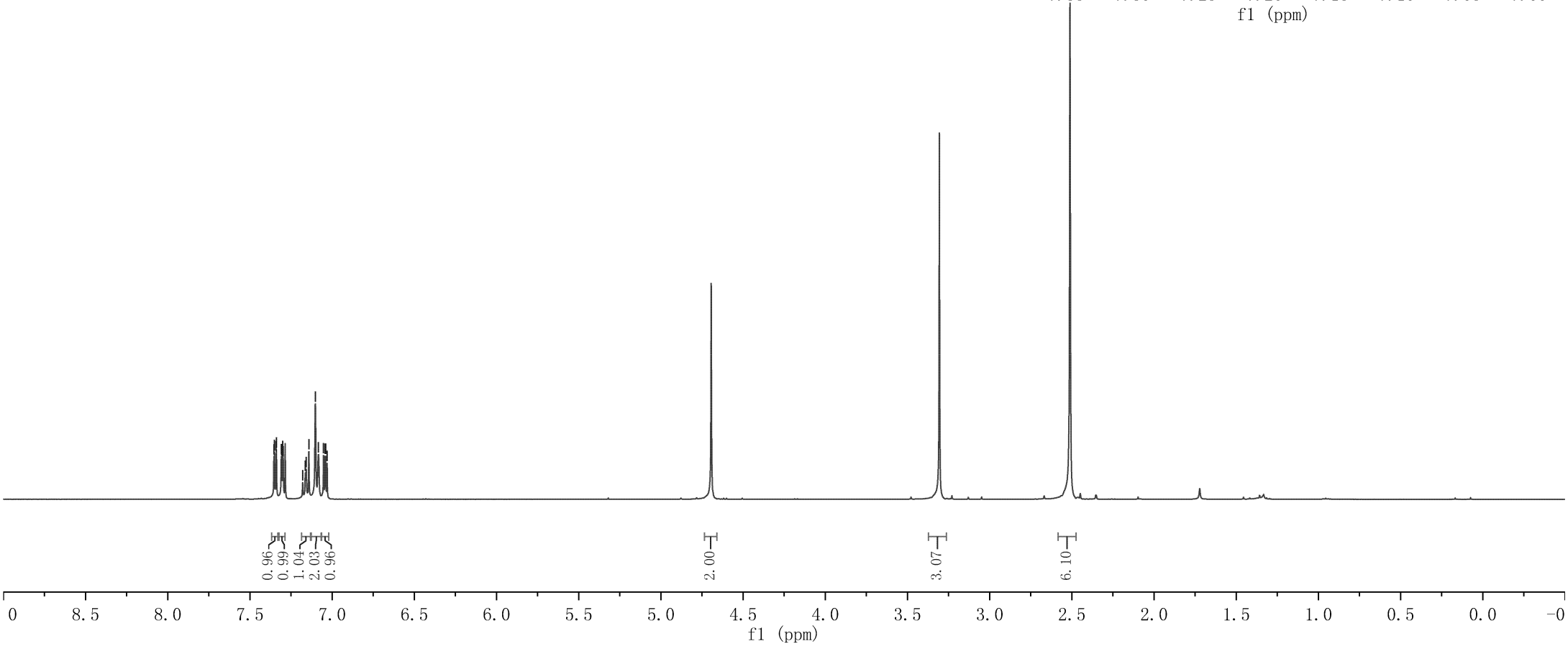
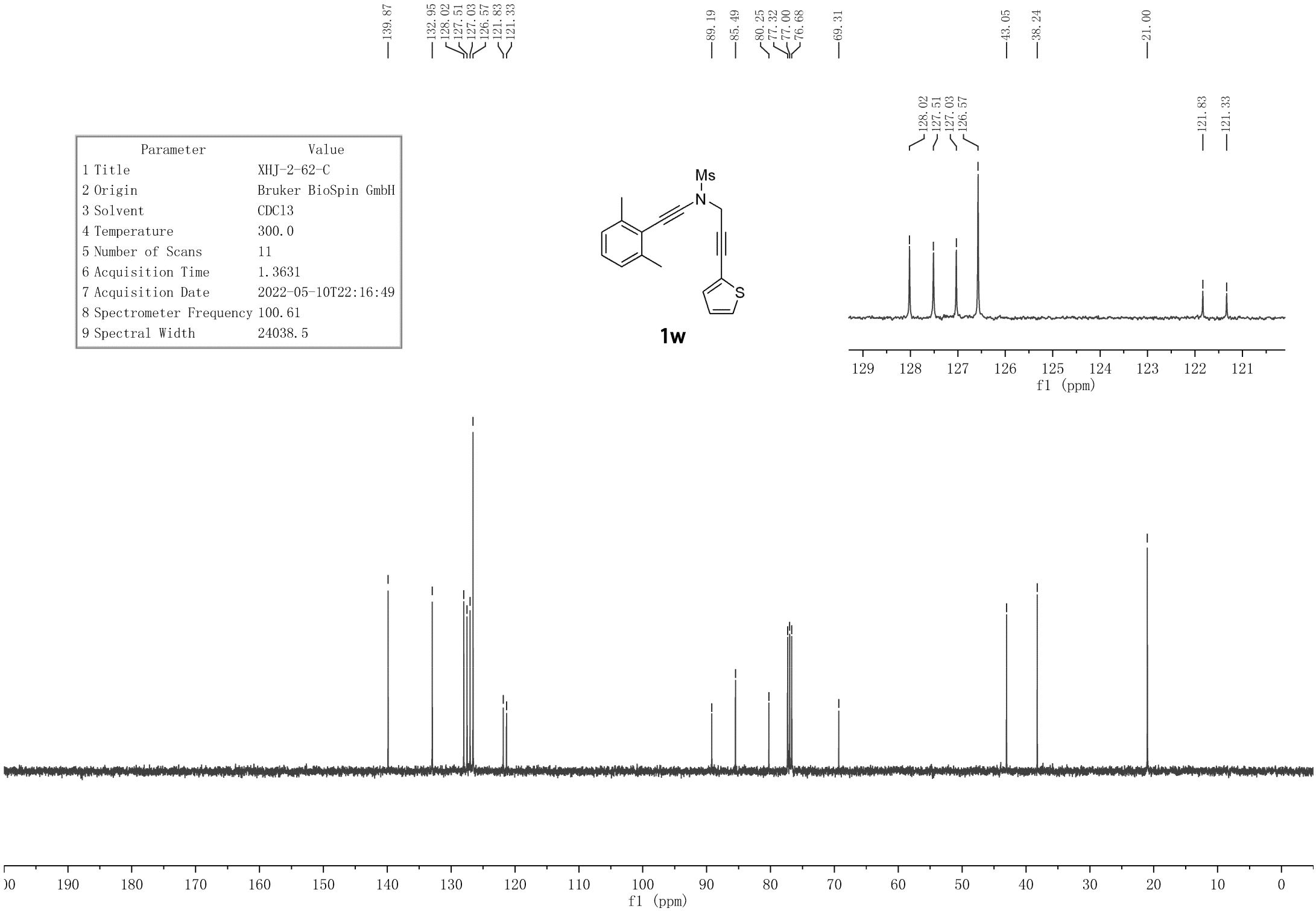
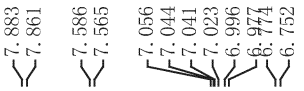
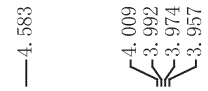




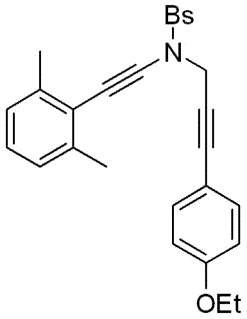


Parameter	Value
1 Title	XHJ-2-62-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	11
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-10T22:16:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

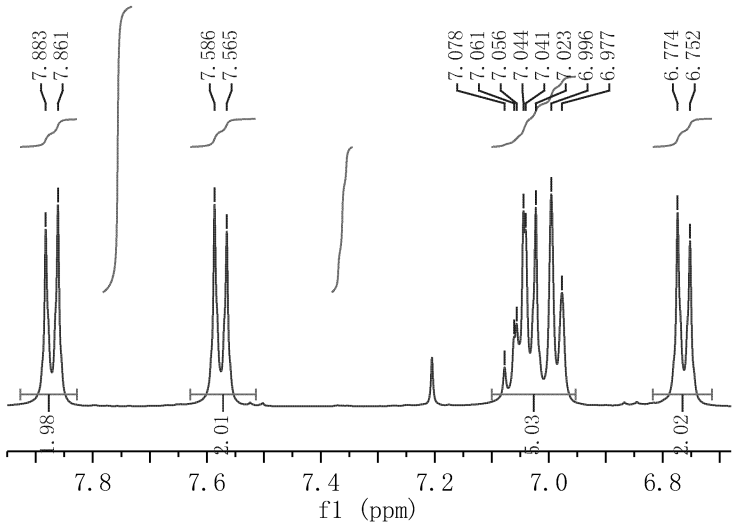


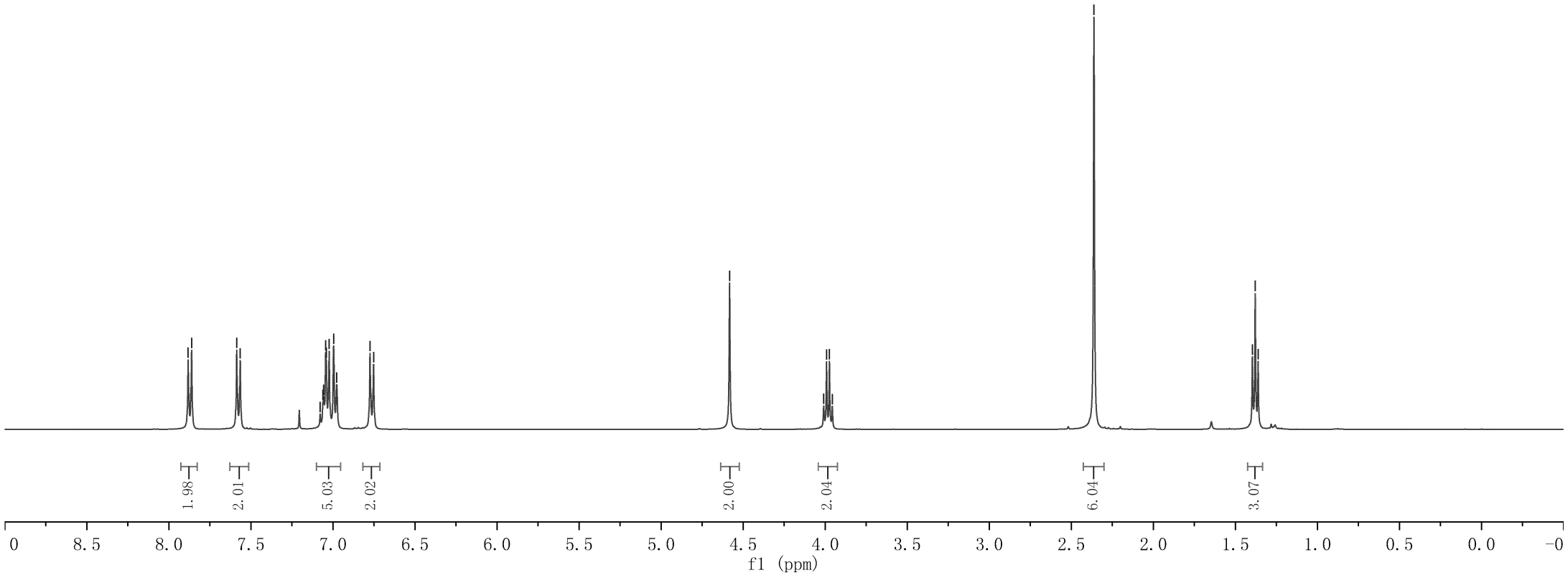


Parameter	Value
1 Title	XHJ-2-128-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-06-23T21:17:06
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



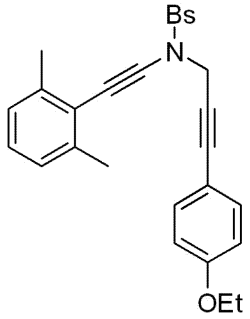
1y



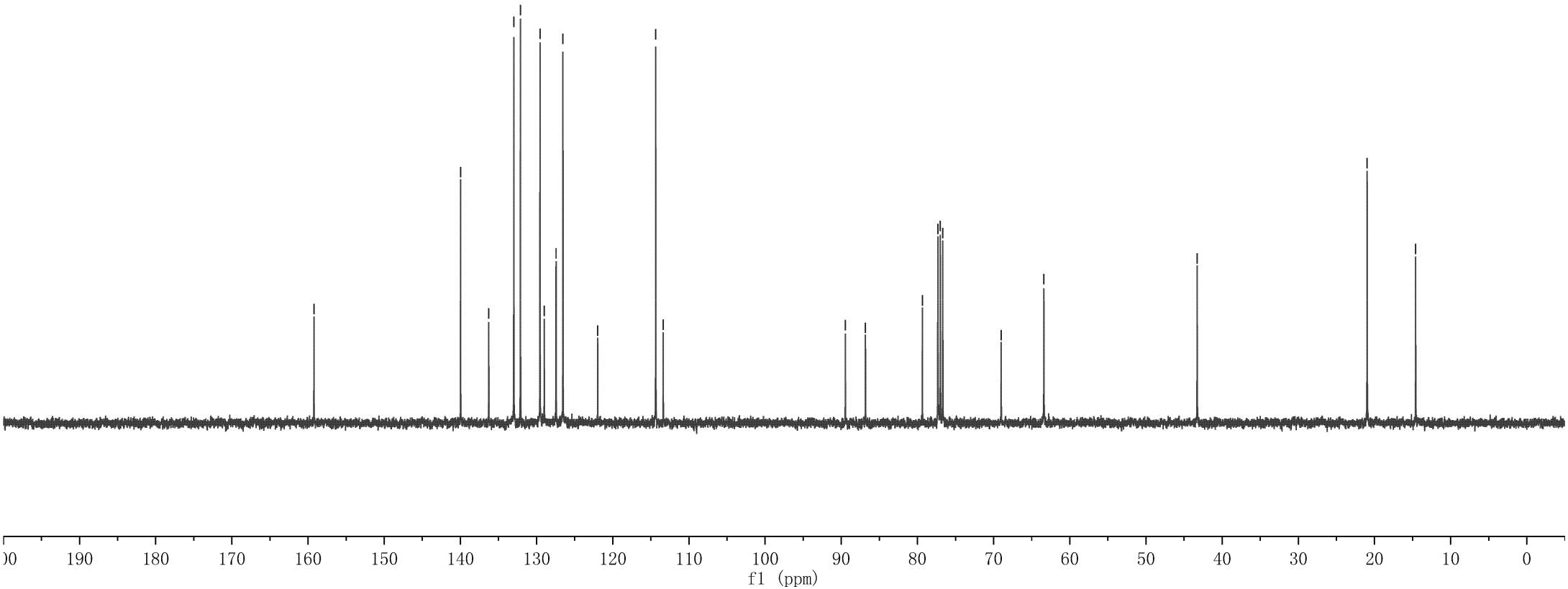


159.22
139.97
136.27
132.99
132.12
129.55
128.99
127.44
126.54
121.97
114.36
113.37
89.46
86.82
79.35
77.32
77.00
76.68
69.01
63.40
43.28
20.97
14.60

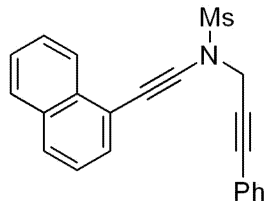
Parameter	Value
1 Title	XHJ-2-128-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	20
6 Acquisition Time	1.3631
7 Acquisition Date	2022-06-23T21:19:09
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



1y



Parameter	Value
1 Title	XHJ-3-116-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-10-29T11:58:41
8 Spectrometer Frequency	399.90
9 Spectral Width	8012.0



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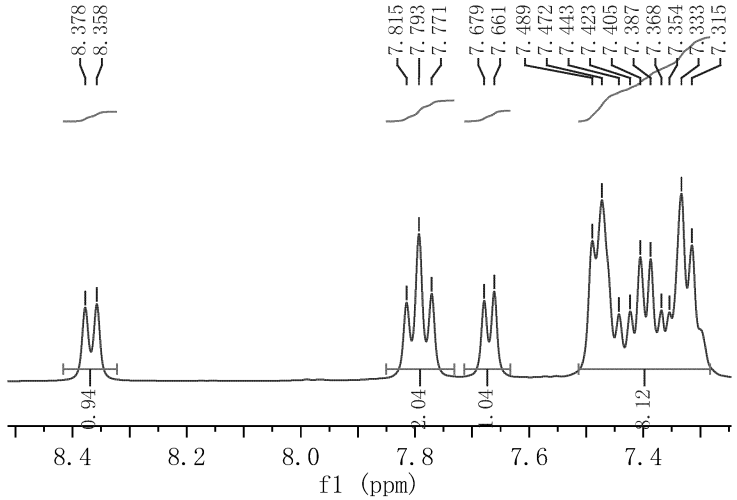
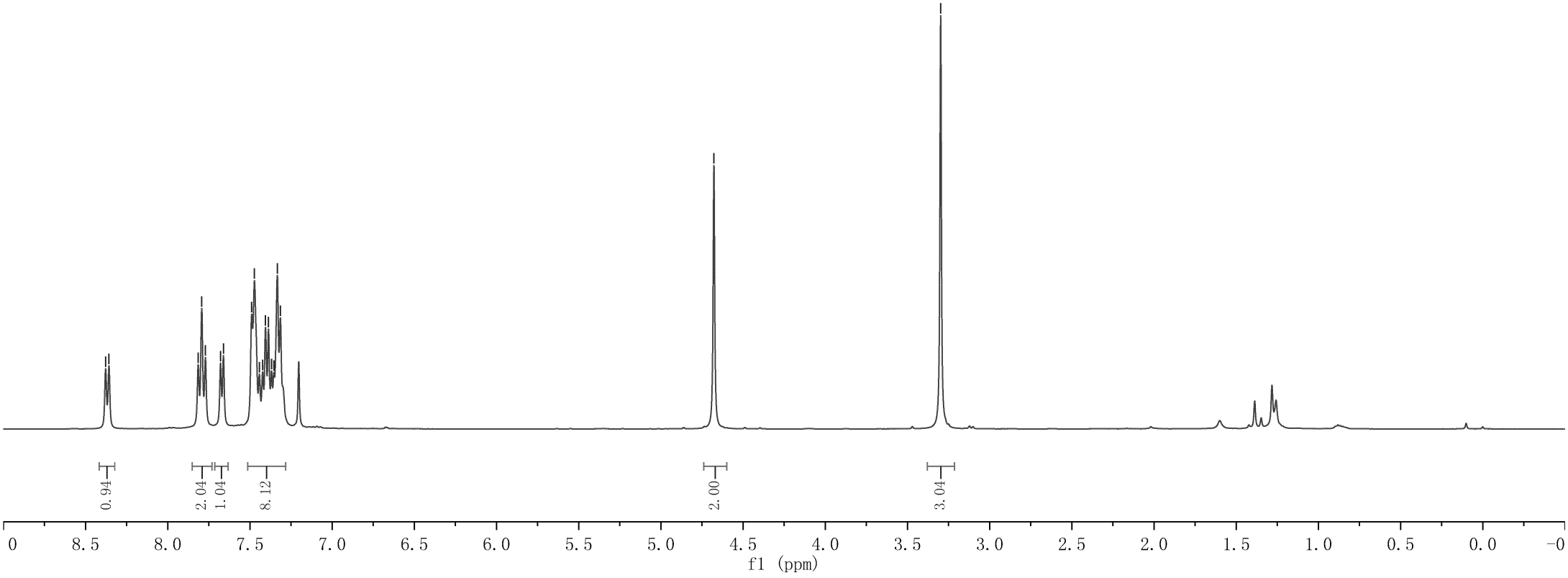
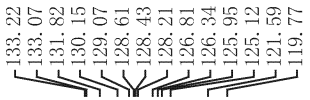
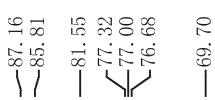
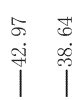


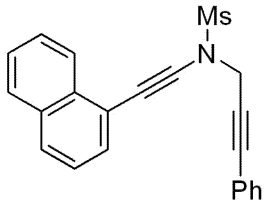








Parameter	Value
1 Title	XHJ-3-116-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.4
5 Number of Scans	500
6 Acquisition Time	1.0000
7 Acquisition Date	2022-10-29T12:18:14
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



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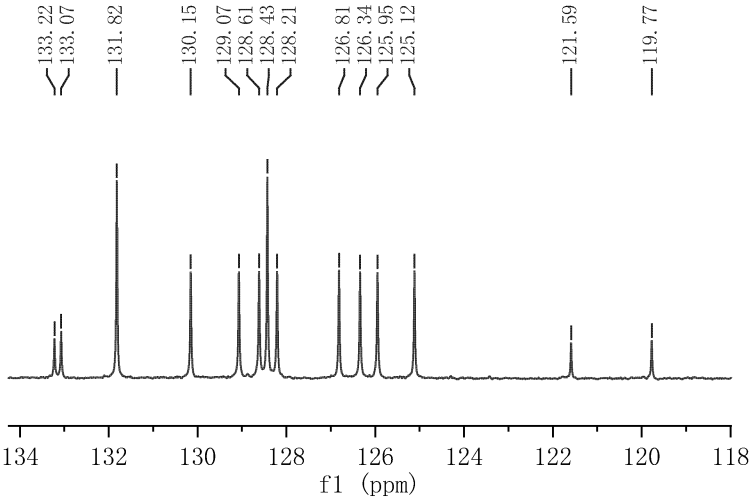

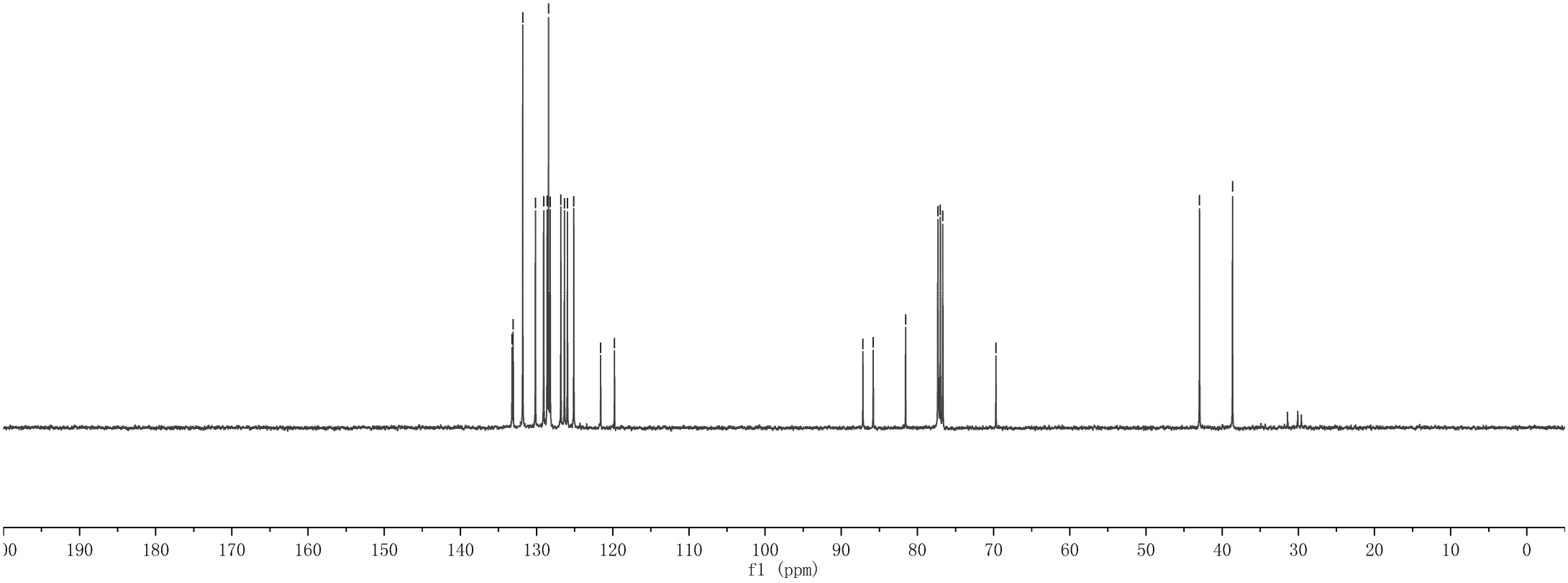

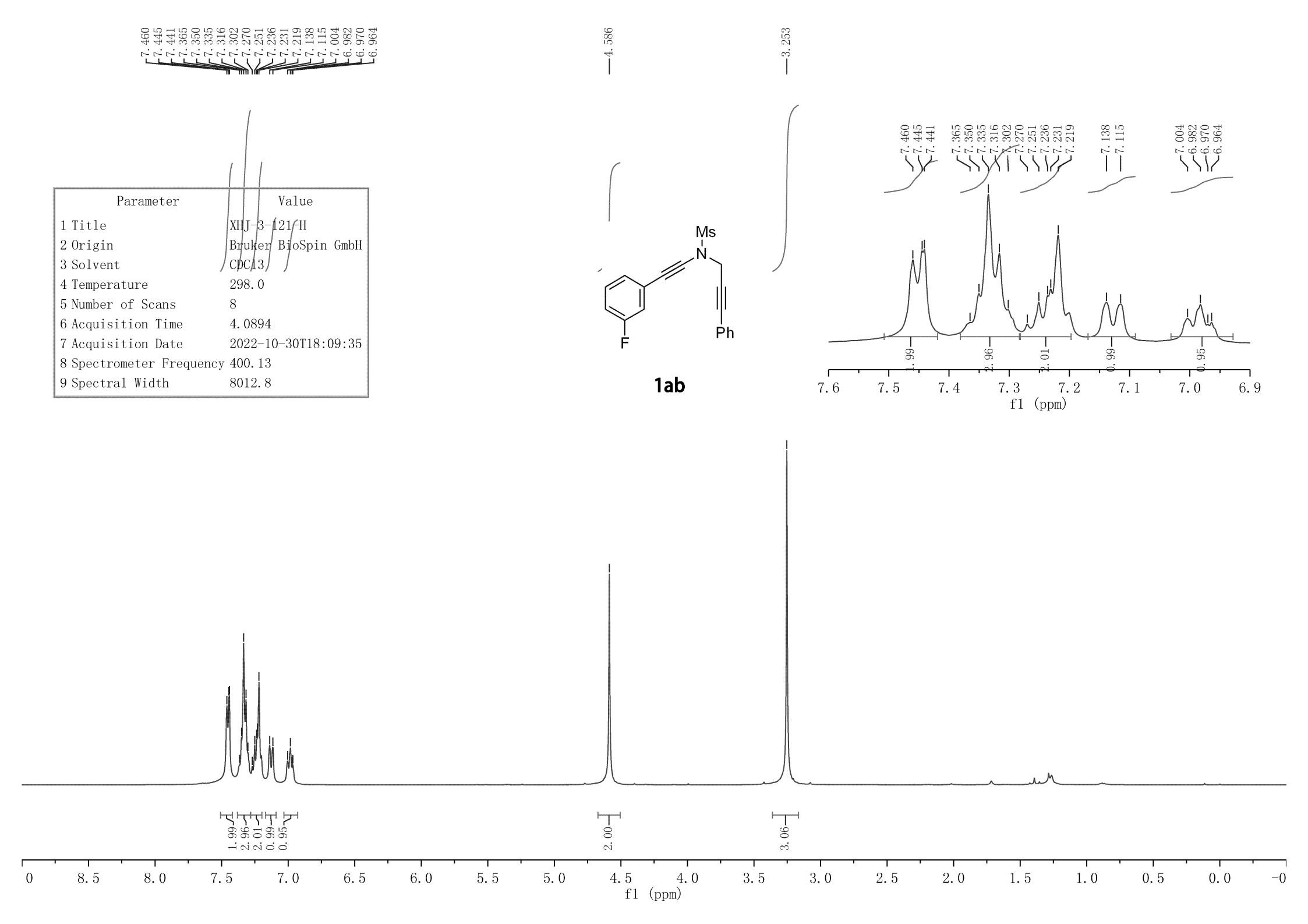
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7.335
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7.302
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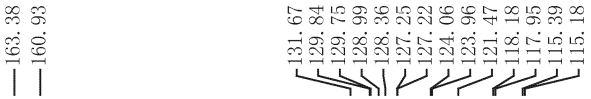
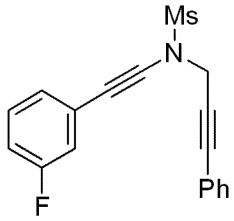
7.251
7.236
7.231
7.219
7.138
7.115
7.004
6.982
6.970
6.964
4.586
3.253
Parameter Value
1 Title XHJ-3-121-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-10-30T18:09:35
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
Ph
F
1ab
1.99
2.96
2.01
0.99
0.95
2.00
3.06
f1 (ppm)



Parameter	Value
1 Title	XHJ-3-121-C-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2022-10-30T18:12:06
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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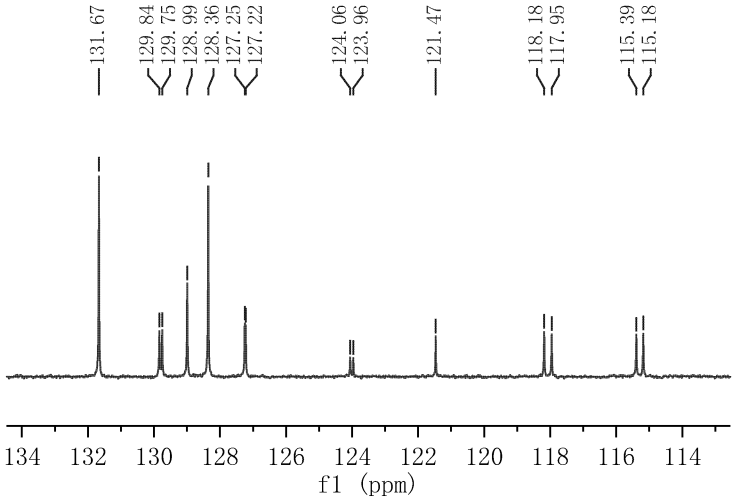
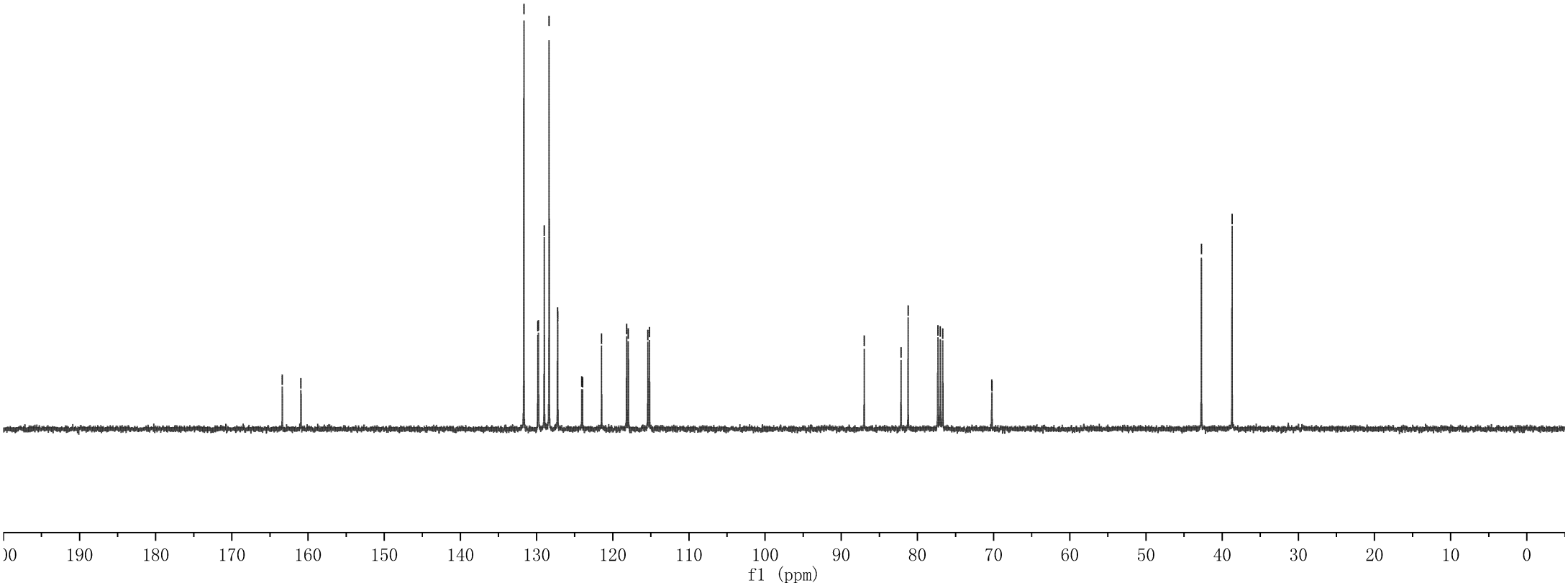
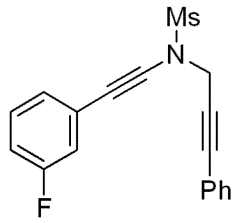
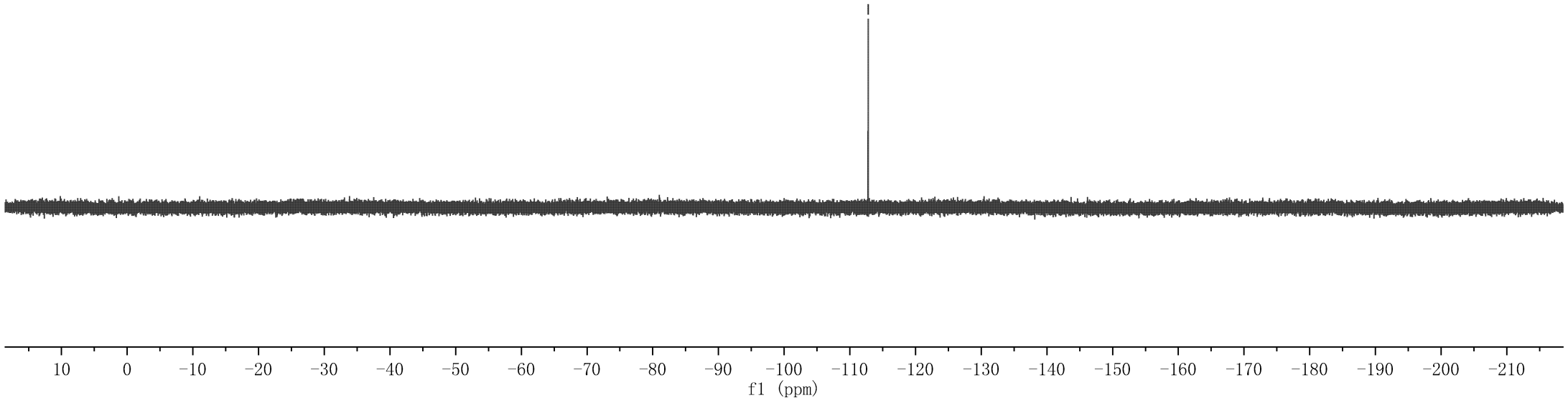




Parameter	Value
1 Title	xhj-3-121-f
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.3
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-11-02T21:50:19
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

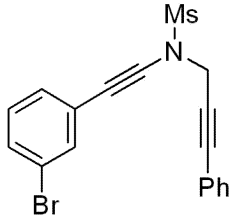


1ab

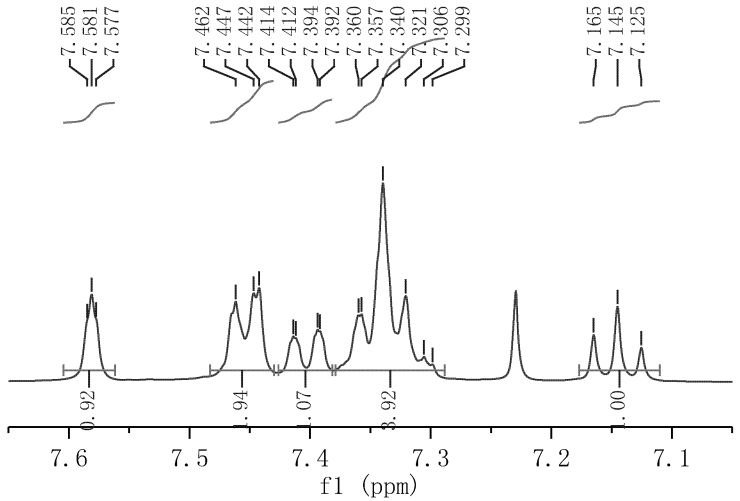


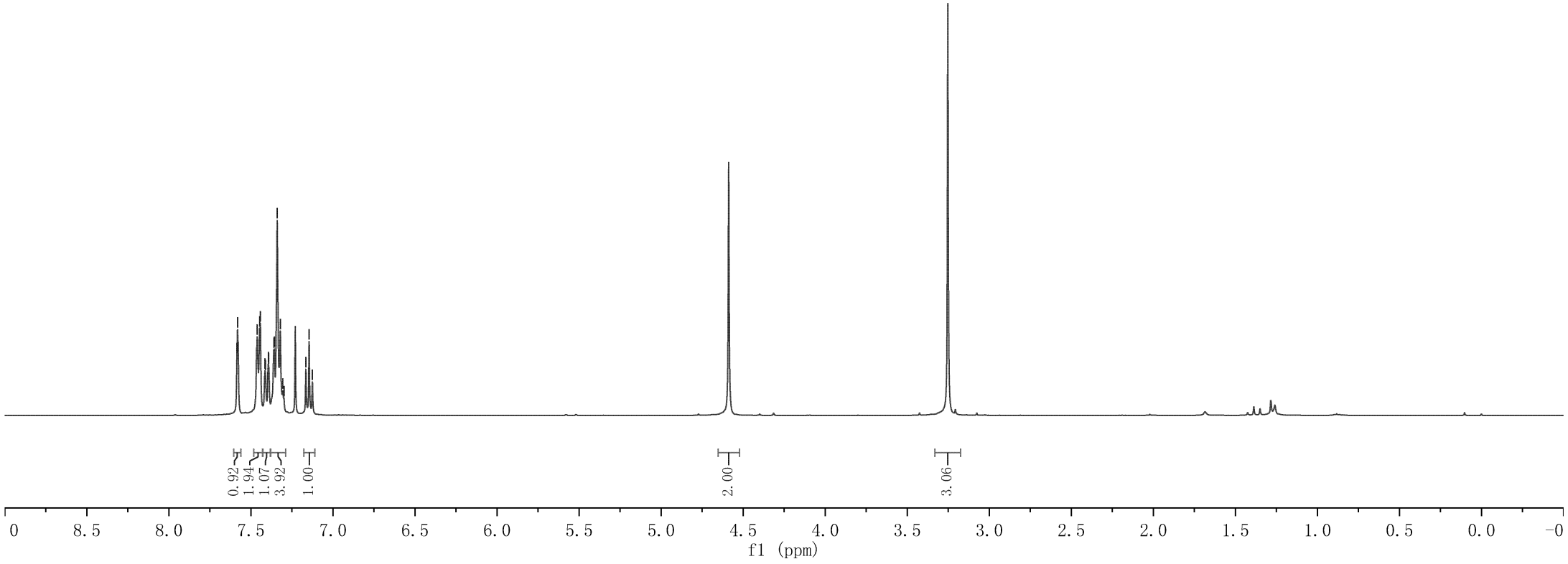
7.585
7.581
7.577
7.462
7.447
7.442
7.414
7.412
7.394
7.392
7.360
7.357
7.340
7.321
7.306
7.299
7.165
7.145
7.125

Parameter	Value
1 Title	XHJ-3-122-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	2022-10-30T18:16:10
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

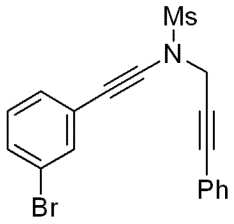


1ac

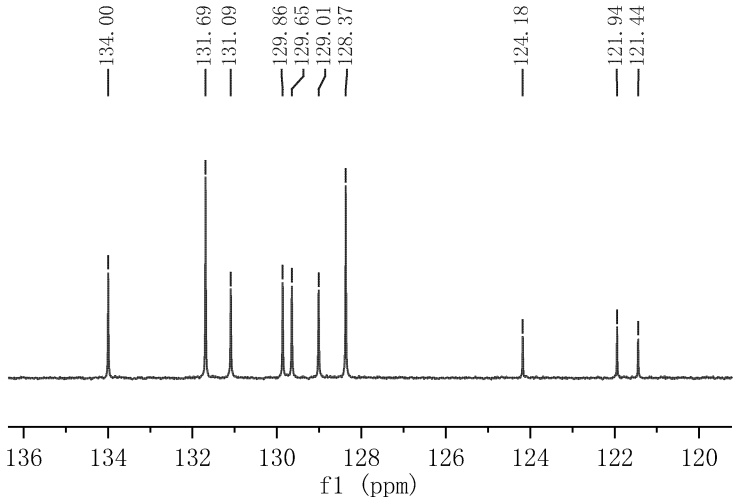


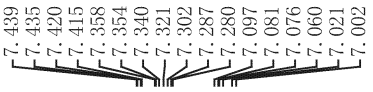


Parameter	Value
1 Title	XHJ-3-122-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	31
6 Acquisition Time	1.3631
7 Acquisition Date	2022-10-30T18:18:30
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

