Supporting Information

Efficient synthesis of tetracyclic γ-lactams via gold-catalyzed oxidative cyclization of alkenyl diynes

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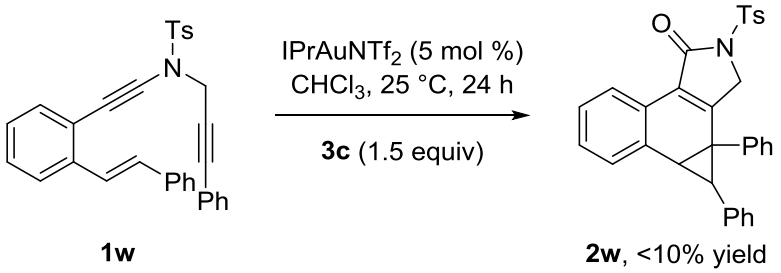
General Information. Ethyl acetate (ACS grade), hexanes (ACS grade) and $HCCl_3$ (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a NicoletAVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass $QTOF_2$ Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

^1H 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. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant(s) in Hz, integration).

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

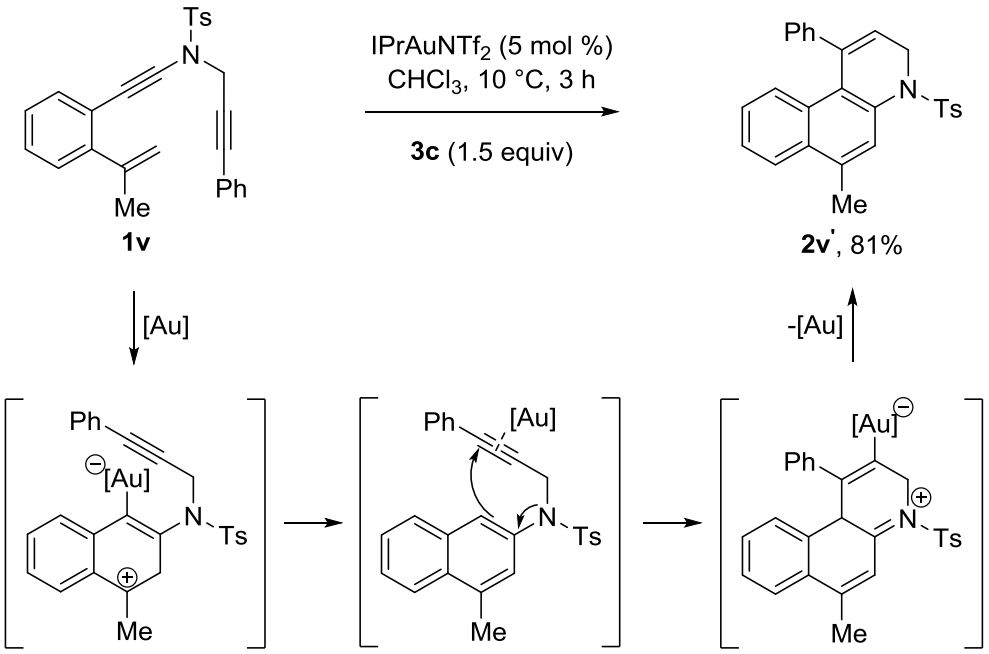
More Substrate Scope Study

1. The use of Ph-substituted alkene-diyne **1w** only led to a complicated mixture of products (<10% yield of the desired product **2w**) under the relevant reaction conditions



1w **2w**, <10% yield

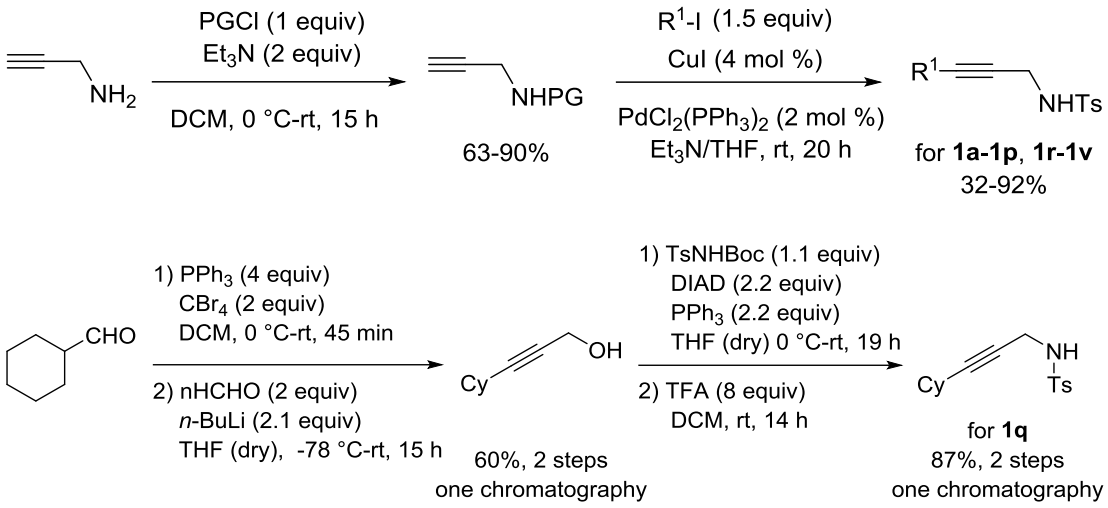
2. In the case of ynamide **1v**, the corresponding tricyclic compound **2v′** was obtained as the main byproduct.



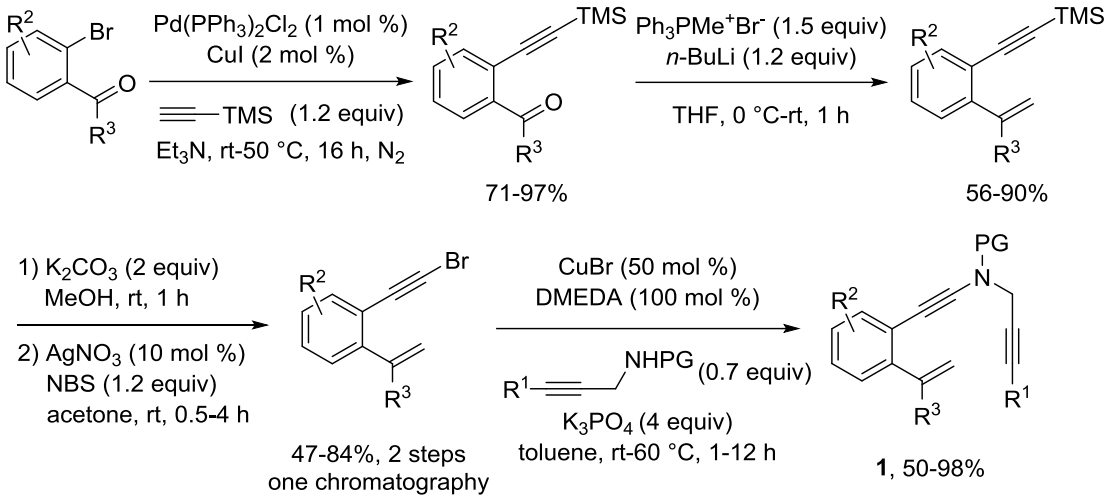
1v **2v′**, 81%

Representative synthetic procedures for the preparation of alkenyl diynes 1.