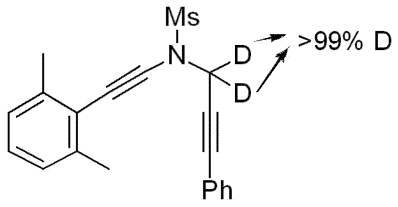


1ac

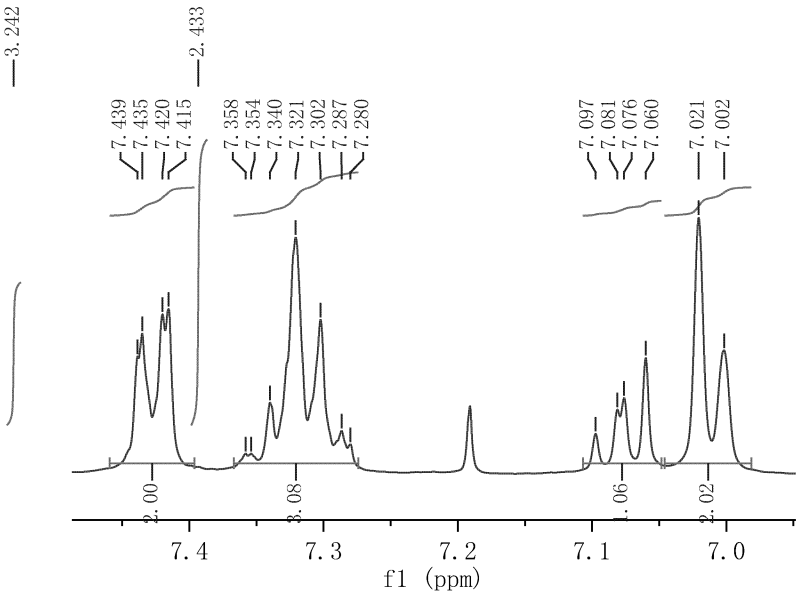


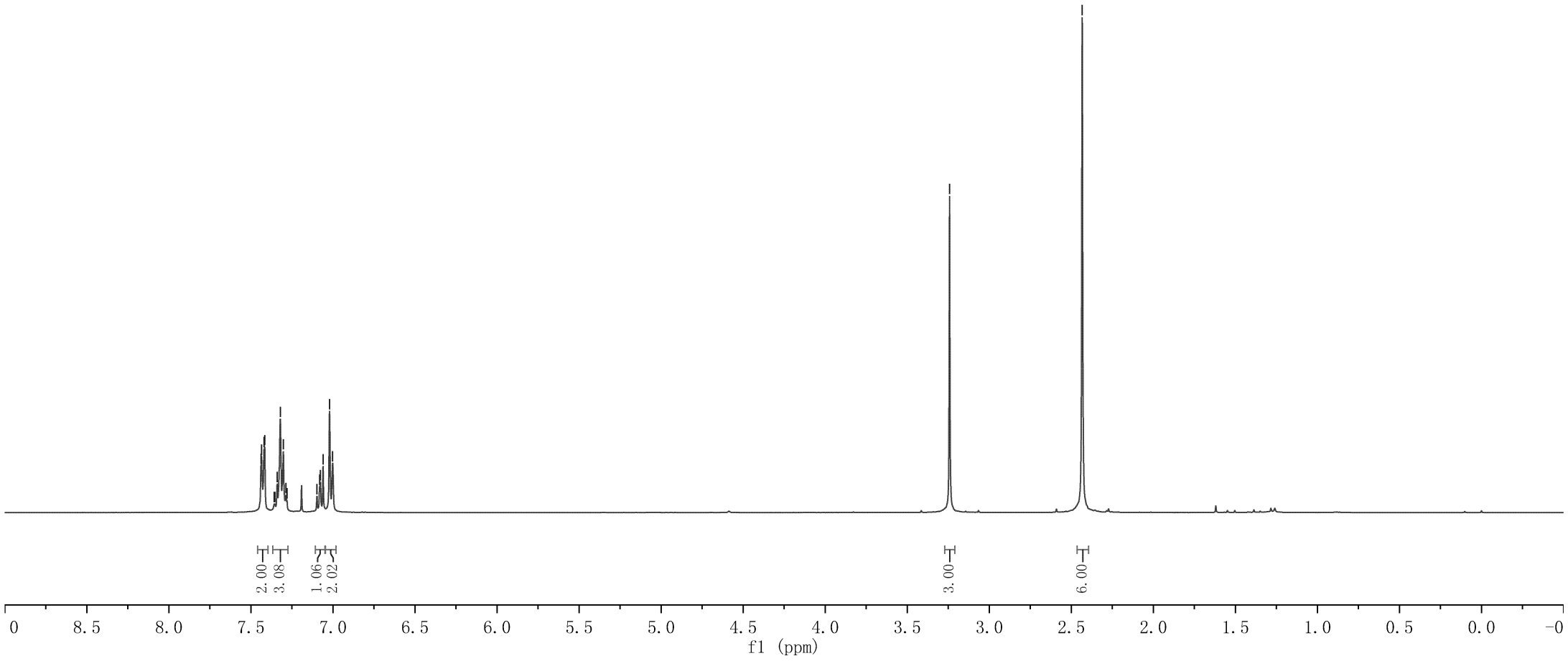


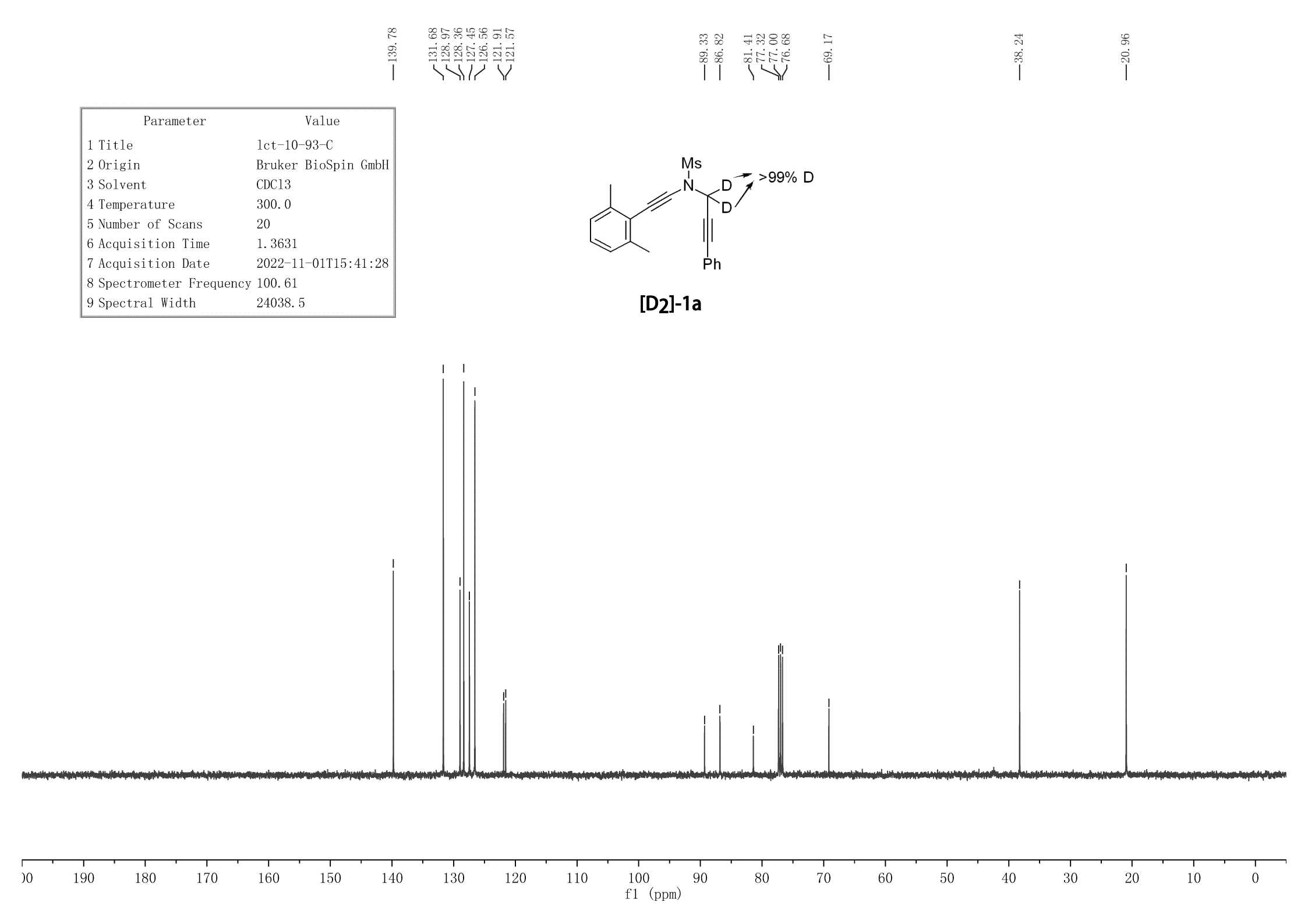
Parameter	Value
1 Title	lct-10-93-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-11-01T15:40:05
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



[D2]-1a



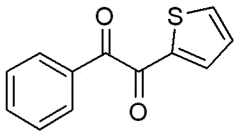




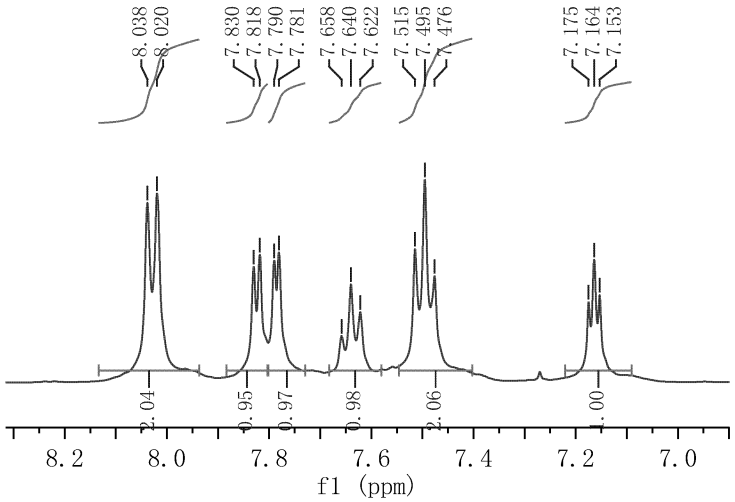
Parameter	Value
1 Title	lct-10-93-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	20
6 Acquisition Time	1.3631
7 Acquisition Date	2022-11-01T15:41:28
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

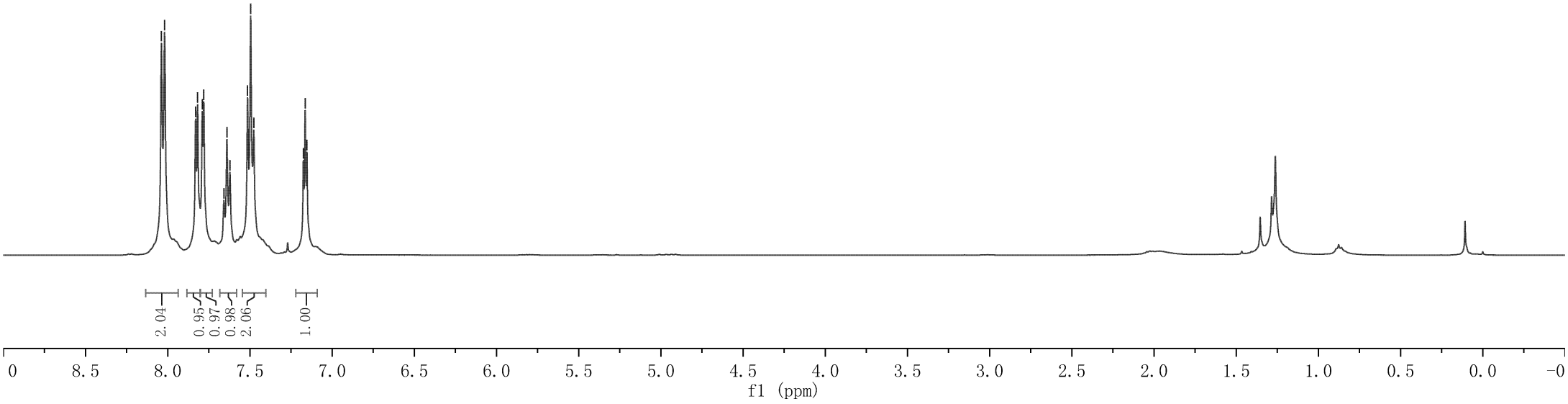
8.038
8.020
7.830
7.818
7.790
7.781
7.658
7.640
7.622
7.515
7.495
7.476
7.175
7.164
7.153

Parameter	Value
1 Title	XHJ-2-DIKETONE-2-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	2022-08-16T15:58:13
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



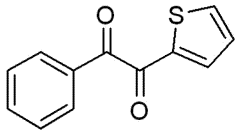
2b



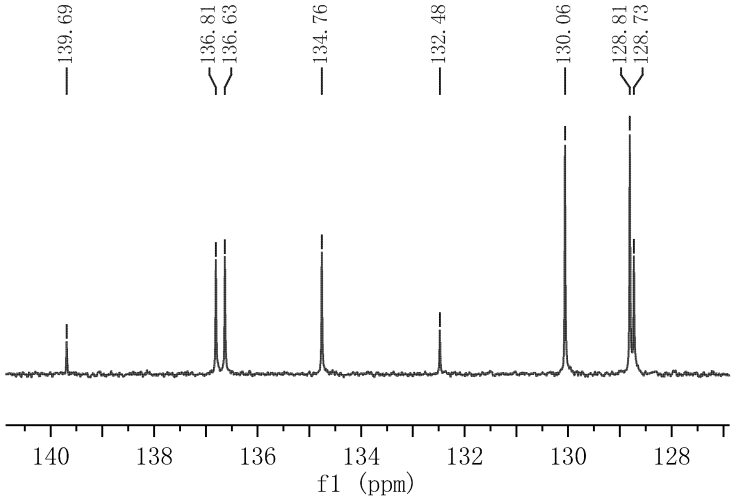


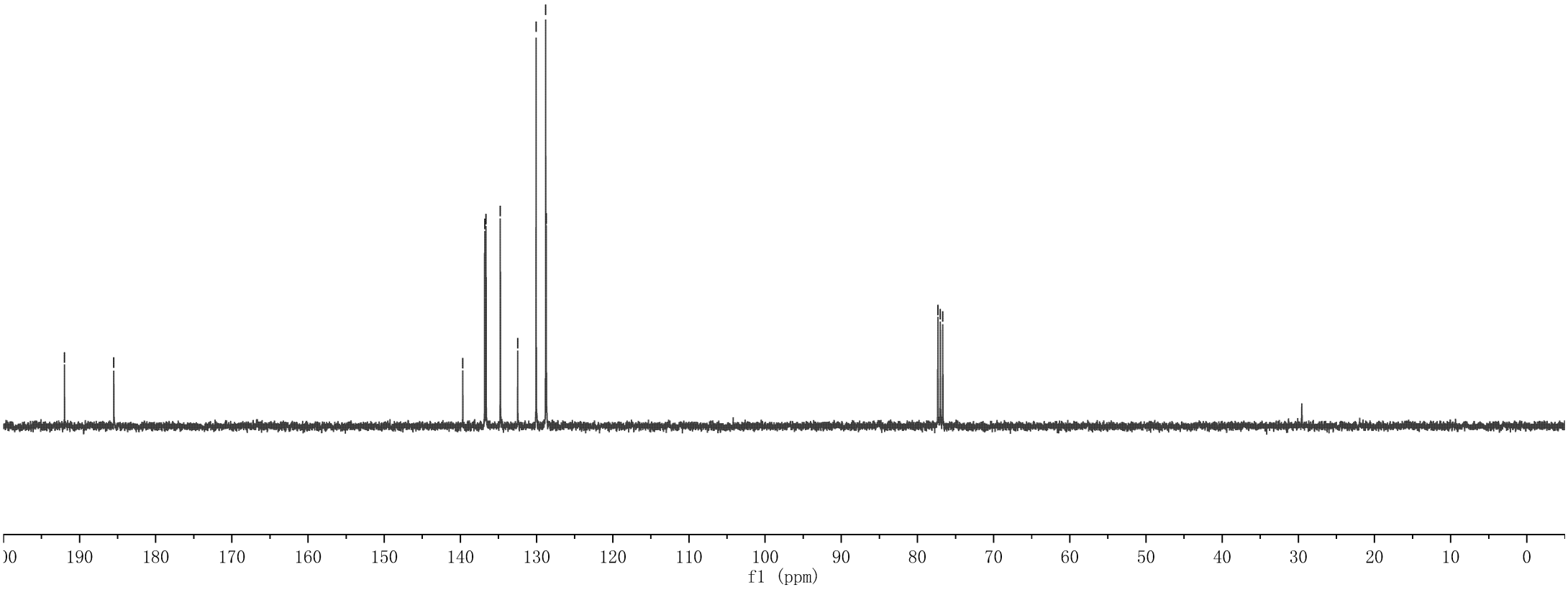
191.98
185.50
139.69
136.81
136.63
134.76
132.48
130.06
128.81
128.73
77.32
77.00
76.68

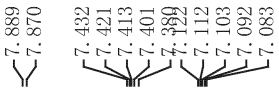
Parameter	Value
1 Title	XHJ-2-DIKETONE-2-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	10
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-16T21:03:16
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

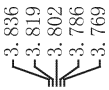


2b

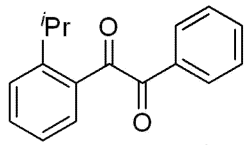




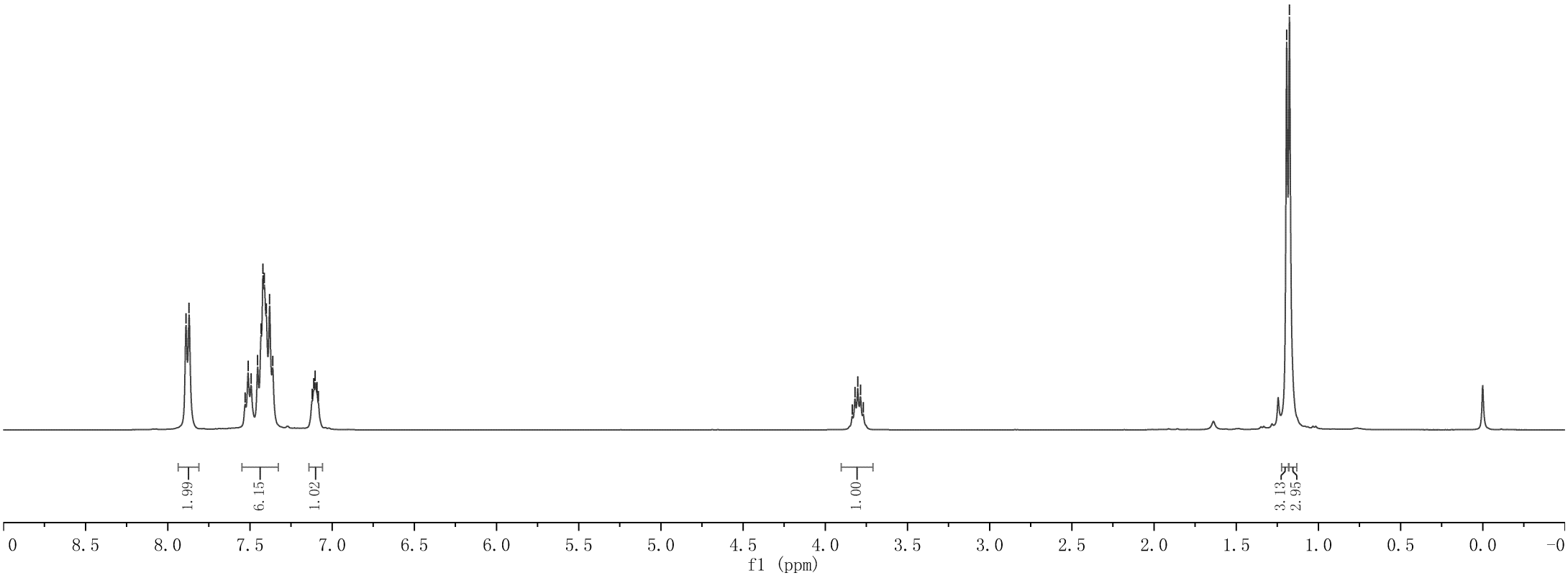




Parameter	Value
1 Title	XHJ-2-diketone-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.6
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-08-11T15:47:48
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0

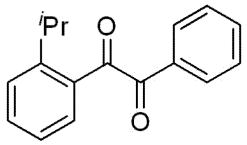


2c

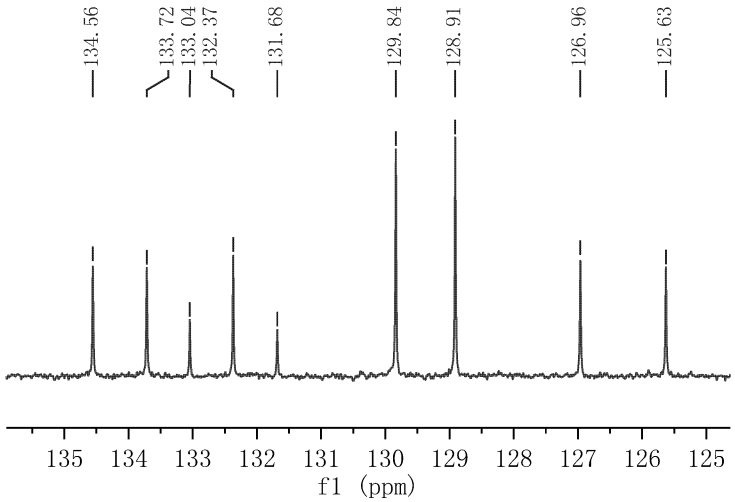


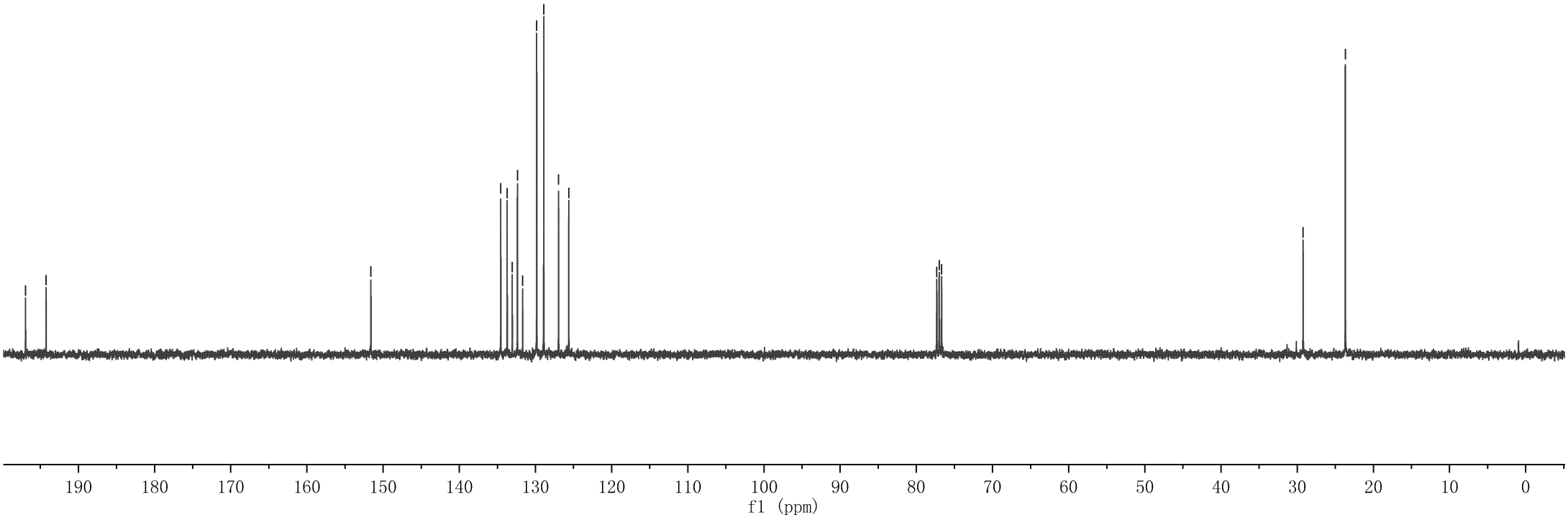
196.94
194.24
151.60
134.56
133.72
133.04
132.37
131.68
129.84
128.91
126.96
125.63
77.32
77.00
76.68
29.22
23.69

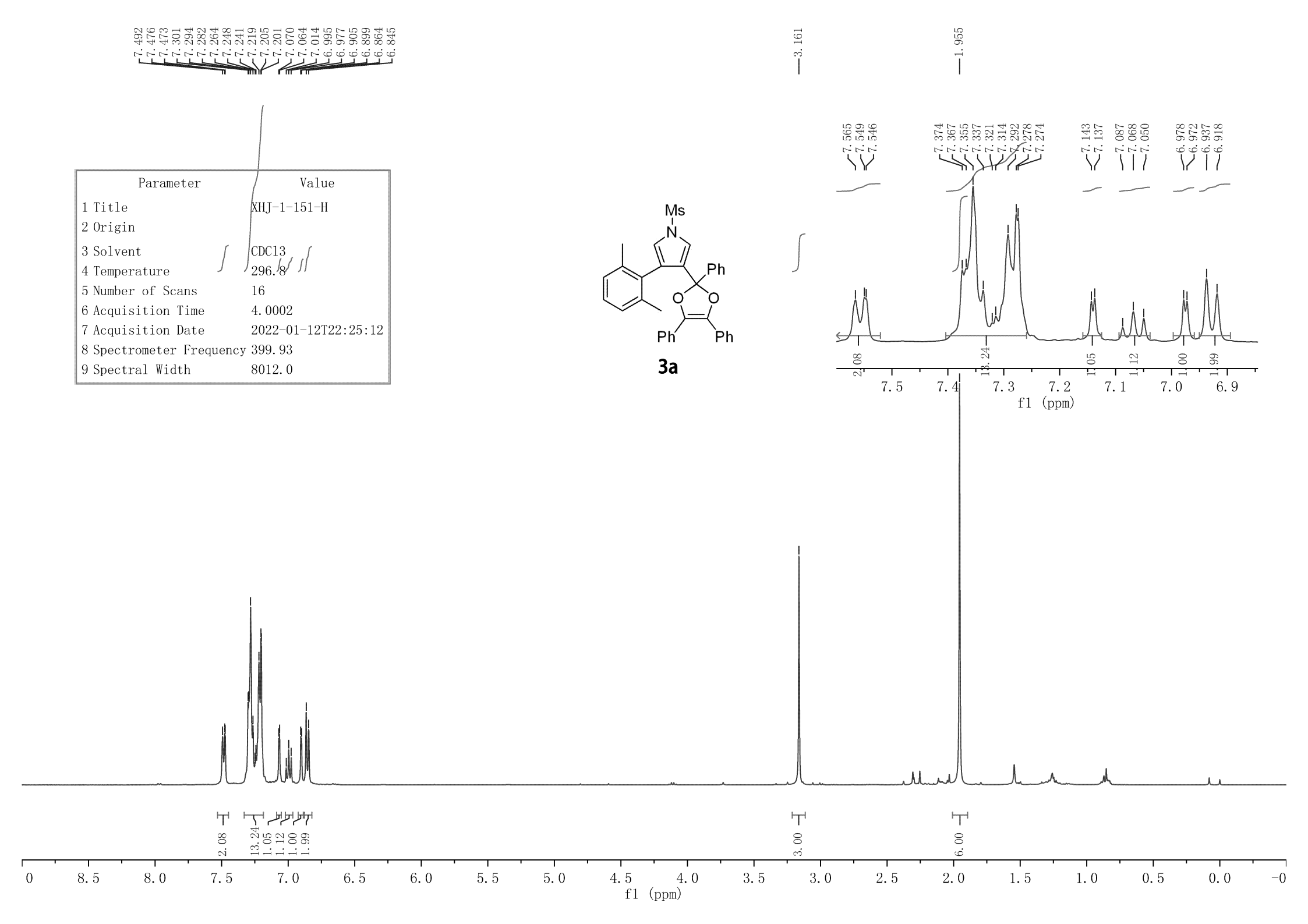
Parameter	Value
1 Title	XHJ-2-DIKETONE-1-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	7
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-16T20:53:27
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

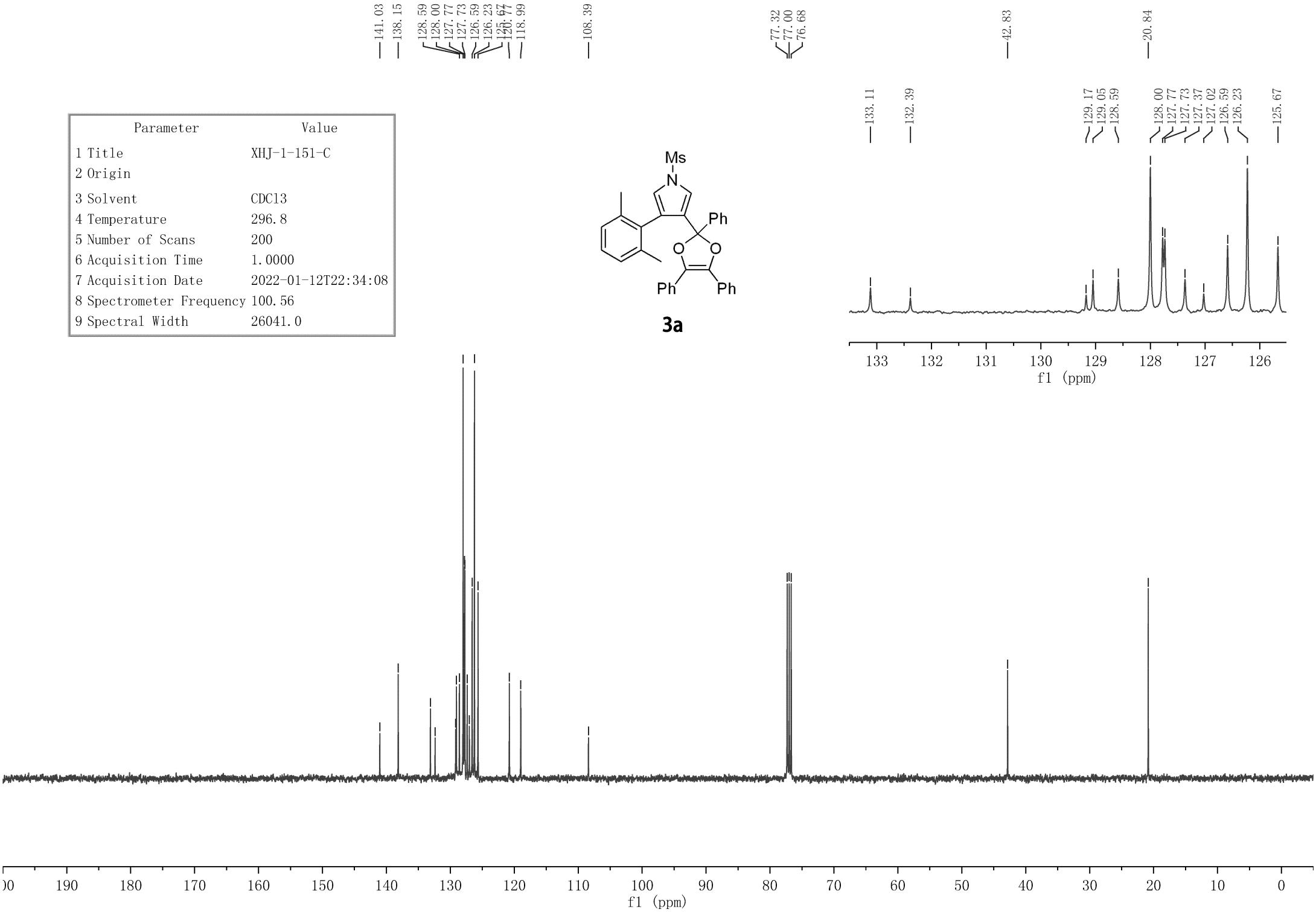


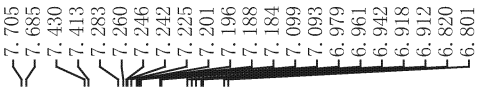
2c



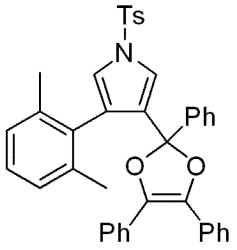



7.492
7.476
7.473
7.301
7.294
7.282
7.264
7.248
7.241
7.219
7.205
7.201
7.070
7.064
7.014
6.995
6.977
6.905
6.899
6.864
6.845
3.161
1.955
Parameter Value
1 Title XHJ-1-151-H
2 Origin
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-01-12T22:25:12
8 Spectrometer Frequency 399.93
9 Spectral Width 8012.0
Ms
N
Ph
O
O
Ph
Ph
3a
7.565
7.549
7.546
7.374
7.367
7.355
7.337
7.321
7.314
7.292
7.278
7.274
7.143
7.137
7.087
7.068
7.050
6.978
6.972
6.937
6.918
2.08
13.24
1.05
1.12
1.00
1.99
f1 (ppm)
2.08
13.24
1.05
1.12
1.00
1.99
3.00
6.00
f1 (ppm)

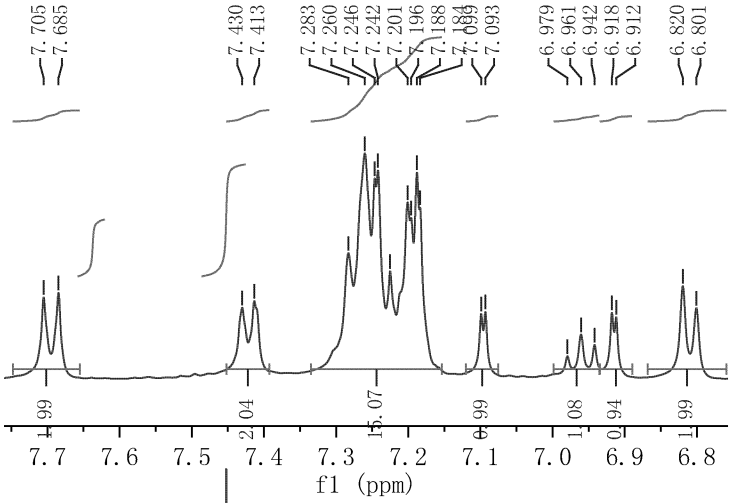

141.03
138.15
128.59
128.00
127.77
127.73
126.59
126.23
118.99
108.39
77.32
77.00
76.68
42.83
20.84
Parameter Value
1 Title XHJ-1-151-C
2 Origin
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-12T22:34:08
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Ph
O
O
Ph
Ph
3a
133.11
132.39
129.17
129.05
128.59
128.00
127.77
127.73
127.37
127.02
126.59
126.23
125.67
133 132 131 130 129 128 127 126
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

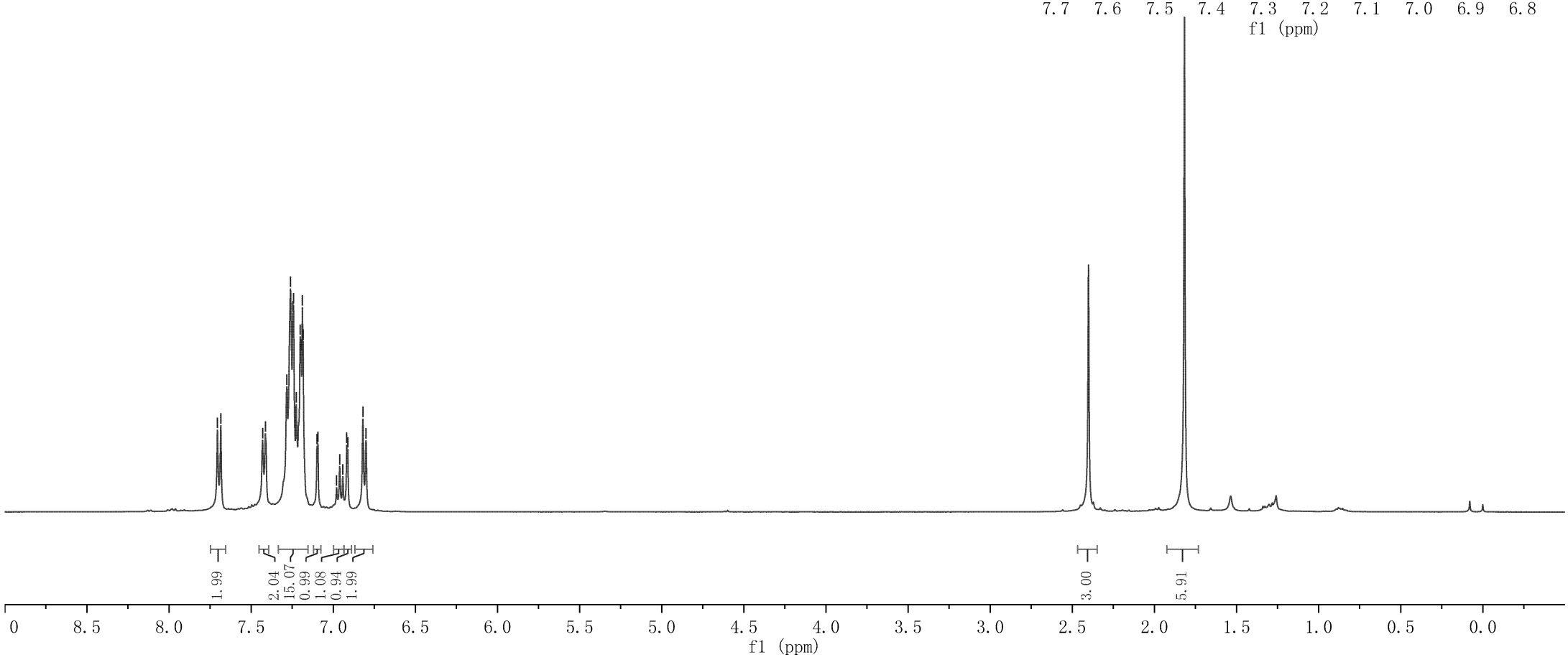


Parameter	Value
1 Title	XHJ-1-136-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	19
6 Acquisition Time	4.0894
7 Acquisition Date	2022-01-06T15:47:59
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

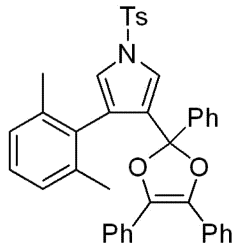


3b

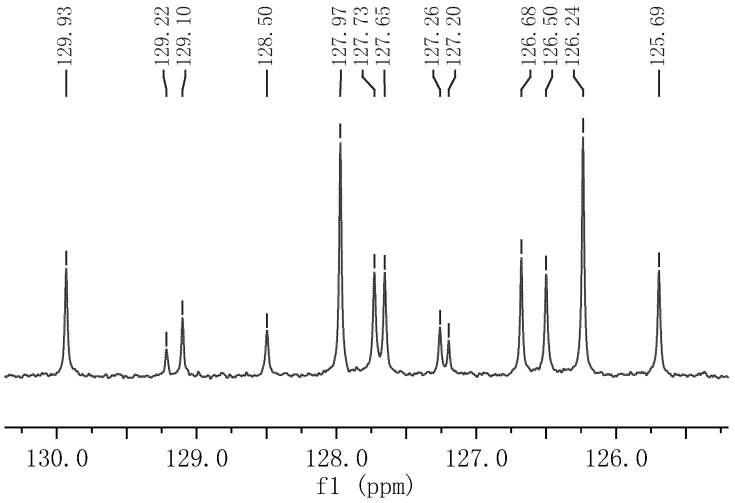


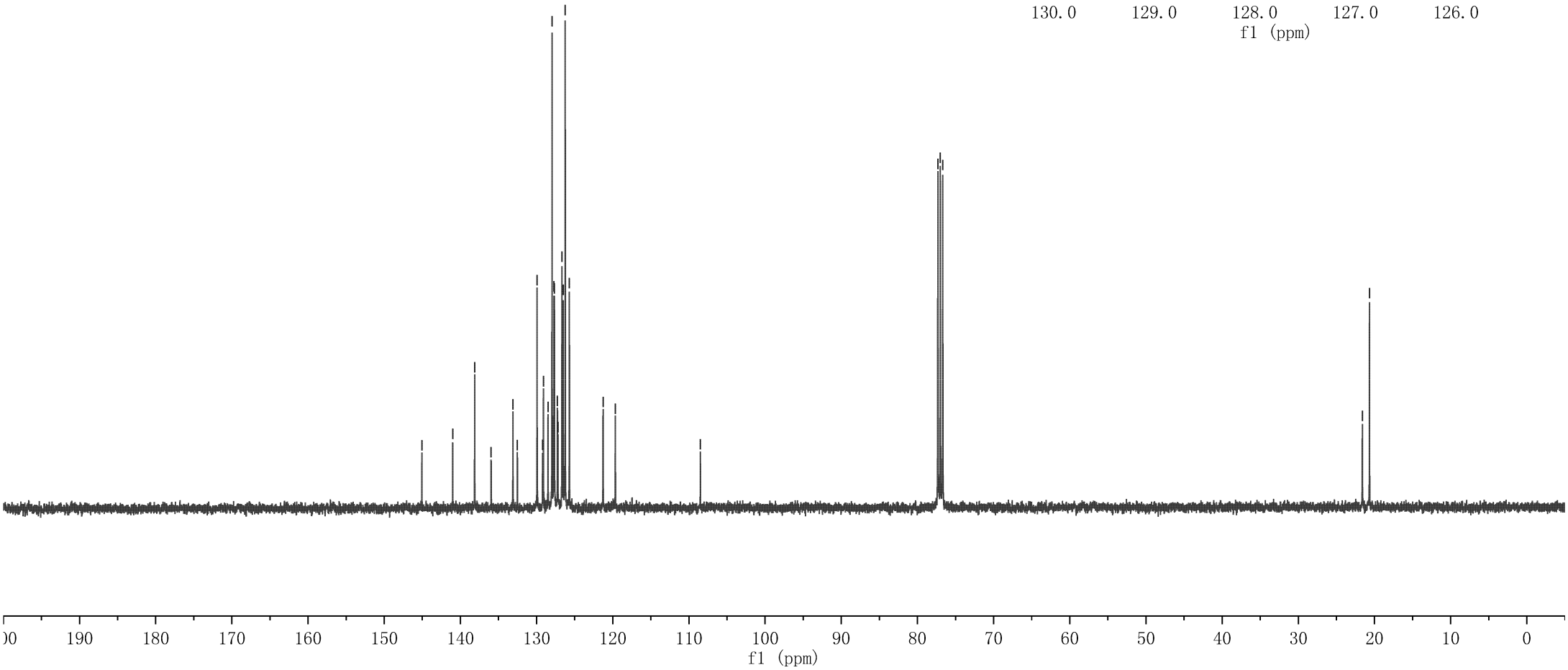


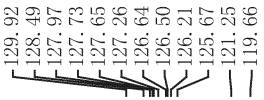
Parameter	Value
1 Title	XHJ-1-136-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	134
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-06T15:50:53
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



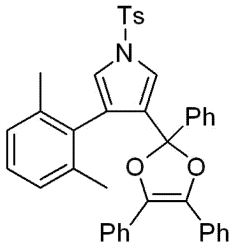
3b



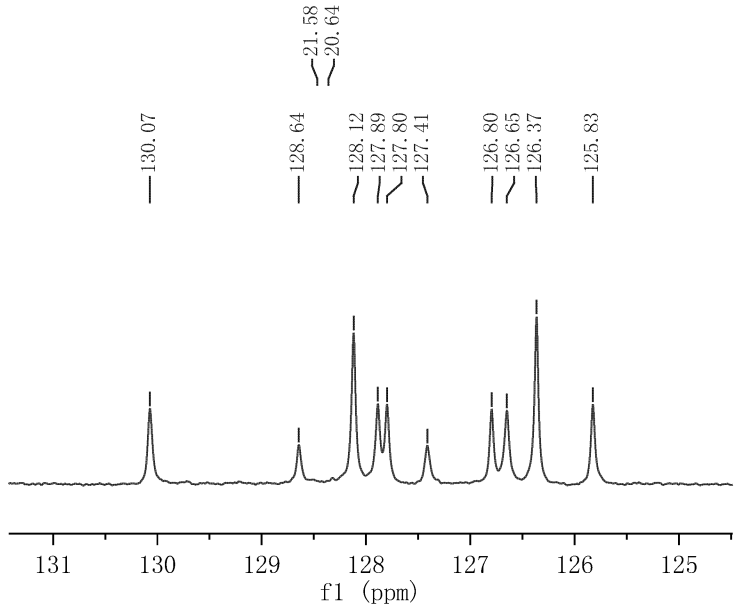


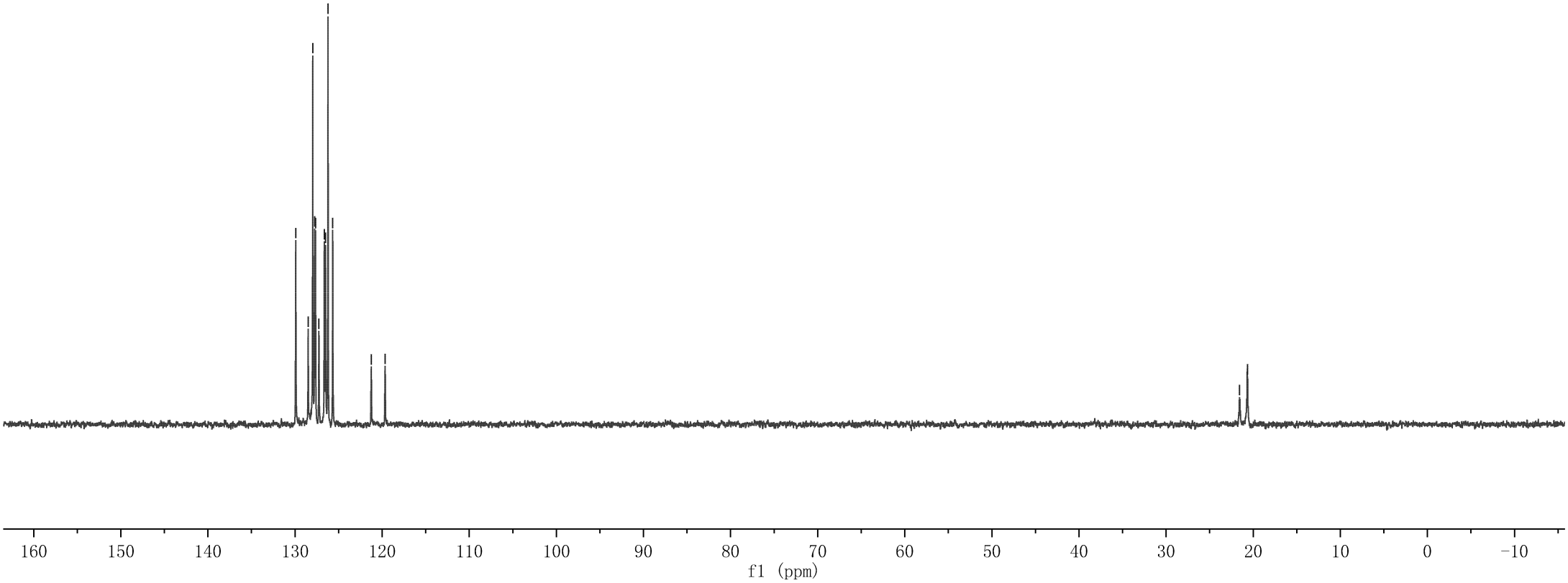


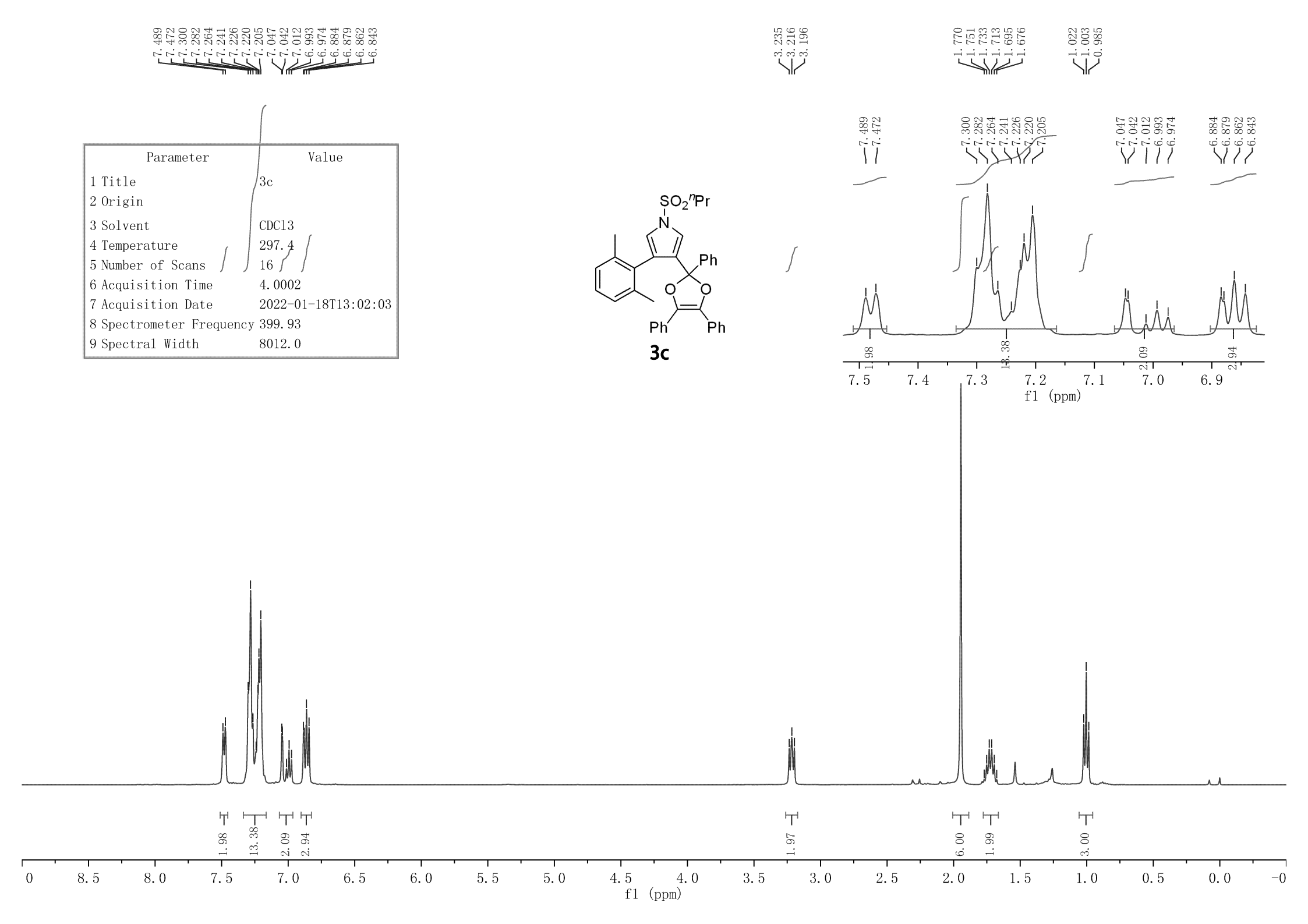
Parameter	Value
1 Title	XHJ-3b-DEPT135
2 Origin	
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	50
6 Acquisition Time	1.0001
7 Acquisition Date	2022-08-28T16:53:40
8 Spectrometer Frequency	100.56
9 Spectral Width	18028.0

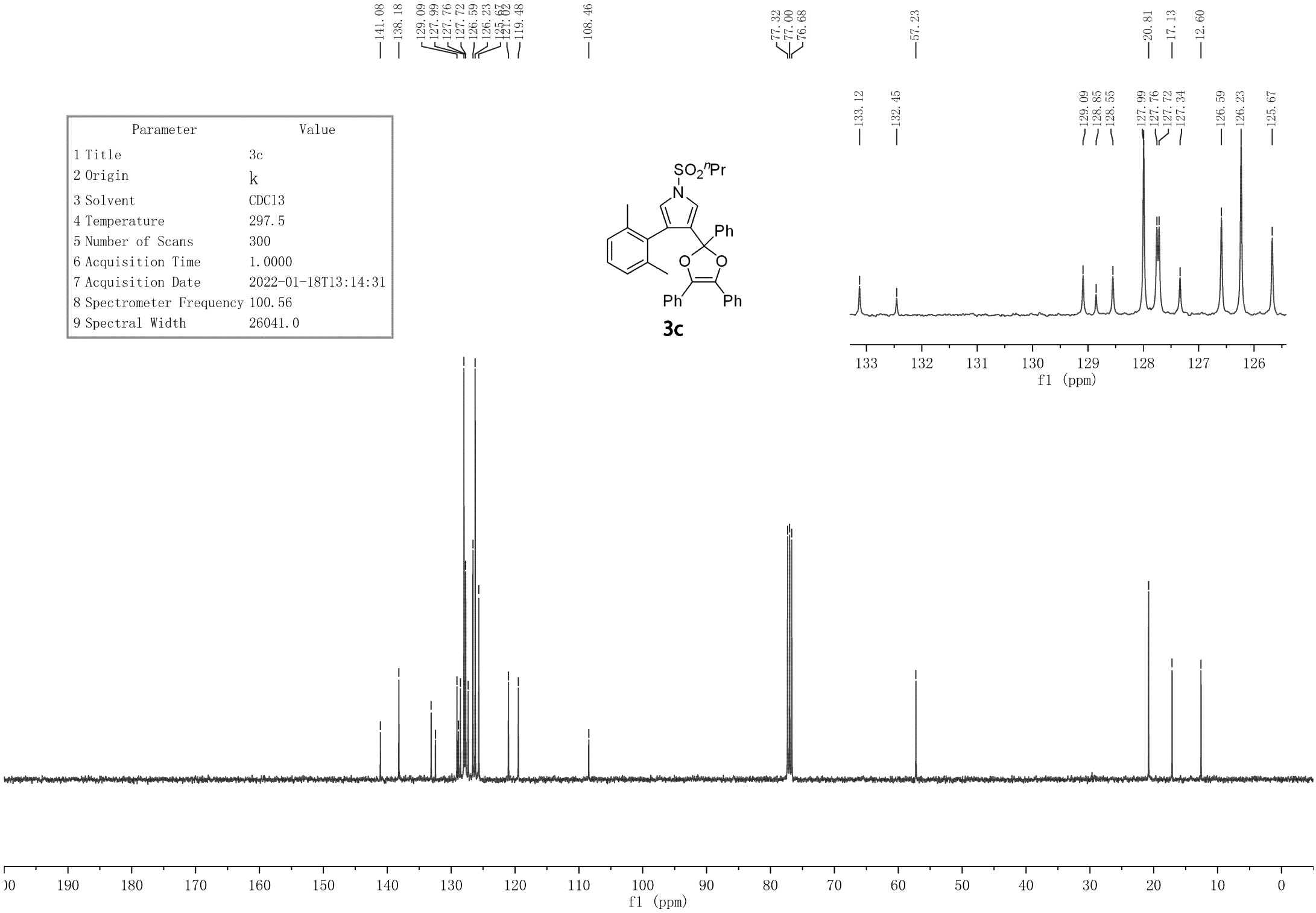


3b

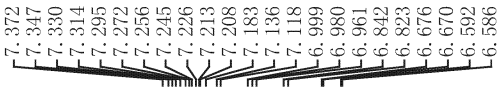




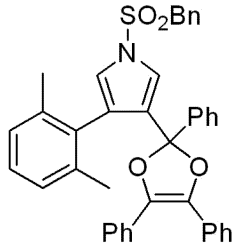

7.489
7.472
7.300
7.282
7.264
7.241
7.226
7.220
7.205
7.047
7.042
7.012
6.993
6.974
6.884
6.879
6.862
6.843
3.235
3.216
3.196
1.770
1.751
1.733
1.713
1.695
1.676
1.022
1.003
0.985
Parameter Value
1 Title 3c
2 Origin
3 Solvent CDCl3
4 Temperature 297.4
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-01-18T13:02:03
8 Spectrometer Frequency 399.93
9 Spectral Width 8012.0
SO2nPr
N
Ph
O
O
Ph
Ph
3c
1.98
13.38
2.09
2.94
1.97
6.00
1.99
3.00
f1 (ppm)



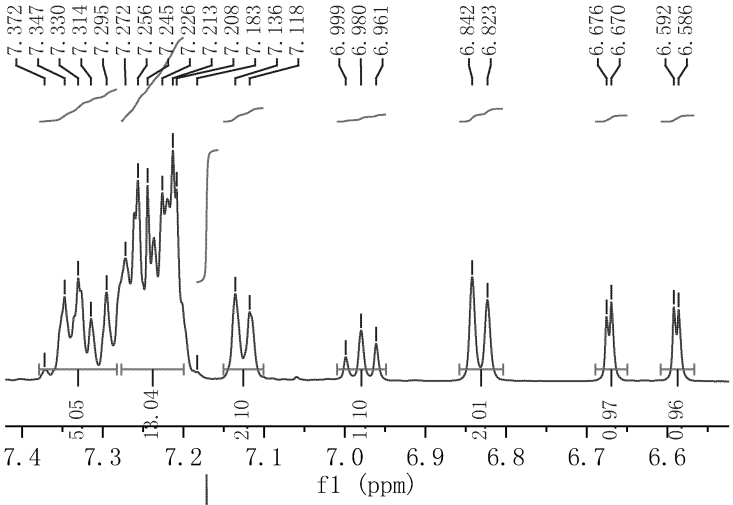
Parameter	Value
1 Title	3c
2 Origin	k
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	300
6 Acquisition Time	1.0000
7 Acquisition Date	2022-01-18T13:14:31
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

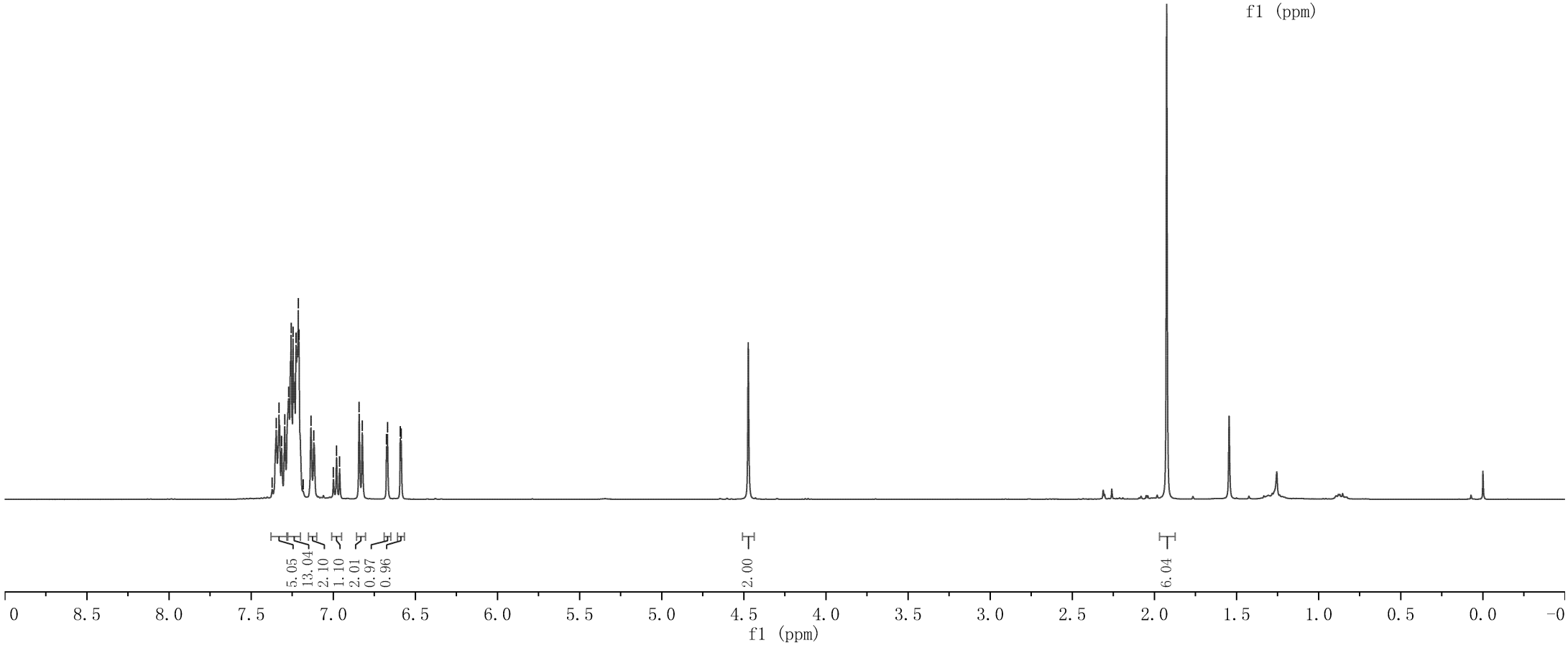


Parameter	Value
1 Title	XHJ-1-161-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	20
6 Acquisition Time	4.0002
7 Acquisition Date	2022-01-17T23:53:35
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0

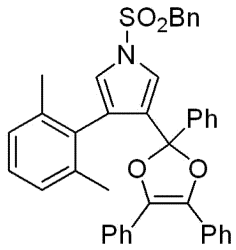


3d

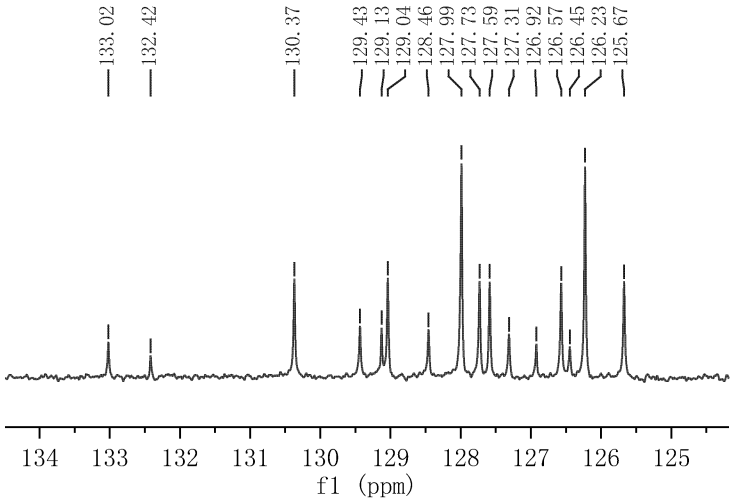


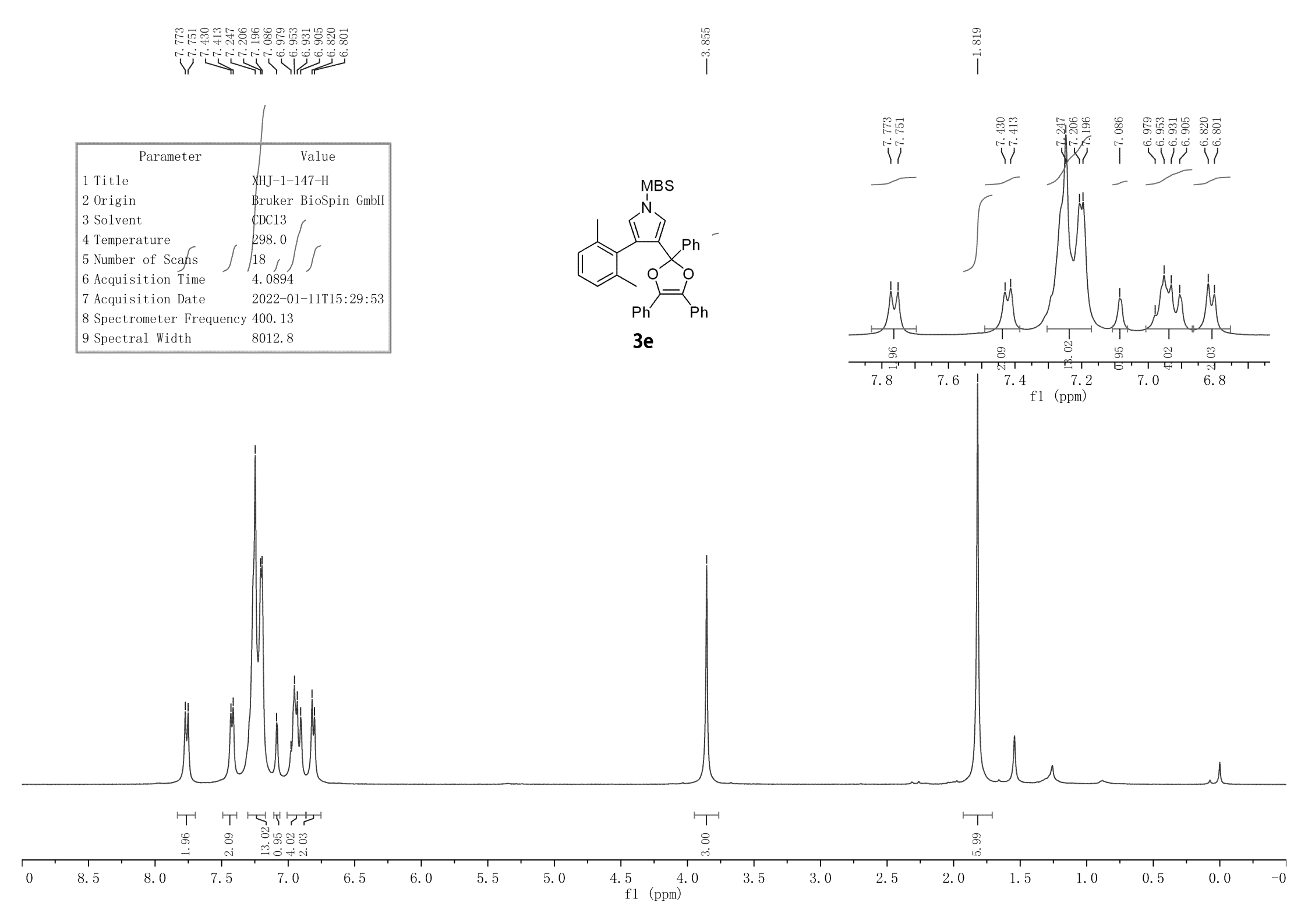


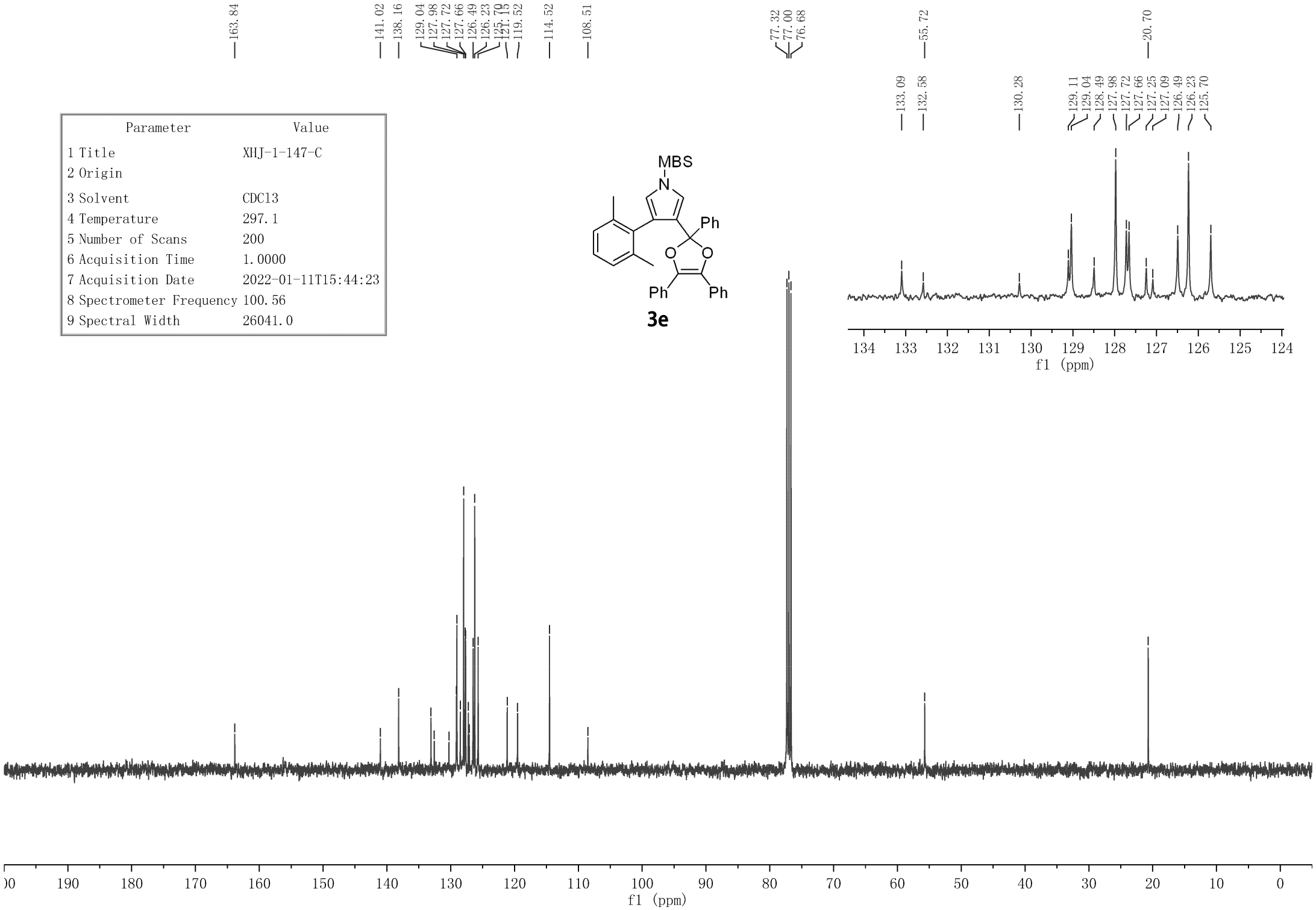
Parameter	Value
1 Title	XHJ-1-161-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	400
6 Acquisition Time	1.0000
7 Acquisition Date	2022-01-18T00:09:10
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



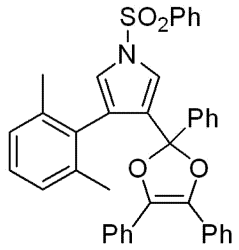
3d



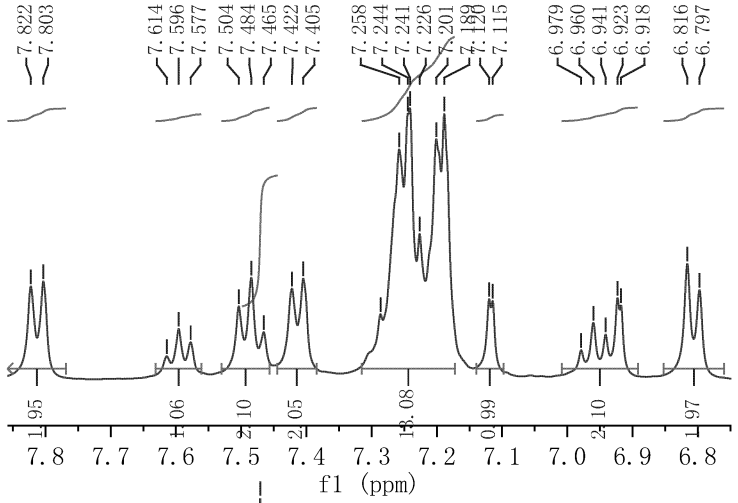

7.773
7.751
7.430
7.413
7.247
7.206
7.196
7.086
6.979
6.953
6.931
6.905
6.820
6.801
3.855
1.819
Parameter Value
1 Title XHJ-1-147-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 18
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-11T15:29:53
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
MBS
N
Ph
O
O
Ph
Ph
3e
1.96
2.09
13.02
0.95
4.02
2.03
3.00
5.99
f1 (ppm)

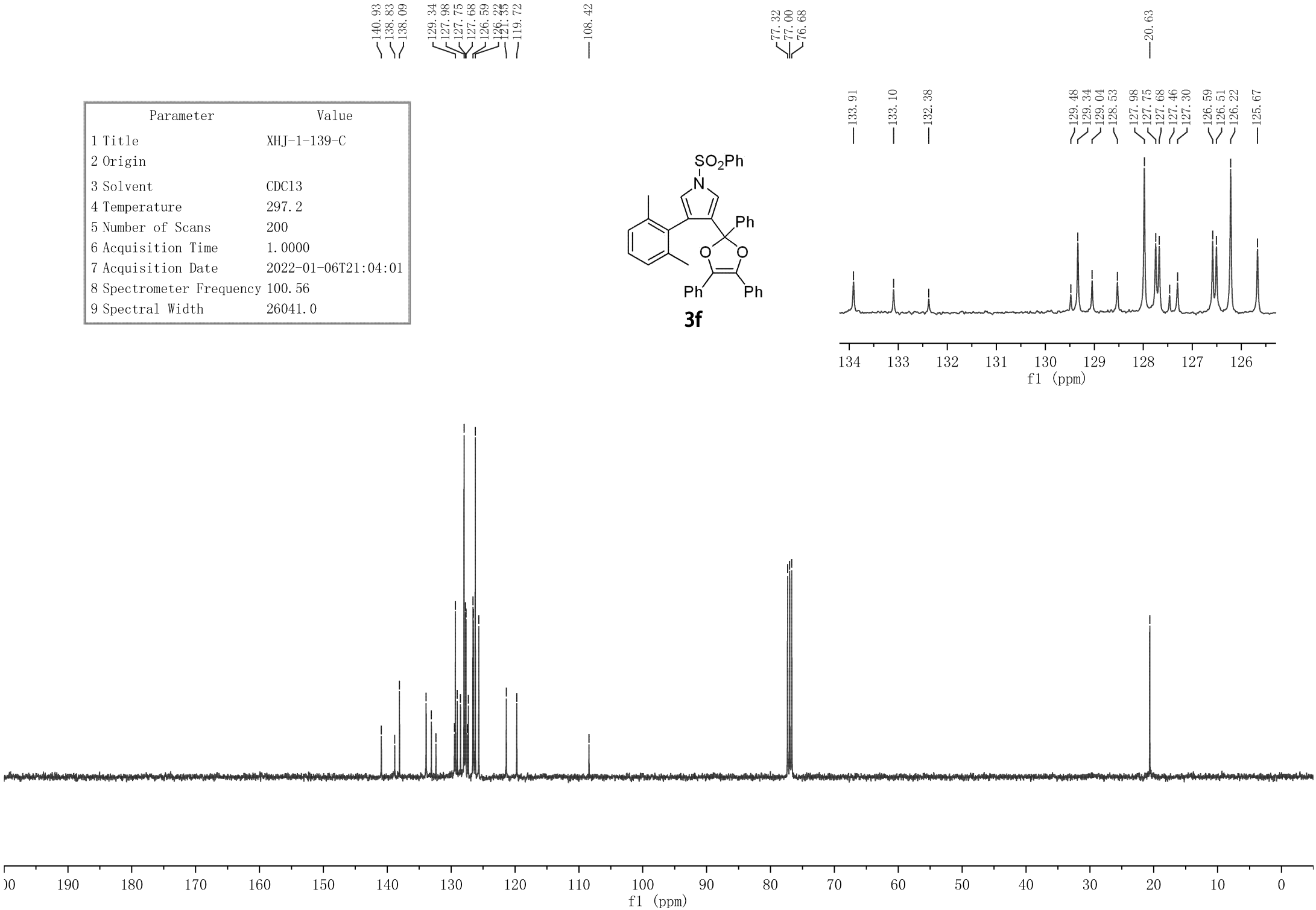

163.84
141.02
138.16
129.04
127.98
127.72
127.66
126.49
126.23
125.70
121.15
119.52
114.52
108.51
77.32
77.00
76.68
55.72
20.70
133.09
132.58
130.28
129.11
129.04
128.49
127.98
127.72
127.66
127.25
127.09
126.49
126.23
125.70
MBS
N
Ph
O
O
Ph
Ph
3e
Parameter Value
1 Title XHJ-1-147-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.1
5 Number of Scans 200
6 Acquisition Time 1.0000
7 Acquisition Date 2022-01-11T15:44:23
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	XHJ-1-139-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	2022-01-06T16:02:43
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



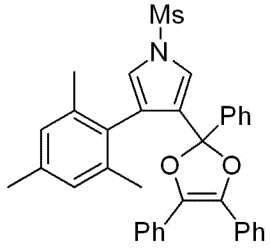
3f





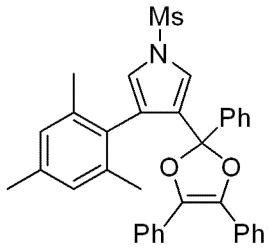
Parameter	Value
1 Title	XHJ-1-139-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.2
5 Number of Scans	200
6 Acquisition Time	1.0000
7 Acquisition Date	2022-01-06T21:04:01
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

Parameter	Value
1 Title	XHJ-1-185-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-02-22T17:00:03
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0

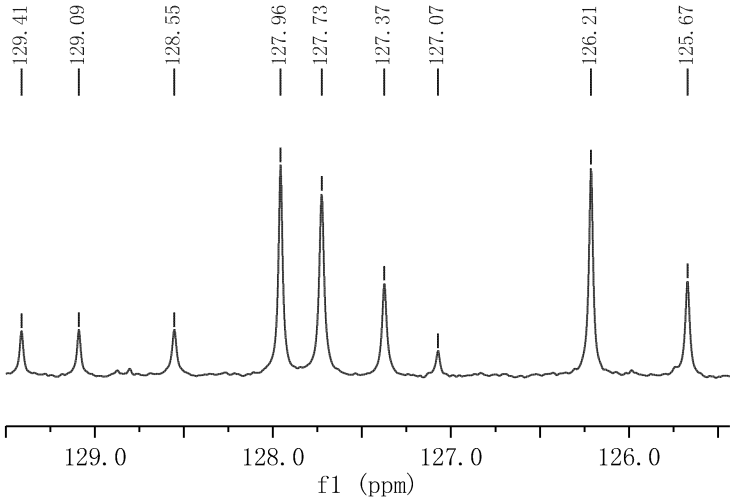


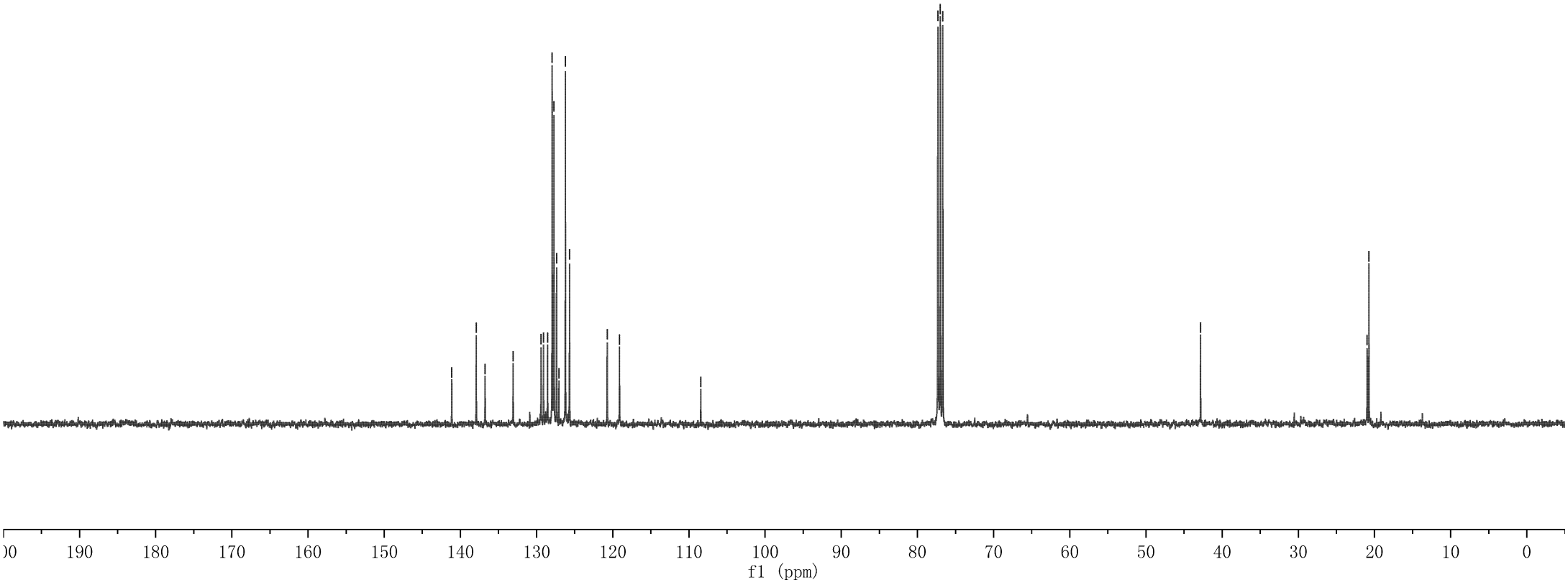
3g

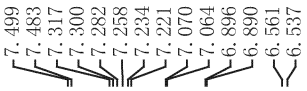
Parameter	Value
1 Title	XHJ-1-185-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	400
6 Acquisition Time	1.0000
7 Acquisition Date	2022-02-22T17:15:32
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