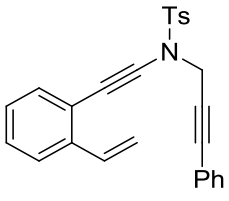
1. Propargyl amide derivatives were prepared according to the following procedures.[1]



2. Alkenyl diynes 1a-1v were prepared according to the following procedures.[2-3]



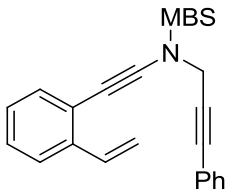
4-methyl-*N*-(3-phenylprop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1a)



1a

The product **1a** was afforded as a pale yellow oil (74%, 304.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.39 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.31 – 7.20 (m, 6H), 7.20 – 7.07 (m, 4H), 5.72 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.11 (dd, *J* = 11.2, 1.2 Hz, 1H), 4.58 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 138.9, 134.8, 134.2, 132.3, 131.6, 129.6, 128.6, 128.2, 128.1, 127.4, 124.4, 121.9, 121.3, 115.3, 86.5, 86.3, 81.1, 69.6, 42.9, 21.5; IR (neat): 3063, 2923, 2232, 1596, 1485, 1367, 1169, 1089, 920, 595; HRESIMS Calcd for $[C_{26}H_{21}NNaO_2S]^+$ (M + Na^+) 434.1185, found 434.1182.

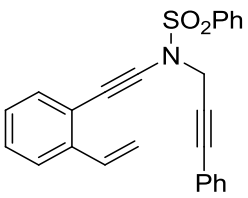
4-methoxy-*N*-(3-phenylprop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1b)



1b

The product **1b** was afforded as a pale yellow oil (81%, 345.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.90 (m, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.38 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 – 7.09 (m, 8H), 6.92 – 6.82 (m, 2H), 5.72 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.11 (dd, *J* = 10.8, 0.8 Hz, 1H), 4.55 (s, 2H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 138.7, 134.6, 132.2, 131.5, 130.3, 128.5, 128.3, 127.9(9), 127.9(7), 127.3, 124.3, 121.7, 121.1, 115.2, 114.0, 86.4(1), 86.3(8), 81.2, 69.4, 55.4, 42.6; IR (neat): 2926, 2231, 1595, 1497, 1366, 1163, 1090, 920, 755, 593; HRESIMS Calcd for $[C_{26}H_{21}NNaO_3S]^+$ (M + Na^+) 450.1134, found 450.1130.

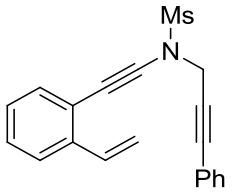
***N*-(3-phenylprop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1c)**



1c

The product **1c** was afforded as a pale yellow oil (98%, 389.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.2 Hz, 2H), 7.66 – 7.44 (m, 4H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.35 – 7.04 (m, 8H), 5.72 (d, *J* = 17.2 Hz, 1H), 5.10 (d, *J* = 10.8 Hz, 1H), 4.61 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.9, 137.2, 134.8, 133.8, 132.4, 131.6, 129.0, 128.7, 128.2, 128.1, 127.4, 124.5, 121.8, 121.1, 115.4, 86.7, 86.0, 81.0, 69.7, 42.9; IR (neat): 2925, 2232, 1698, 1489, 1367, 1171, 1089, 920, 756, 596; HRESIMS Calcd for $[C_{25}H_{19}NNaO_2S]^+$ (M + Na^+) 420.1029, found 420.1025.

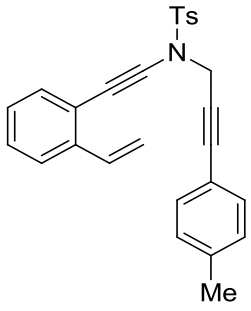
***N*-(3-phenylprop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)methanesulfonamide (1d)**



1d

The product **1d** was afforded as a pale yellow oil (75%, 251.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.53 (m, 1H), 7.49 – 7.41 (m, 3H), 7.37 – 7.16 (m, 6H), 5.78 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.23 (dd, *J* = 10.8, 0.8 Hz, 1H), 4.62 (s, 2H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 134.7, 132.3, 131.8, 129.1, 128.4, 128.3, 127.4, 124.6, 121.6, 120.8, 115.7, 87.1, 85.6, 81.5, 69.9, 42.9, 38.6; IR (neat): 2928, 2233, 1698, 1490, 1360, 1165, 1038, 920, 759, 517; HRESIMS Calcd for $[C_{20}H_{17}NNaO_2S]^+$ (M + Na^+) 358.0872, found 358.0874.

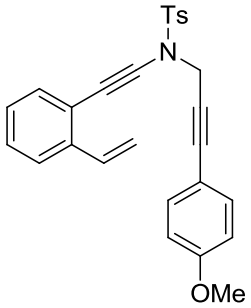
4-methyl-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1e)



1e

The product **1e** was afforded as a pale yellow oil (98%, 416.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.33 – 6.99 (m, 9H), 5.72 (d, *J* = 17.6 Hz, 1H), 5.12 (d, *J* = 10.8 Hz, 1H), 4.57 (s, 2H), 2.35 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 138.9, 138.7, 134.9, 134.2, 132.3, 131.5, 129.6, 128.8, 128.2, 128.0, 127.3, 124.4, 121.3, 118.8, 115.3, 86.7, 86.3, 80.4, 69.6, 42.9, 21.5, 21.4; IR (neat): 2922, 2232, 1597, 1509, 1367, 1170, 1089, 919, 669, 588; HRESIMS Calcd for $[C_{27}H_{23}NNaO_2S]^+$ (M + Na^+) 448.1342, found 448.1340.

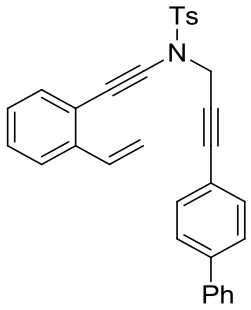
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1f)**



1f

The product **1f** was afforded as a pale yellow oil (90%, 396.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.87 (m, 2H), 7.56 – 7.50 (m, 1H), 7.38 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.30 – 7.07 (m, 7H), 6.81 – 6.72 (m, 2H), 5.73 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.12 (dd, *J* = 10.8, 0.8 Hz, 1H), 4.56 (s, 2H), 3.77 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 144.8, 138.8, 134.9, 134.2, 133.1, 132.3, 129.6, 128.2, 128.0, 127.3, 124.4, 121.3, 115.3, 114.0, 113.7, 86.5, 86.4, 79.7, 69.6, 55.2, 43.0, 21.5; IR (neat): 2924, 2232, 1605, 1509, 1366, 1292, 1249, 1168, 1088, 589; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1293.