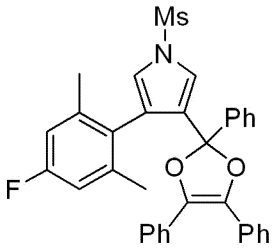
3g



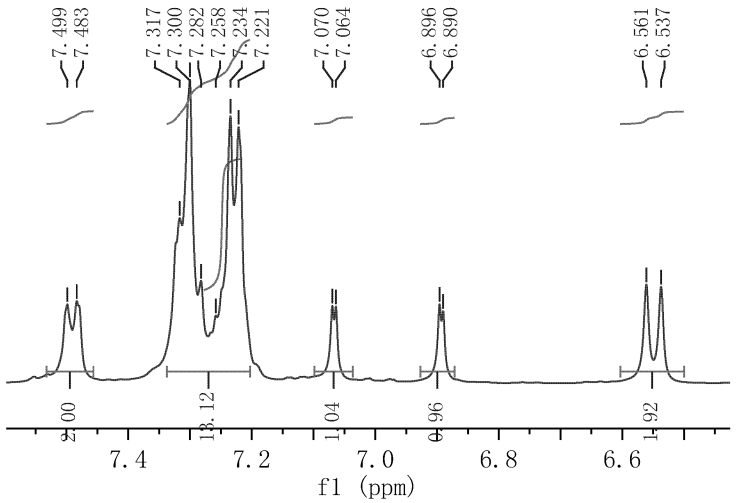


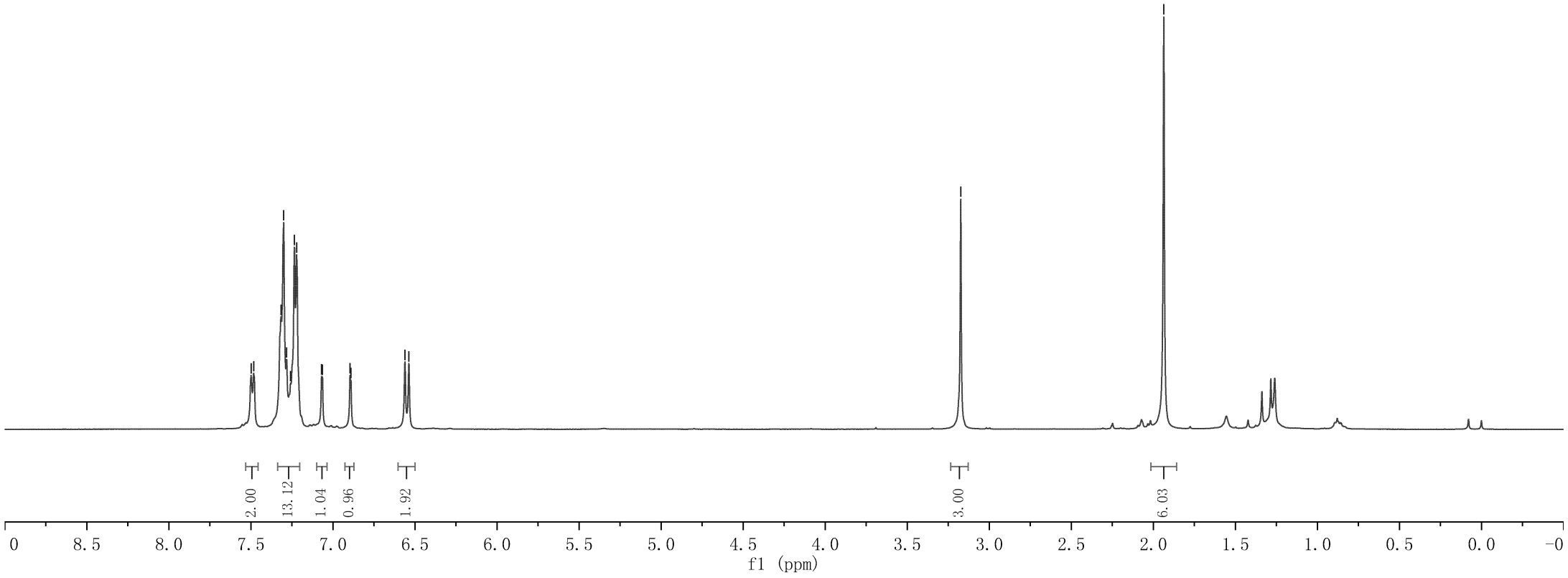


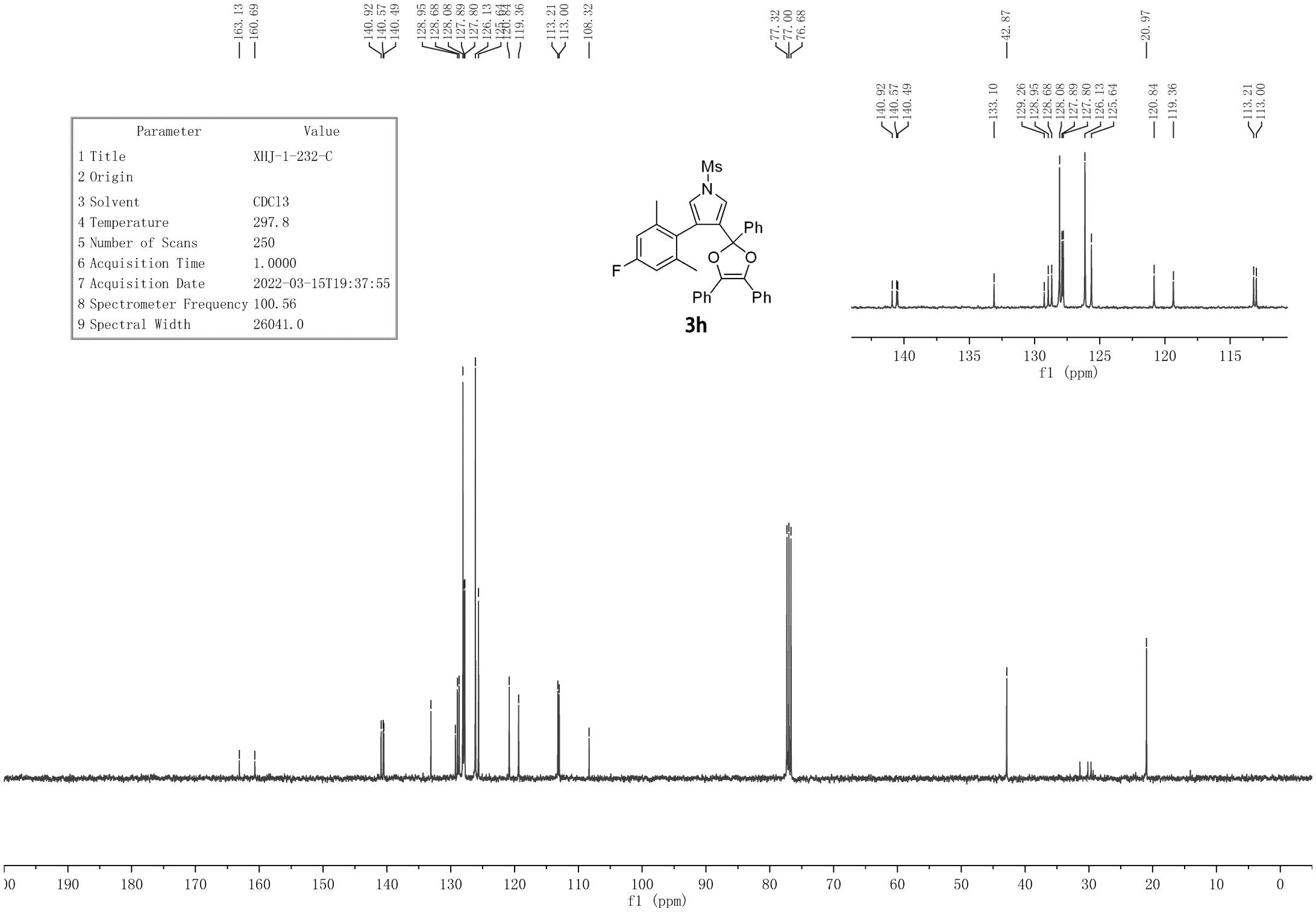
Parameter	Value
1 Title	XHJ-1-232-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	17
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-15T15:37:06
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



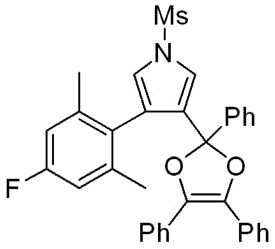
3h





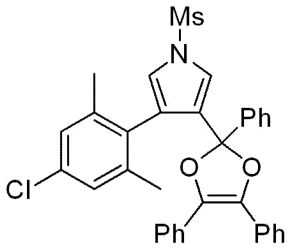

163.13
160.69
140.92
140.57
140.49
128.95
128.68
128.08
127.89
127.80
126.13
119.36
113.21
113.00
108.32
77.32
77.00
76.68
42.87
20.97
Parameter Value
1 Title XHJ-1-232-C
2 Origin
3 Solvent CDCl3
4 Temperature 297.8
5 Number of Scans 250
6 Acquisition Time 1.0000
7 Acquisition Date 2022-03-15T19:37:55
8 Spectrometer Frequency 100.56
9 Spectral Width 26041.0
Ms
N
Ph
O
O
F
Ph
Ph
3h
140.92
140.57
140.49
133.10
129.26
128.95
128.68
128.08
127.89
127.80
126.13
125.64
120.84
119.36
113.21
113.00
140
135
130
125
120
115
f1 (ppm)
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	XHJ-1-232-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.1
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-08-16T20:07:25
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

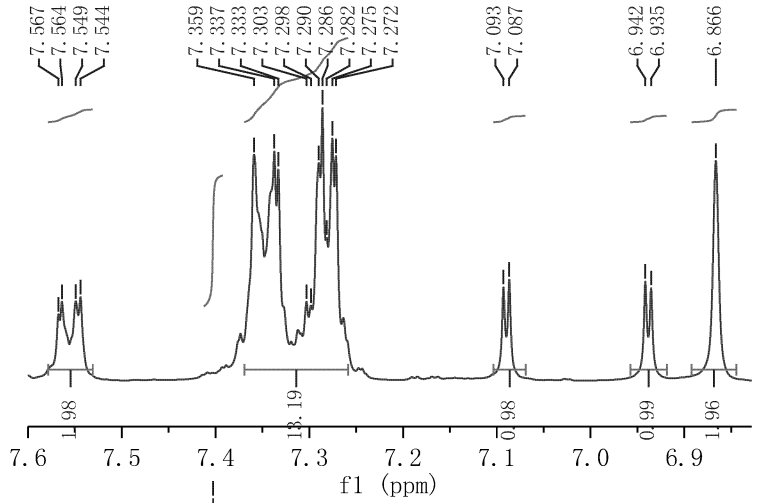


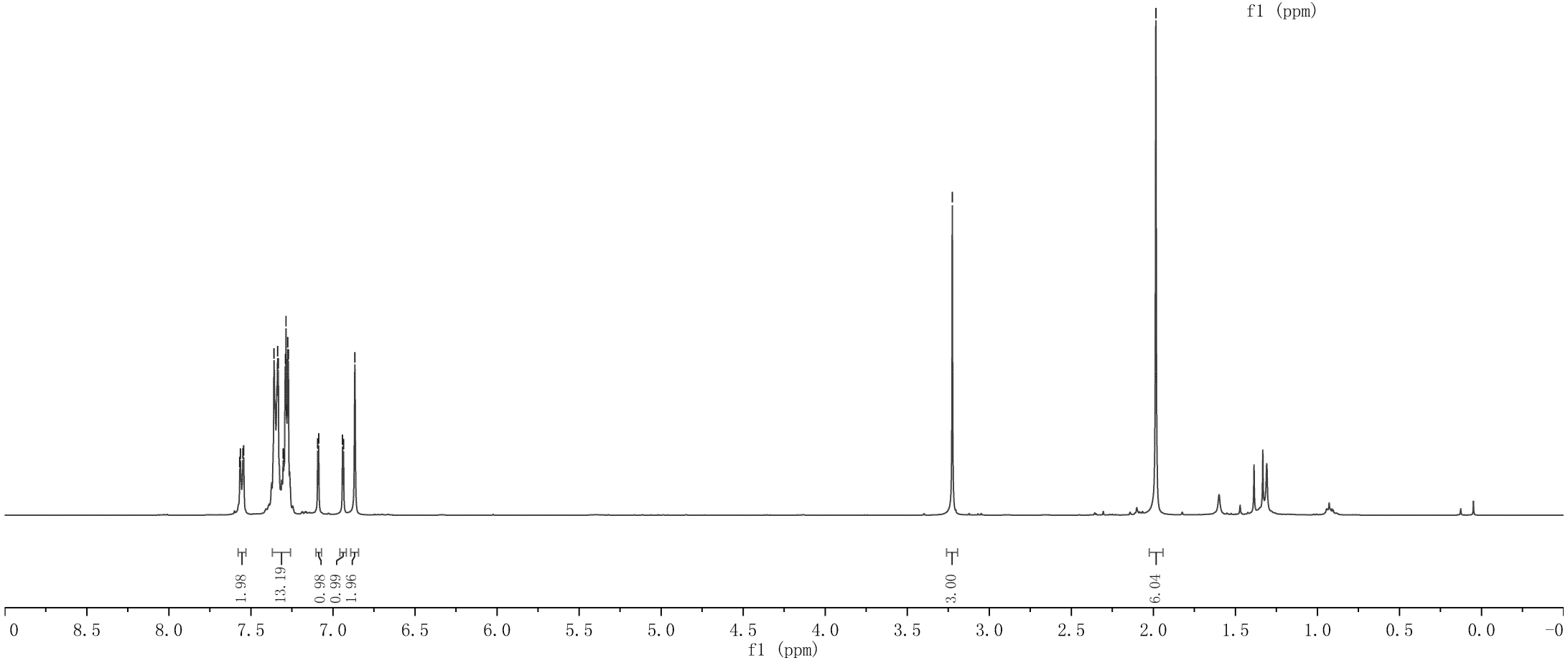
3h

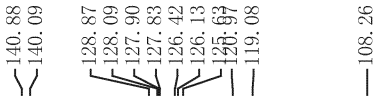
Parameter	Value
1 Title	XHJ-1-224-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-11T22:33:28
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



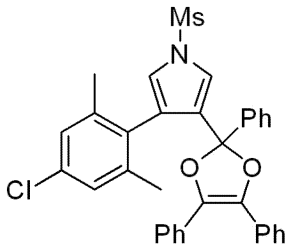
3i



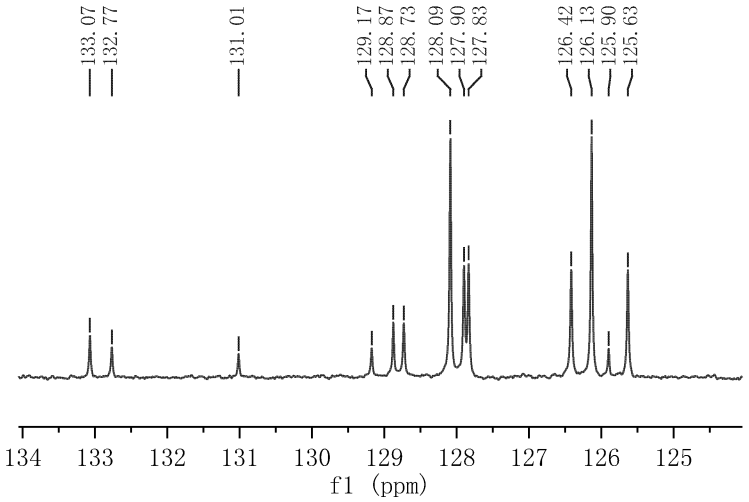


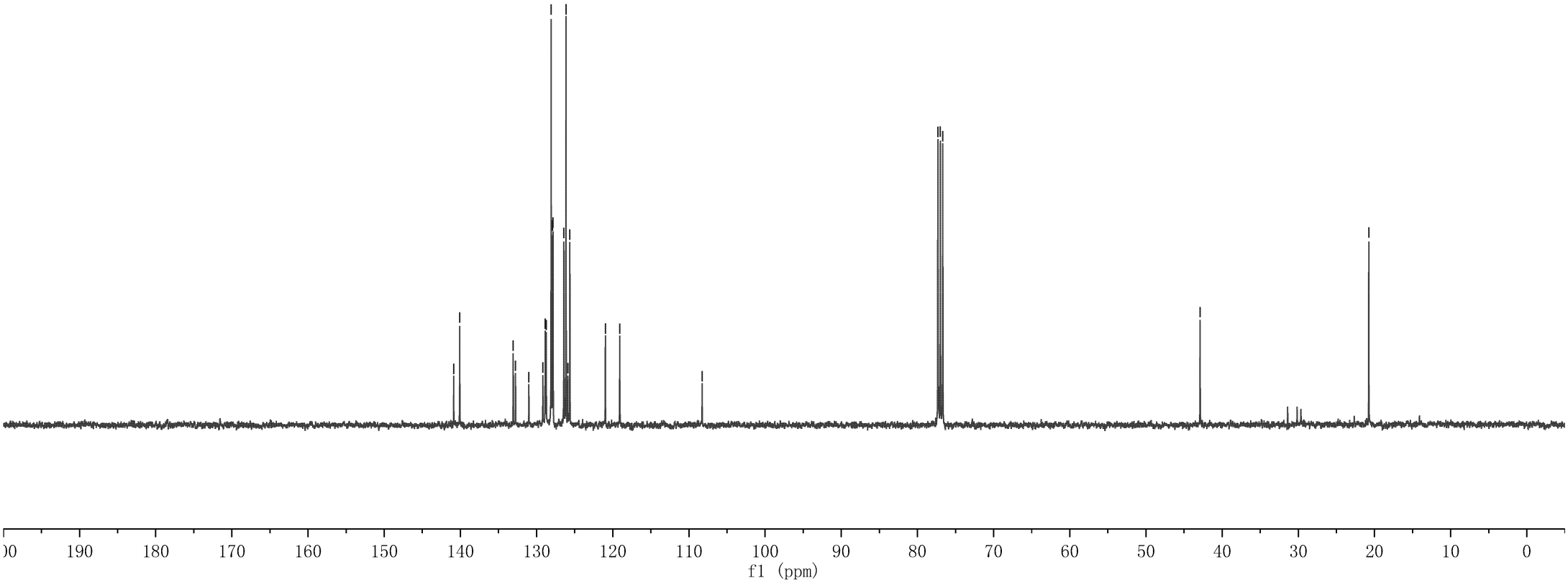


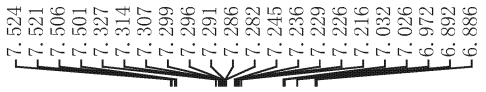
Parameter	Value
1 Title	XHJ-1-224-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	296.8
5 Number of Scans	250
6 Acquisition Time	1.0000
7 Acquisition Date	2022-03-12T02:05:30
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



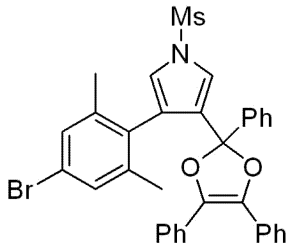
3i



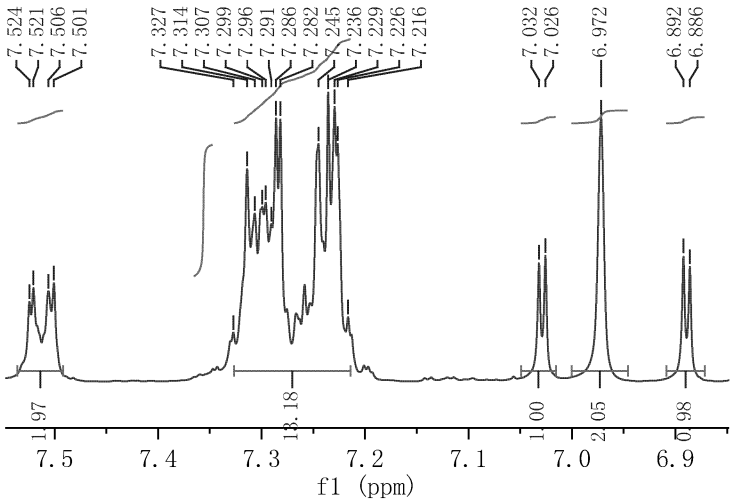


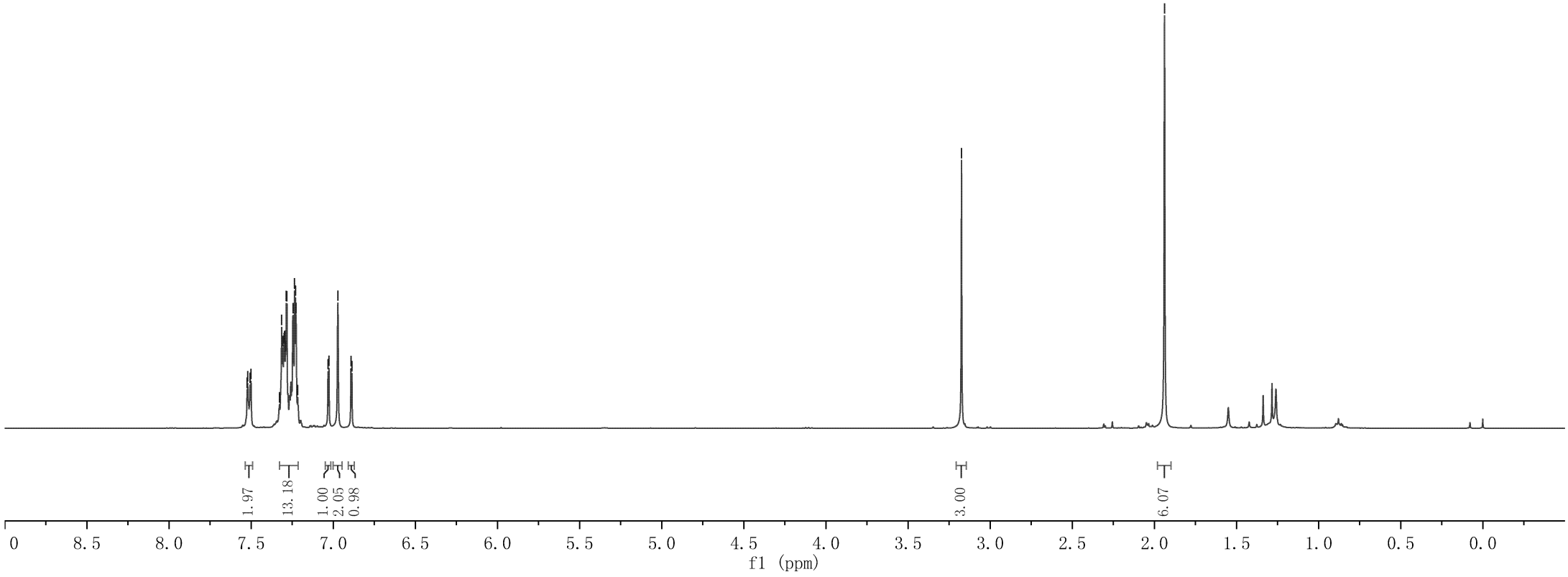


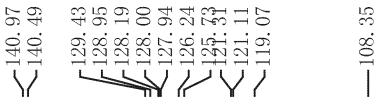
Parameter	Value
1 Title	XHJ-1-221-H-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-03-10T20:18:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

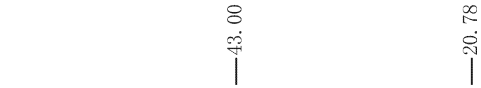


3j

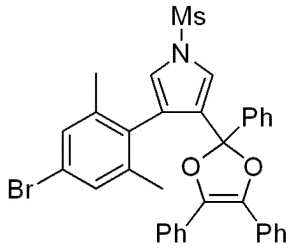




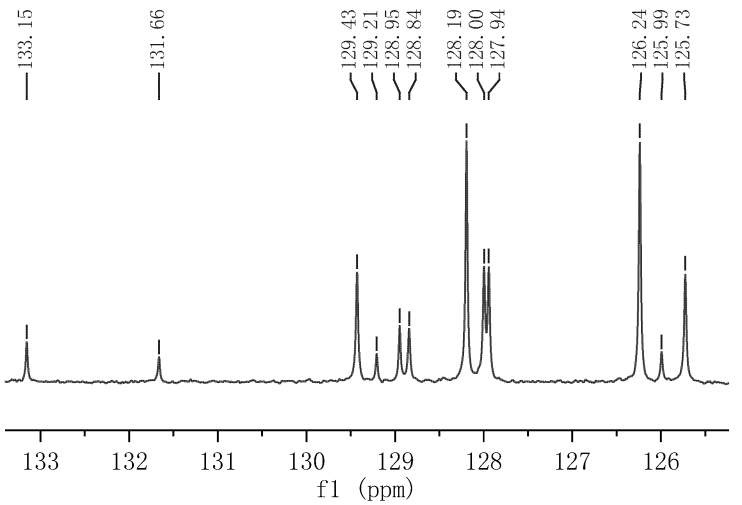


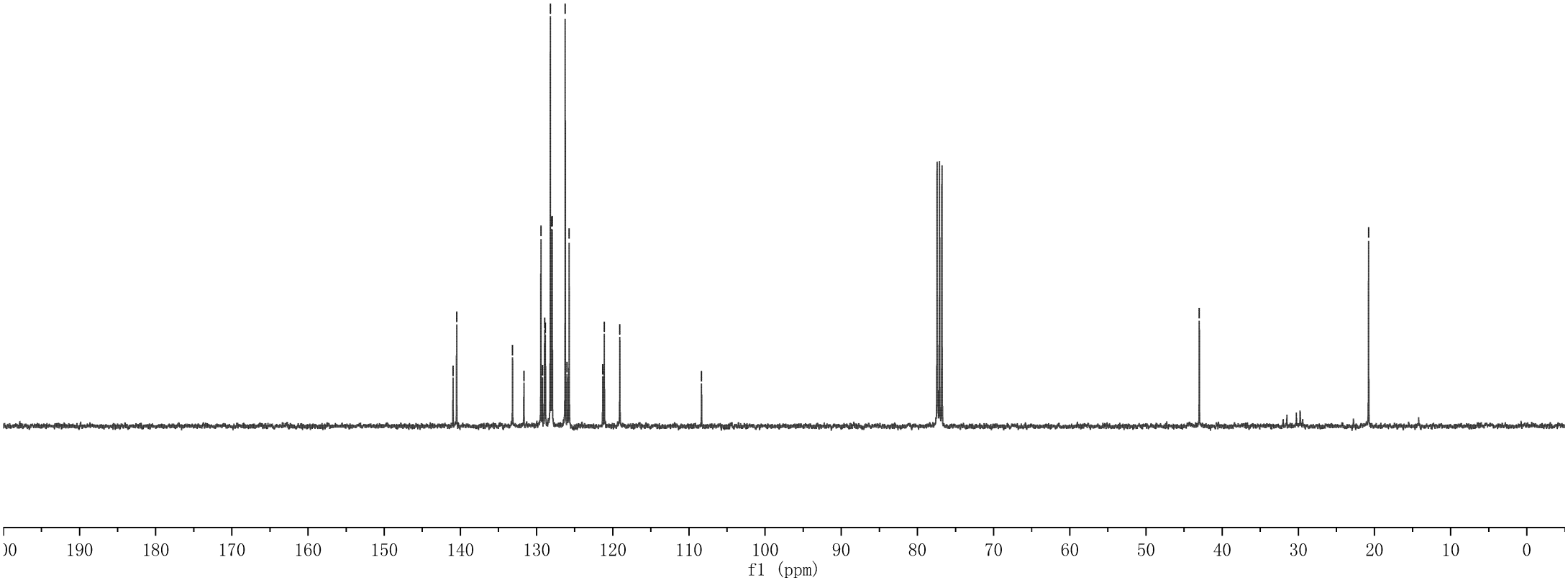


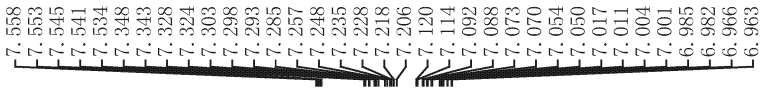
Parameter	Value
1 Title	XHJ-1-221-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	400
6 Acquisition Time	1.0000
7 Acquisition Date	2022-03-10T11:13:17
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



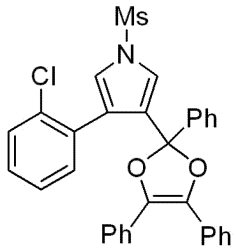
3j



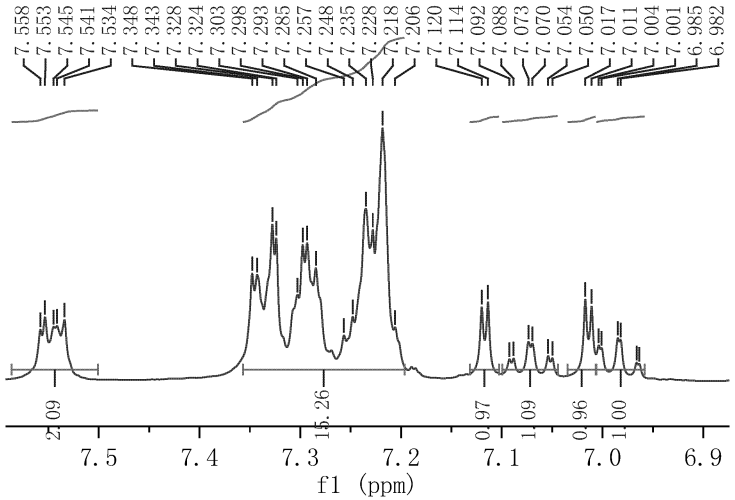


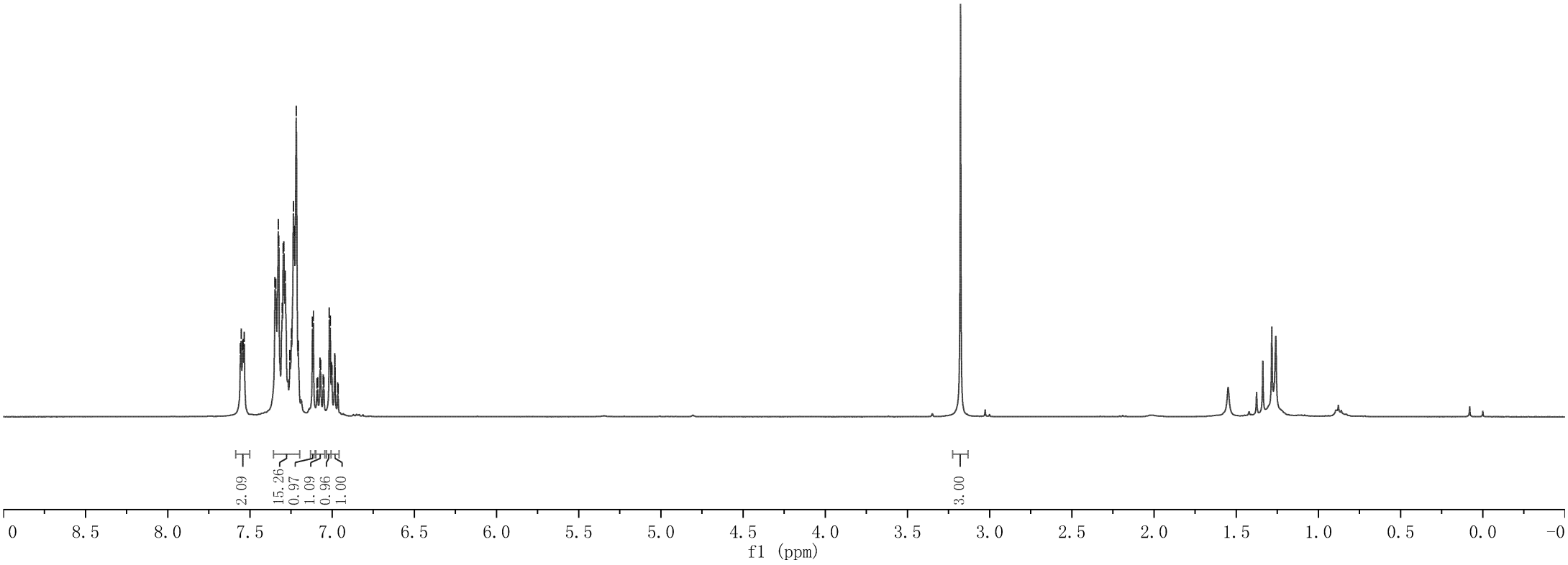


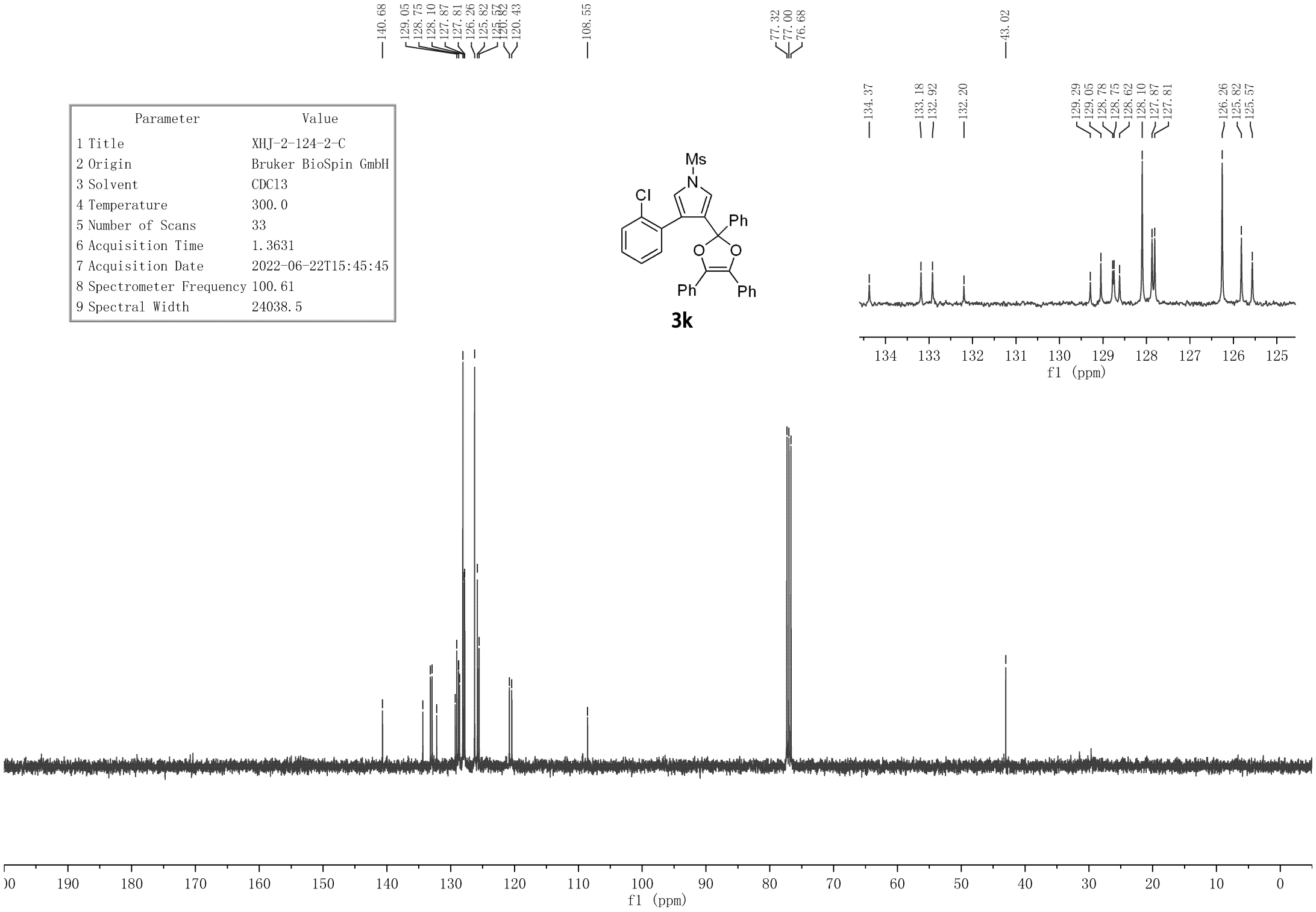
Parameter	Value
1 Title	XHJ-2-124-2-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-06-22T15:44:05
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

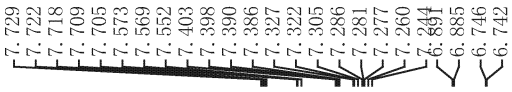


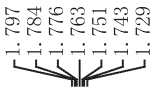
3k

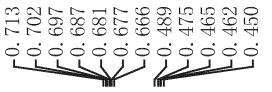




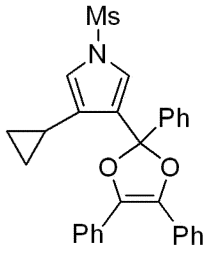

140.68
129.05
128.75
128.10
127.87
127.81
126.26
125.82
125.57
120.82
120.43
108.55
77.32
77.00
76.68
43.02
Parameter Value
1 Title XHJ-2-124-2-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 33
6 Acquisition Time 1.3631
7 Acquisition Date 2022-06-22T15:45:45
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Cl
Ph
O
O
Ph
Ph
3k
134.37
133.18
132.92
132.20
129.29
129.05
128.78
128.75
128.62
128.10
127.87
127.81
126.26
125.82
125.57
134 133 132 131 130 129 128 127 126 125
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



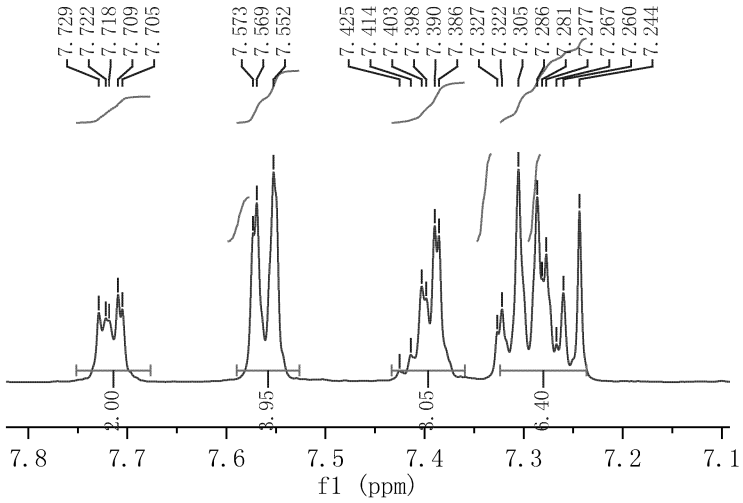


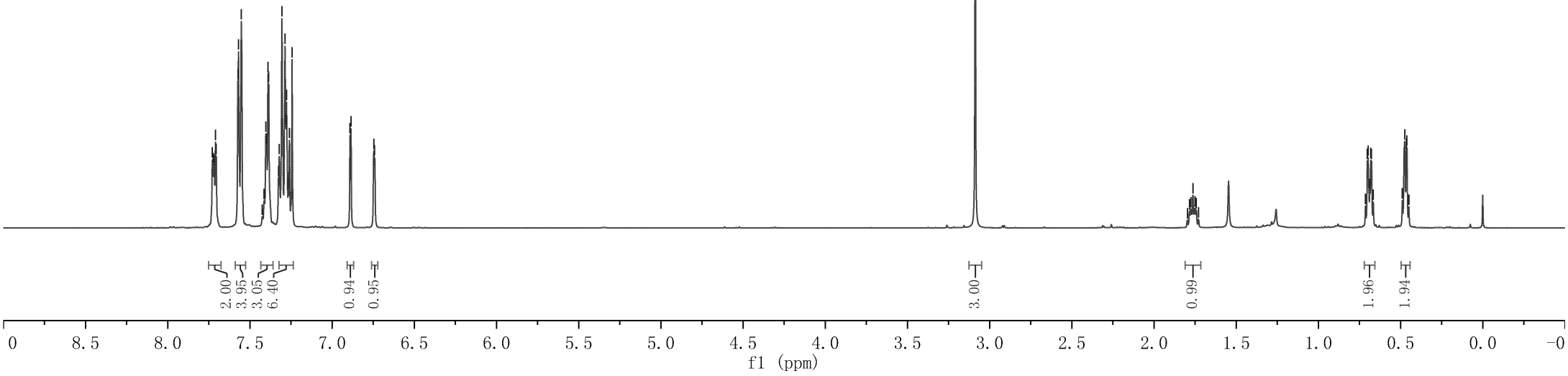


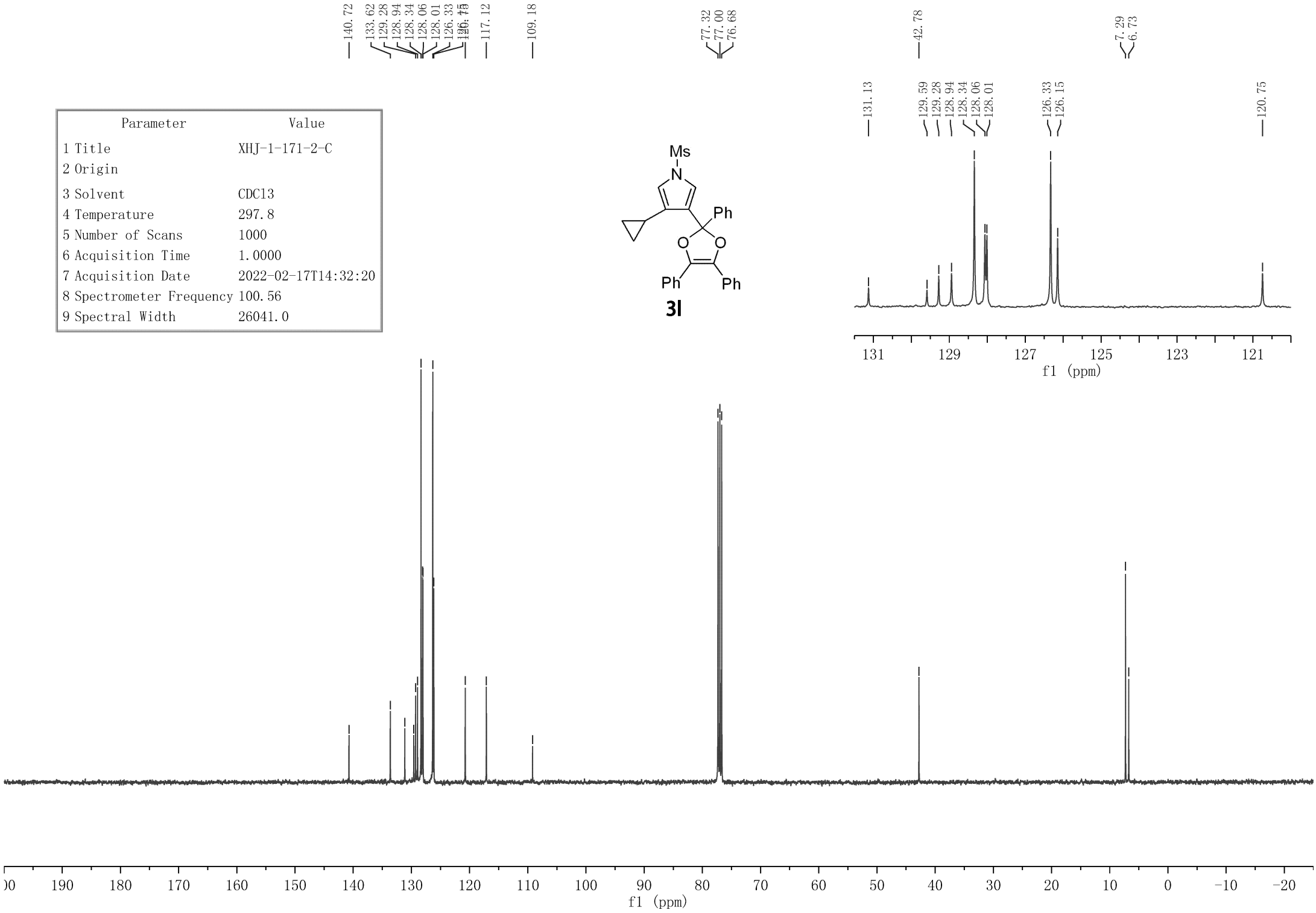
Parameter	Value
1 Title	XHJ-1-171-2-H
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.8
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-02-17T13:56:39
8 Spectrometer Frequency	399.93
9 Spectral Width	8012.0



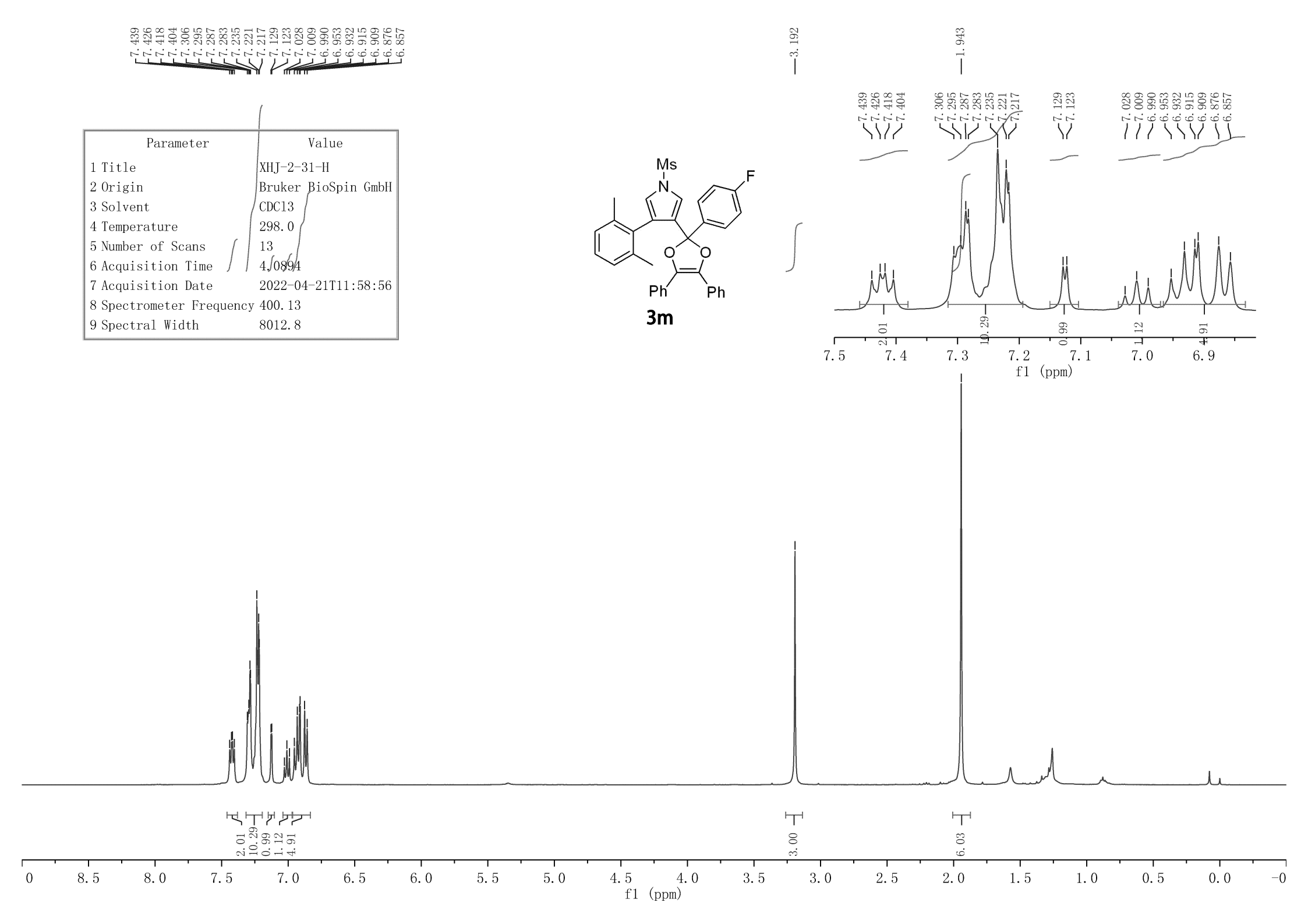
3l

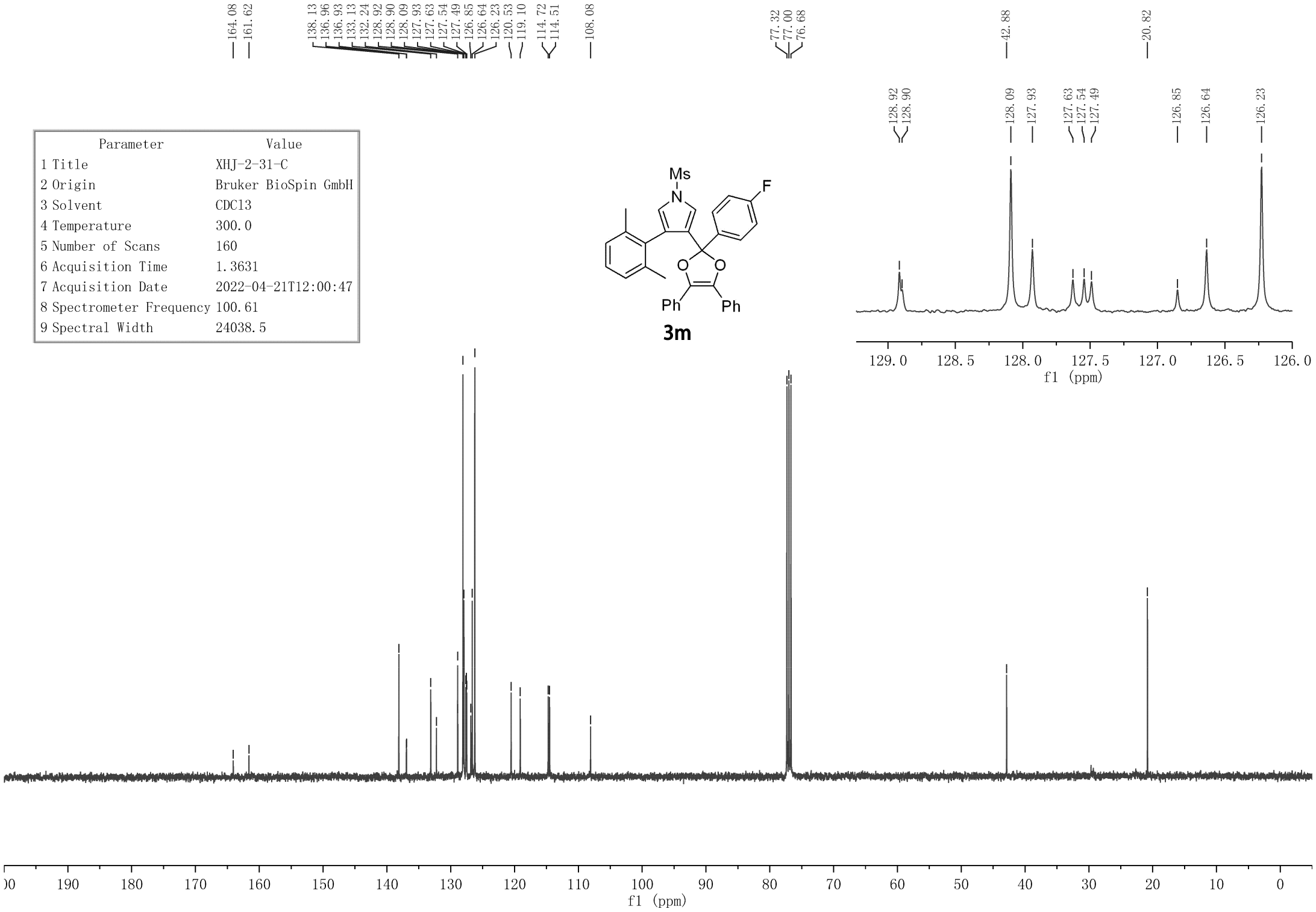




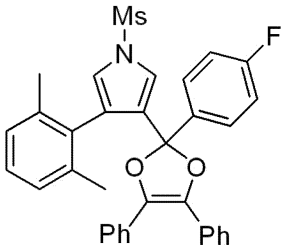


Parameter	Value
1 Title	XHJ-1-171-2-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.8
5 Number of Scans	1000
6 Acquisition Time	1.0000
7 Acquisition Date	2022-02-17T14:32:20
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

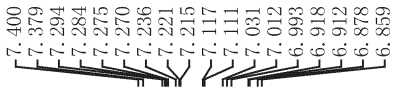

7.439
7.426
7.418
7.404
7.306
7.295
7.287
7.283
7.235
7.221
7.217
7.129
7.123
7.028
7.009
6.990
6.953
6.932
6.915
6.909
6.876
6.857
3.192
1.943
Parameter Value
1 Title XHJ-2-31-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 13
6 Acquisition Time 4.0894
7 Acquisition Date 2022-04-21T11:58:56
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
F
O
O
Ph
Ph
3m
2.01
10.29
0.99
1.12
4.91
3.00
6.03
f1 (ppm)


164.08
161.62
138.13
136.96
136.93
133.13
132.24
128.92
128.90
128.09
127.93
127.63
127.54
127.49
126.85
126.64
126.23
120.53
119.10
114.72
114.51
108.08
77.32
77.00
76.68
42.88
20.82
Parameter Value
1 Title XHJ-2-31-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 2022-04-21T12:00:47
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
F
O
O
Ph
Ph
3m
f1 (ppm)
f1 (ppm)

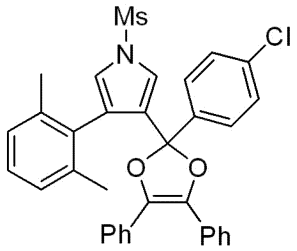
Parameter	Value
1 Title	XHJ-2-31-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.3
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-08-16T20:23:01
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



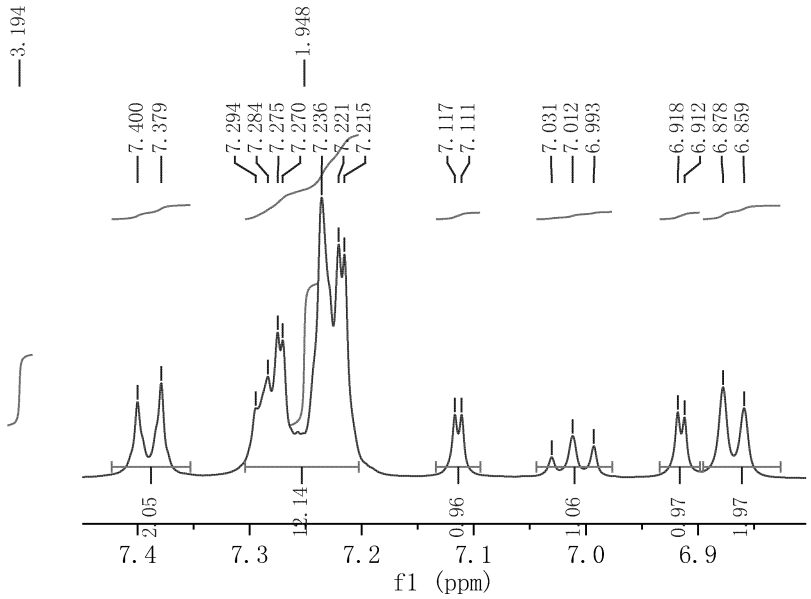
3m

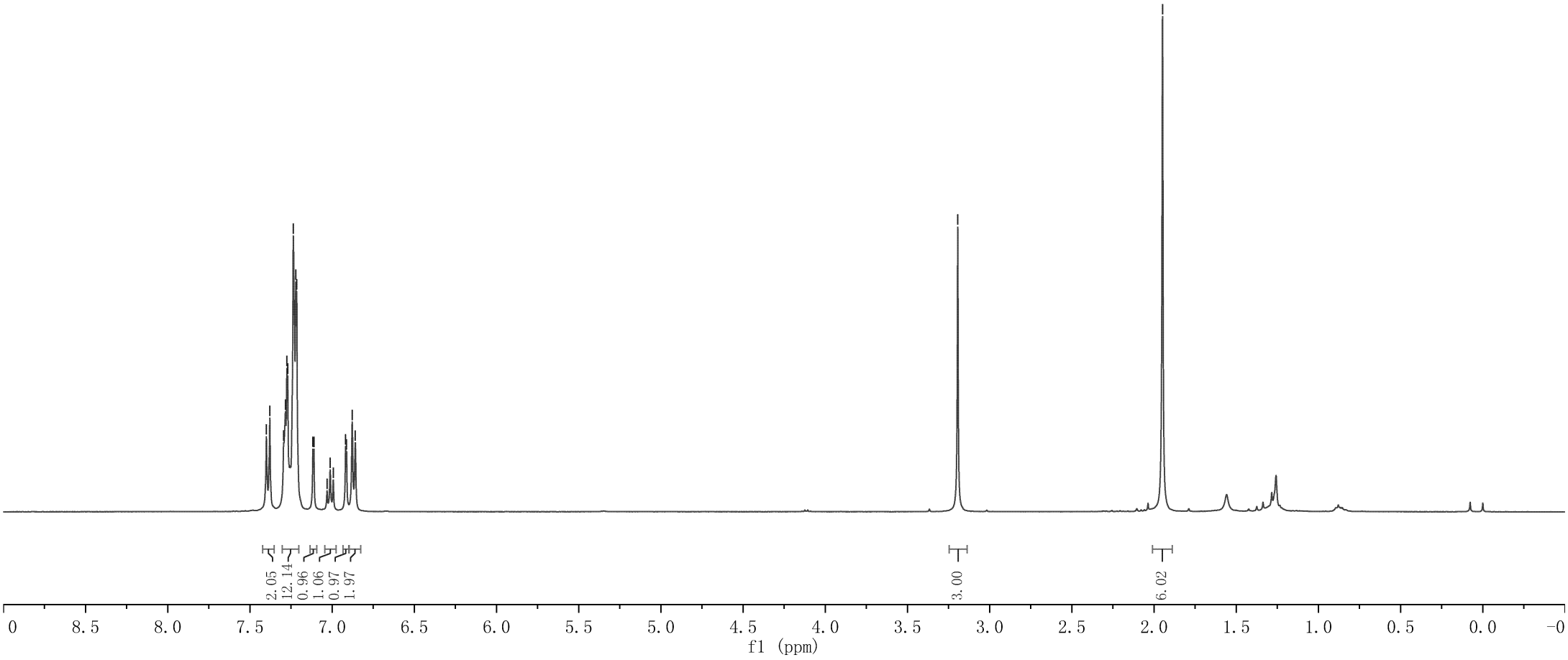


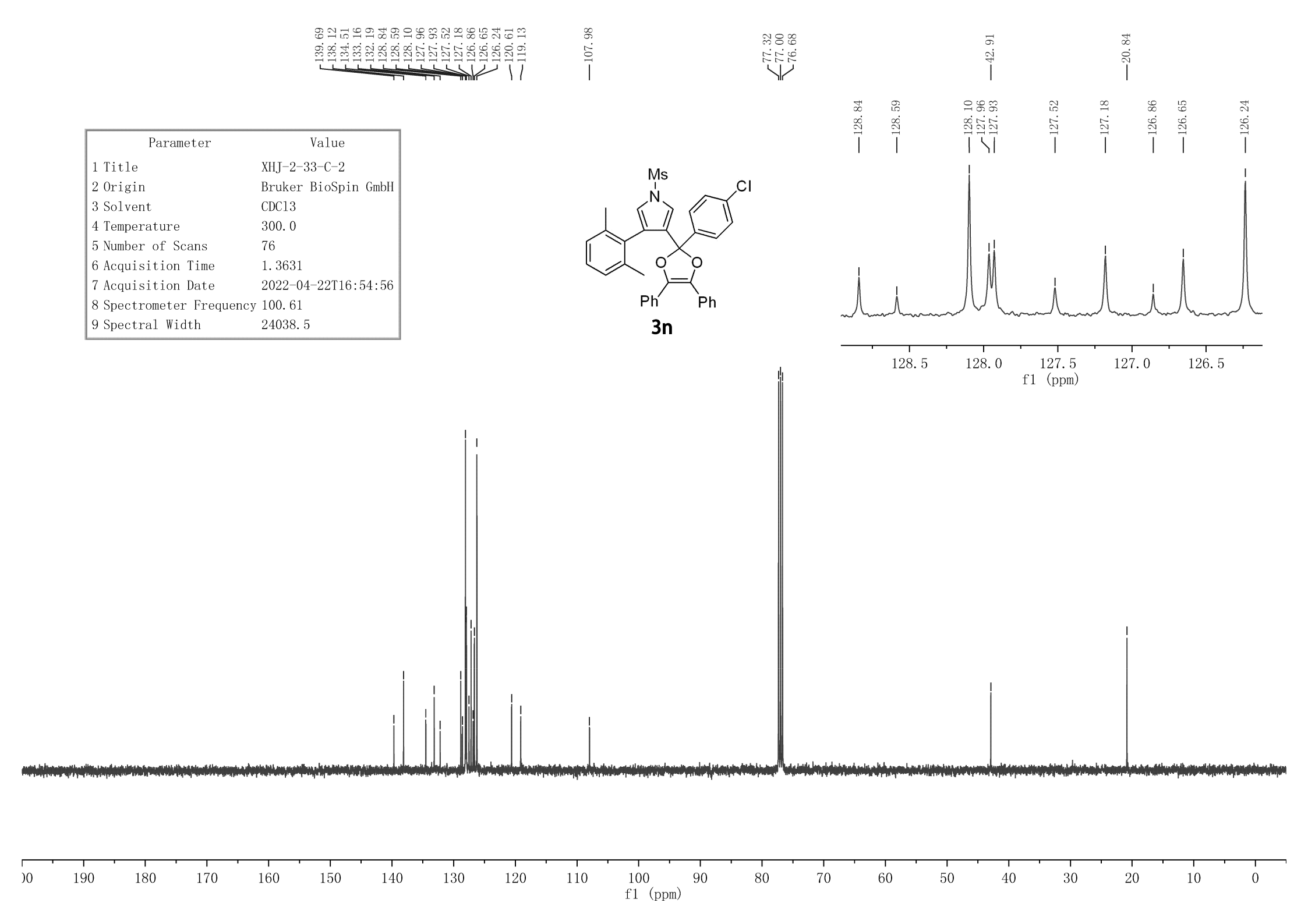
Parameter	Value
1 Title	XHJ-2-33-H-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-21T16:30:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



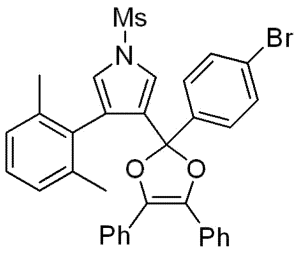
3n



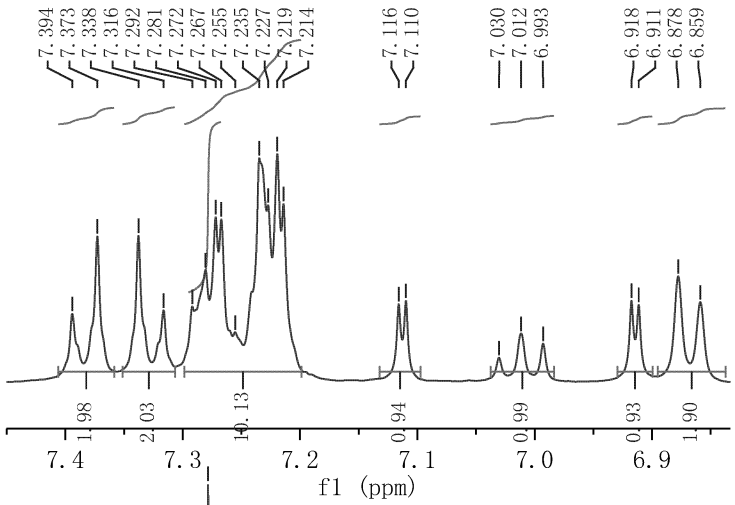


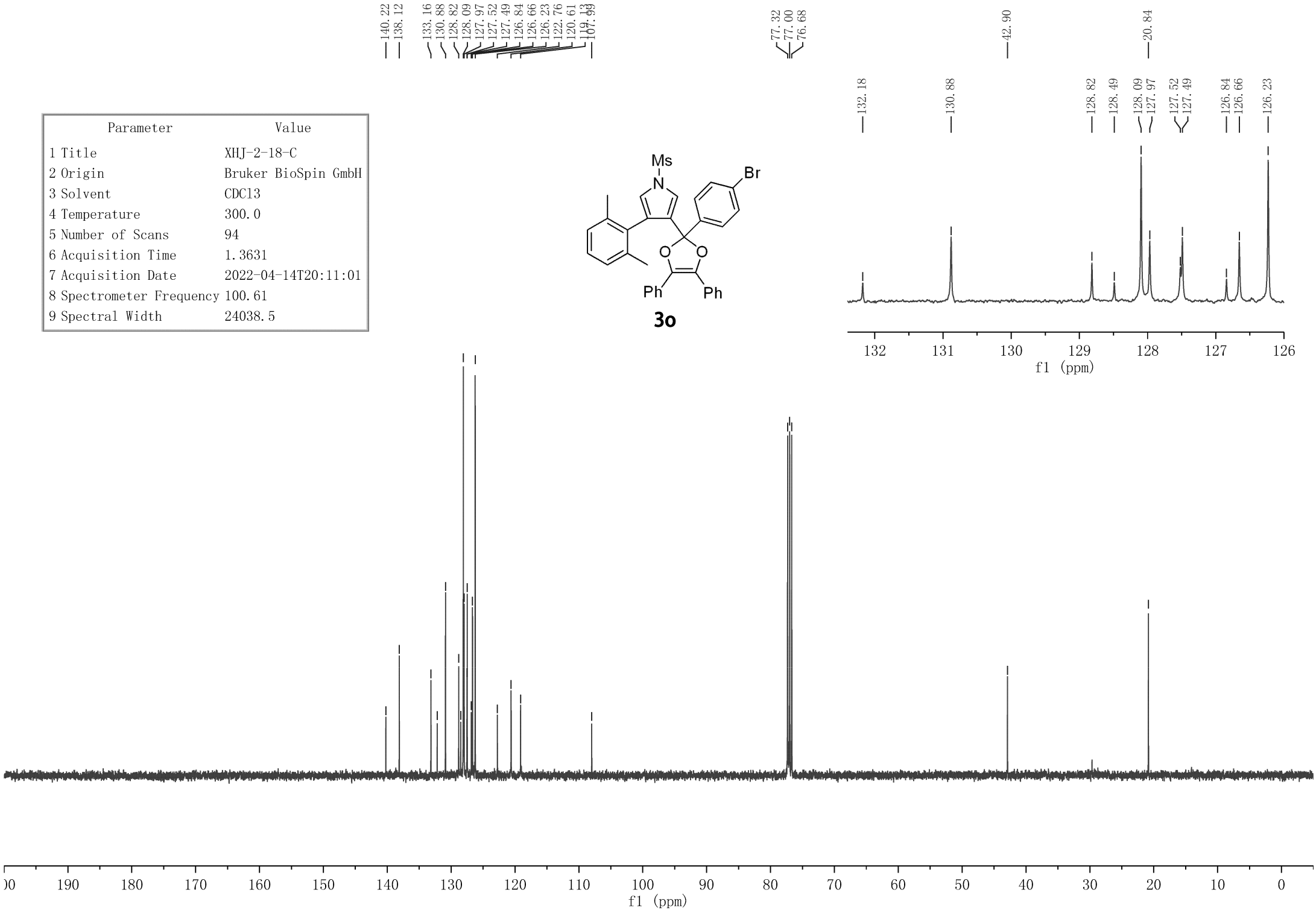

139.69
138.12
134.51
133.16
132.19
128.84
128.59
128.10
127.96
127.93
127.52
127.18
126.86
126.65
126.24
120.61
119.13
107.98
77.32
77.00
76.68
42.91
20.84
Parameter Value
1 Title XHJ-2-33-C-2
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 76
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-22T16:54:56
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Cl
O
O
Ph
Ph
3n
f1 (ppm)
f1 (ppm)

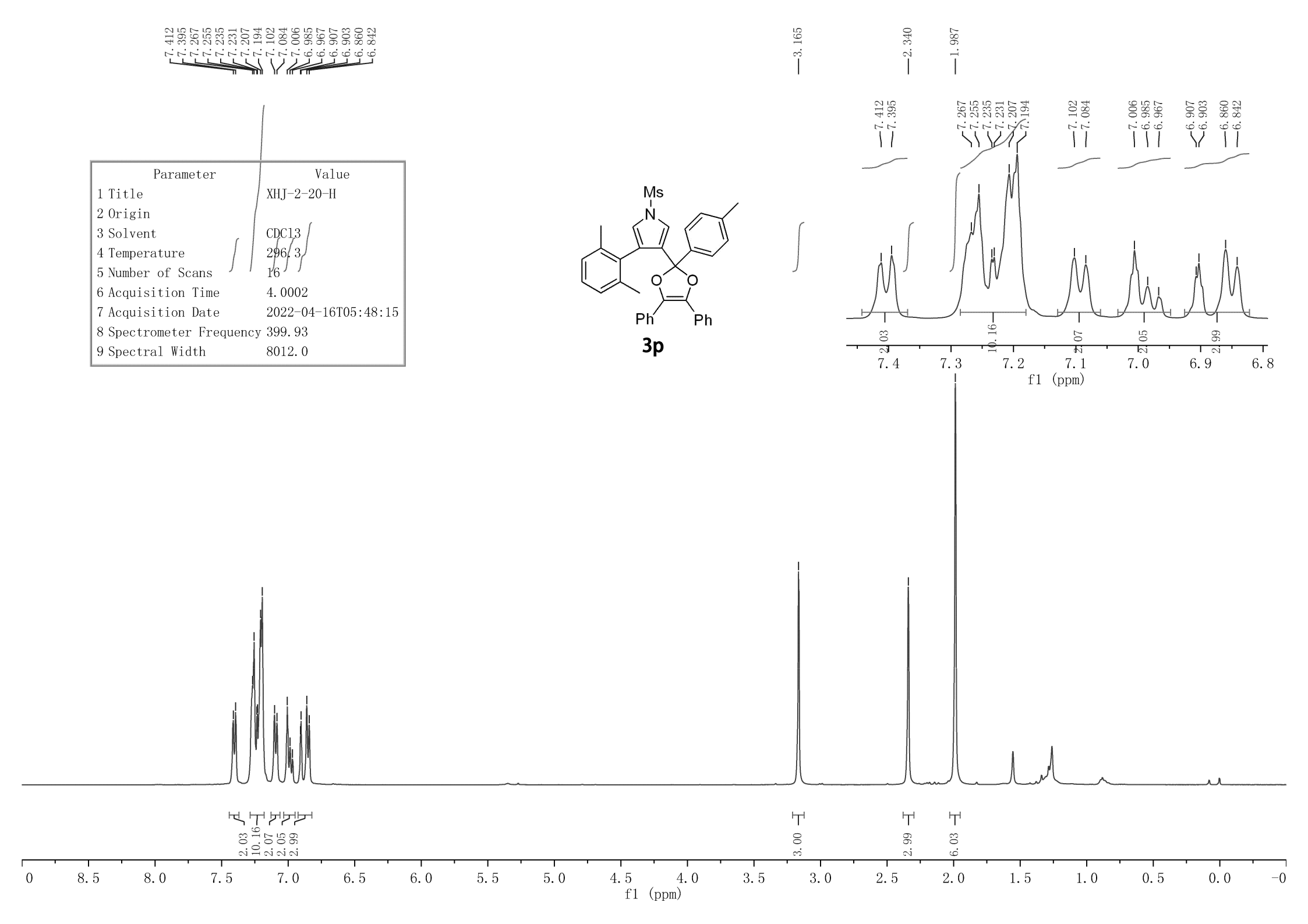
Parameter	Value
1 Title	XHJ-2-18-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-14T16:58:12
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



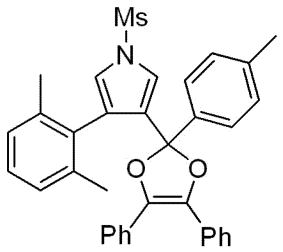
3o



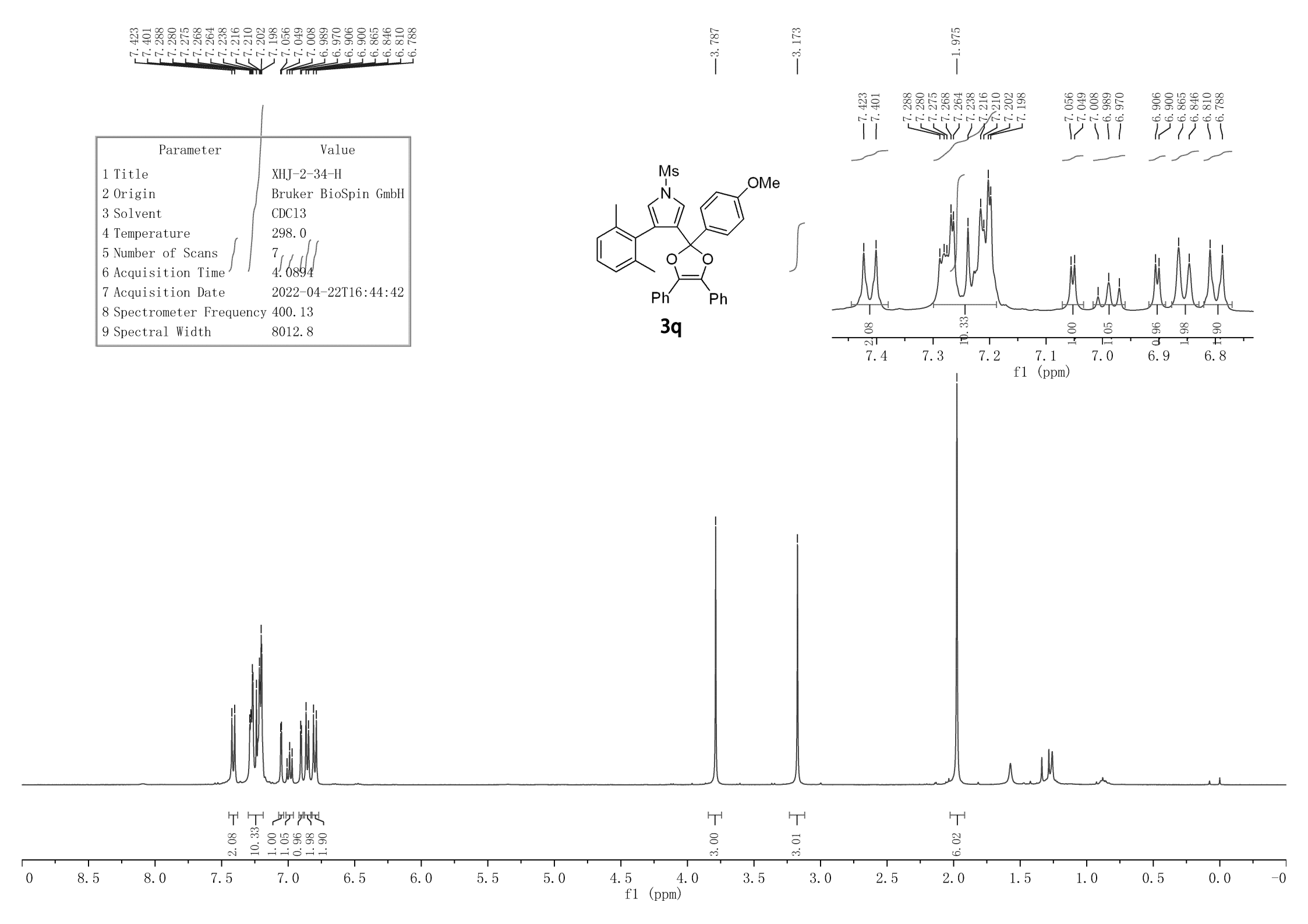

140.22
138.12
133.16
130.88
128.82
128.09
127.97
127.52
127.49
126.84
126.66
126.23
122.76
120.61
77.32
77.00
76.68
42.90
20.84
Parameter Value
1 Title XHJ-2-18-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 94
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-14T20:11:01
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
Br
O
O
Ph
Ph
3o
f1 (ppm)
f1 (ppm)

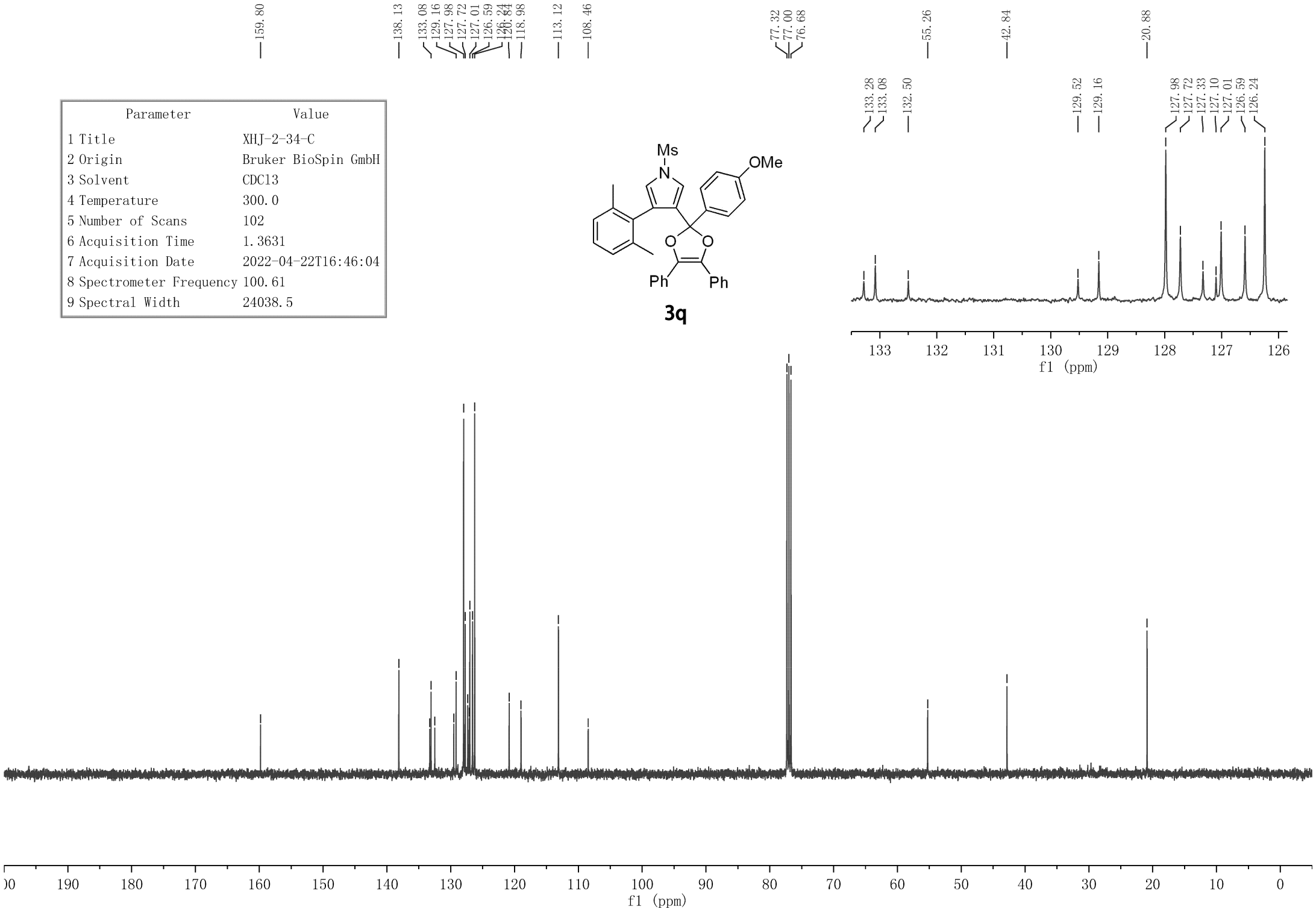

7.412
7.395
7.267
7.255
7.235
7.231
7.207
7.194
7.102
7.084
7.006
6.985
6.967
6.907
6.903
6.860
6.842
3.165
2.340
1.987
Parameter Value
1 Title XHJ-2-20-H
2 Origin
3 Solvent CDCl3
4 Temperature 296.3
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-04-16T05:48:15
8 Spectrometer Frequency 399.93
9 Spectral Width 8012.0
Ms
N
O
O
Ph
Ph
3p
2.03
10.16
2.07
2.05
2.99
3.00
2.99
6.03
f1 (ppm)

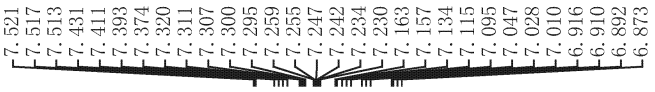
Parameter	Value
1 Title	XHJ-2-20-C
2 Origin	
3 Solvent	CDCl3
4 Temperature	296.8
5 Number of Scans	300
6 Acquisition Time	1.0000
7 Acquisition Date	2022-04-16T06:00:38
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