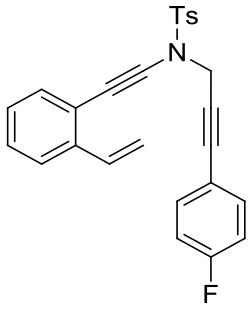
***N*-(3-([1,1'-biphenyl]-4-yl)prop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1g)**



1g

The product **1g** was afforded as a pale yellow oil (96%, 467.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.87 (m, 2H), 7.64 – 7.05 (m, 16H), 5.73 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.14 (dd, *J* = 11.2, 0.8 Hz, 1H), 4.58 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 141.2, 139.9, 138.8, 134.8, 134.1, 132.3, 132.0, 129.6, 128.8, 128.2, 128.1, 127.7, 127.3, 126.8, 126.7, 124.4, 121.2, 120.7, 115.3, 86.4, 86.3, 81.8, 69.6, 42.8, 21.5; IR (neat): 3060, 2923, 2232, 1597, 1486, 1367, 1169, 1089, 919, 592; HRESIMS Calcd for $[C_{32}H_{25}NNaO_2S]^+$ (M + Na^+) 510.1498, found 510.1496.

***N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benze nesulfonamide (1h)**

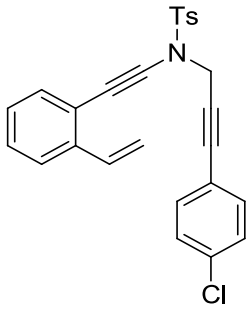


1h

The product **1h** was afforded as a pale yellow oil (69%, 296.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.05 (m, 7H), 6.99 – 6.85 (m, 2H), 5.73 (d, *J* = 17.6 Hz, 1H), 5.11 (d, *J* = 10.8 Hz, 1H), 4.55 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4 (d, *J* = 249.0 Hz), 144.8, 138.7, 134.6, 134.0, 133.5 (d, *J* = 8.0 Hz), 132.1, 129.5, 128.1, 127.3, 124.3, 121.0, 117.8 (d, *J* = 3.0 Hz), 115.3 (d, *J* = 22.0 Hz), 115.2, 86.2, 85.3, 80.9, 69.5, 42.6, 21.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.1; IR (neat): 3064, 2924,

2232, 1599, 1368, 1231, 1171, 920, 670, 589; HRESIMS Calcd for $[C_{26}H_{20}FNNaO_2S]^+$ (M + Na^+) 452.1091, found 452.1094.

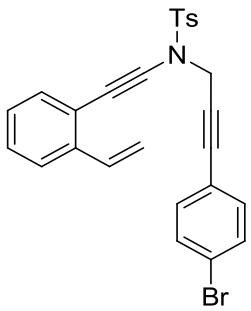
***N*-(3-(4-chlorophenyl)prop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1i)**



1i

The product **1i** was afforded as a pale yellow oil (79%, 351.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.03 (m, 9H), 5.73 (d, *J* = 17.6 Hz, 1H), 5.12 (d, *J* = 11.2 Hz, 1H), 4.56 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 138.8, 134.7, 134.6, 134.1, 132.8, 132.2, 129.5, 128.4, 128.1(4), 128.1(0), 127.4, 124.4, 121.1, 120.3, 115.3, 86.1, 85.3, 82.2, 69.6, 42.7, 21.4; IR (neat): 2924, 2232, 1595, 1489, 1369, 1170, 1089, 920, 753, 600; HRESIMS Calcd for $[C_{26}H_{20}ClNNaO_2S]^+$ (M + Na^+) 468.0795, found 468.0792.

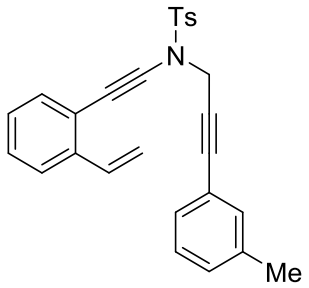
***N*-(3-(4-bromophenyl)prop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1j)**



1j

The product **1j** was afforded as a pale yellow oil (92%, 449.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.30 – 7.20 (m, 3H), 7.20 – 7.06 (m, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 5.73 (d, *J* = 17.6 Hz, 1H), 5.12 (d, *J* = 10.8 Hz, 1H), 4.55 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 138.8, 134.8, 134.1, 133.0, 132.3, 131.3, 129.6, 128.2, 128.1, 127.4, 124.5, 122.9, 121.1, 120.8, 115.3, 86.2, 85.4, 82.4, 69.7, 42.7, 21.5; IR (neat): 3063, 2923, 2232, 1596, 1369, 1170, 1088, 920, 751, 662; HRESIMS Calcd for $[C_{26}H_{20}BrNNaO_2S]^+$ (M + Na^+) 512.0290, found 512.0293.

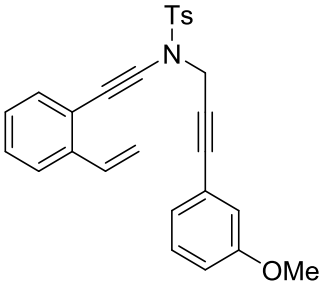
4-methyl-*N*-(3-(*m*-tolyl)prop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1k)



1k

The product **1k** was afforded as a pale yellow oil (93%, 395.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.87 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.39 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.30 – 7.20 (m, 3H), 7.20 – 7.06 (m, 4H), 7.01 – 6.93 (m, 2H), 5.73 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.12 (dd, *J* = 10.8, 0.8 Hz, 1H), 4.57 (s, 2H), 2.34 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 138.9, 137.7, 134.9, 134.2, 132.4, 132.2, 129.6, 129.5, 128.7, 128.2, 128.1, 128.0, 127.4, 124.4, 121.7, 121.3, 115.3, 86.8, 86.3, 80.7, 69.6, 42.9, 21.5, 21.1; IR (neat): 3059, 2922, 2232, 1597, 1484, 1367, 1170, 1089, 921, 594; HRESIMS Calcd for $[C_{27}H_{23}NNaO_2S]^+$ (M + Na^+) 448.1342, found 448.1340.

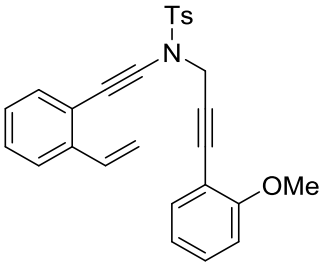
***N*-(3-(3-methoxyphenyl)prop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1l)**



1l

The product **1a** was afforded as a pale yellow oil (89%, 392.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.38 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.27 – 7.08 (m, 6H), 6.82 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.78 – 6.73 (m, 1H), 6.71 – 6.66 (m, 1H), 5.72 (d, *J* = 17.6 Hz, 1H), 5.13 (d, *J* = 10.8 Hz, 1H), 4.56 (s, 2H), 3.69 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 144.9, 138.7, 134.7, 134.0, 132.2, 129.5, 129.1, 128.0(3), 128.0(1), 127.3, 124.3, 123.9, 122.7, 121.1, 116.8, 115.3, 114.6, 86.4, 86.2, 80.8, 69.5, 55.0, 42.7, 21.3; IR (neat): 2926, 2232, 1596, 1480, 1368, 1290, 1169, 1046, 920, 685, 592; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1294.