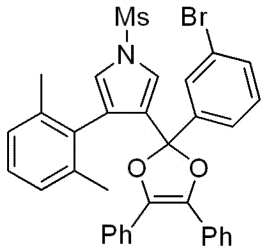
3p


7.423
7.401
7.288
7.280
7.275
7.268
7.264
7.238
7.216
7.210
7.202
7.198
7.056
7.049
7.008
6.989
6.970
6.906
6.900
6.865
6.846
6.810
6.788
3.787
3.173
1.975
Parameter
Value
1 Title
XHJ-2-34-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
2022-04-22T16:44:42
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
Ms
N
OMe
O
O
Ph
Ph
3q
2.08
10.33
1.00
1.05
0.96
1.98
1.90
3.00
3.01
6.02
f1 (ppm)

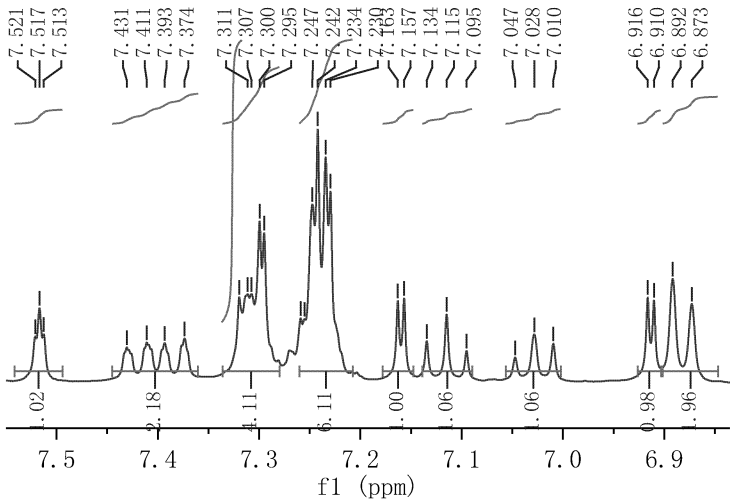

159.80
138.13
133.08
129.16
127.98
127.72
127.01
126.59
118.98
113.12
108.46
77.32
77.00
76.68
55.26
42.84
20.88
Parameter Value
1 Title XHJ-2-34-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 102
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-22T16:46:04
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
OMe
O
O
Ph
Ph
3q
133.28
133.08
132.50
129.52
129.16
127.98
127.72
127.33
127.10
127.01
126.59
126.24
f1 (ppm)
f1 (ppm)

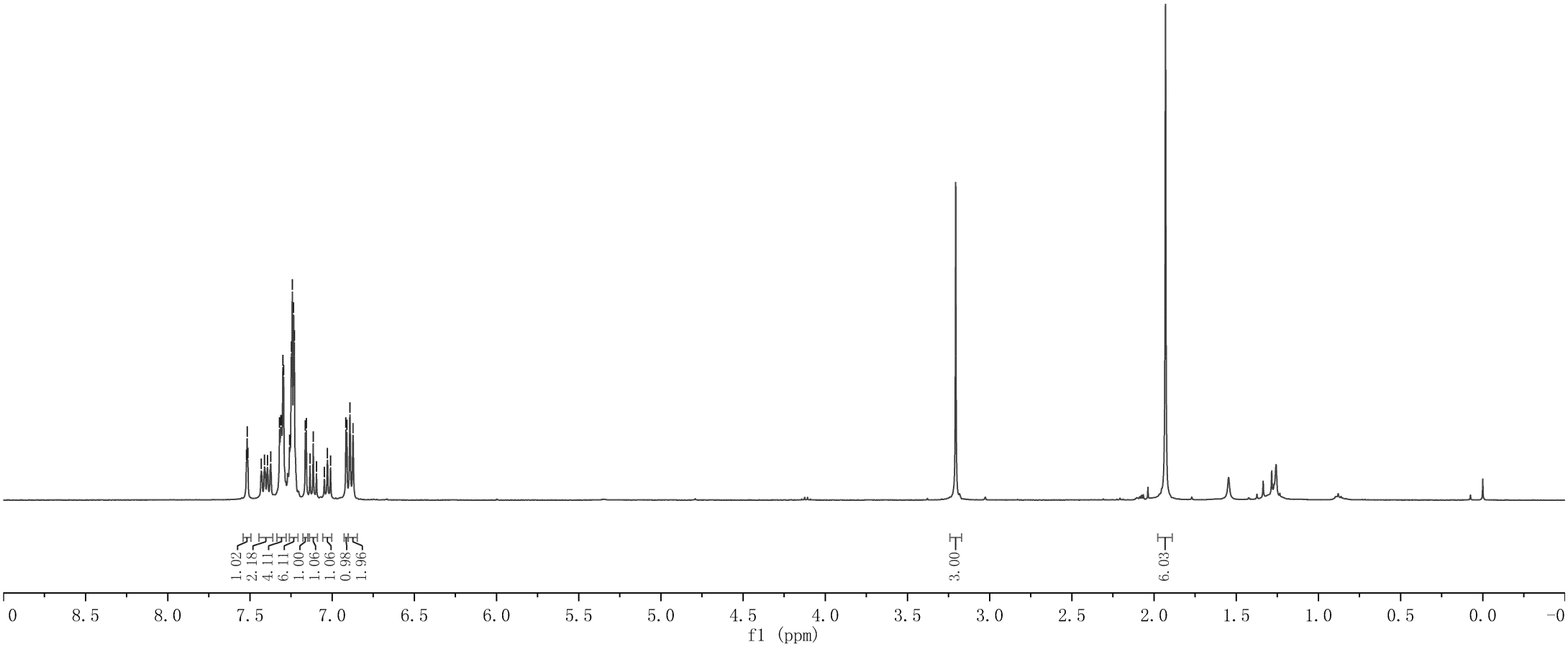


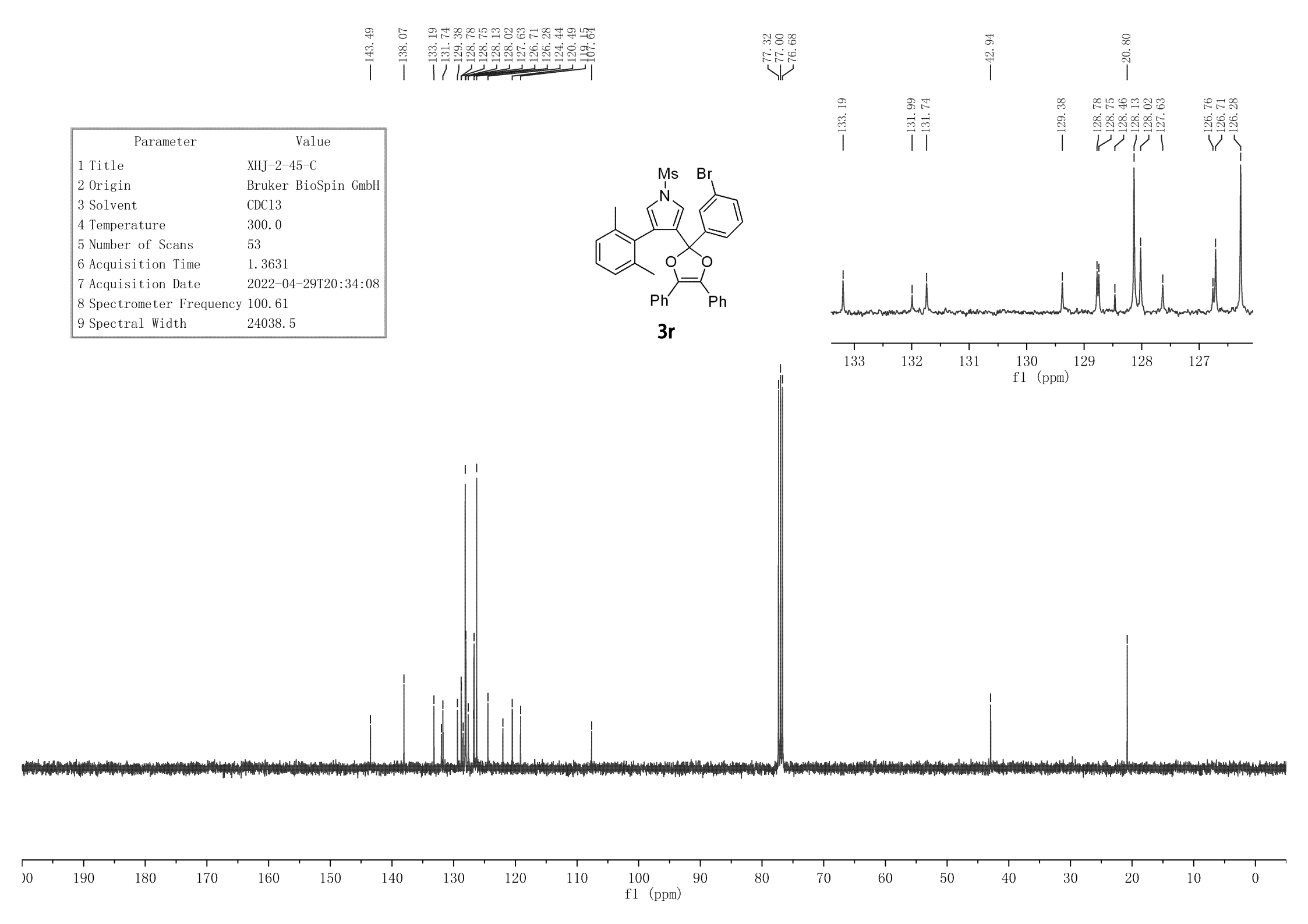
Parameter	Value
1 Title	XHJ-2-45-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-29T20:32:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



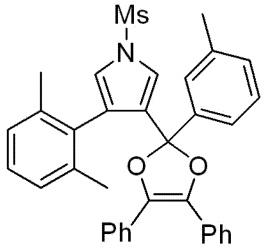
3r





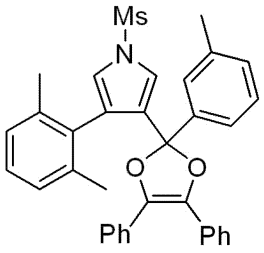

143.49
138.07
133.19
131.74
129.38
128.78
128.75
128.13
128.02
127.63
126.71
126.28
124.44
120.49
77.32
77.00
76.68
42.94
20.80
Parameter Value
1 Title XHJ-2-45-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 53
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-29T20:34:08
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
Br
N
O
O
Ph
Ph
3r
133.19
131.99
131.74
129.38
128.78
128.75
128.46
128.13
128.02
127.63
126.76
126.71
126.28
133
132
131
130
129
128
127
f1 (ppm)
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	XHJ-2-58-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	2022-05-10T14:29:39
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

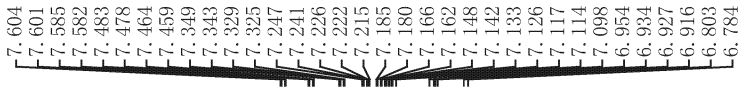


3s

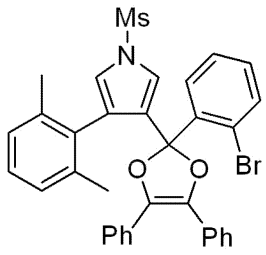
Parameter	Value
1 Title	XHJ-2-58-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-10T14:31:21
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



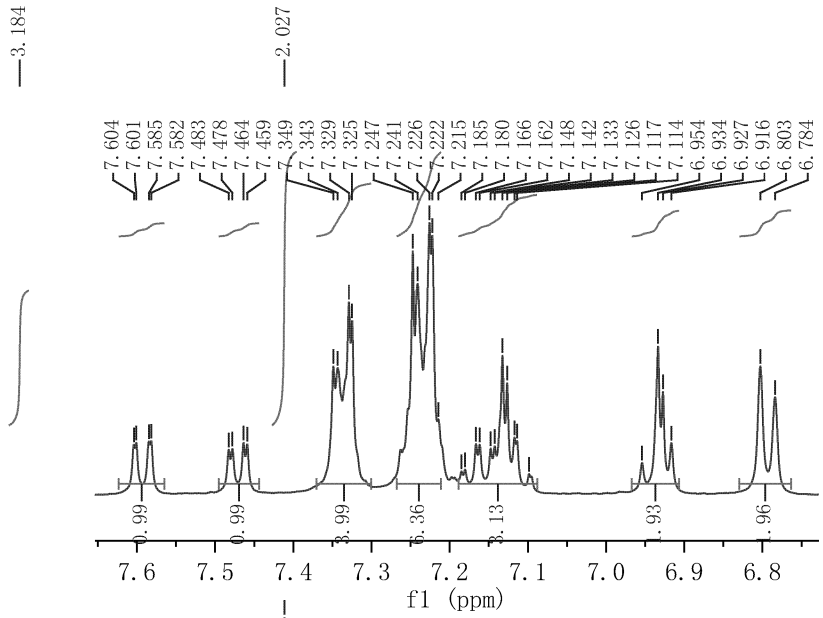
3s

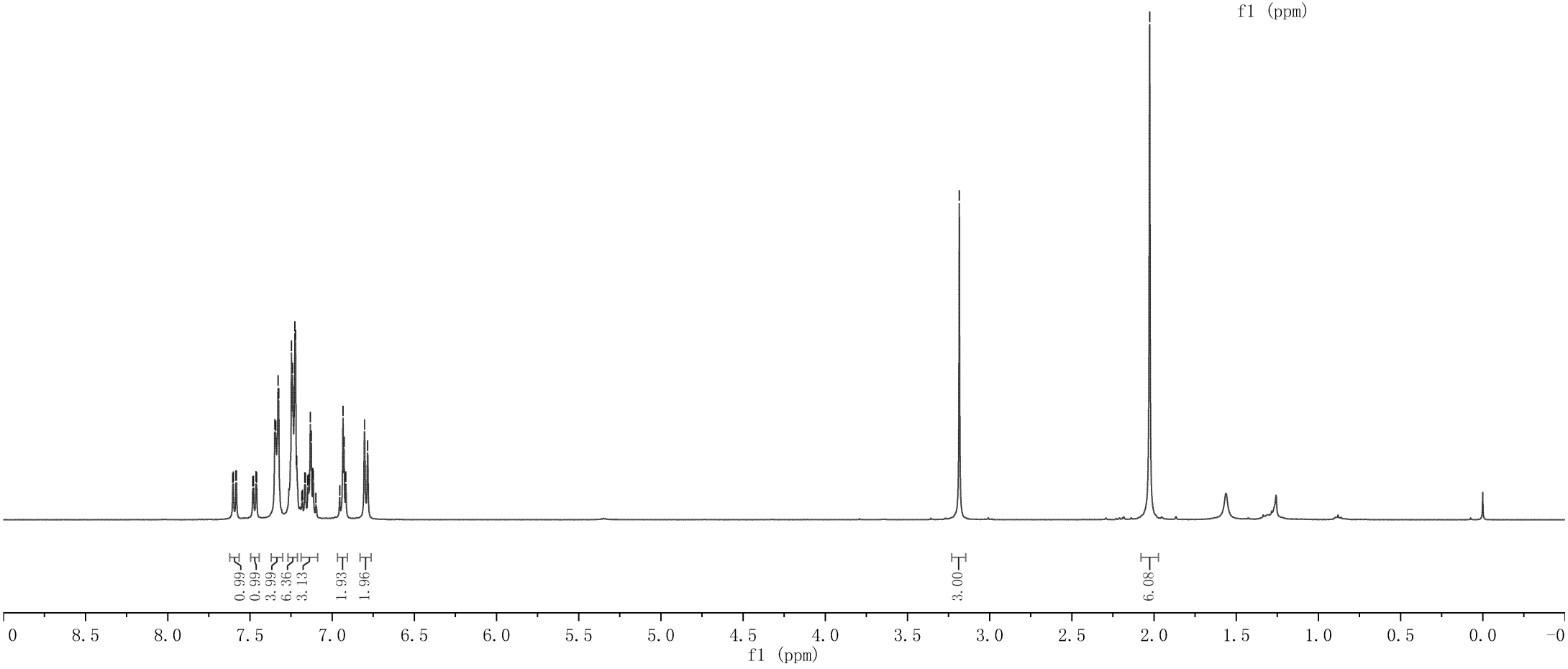


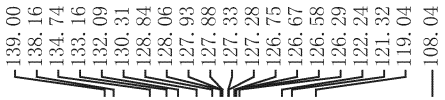
Parameter	Value
1 Title	XHJ-2-44-H-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-12T14:01:58
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



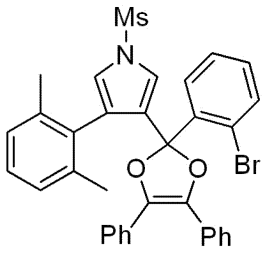
3t



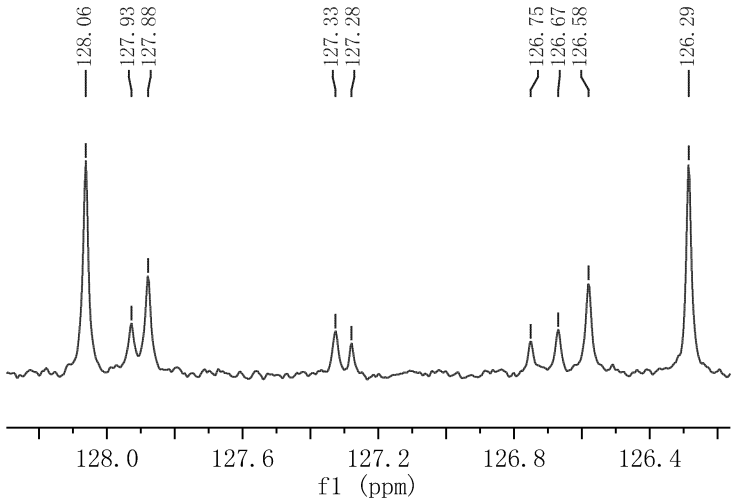


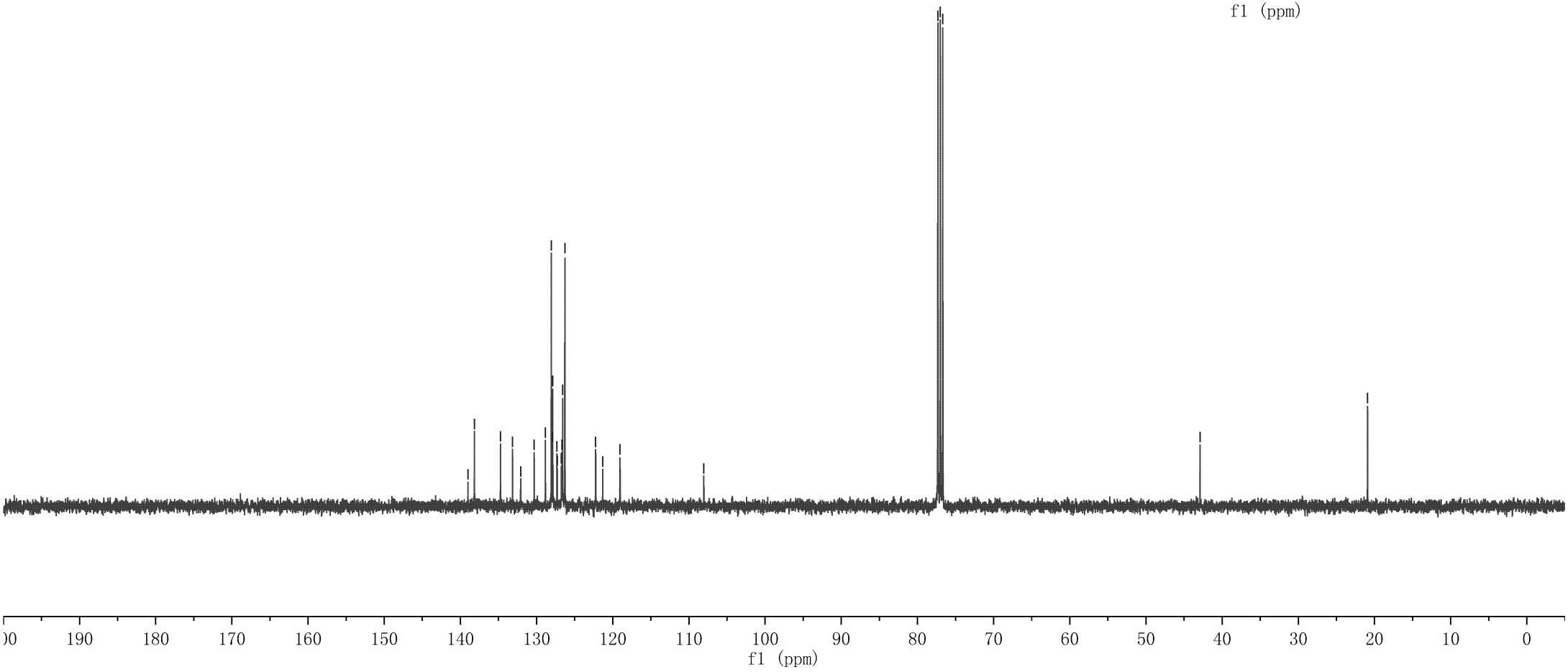


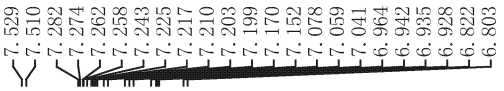
Parameter	Value
1 Title	XHJ-2-44-C-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	77
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-12T14:03:04
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



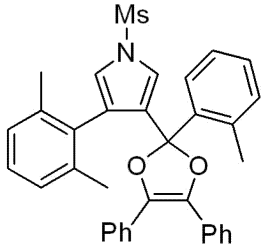
3t



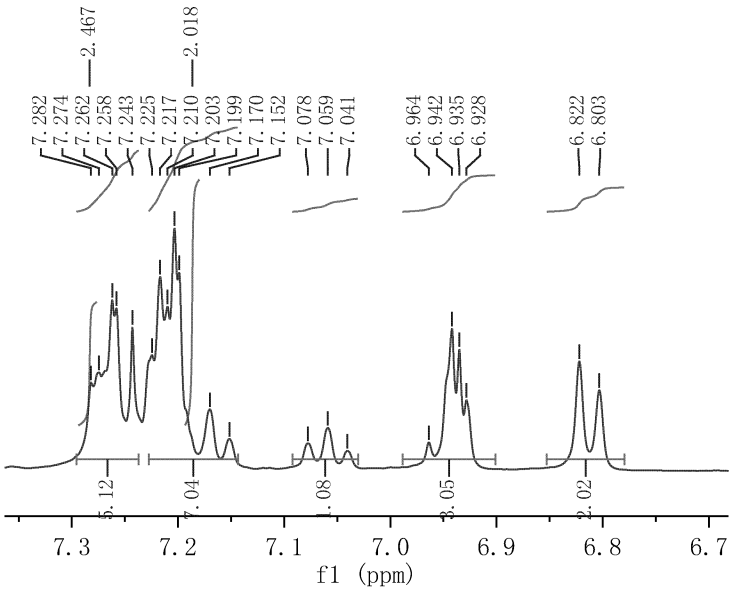


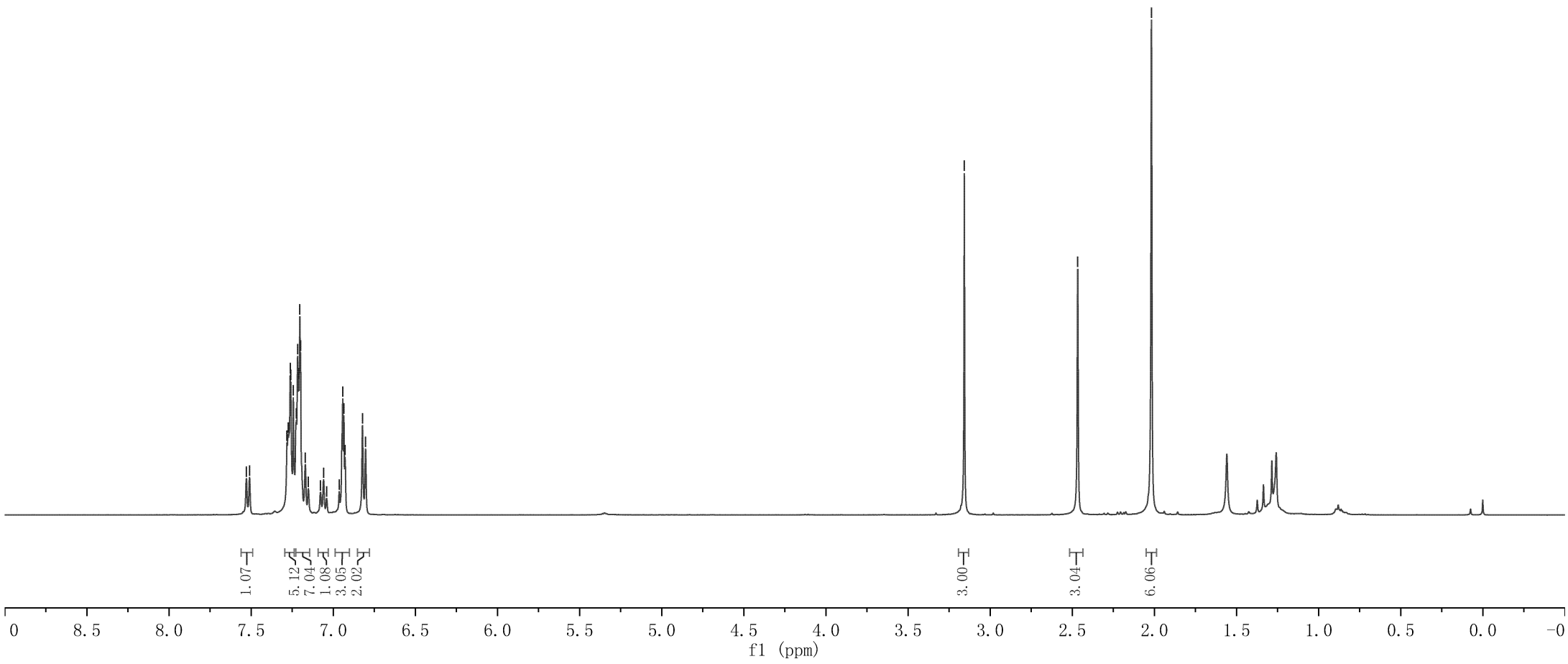


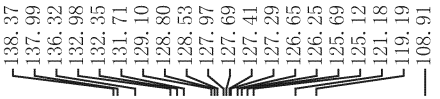
Parameter	Value
1 Title	XHJ-2-59-H-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-11T20:56:14
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



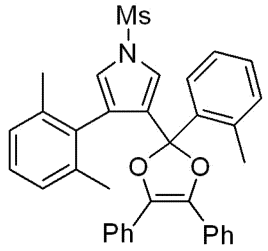
3u



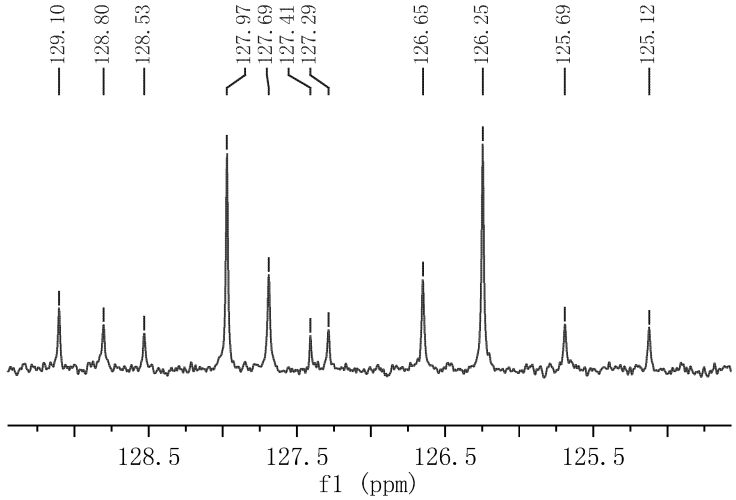


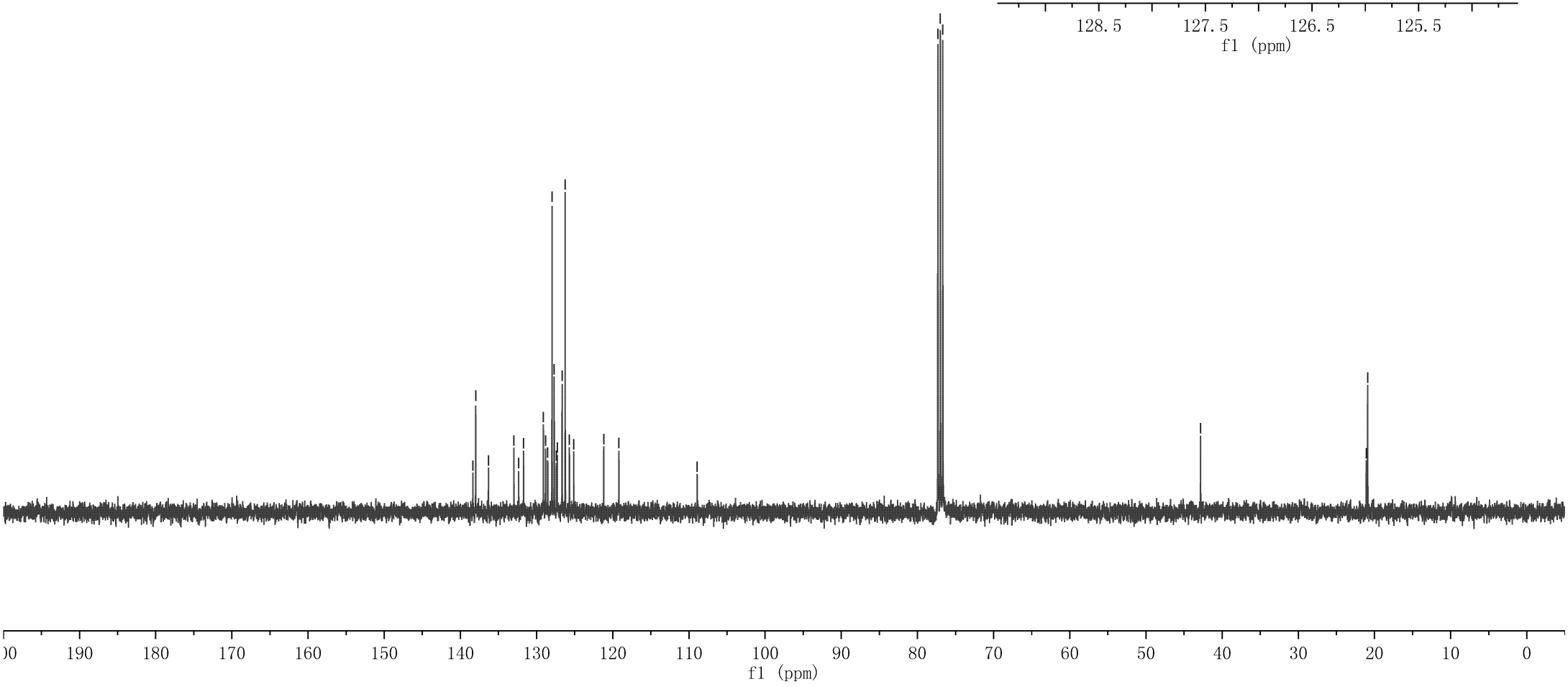


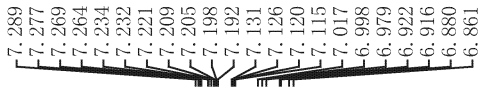
Parameter	Value
1 Title	XHJ-2-59-C-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	40
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-11T20:57:31
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



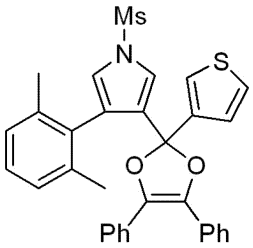
3u



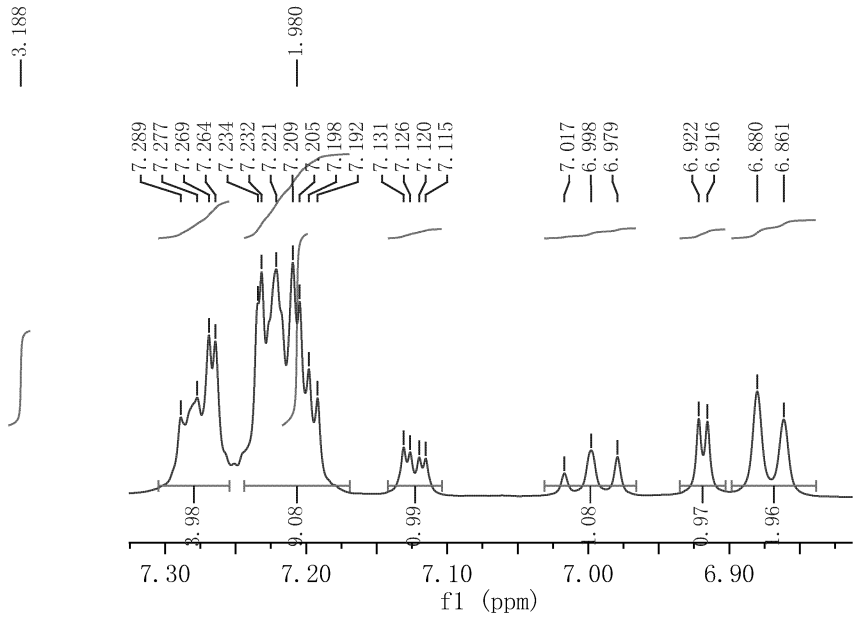


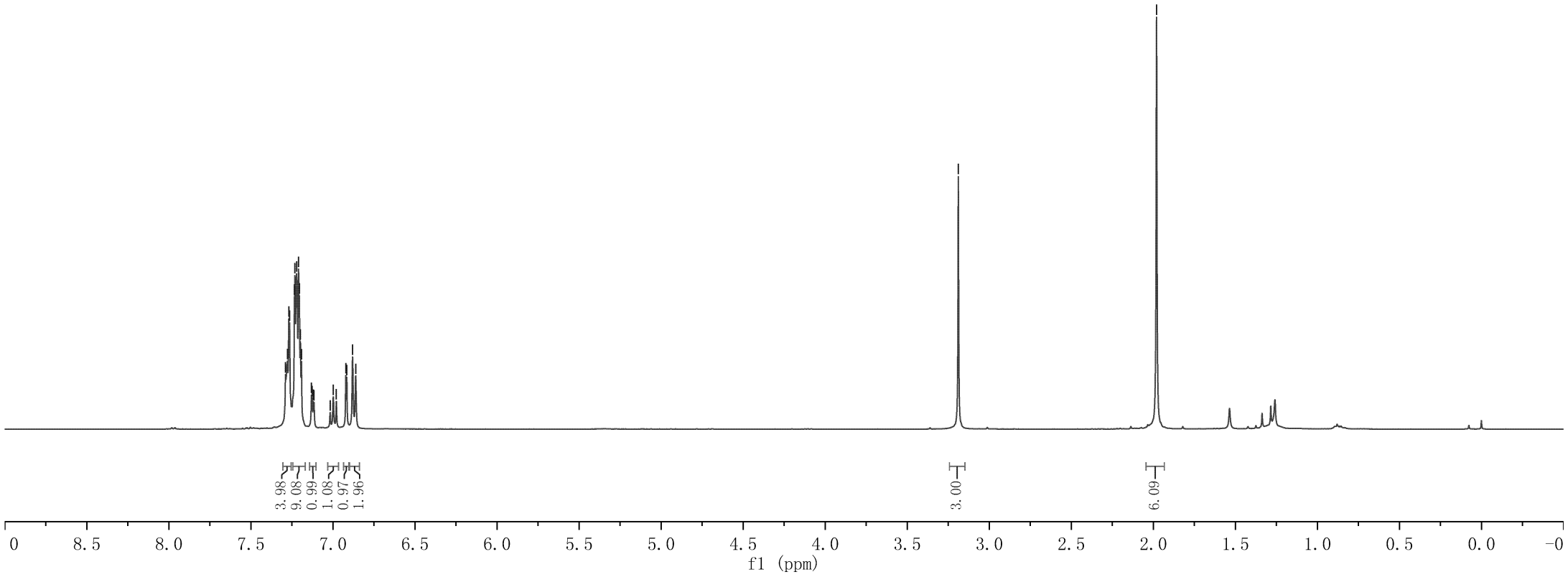


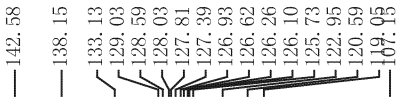
Parameter	Value
1 Title	XHJ-2-48-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-04-30T10:19:48
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

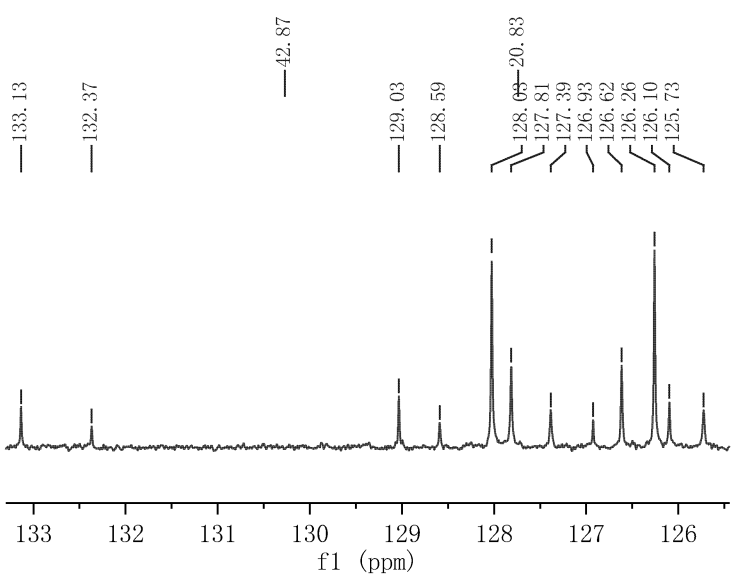


3v

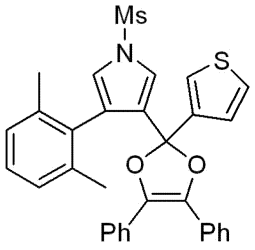




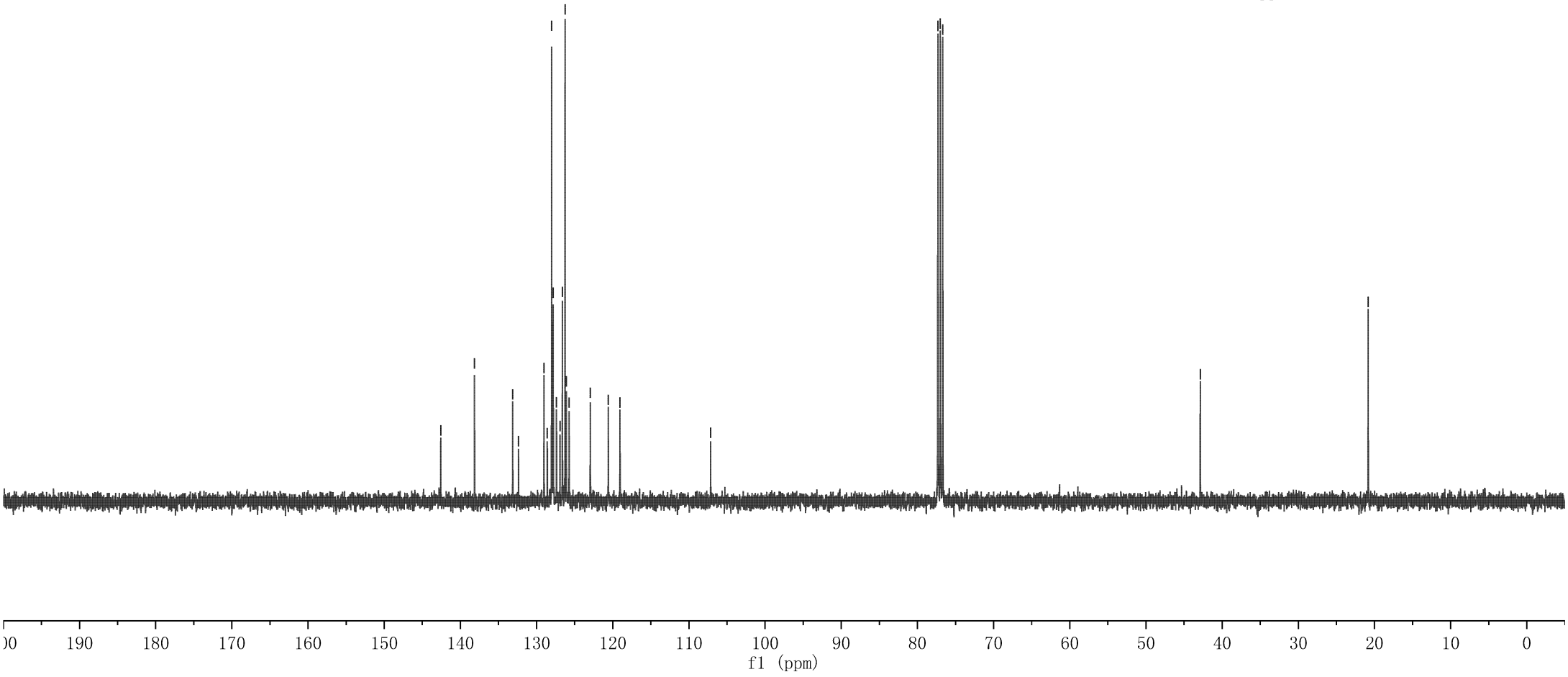


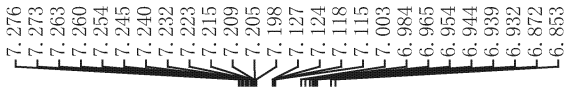


Parameter	Value
1 Title	XHJ-2-48-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	40
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-30T10:21:09
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

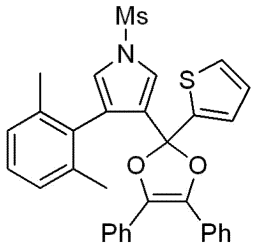


3v





Parameter	Value
1 Title	XHJ-2-66-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	2022-05-12T14:09:59
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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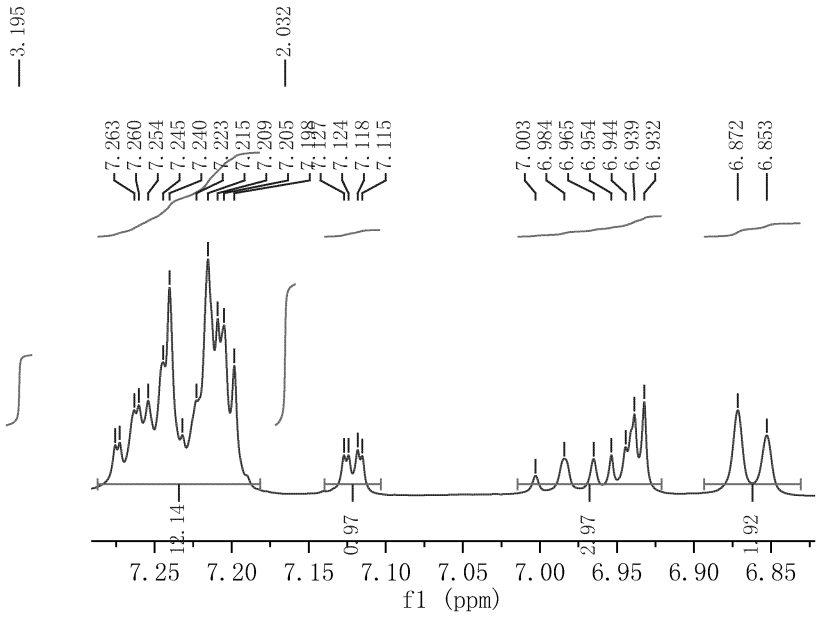
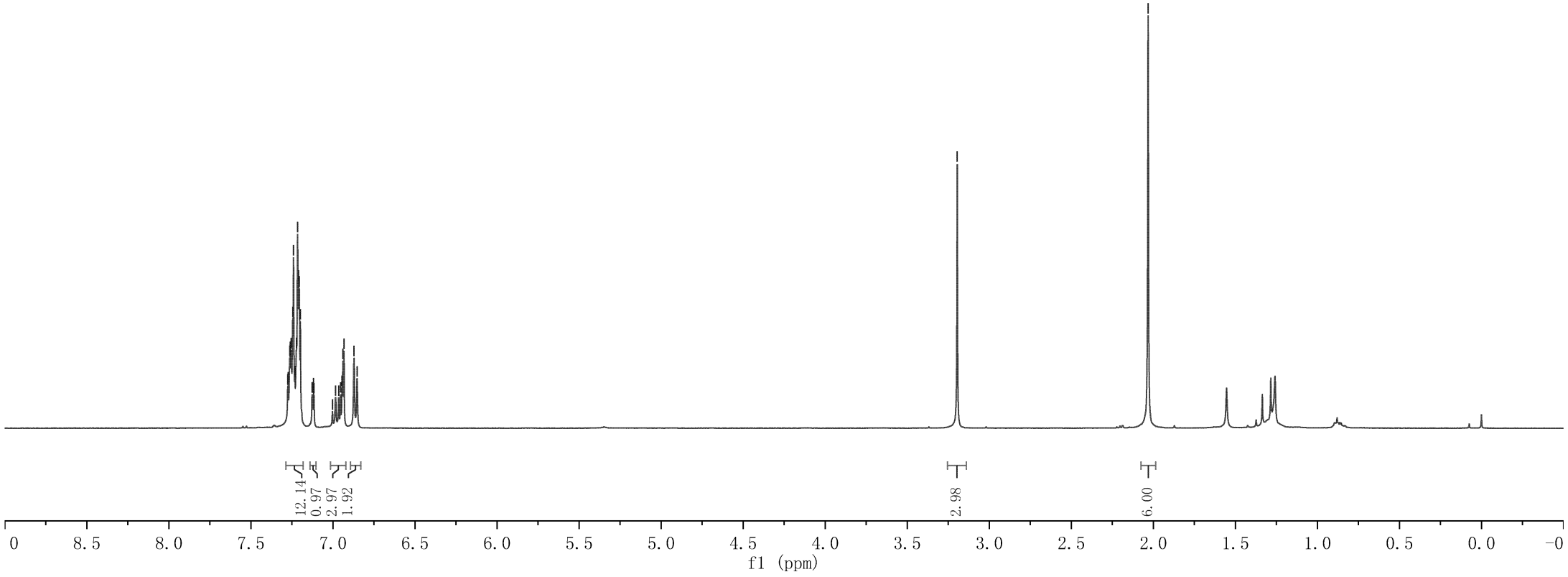
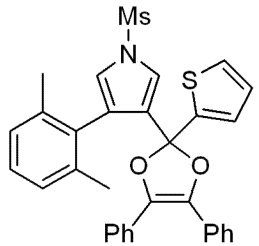


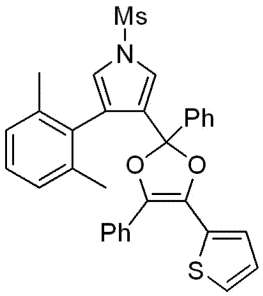


Parameter	Value
1 Title	XHJ-2-66-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	39
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-12T14:10:55
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

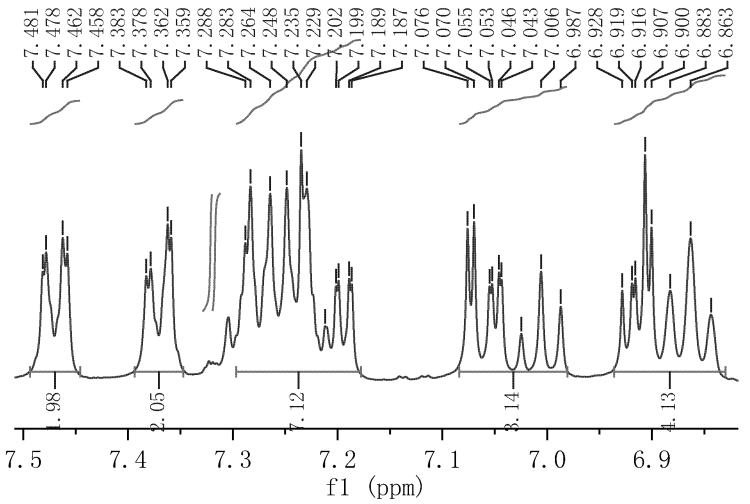


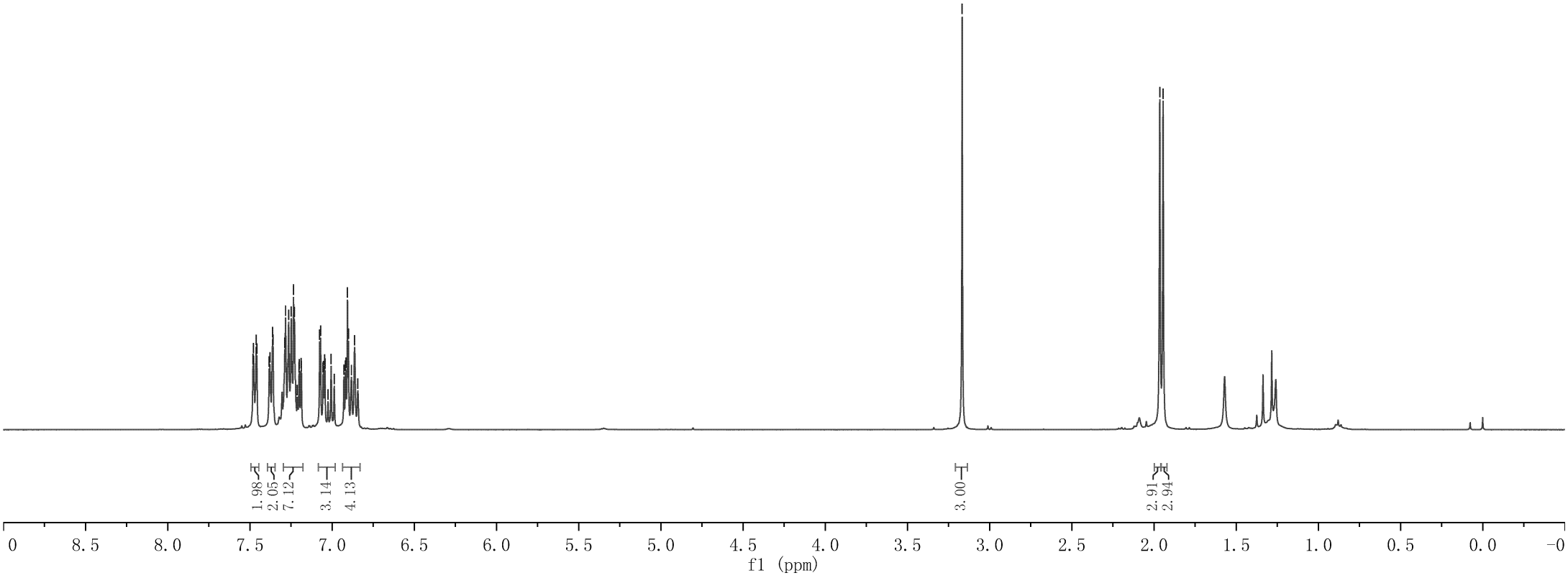
3w

Parameter	Value
1 Title	XHJ-2-105-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	2022-06-13T15:32:10
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

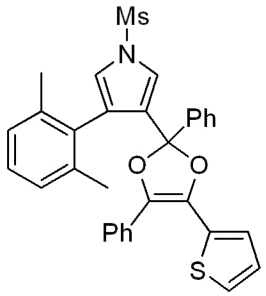


3x



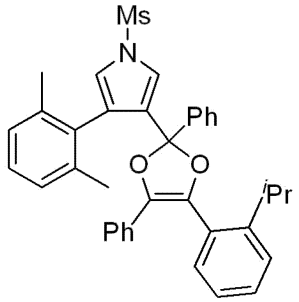


Parameter	Value
1 Title	XHJ-2-105-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	31
6 Acquisition Time	1.3631
7 Acquisition Date	2022-06-13T15:34:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

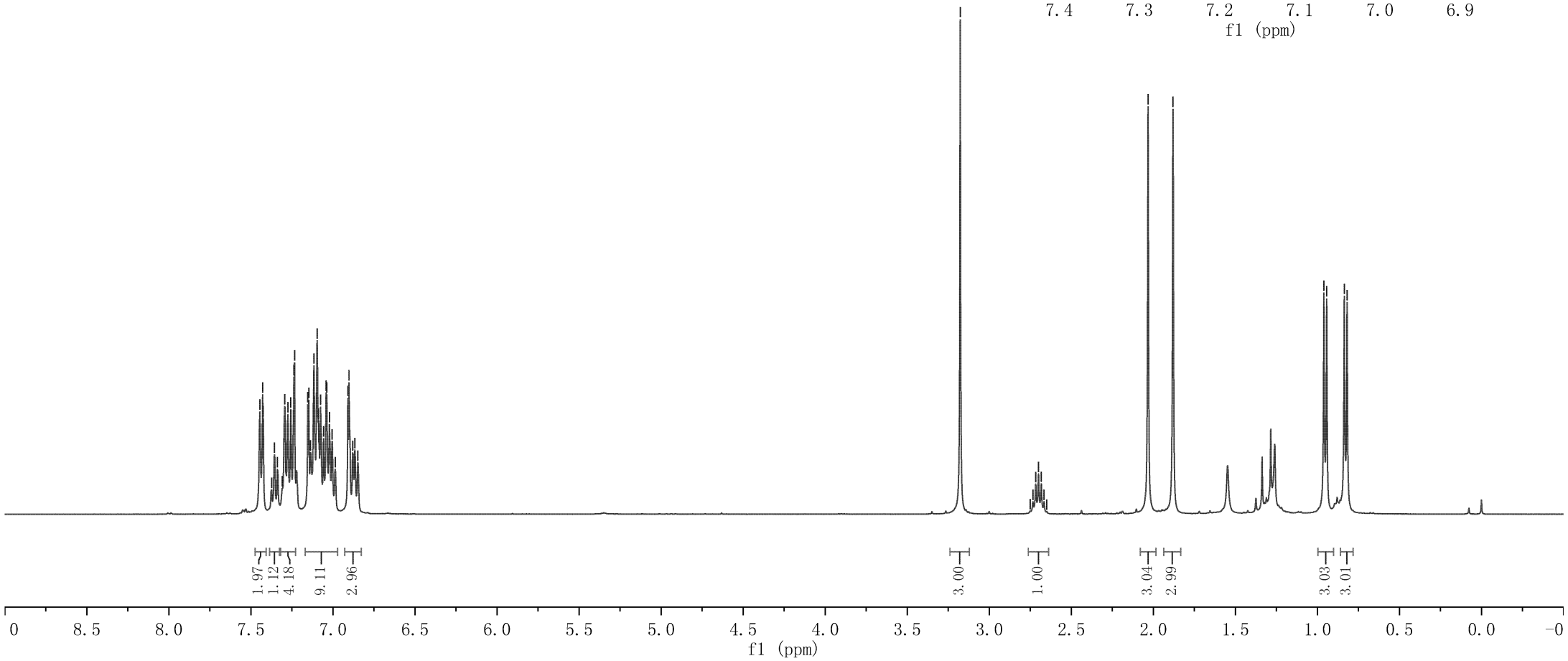


3x

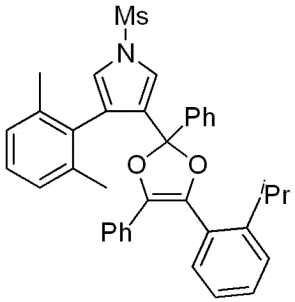
Parameter	Value
1 Title	XHJ-2-91-2-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	10
6 Acquisition Time	4.0894
7 Acquisition Date	2022-06-03T15:34:37
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



3y



Parameter	Value
1 Title	XHJ-2-91-2-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	2022-06-03T15:36:16
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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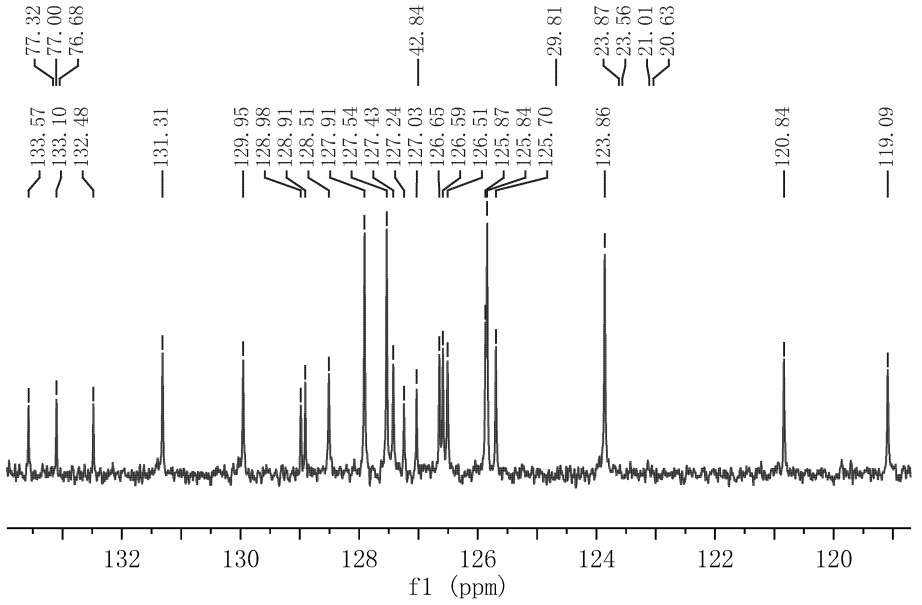
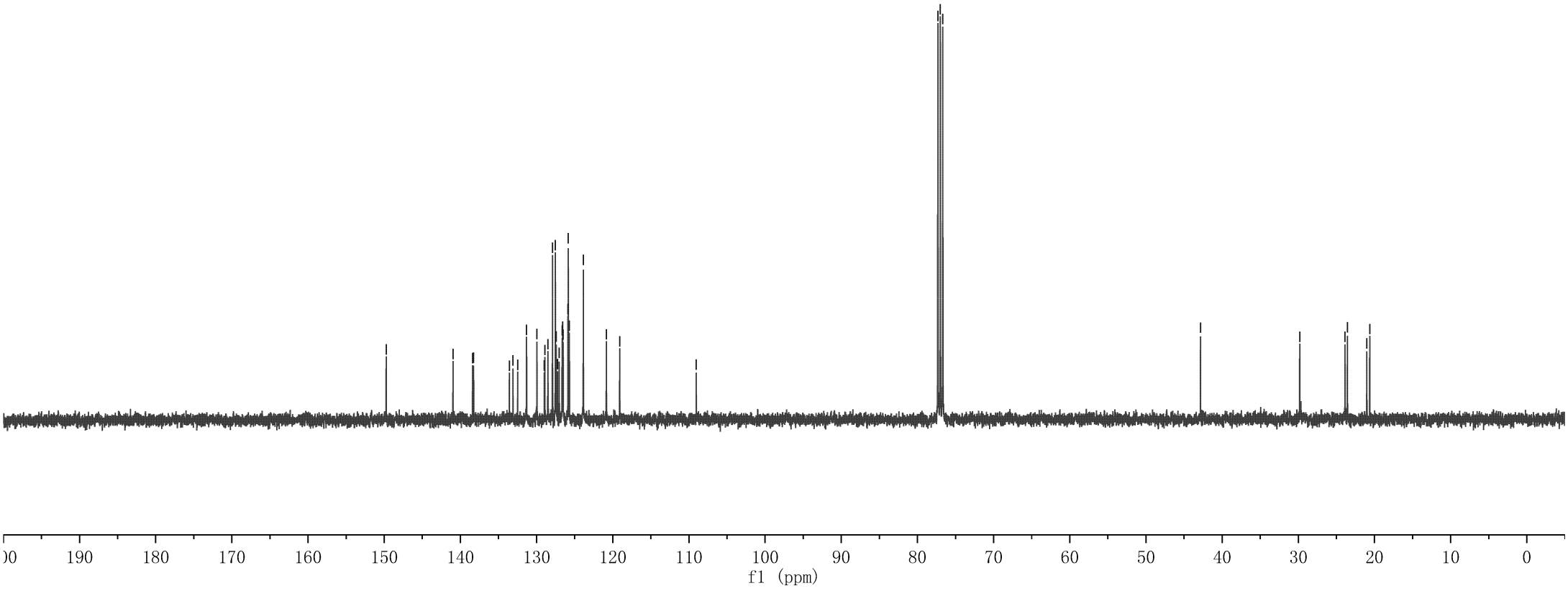




7.692 7.672 7.651 7.631 7.350 7.332 7.279 7.260 7.164 7.100 7.082 7.047 7.028 7.000 6.983 6.966 6.916 6.844 6.830 6.757 6.737

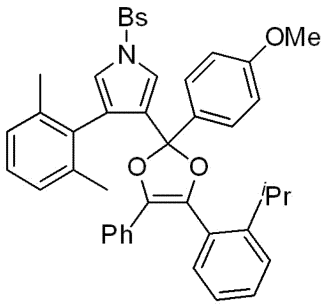
3.791

2.733 2.717 2.701

1.896 1.745

0.963 0.947 0.859 0.842

Parameter	Value
1 Title	XHJ-2-134-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	2022-06-28T10:54:01
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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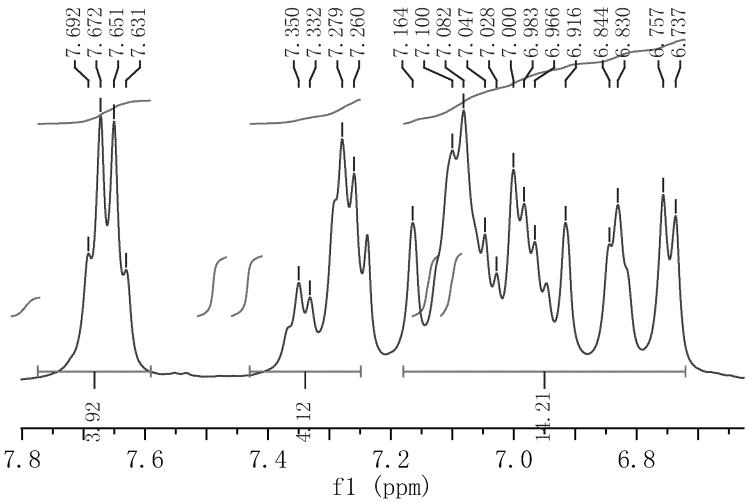
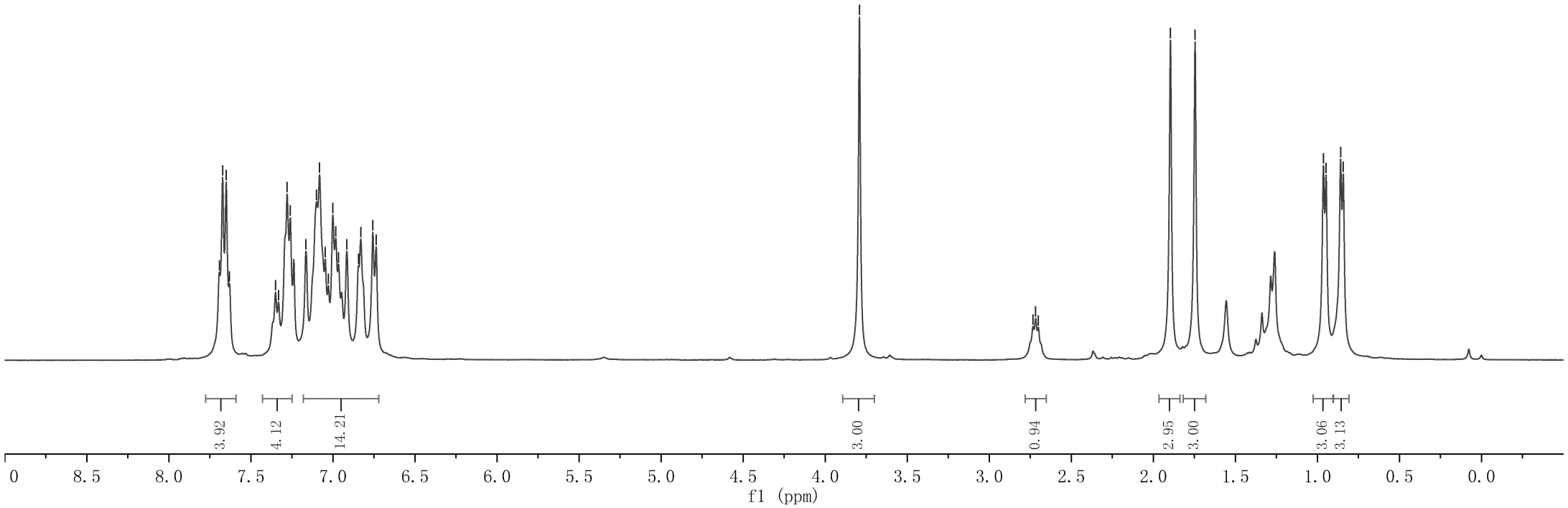
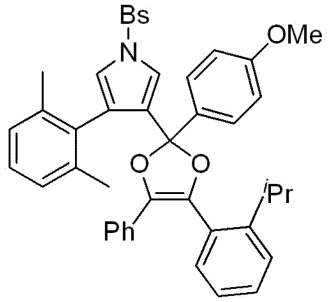




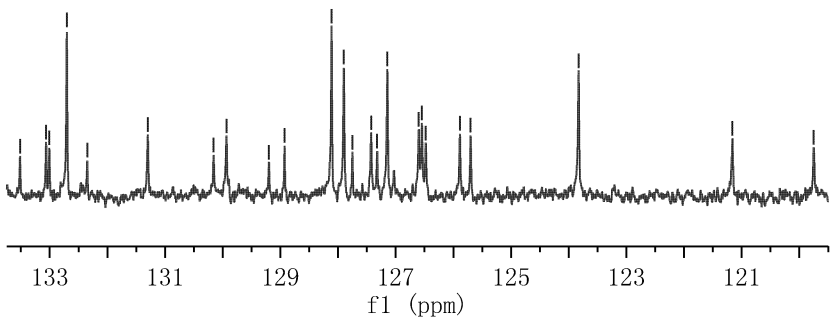
Parameter	Value
1 Title	XHJ-2-125-C-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	192
6 Acquisition Time	1.3631
7 Acquisition Date	2022-06-23T15:35:08
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

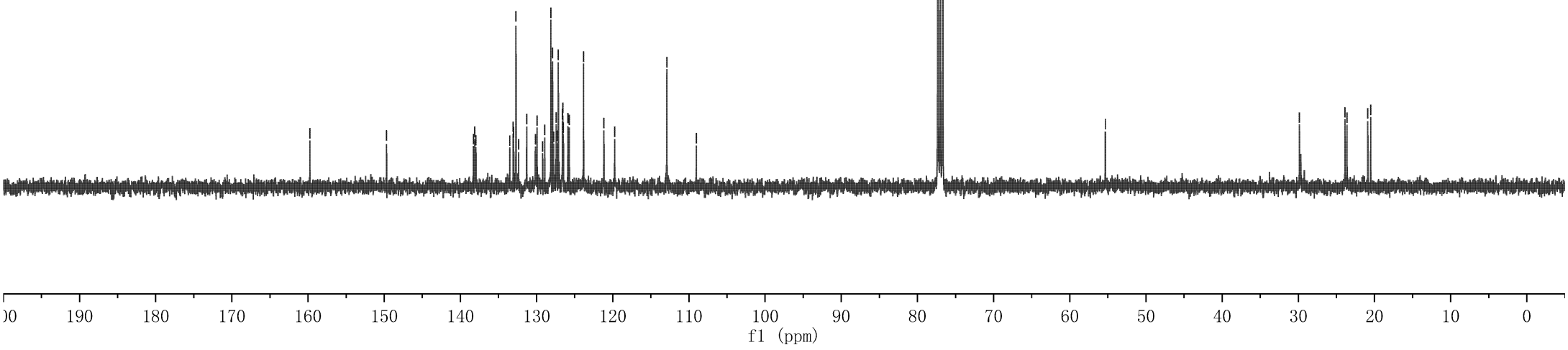


3z

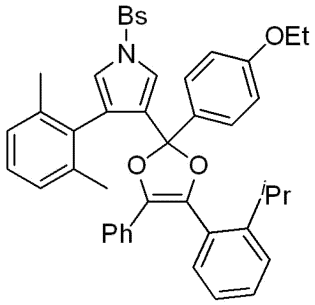
159.76 149.69 138.29 138.12 137.96 132.70 131.30 128.11 127.90 127.43 127.14 126.60 126.55 125.89 125.70 109.02 77.32 77.00 76.68 55.33 29.85 23.87 23.62 20.88 20.50

133.51 133.06 133.01 132.70 132.35 131.30 130.16 129.94 129.20 128.93 128.11 127.90 127.75 127.43 127.32 127.14 126.60 126.55 126.48 125.89 125.70 123.83 121.16 119.75





Parameter	Value
1 Title	XHJ-2-132-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	2022-06-27T15:38:22
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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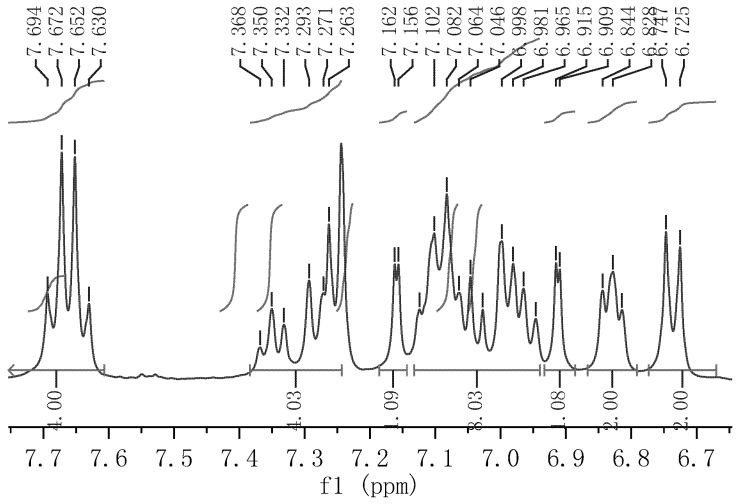
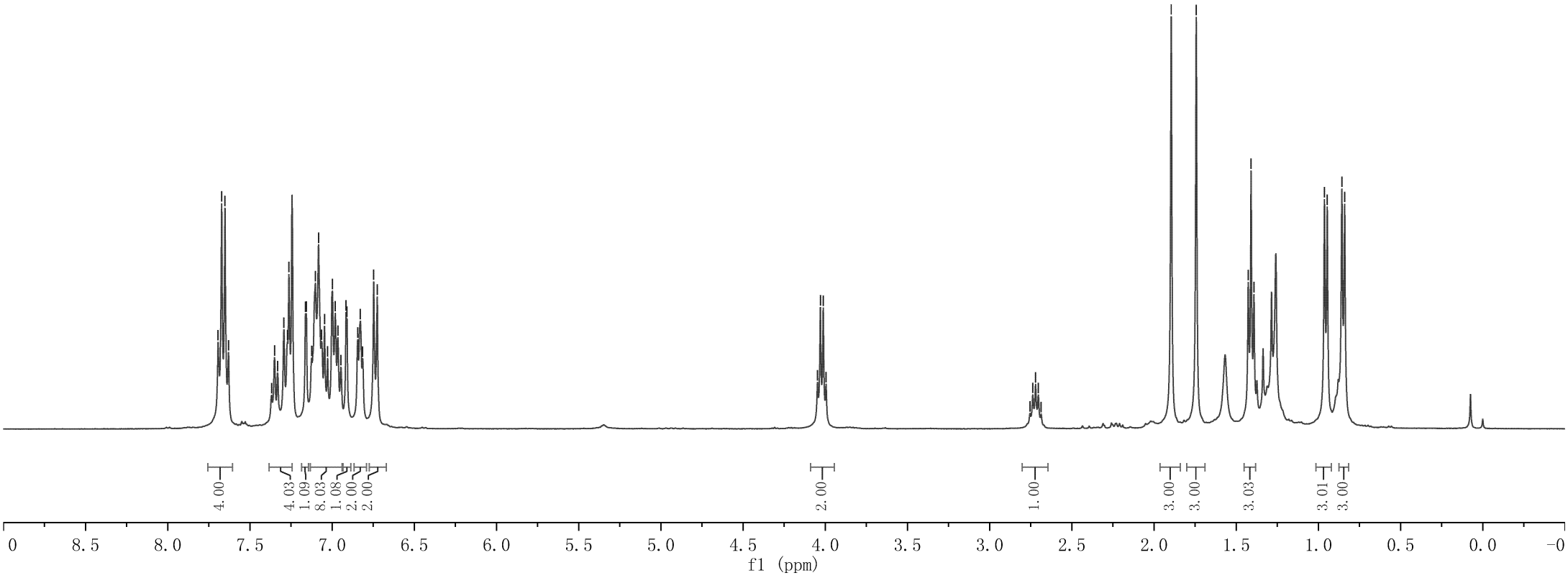
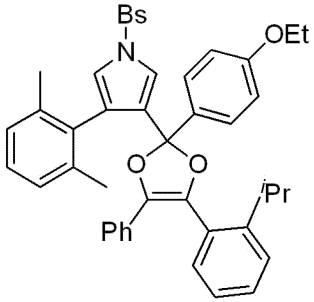




Parameter	Value
1 Title	XHJ-2-132-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	100
6 Acquisition Time	1.3631
7 Acquisition Date	2022-06-27T15:40:30
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

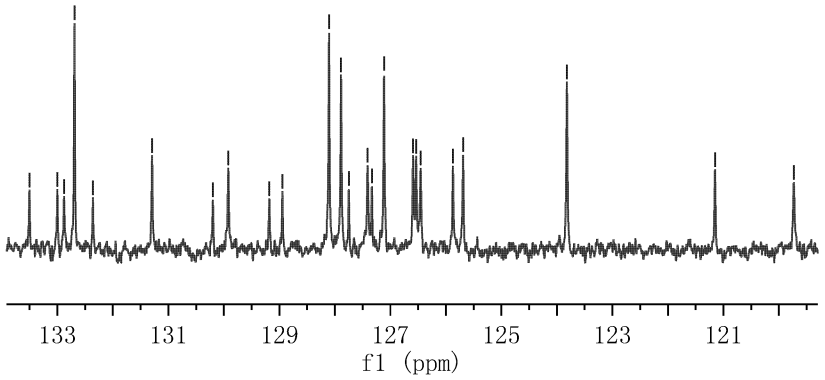


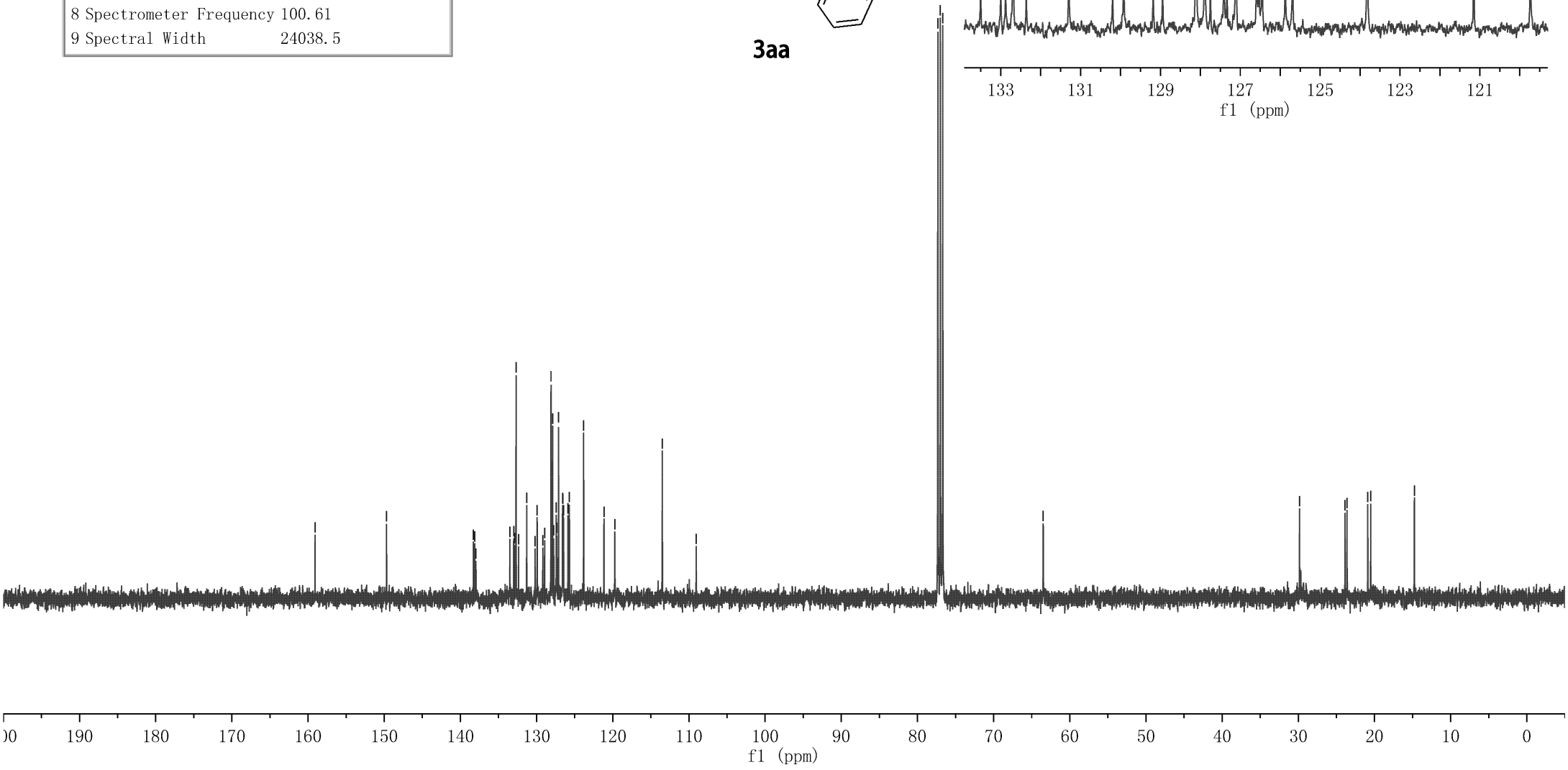
3aa

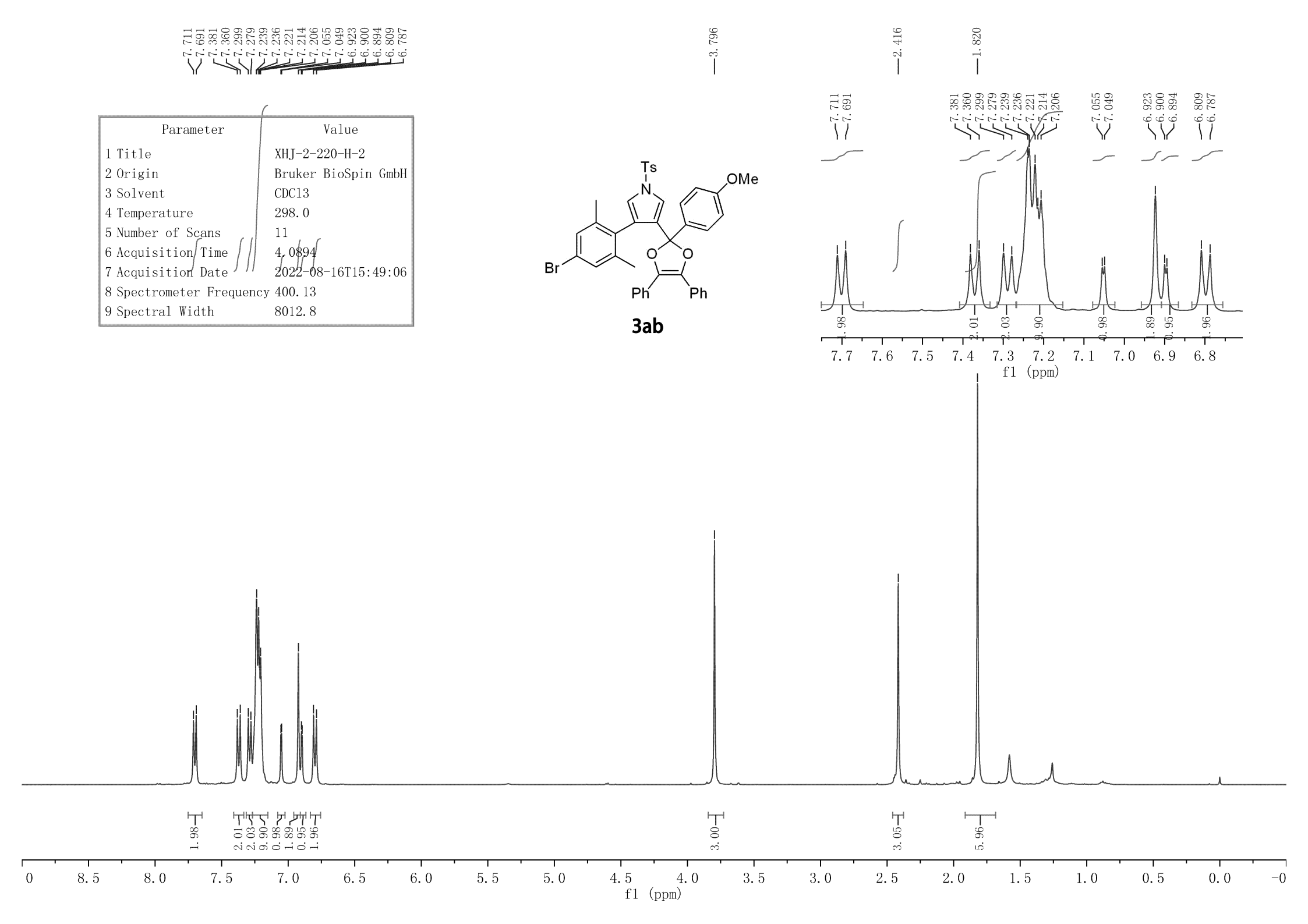
159.08 149.69 138.29 138.13 137.96 132.69 131.29 128.11 127.89 127.41 127.11 126.59 126.54 125.69 109.05