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

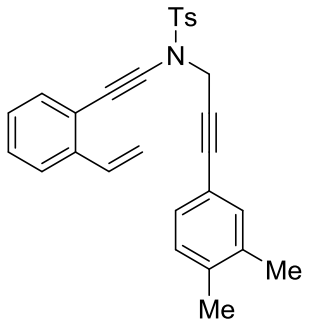


1m

The product **1m** was afforded as a pale yellow oil (98%, 432.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.37 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.28 – 7.18 (m, 4H), 7.18 – 7.08 (m, 2H), 7.02 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.83 – 6.74 (m, 2H), 5.71 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.11 (dd, *J* = 11.2, 0.8 Hz, 1H), 4.62 (s, 2H), 3.73 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 144.7, 138.7, 134.7, 134.0, 133.6, 132.1, 130.0, 129.4, 128.1, 127.9, 127.2, 124.3, 121.2,

120.0, 115.1, 110.9, 110.4, 86.2, 84.8, 83.1, 69.6, 55.4, 43.0, 21.4; IR (neat): 2927, 2232, 1596, 1493, 1366, 1265, 1169, 1089, 921, 753, 594; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1293.

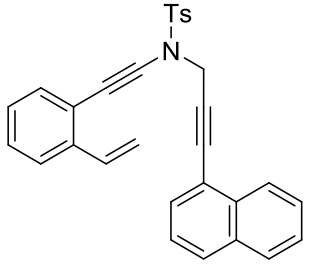
_N_-(3-(3,4-dimethylphenyl)prop-2-yn-1-yl)-4-methyl-_N_-((2-vinylphenyl)ethynyl)benzenesulfonamide (1n)



1n

The product **1n** was afforded as a pale yellow solid (96%, 421.4 mg; mp 84-85 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.39 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.31 – 7.20 (m, 3H), 7.20 – 7.08 (m, 2H), 7.03 – 6.96 (m, 1H), 6.97 – 6.88 (m, 2H), 5.73 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.13 (dd, *J* = 11.2, 0.8 Hz, 1H), 4.57 (s, 2H), 2.36 (s, 3H), 2.22 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 138.9, 137.5, 136.4, 134.9, 134.3, 132.7, 132.4, 129.6, 129.4, 129.1, 128.3, 128.0, 127.3, 124.5, 121.4, 119.2, 115.3, 86.9, 86.4, 80.1, 69.6, 43.0, 21.5, 19.7, 19.5; IR (neat): 2921, 2232, 1596, 1499, 1368, 1170, 1088, 921, 813, 670, 592; HRESIMS Calcd for $[C_{28}H_{25}NNaO_2S]^+$ (M + Na^+) 462.1498, found 462.1496.

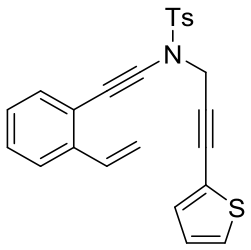
4-methyl-_N_-(3-(naphthalen-1-yl)prop-2-yn-1-yl)-_N_-((2-vinylphenyl)ethynyl)benzenesulfonamide (1o)



1o

The product **1o** was afforded as a pale yellow oil (96%, 442.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.87 (m, 3H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.45 – 7.37 (m, 3H), 7.35 – 7.10 (m, 5H), 7.06 (d, *J* = 8.4 Hz, 2H), 5.70 (dd, *J* = 17.6, 0.8 Hz, 1H), 5.09 (dd, *J* = 10.8, 0.8 Hz, 1H), 4.72 (s, 2H), 2.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 138.8, 134.7, 133.9, 132.8(4), 132.8(0), 132.3, 130.5, 129.5, 129.0, 128.1, 128.0, 127.3, 126.6, 126.3, 125.9, 124.8, 124.4, 121.2, 119.5, 115.4, 86.4, 85.9, 84.8, 69.9, 43.1, 21.2; IR (neat): 3059, 2232, 1596, 1368, 1170, 1088, 918, 801, 773, 675, 594; HRESIMS Calcd for $[C_{30}H_{23}NNaO_2S]^+$ (M + Na^+) 484.1342, found 484.1344.

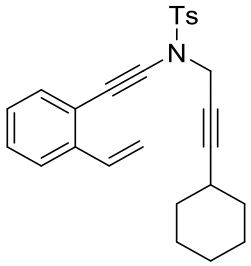
4-methyl-*N*-(3-(thiophen-2-yl)prop-2-yn-1-yl)-*N*-((2-vinylphenyl)ethynyl)benzene sulfonamide (1p)



1p

The product **1p** was afforded as a pale yellow oil (96%, 400.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.38 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.33 – 7.06 (m, 6H), 7.04 – 6.97 (m, 1H), 6.93 – 6.87 (m, 1H), 5.73 (d, *J* = 17.6 Hz, 1H), 5.16 (d, *J* = 11.2 Hz, 1H), 4.58 (s, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 138.9, 134.8, 134.0, 132.7, 132.3, 129.6, 128.1(2), 128.0(9), 127.6, 127.3, 126.8, 124.5, 121.7, 121.1, 115.3, 86.1, 85.0, 79.8, 69.7, 43.0, 21.6; IR (neat): 2922, 2229, 1367, 1168, 1089, 666, 594, 545; HRESIMS Calcd for $[C_{24}H_{19}NNaO_2S_2]^+$ (M + Na^+) 440.0749, found 440.0751.

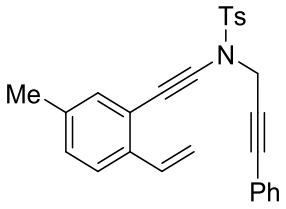
***N*-(3-cyclohexylprop-2-yn-1-yl)-4-methyl-*N*-((2-vinylphenyl)ethynyl)benzenesulfonamide (1q)**



1q

The product **1q** was afforded as a pale yellow oil (84%, 350.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.84 (m, 2H), 7.58 – 7.51 (m, 1H), 7.37 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.28 – 7.21 (m, 1H), 7.21 – 7.08 (m, 2H), 5.78 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.27 (dd, *J* = 11.2, 1.2 Hz, 1H), 4.35 (d, *J* = 2.0 Hz, 2H), 2.42 (s, 3H), 2.26 – 2.12 (m, 1H), 1.63 – 1.48 (m, 4H), 1.47 – 1.36 (m, 1H), 1.27 – 1.10 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 138.7, 135.0, 134.5, 132.2, 129.5, 128.1, 127.9, 127.3, 124.4, 121.5, 115.1, 91.4, 86.3, 71.9, 69.5, 42.4, 32.1, 28.7, 25.7, 24.5, 21.5; IR (neat): 2929, 2853, 2232, 1448, 1368, 1170, 1089, 922, 751, 661, 593; HRESIMS Calcd for $[C_{26}H_{27}NNaO_2S]^+$ ($M + Na^+$) 440.1655, found 440.1660.