77.32 77.00 76.68 63.49 29.84 23.87 23.61 20.88 20.50 14.77

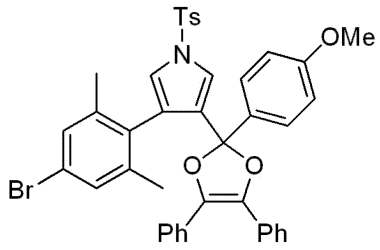
133.50 133.00 132.88 132.69 132.36 131.29 130.20 129.92 129.18 128.95 128.11 127.89 127.75 127.41 127.33 127.11 126.59 126.54 126.46 125.87 125.69 123.82 121.15 119.73





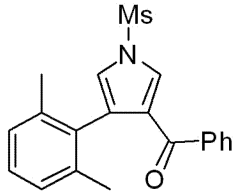

7.711
7.691
7.381
7.360
7.299
7.279
7.239
7.236
7.221
7.214
7.206
7.055
7.049
6.923
6.900
6.894
6.809
6.787
3.796
2.416
1.820
Parameter
Value
1 Title
XHJ-2-220-H-2
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
298.0
5 Number of Scans
11
6 Acquisition Time
4.0894
7 Acquisition Date
2022-08-16T15:49:06
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
Ts
N
OMe
Br
O
O
Ph
Ph
3ab
1.98
2.01
2.03
9.90
0.98
1.89
0.95
1.96
3.00
3.05
5.96
f1 (ppm)

Parameter	Value
1 Title	XHJ-2-220-C-3
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	51
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-16T15:51:41
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

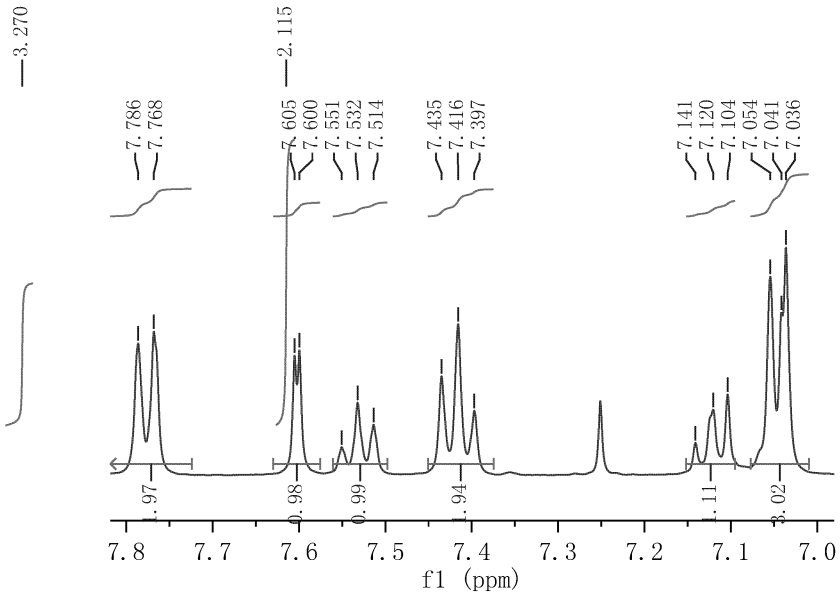


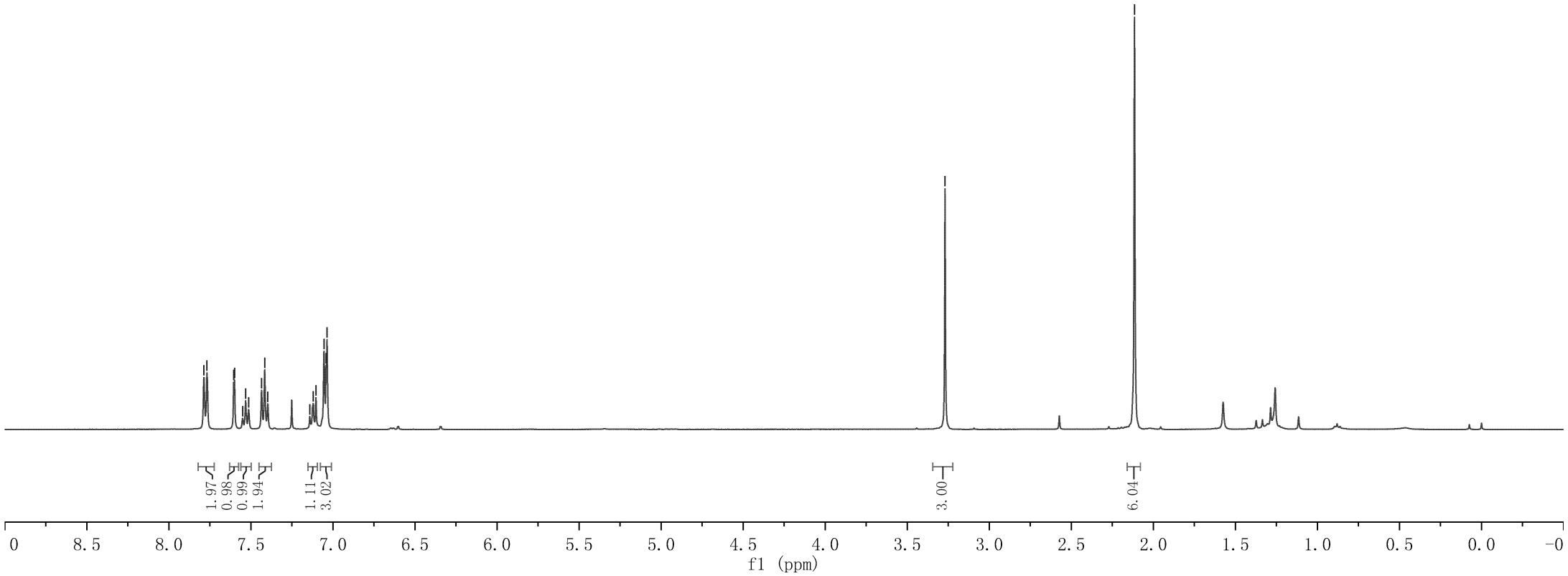
3ab

Parameter	Value
1 Title	XHJ-3-132-H-2
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	2022-11-02T20:57:18
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



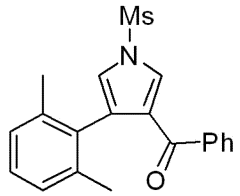
3a′



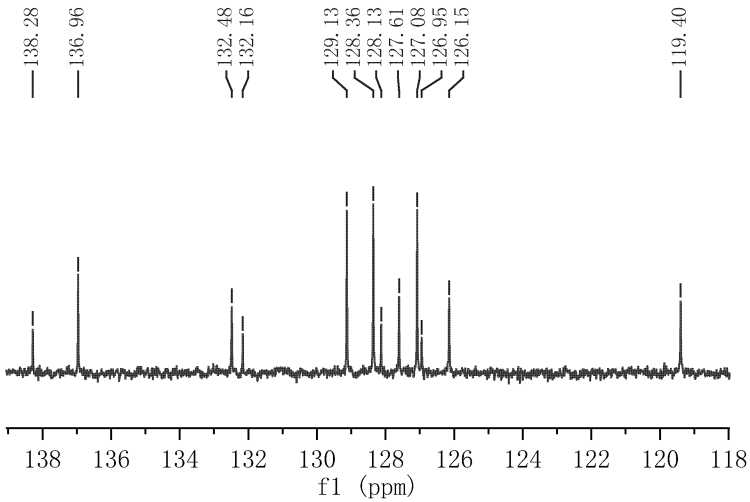


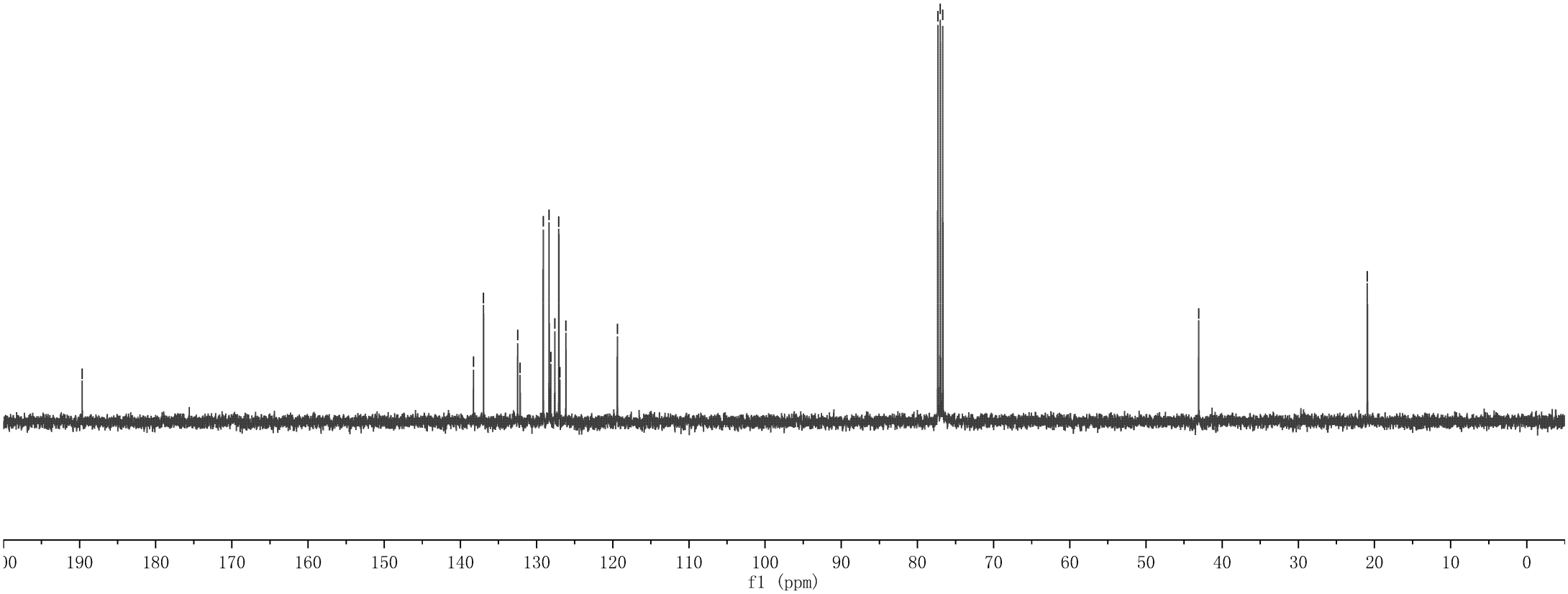
189.65
138.28
136.96
132.48
129.13
128.36
128.13
127.61
127.08
126.15
119.40
77.32
77.00
76.68
43.08
20.94

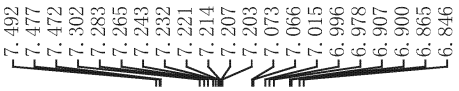
Parameter	Value
1 Title	XHJ-3-132-C-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	52
6 Acquisition Time	1.3631
7 Acquisition Date	2022-11-02T20:58:31
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



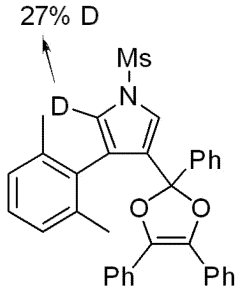
3a′



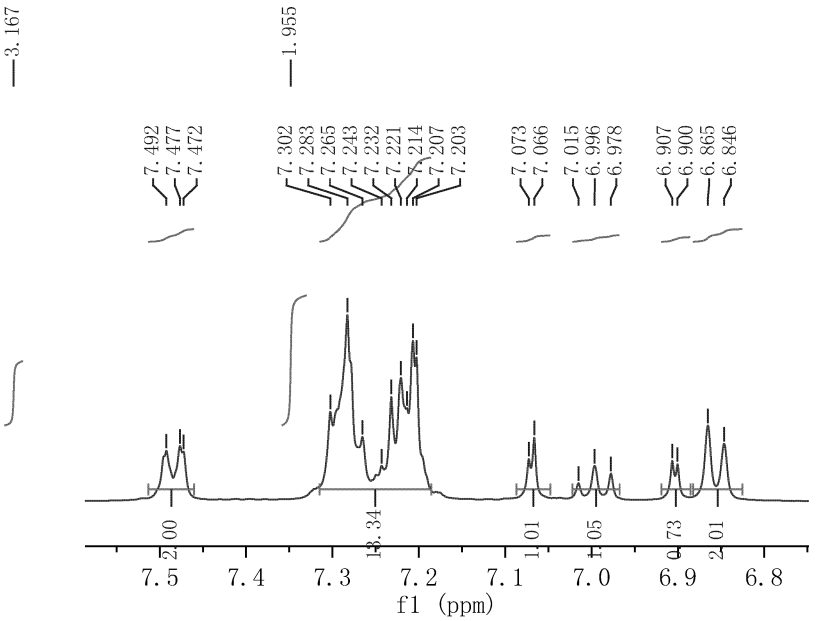


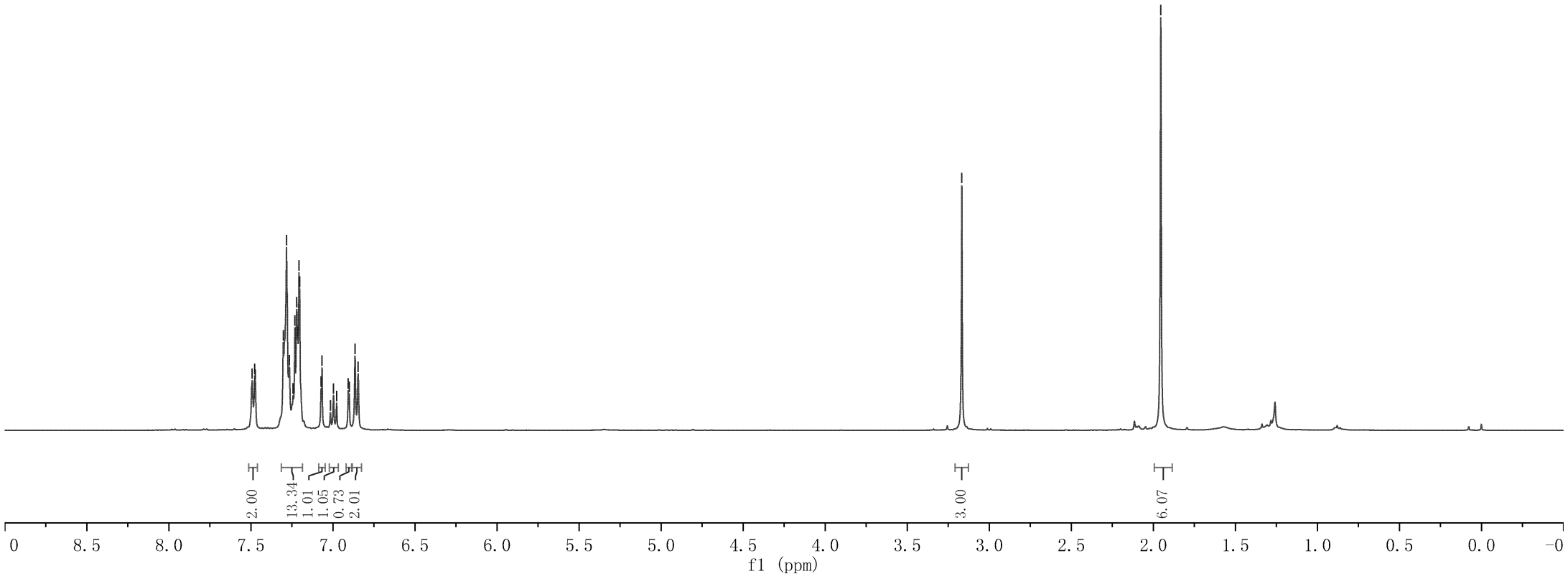


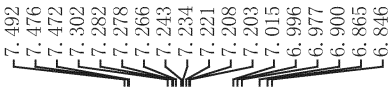
Parameter	Value
1 Title	XHJ-3-130-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	11
6 Acquisition Time	4.0894
7 Acquisition Date	2022-11-02T08:01:07
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



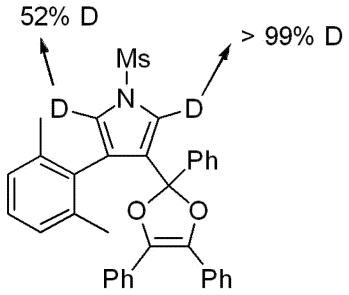
[D1]-3a







Parameter	Value
1 Title	XHJ-3-131-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	2022-11-02T14:22:57
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



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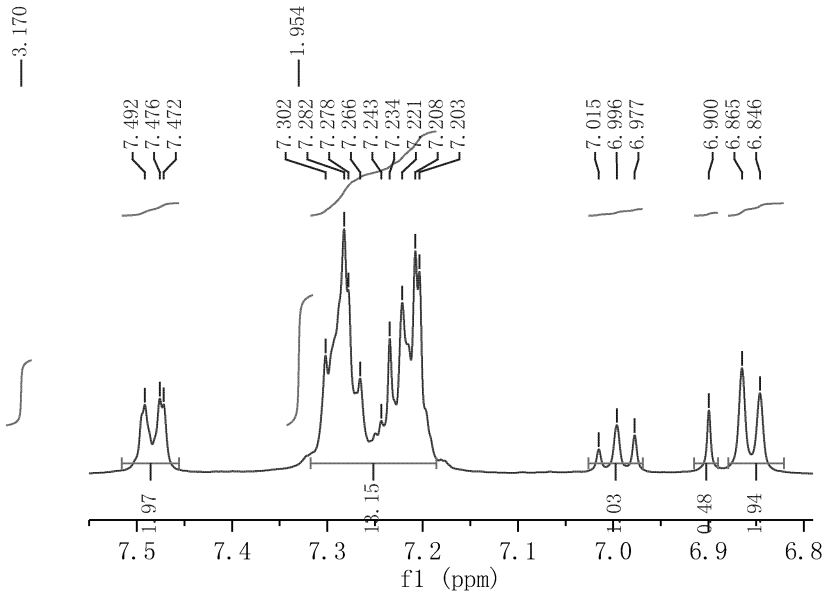
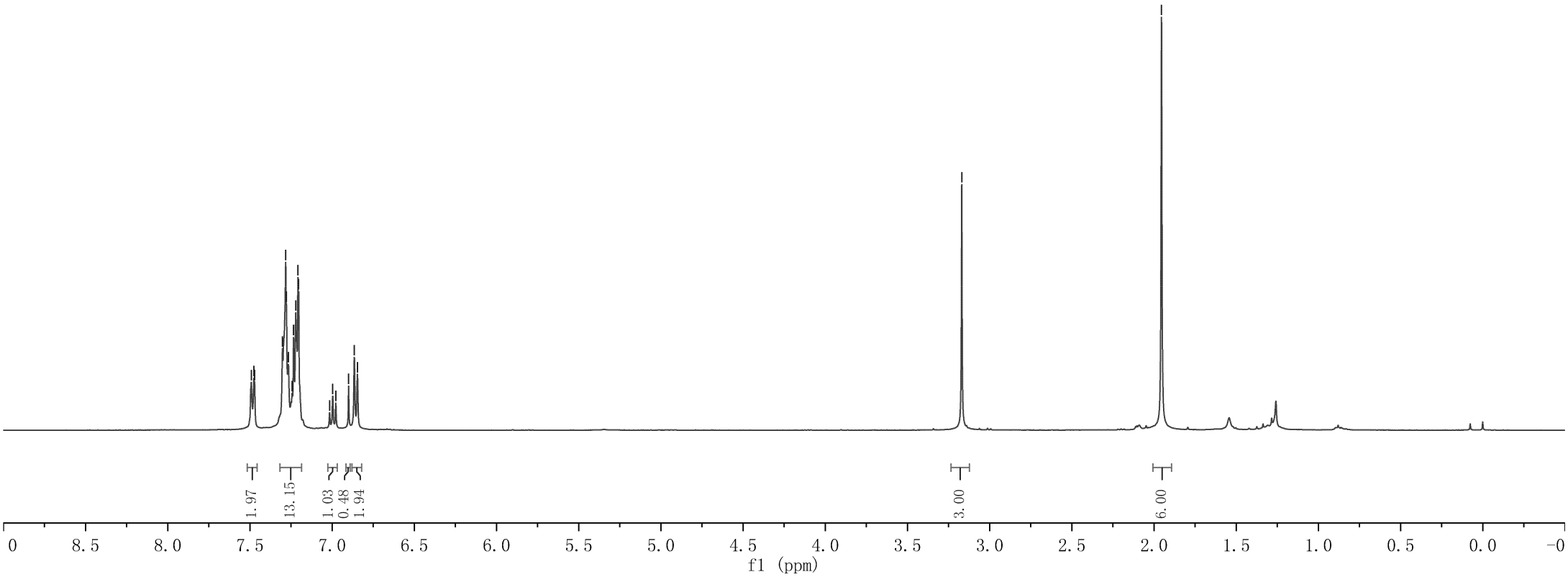
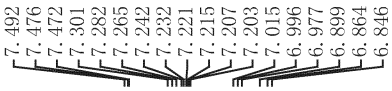
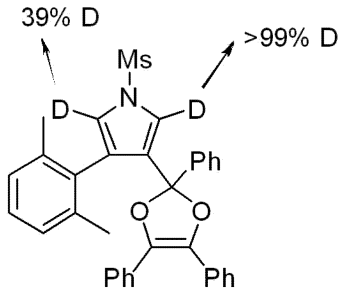


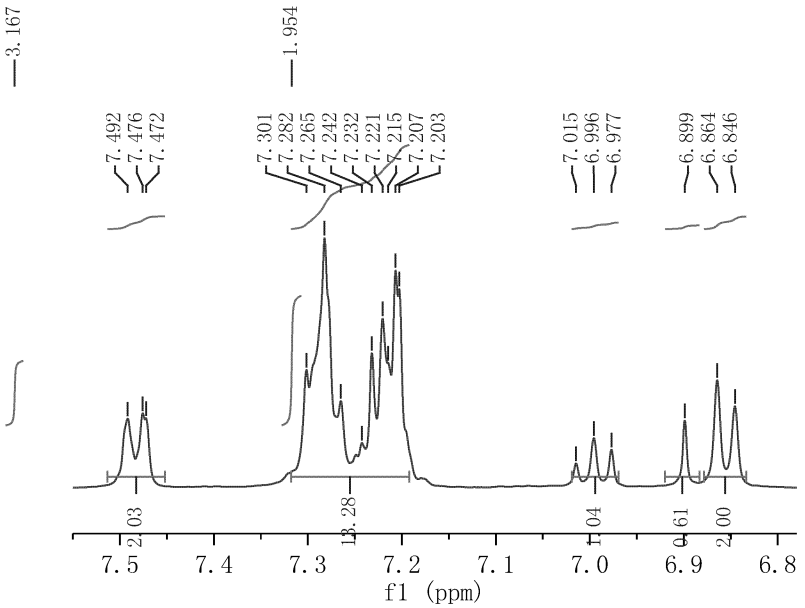


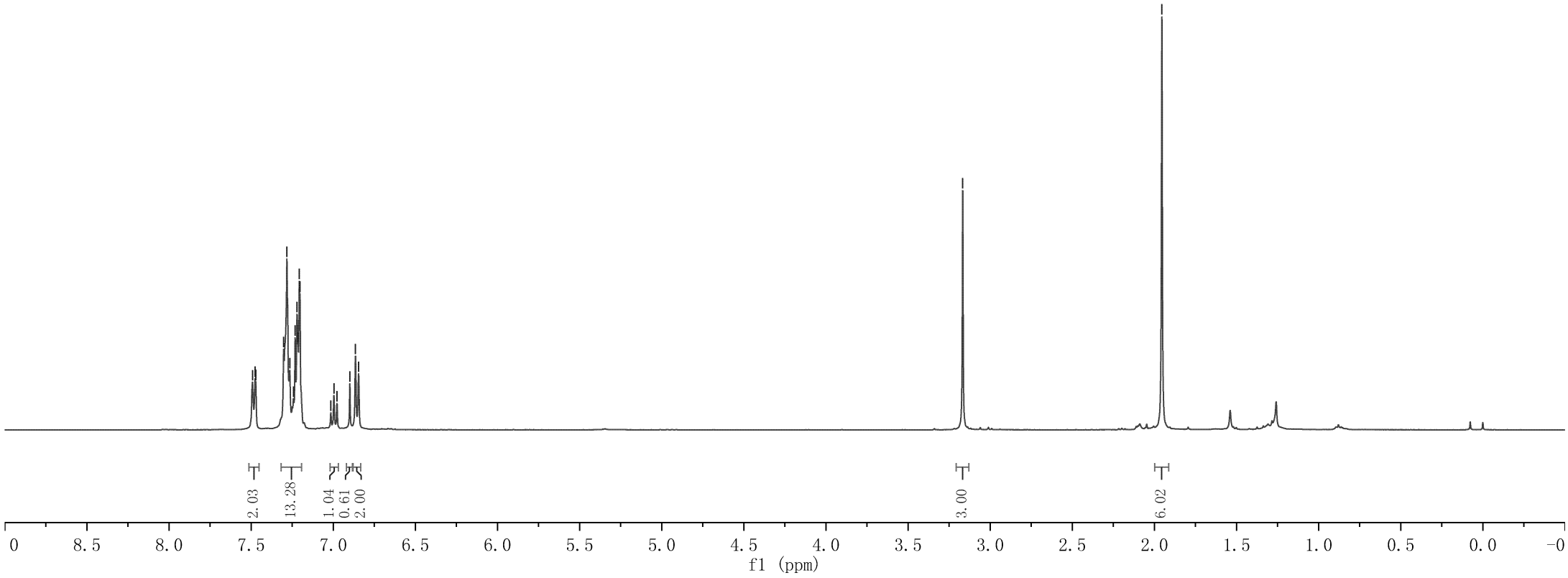


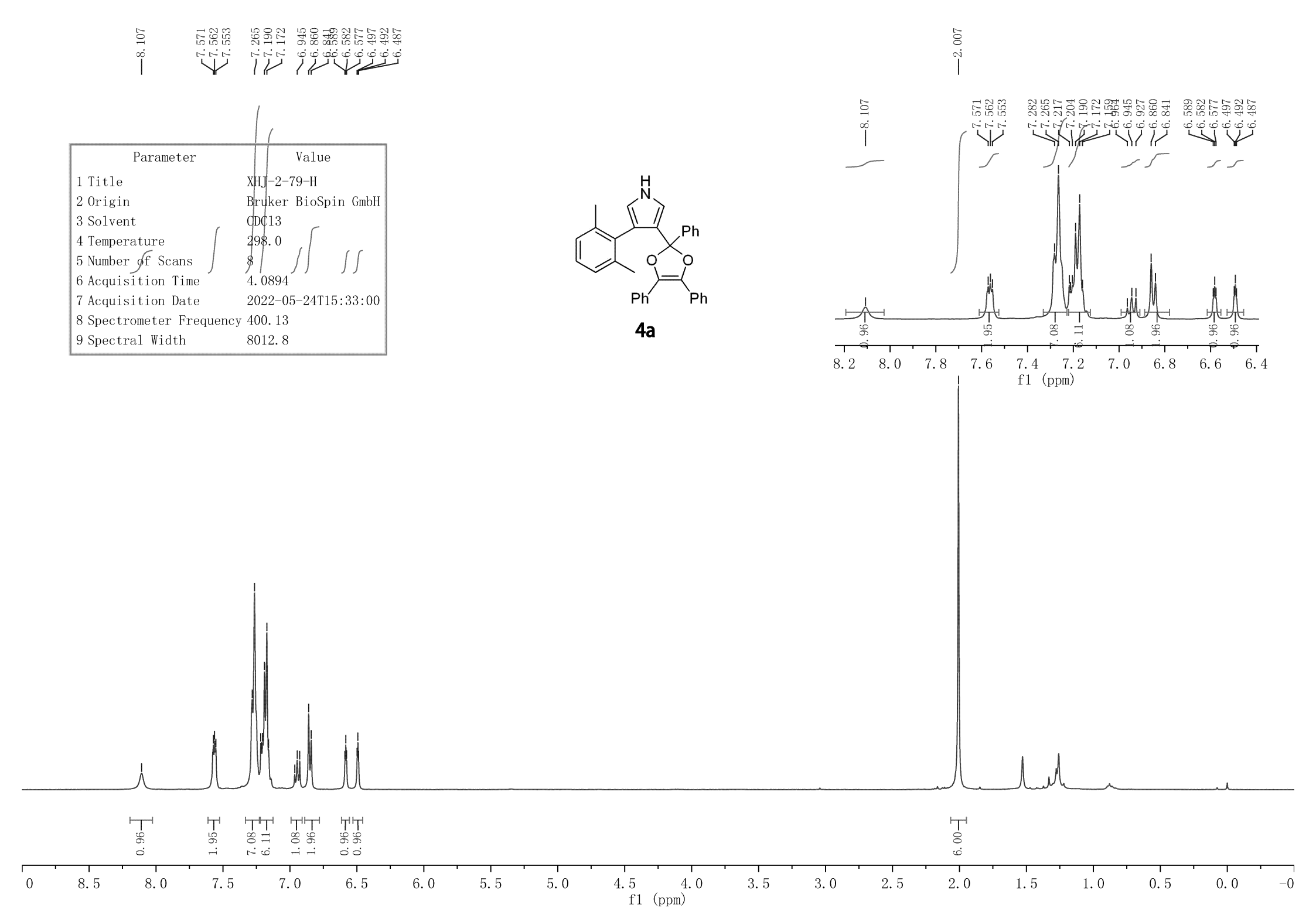
Parameter	Value
1 Title	XHJ-3-142-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	5
6 Acquisition Time	4.0894
7 Acquisition Date	2022-11-08T18:16:42
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

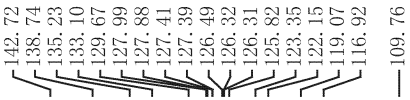


[D2]-3a

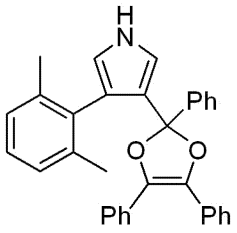




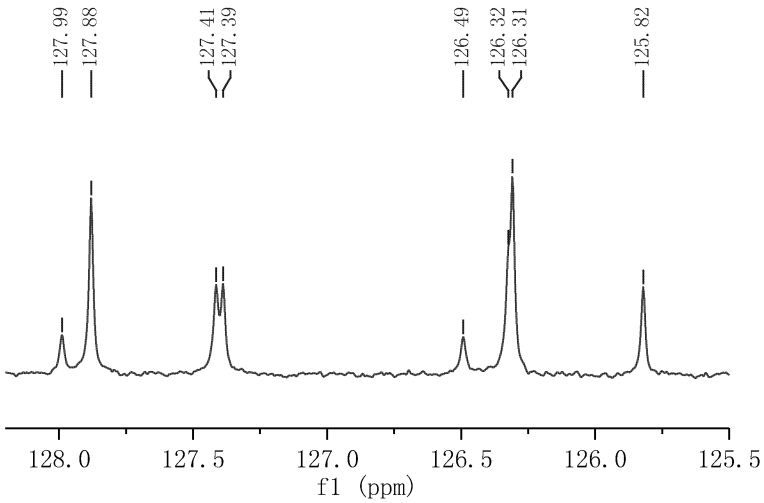

8.107
7.571
7.562
7.553
7.265
7.190
7.172
6.945
6.860
6.841
6.589
6.582
6.577
6.497
6.492
6.487
2.007
Parameter Value
1 Title XHJ-2-79-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-05-24T15:33:00
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
H
N
Ph
O
O
Ph
Ph
4a
0.96
1.95
7.08
6.11
1.08
1.96
0.96
0.96
6.00
f1 (ppm)

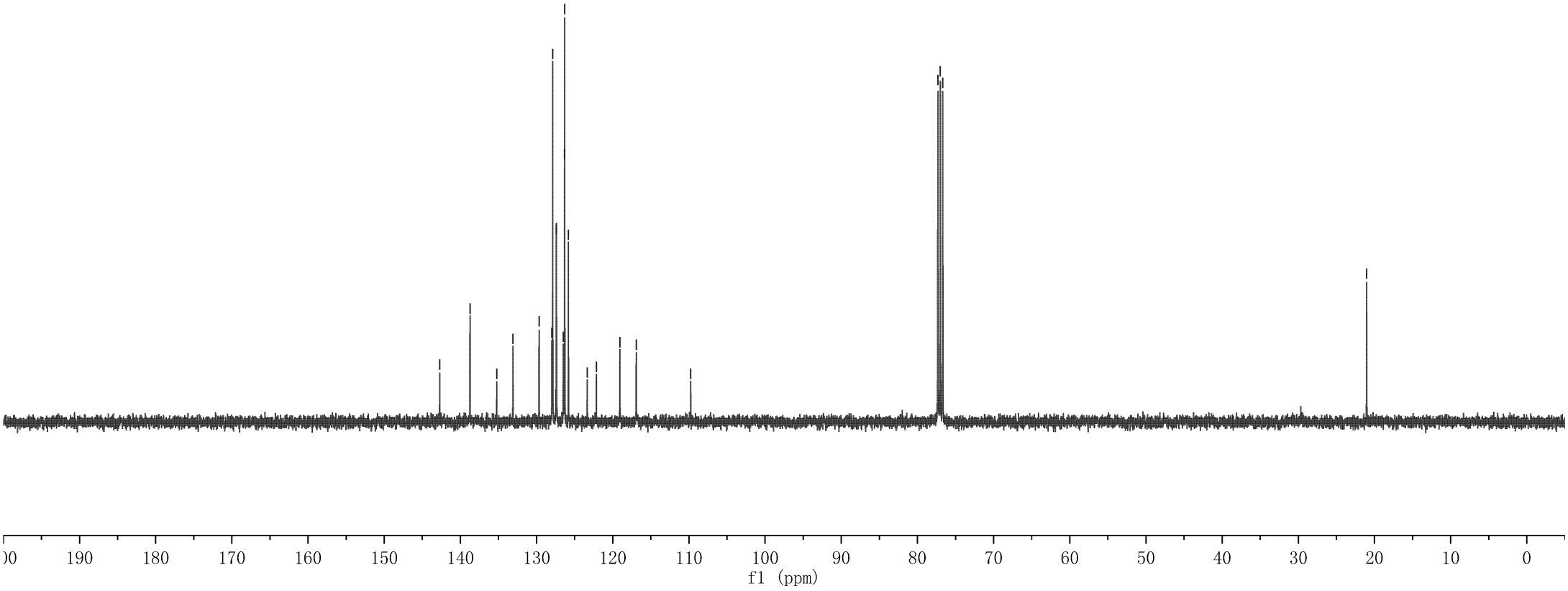


Parameter	Value
1 Title	XHJ-2-79-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	44
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-24T15:34:47
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

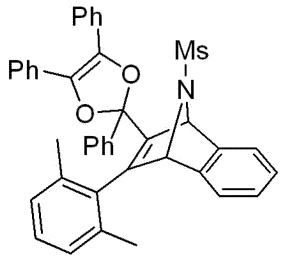


4a

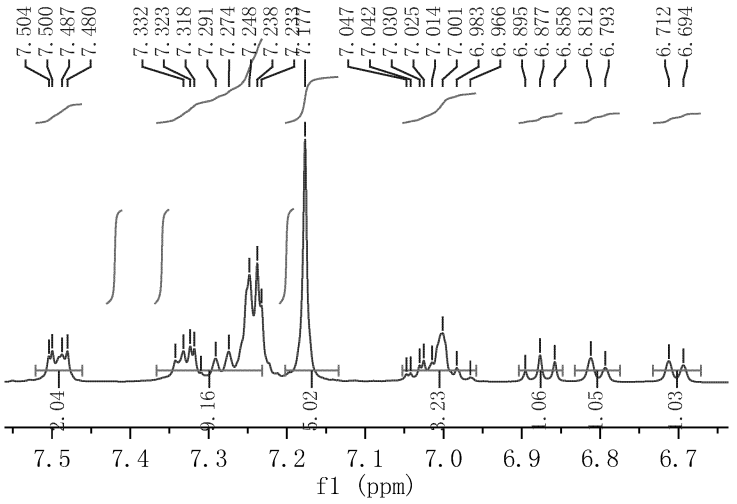


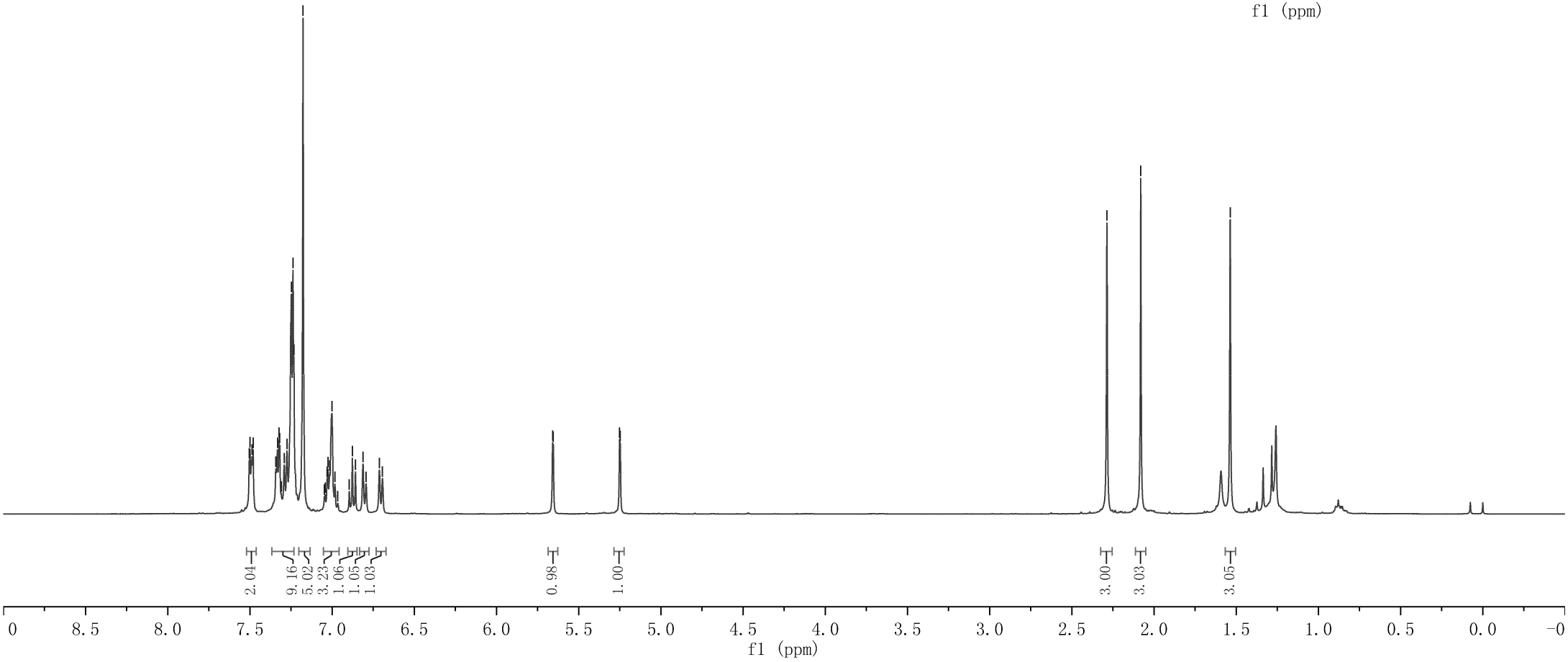


Parameter	Value
1 Title	XHJ-2-78-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	16
6 Acquisition Time	4.0894
7 Acquisition Date	2022-05-25T15:29:15
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

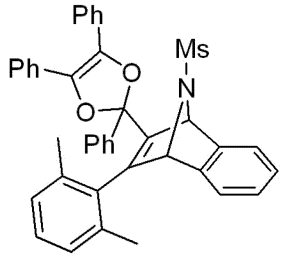


4b





Parameter	Value
1 Title	XHJ-2-78-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	2022-05-25T15:31:10
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



4b