4-methyl-*N*-((5-methyl-2-vinylphenyl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)benze nesulfonamide (1r)

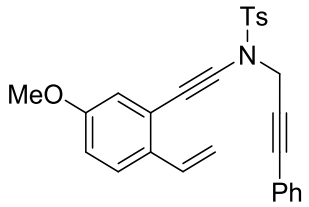


1r

The product **1r** was afforded as a pale yellow oil (82%, 341.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.29 – 7.17 (m, 6H), 7.17 – 7.05 (m, 3H), 7.05 – 6.99 (m, 1H), 5.67 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.05 (dd, *J* = 11.2, 1.2 Hz, 1H), 4.55 (s, 2H), 2.29 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 137.1, 136.0, 134.5, 134.1, 132.6, 131.5, 129.5, 129.0, 128.5, 128.1, 128.0, 124.3, 121.8, 120.9, 114.2, 86.5, 85.9, 81.1, 69.7, 42.7, 21.4, 20.7; IR (neat):

2922, 2235, 1700, 1490, 1364, 1168, 1089, 814, 758, 660, 591; HRESIMS Calcd for $[C_{27}H_{23}NNaO_2S]^+$ (M + Na^+) 448.1342, found 440.1340.

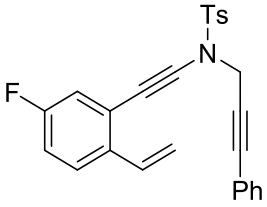
_N_-((5-methoxy-2-vinylphenyl)ethynyl)-4-methyl-_N_-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1s)



1s

The product **1s** was afforded as a pale yellow oil (95%, 403.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.88 (m, 2H), 7.46 (d, *J* = 8.8 Hz, 1H), 7.32 – 7.20 (m, 5H), 7.19 – 7.13 (m, 2H), 7.05 (dd, *J* = 17.6, 10.8 Hz, 1H), 6.89 (d, *J* = 2.8 Hz, 1H), 6.82 (dd, *J* = 8.8, 2.8 Hz, 1H), 5.59 (dd, *J* = 17.6, 0.8 Hz, 1H), 4.99 (dd, *J* = 10.8, 0.8 Hz, 1H), 4.58 (s, 2H), 3.74 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 144.9, 134.2(0), 134.1(5), 131.9, 131.6, 129.6, 128.6, 128.2, 128.1, 125.7, 122.2, 121.9, 116.0, 115.4, 113.1, 86.6, 86.1, 81.1, 69.7, 55.3, 42.8, 21.5; IR (neat): 2930, 2236, 1600, 1490, 1366, 1168, 1089, 758, 660, 590; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1299.

_N_-((5-fluoro-2-vinylphenyl)ethynyl)-4-methyl-_N_-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1t)

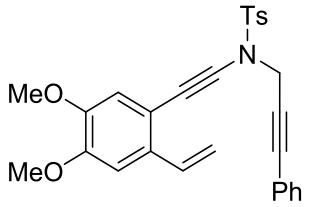


1t

The product **1t** was afforded as a pale yellow oil (93%, 399.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.86 (m, 2H), 7.51 – 7.43 (m, 1H), 7.31 – 7.20 (m, 5H), 7.19 – 7.13 (m, 2H), 7.12 – 7.01 (m, 2H), 6.98 – 6.89 (m, 1H), 5.65 (d, *J* = 17.6 Hz, 1H),

5.10 (d, *J* = 11.2 Hz, 1H), 4.57 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6 (d, *J* = 246.0 Hz), 145.1, 135.1 (d, *J* = 3.0 Hz), 134.2, 133.8, 131.6, 129.7, 128.7, 128.1(3), 128.0(9), 126.2 (d, *J* = 9.0 Hz), 122.9 (d, *J* = 10.0 Hz), 121.8, 118.2 (d, *J* = 23.0 Hz), 115.5 (d, *J* = 21.0 Hz), 115.0, 87.2, 86.7, 80.9, 68.9, 42.7, 21.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.7; IR (neat): 2921, 2237, 1600, 1488, 1369, 1169, 662, 589, 544; HRESIMS Calcd for $[C_{26}H_{20}FNNaO_2S]^+$ (M + Na^+) 452.1091, found 452.1095.

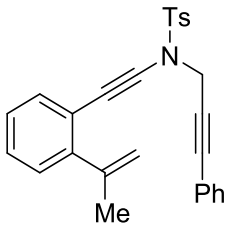
_N_-((4,5-dimethoxy-2-vinylphenyl)ethynyl)-4-methyl-_N_-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1u)



1u

The product **1u** was afforded as a pale yellow oil (80%, 376.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.33 – 6.97 (m, 9H), 6.85 (s, 1H), 5.60 (d, *J* = 17.6 Hz, 1H), 4.99 (d, *J* = 10.8 Hz, 1H), 4.57 (s, 2H), 3.87 (s, 3H), 3.78 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 148.3, 144.7, 134.3, 134.0, 132.9, 131.4, 129.4, 128.4, 128.1, 127.9, 121.7, 114.5, 113.4, 113.1, 106.5, 86.4, 84.8, 81.2, 69.2, 55.6(3), 55.6(0), 42.8, 21.3; IR (neat): 2928, 2235, 1598, 1361, 1266, 1212, 1167, 1089, 663, 588; HRESIMS Calcd for $[C_{28}H_{25}NNaO_4S]^+$ (M + Na^+) 494.1397, found 494.1395.

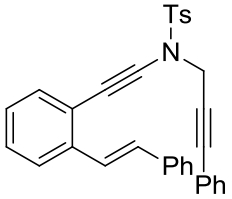
4-methyl-_N_-(3-phenylprop-2-yn-1-yl)-_N_-((2-(prop-1-en-2-yl)phenyl)ethynyl)benzenesulfonamide (1v)



1v

The product **1v** was afforded as a pale yellow oil (90%, 382.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.17 – 6.97 (m, 10H), 5.08 – 4.92 (m, 2H), 4.41 (s, 2H), 2.18 (s, 3H), 1.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 144.7, 144.6, 134.3, 132.5, 131.4, 129.4, 128.4, 128.0, 127.9, 127.7, 127.6, 126.6, 121.8, 120.0, 115.6, 86.2, 85.0, 81.2, 70.4, 42.7, 23.2, 21.3; IR (neat): 3061, 2919, 2232, 1597, 1490, 1368, 1170, 1038, 916, 757, 593; HRESIMS Calcd for $[C_{27}H_{23}NNaO_2S]^+$ (M + Na^+) 448.1342, found 448.1346.

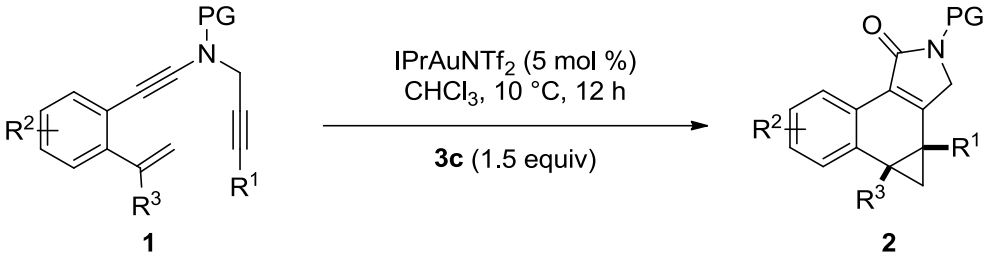
(*E*)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)-*N*-((2-styrylphenyl)ethynyl)benzenesulfonamide (1w)



1w

The product **1w** was afforded as a pale yellow oil (93%, 273.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.66 – 7.58 (m, 1H), 7.53 – 7.45 (m, 2H), 7.45 – 7.38 (m, 1H), 7.33 – 7.26 (m, 2H), 7.23 – 7.10 (m, 11H), 4.62 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 138.6, 137.1, 134.3, 132.3, 131.6, 130.4, 129.6, 128.5, 128.1, 127.7, 127.1, 126.8, 126.4, 124.6, 121.8, 121.5, 86.7, 86.5, 81.0, 69.8, 42.8, 21.4; IR (neat): 3059, 3030, 2231, 1596, 1367, 1169, 1088, 758, 690, 592; HRESIMS Calcd for $[C_{32}H_{25}NNaO_2S]^+$ (M + Na^+) 510.1498, found 510.1500.

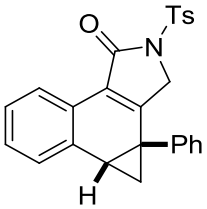
3. General procedure for the synthesis of tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-ones 2.



1 2

Compound **3c** (0.3 mmol, 49.2 mg) was added to a solution of the diyne **1** (0.2 mmol) in $CHCl_3$ (2 ml) at 10 ^oC temperature, then $IPrAuNTf_2$ (0.01 mmol, 8.7 mg) was added into the mixture. Next, the reaction was stirred at 10 ^oC for about 12 h and the progress of the reaction was monitored by TLC. Upon completed, the mixture was evaporated in vacuum. The residue was purified by flash chromatography on silica gel (eluent: PE/EtOAc) to afford the desired product **2**.

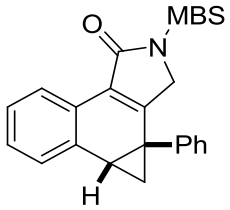
3b-phenyl-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (1a)



2a

Compound **2a** was prepared in 71% yield (60.6 mg) according to the general procedure. Pale yellow solid (mp 121-123 ^oC). ^1H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.6 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.18 (m, 10H), 4.48 (d, *J* = 19.2 Hz, 1H), 4.11 (d, *J* = 19.2 Hz, 1H), 2.83 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.39 (s, 3H), 2.28 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.46 – 0.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 156.5, 144.9, 139.4, 135.5, 134.9, 129.6, 129.5, 129.0, 128.5, 128.1, 128.0, 127.6, 126.4, 124.4, 124.2, 121.9, 50.7, 31.8, 31.6, 21.6, 16.8; IR (neat): 2924, 1720, 1579, 1493, 1365, 1243, 1170, 1091, 676, 582, 545; HRESIMS Calcd for $[C_{26}H_{21}NNaO_3S]^+$ (M + Na^+) 450.1134, found 450.1135.

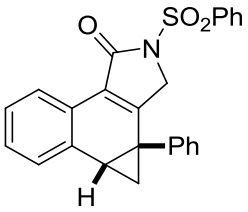
2-((4-methoxyphenyl)sulfonyl)-3b-phenyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2b)



2b

Compound **2b** was prepared in 69% yield (61.1 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.43 (m, 1H), 8.01 (d, *J* = 8.8 Hz, 2H), 7.45 – 7.21 (m, 8H), 6.97 (d, *J* = 8.8 Hz, 2H), 4.48 (d, *J* = 19.2 Hz, 1H), 4.10 (d, *J* = 19.2 Hz, 1H), 3.84 (s, 3H), 2.84 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.29 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.43 (dd, *J* = 5.6, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 163.9, 156.4, 139.6, 134.9, 130.4, 130.1, 129.6, 129.0, 128.6, 128.2, 127.7, 126.5, 124.5, 124.3, 122.0, 114.2, 55.6, 50.7, 31.9, 31.7, 16.9; IR (neat): 3062, 2929, 1717, 1594, 1496, 1361, 1262, 1162, 1091, 677, 583; HRESIMS Calcd for $[C_{26}H_{21}NNaO_4S]^+$ (M + Na^+) 466.1083, found 466.1086.

3b-phenyl-2-(phenylsulfonyl)-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2c)

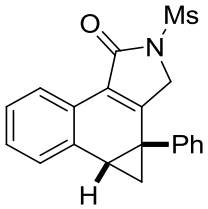


2c

Compound **2c** was prepared in 73% yield (60.3 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.45 (m, 1H), 8.11 – 8.04 (m, 2H), 7.66 – 7.58 (m, 1H), 7.57 – 7.48 (m, 2H), 7.45 – 7.23 (m, 8H), 4.50 (d, *J* = 19.2 Hz, 1H), 4.12 (d, *J* = 19.2 Hz, 1H), 2.85 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.29 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.44 (dd, *J* = 5.6, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

166.9, 156.6, 139.5, 138.5, 134.9, 133.8, 129.6, 129.1, 128.6, 128.2, 128.0, 127.7, 126.5, 124.4, 124.2, 121.9, 50.8, 31.9, 31.7, 16.9; IR (neat): 3064, 1719, 1492, 1447, 1362, 1170, 1117, 1091, 604, 588, 567; HRESIMS Calcd for $[C_{25}H_{19}NNaO_3S]^+$ (M + Na^+) 436.0978, found 436.0980.

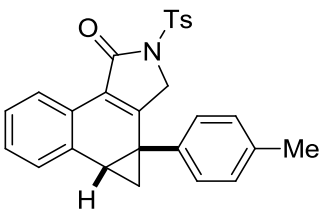
2-(methylsulfonyl)-3b-phenyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2d)



2d

Compound **2d** was prepared in 60% yield (42.1 mg) according to the general procedure. Pale yellow solid. (mp 169-171 ^oC). ^1H NMR (400 MHz, $CDCl_3$) δ 8.57 – 8.51 (m, 1H), 7.50 – 7.44 (m, 1H), 7.40 – 7.29 (m, 7H), 4.46 (d, *J* = 19.2 Hz, 1H), 4.08 (d, *J* = 19.2 Hz, 1H), 3.34 (s, 3H), 2.90 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.34 (dd, *J* = 9.2, 4.4 Hz, 1H), 0.49 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 157.1, 139.4, 135.0, 129.6, 129.1, 128.7, 128.3, 127.8, 126.7, 124.4, 124.2, 121.9, 50.1, 41.0, 32.0, 31.8, 17.0; IR (neat): 2927, 1715, 1493, 1446, 1349, 1167, 1119, 1044, 701, 570, 543; HRESIMS Calcd for $[C_{20}H_{17}NNaO_3S]^+$ (M + Na^+) 374.0821, found 374.0825.

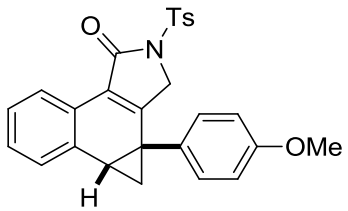
3b-(*p*-tolyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2e)



2e

Compound **2e** was prepared in 71% yield (62.6 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.43 (m, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.34 – 7.13 (m, 8H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.11 (d, *J* = 19.2 Hz, 1H), 2.80 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.40 (s, 3H), 2.37 (s, 3H), 2.26 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.38 (dd, *J* = 5.6, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 156.9, 144.9, 138.0, 136.6, 135.6, 135.0, 129.7, 129.6, 129.4, 128.5, 128.0, 127.6, 126.4, 124.4, 124.2, 121.8, 50.7, 31.8, 31.6, 21.6, 21.1, 17.0; IR (neat): 3028, 2922, 1720, 1597, 1493, 1362, 1170, 1091, 675, 582, 545; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1292.

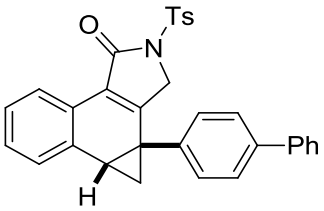
3b-(4-methoxyphenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2f)



2f

Compound **2f** was prepared in 70% yield (64.0 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.35 – 7.21 (m, 6H), 6.93 – 6.85 (m, 2H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.10 (d, *J* = 19.2 Hz, 1H), 3.83 (s, 3H), 2.81 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.41 (s, 3H), 2.25 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.39 (dd, *J* = 5.6, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 159.5, 157.0, 144.9, 135.7, 135.1, 131.8, 130.7, 129.7, 128.5, 128.1, 127.6, 126.5, 124.5, 124.3, 121.8, 114.4, 55.4, 50.8, 32.0, 31.3, 21.6, 17.2; IR (neat): 2922, 1513, 1369, 1246, 1172, 1093, 1060, 669, 608, 582, 538; HRESIMS Calcd for $[C_{27}H_{23}NNaO_4S]^+$ (M + Na^+) 480.1240, found 480.1244.

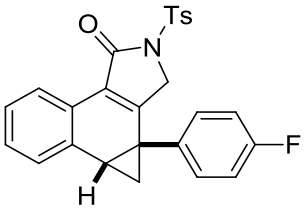
3b-([1,1'-biphenyl]-4-yl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2g)



2g

Compound **2g** was prepared in 65% yield (65.4 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.46 (m, 1H), 7.96 (d, *J* = 8.4 Hz, 2H), 7.62 – 7.55 (m, 4H), 7.50 – 7.19 (m, 10H), 4.52 (d, *J* = 19.2 Hz, 1H), 4.19 (d, *J* = 19.2 Hz, 1H), 2.86 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.39 (s, 3H), 2.31 (dd, *J* = 9.2, 4.4 Hz, 1H), 0.44 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 156.4, 144.9, 141.2, 140.2, 138.4, 135.6, 134.9, 130.0, 129.7, 128.8, 128.6, 128.0, 127.7(1), 127.6(7), 127.6, 127.1, 126.5, 124.5, 124.2, 122.0, 50.8, 31.8, 31.5, 21.6, 16.9; IR (neat): 3029, 2922, 1719, 1597, 1489, 1362, 1169, 1091, 675, 600, 582, 545; HRESIMS Calcd for $[C_{32}H_{25}NNaO_3S]^+$ (M + Na^+) 526.1447, found 526.1450.

3b-(4-fluorophenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2h)

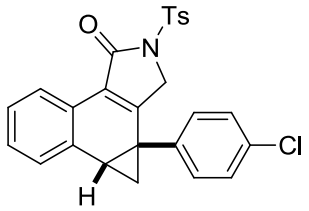


2h

Compound **2h** was prepared in 72% yield (64.1 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.38 (m, 1H), 7.36 – 7.20 (m, 6H), 7.11 – 7.01 (m, 2H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.08 (d, *J* = 19.2 Hz, 1H), 2.82 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.40 (s, 3H), 2.24 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.46 – 0.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 162.4 (d, *J* = 246.0 Hz), 155.9, 145.0, 135.5(4), 135.4(5) (d, *J* = 4.0 Hz), 134.7, 131.3 (d, *J* = 9.0 Hz), 129.7, 128.6, 128.0, 127.6, 126.6, 124.5, 124.1, 122.1, 116.0 (d, *J* = 21.0 Hz), 50.6, 31.7, 31.0, 21.6, 17.1; ^{19}F NMR (376 MHz,

$CDCl_3$) δ -113.0; IR (neat): 2924, 1720, 1597, 1511, 1362, 1222, 1170, 1091, 675, 582, 545; HRESIMS Calcd for $[C_{26}H_{20}FNNaO_3S]^+$ (M + Na^+) 468.1040, found 468.1045.

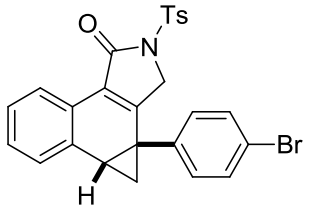
3b-(4-chlorophenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2i)



2i

Compound **2i** was prepared in 82% yield (75.6 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.43 (m, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.46 – 7.19 (m, 9H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.09 (d, *J* = 19.2 Hz, 1H), 2.82 (dd, *J* = 9.6, 5.6 Hz, 1H), 2.41 (s, 3H), 2.24 (dd, *J* = 9.6, 4.4 Hz, 1H), 0.44 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 155.5, 145.0, 138.0, 135.5, 134.6, 134.3, 131.0, 129.7, 129.3, 128.7, 128.1, 127.7, 126.7, 124.5, 124.1, 122.3, 50.6, 31.7, 31.1, 21.6, 16.9; IR (neat): 2922, 1719, 1491, 1362, 1169, 1118, 1091, 1013, 679, 582, 545; HRESIMS Calcd for $[C_{26}H_{20}ClNNaO_3S]^+$ (M + Na^+) 484.0745, found 484.0743.

3b-(4-bromophenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2j)

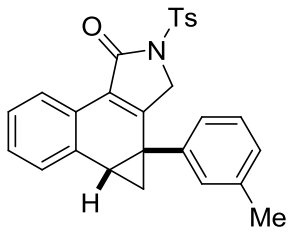


2j

Compound **2j** was prepared in 70% yield (70.7 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 7.6, 1.2 Hz,

1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.55 – 7.46 (m, 2H), 7.41 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.36 – 7.17 (m, 6H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.09 (d, *J* = 19.2 Hz, 1H), 2.82 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.41 (s, 3H), 2.24 (dd, *J* = 9.2, 4.4 Hz, 1H), 0.44 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 155.4, 145.0, 138.5, 135.5, 134.6, 132.2, 131.3, 129.7, 128.7, 128.1, 127.7, 126.7, 124.5, 124.1, 122.4, 122.3, 50.6, 31.7, 31.1, 21.6, 16.8; IR (neat): 2925, 1733, 1596, 1489, 1361, 1169, 1118, 1091, 667, 583, 546; HRESIMS Calcd for $[C_{26}H_{20}BrNNaO_3S]^+$ (M + Na^+) 528.0239, found 528.0237.

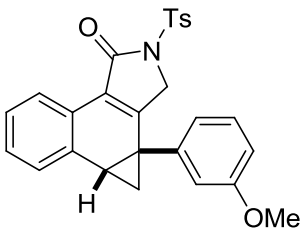
3b-(*m*-tolyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2k)



2k

Compound **2k** was prepared in 69% yield (60.9 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.44 (m, 1H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.46 – 7.38 (m, 1H), 7.36 – 7.21 (m, 5H), 7.19 – 7.07 (m, 3H), 4.48 (d, *J* = 19.2 Hz, 1H), 4.13 (d, *J* = 19.2 Hz, 1H), 2.82 (dd, *J* = 9.6, 5.6 Hz, 1H), 2.41 (s, 3H), 2.36 (s, 3H), 2.27 (dd, *J* = 9.6, 4.4 Hz, 1H), 0.41 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 156.8, 144.9, 139.5, 138.8, 135.7, 135.0, 130.3, 129.7, 129.0, 128.9, 128.5, 128.1, 127.7, 126.6, 126.5, 124.5, 124.3, 121.9, 50.8, 31.9, 31.7, 21.6, 21.3, 16.9; IR (neat): 2923, 2854, 1720, 1597, 1492, 1362, 1170, 1091, 676, 582, 544; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1293.

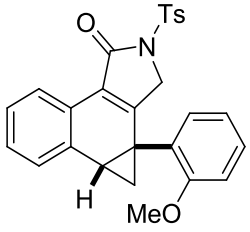
3b-(3-methoxyphenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2l)



2l

Compound **2l** was prepared in 75% yield (68.6 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.36 – 7.17 (m, 5H), 6.95 – 6.79 (m, 3H), 4.49 (d, *J* = 19.2 Hz, 1H), 4.14 (d, *J* = 19.2 Hz, 1H), 3.80 (s, 3H), 2.84 (dd, *J* = 9.6, 5.6 Hz, 1H), 2.40 (s, 3H), 2.27 (dd, *J* = 9.6, 4.4 Hz, 1H), 0.40 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 160.0, 156.5, 144.9, 140.9, 135.5, 134.9, 130.1, 129.7, 128.5, 128.0, 127.7, 126.5, 124.4, 124.2, 121.9, 121.8, 115.4, 113.4, 55.3, 50.7, 31.9, 31.6, 21.6, 16.9; IR (neat): 2923, 1719, 1597, 1489, 1362, 1329, 1169, 1091, 676, 582, 545; HRESIMS Calcd for $[C_{27}H_{23}NNaO_4S]^+$ (M + Na^+) 480.1240, found 480.1244.

3b-(2-methoxyphenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2m)

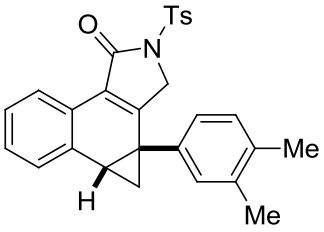


2m

Compound **2m** was prepared in 72% yield (65.8 mg) according to the general procedure. Pale yellow solid. (mp 215-217 ^{o}C). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.5 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 2H), 7.41 (d, *J* = 7.0 Hz, 1H), 7.36 – 7.20 (m, 6H), 6.99 – 6.86 (m, 2H), 4.86 – 4.20 (m, 1H), 4.05 (d, *J* = 19.0 Hz, 1H), 3.96 – 3.48 (m, 3H), 3.04 – 2.54 (m, 1H), 2.40 (s, 3H), 2.32 – 1.97 (m, 1H), 0.61 – 0.27 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.3, 158.7, 158.1, 144.8, 135.7, 135.5, 129.7, 129.6, 128.1, 128.0, 127.5, 126.2, 124.4, 124.2, 120.9, 120.6, 110.8, 55.4, 50.7, 31.7, 28.2,

21.6; IR (neat): 3060, 2925, 1719, 1598, 1492, 1362, 1170, 1091, 937, 676, 583; HRESIMS Calcd for $[C_{27}H_{23}NNaO_4S]^+$ (M + Na^+) 480.1240, found 480.1242.

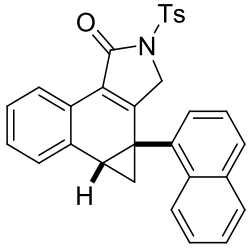
3b-(3,4-dimethylphenyl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2n)



2n

Compound **2n** was prepared in 65% yield (59.2 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.35 – 7.21 (m, 4H), 7.16 – 7.01 (m, 3H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.13 (d, *J* = 19.2 Hz, 1H), 2.80 (dd, *J* = 9.6, 5.6 Hz, 1H), 2.41 (s, 3H), 2.33 – 2.21 (m, 7H), 0.38 (dd, *J* = 5.6, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 157.1, 144.9, 137.3, 137.1, 136.7, 135.7, 135.1, 130.8, 130.2, 129.7, 128.5, 128.1, 127.6, 126.8, 126.4, 124.4, 124.3, 121.7, 50.8, 31.8, 31.7, 21.6, 19.7, 19.4, 16.9; IR (neat): 2922, 1719, 1597, 1493, 1452, 1363, 1170, 1091, 675, 582, 544; HRESIMS Calcd for $[C_{28}H_{25}NNaO_3S]^+$ (M + Na^+) 478.1447, found 478.1448.

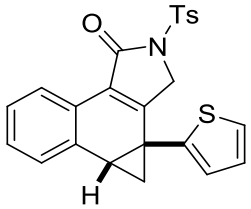
3b-(naphthalen-1-yl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2o)



2o

Compound **2o** was prepared in 70% yield (66.8 mg), d.r. = 6.2:1 according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 – 8.53 (m, 1H), 7.93 – 7.81 (m, 4H), 7.64 (dd, *J* = 7.2, 0.8 Hz, 1H), 7.54 – 7.41 (m, 3H), 7.41 – 7.23 (m, 6H), 4.41 (d, *J* = 19.2 Hz, 1H), 3.75 (d, *J* = 19.2 Hz, 1H), 2.82 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.48 (dd, *J* = 9.2, 4.4 Hz, 1H), 2.40 (s, 3H), 0.59 (dd, *J* = 5.6, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 157.5, 144.9, 135.5, 135.4, 134.7, 134.0, 132.6, 129.6, 129.3, 128.9, 128.8, 128.1, 128.0, 127.3, 127.2, 126.8, 126.2, 125.3, 124.6, 124.4, 123.6, 121.8, 50.7, 32.2, 30.0, 21.6, 17.1; IR (neat): 3060, 2924, 2854, 1720, 1596, 1363, 1170, 1091, 676, 582, 544; HRESIMS Calcd for $[C_{30}H_{23}NNaO_3S]^+$ (M + Na^+) 500.1291, found 500.1294.

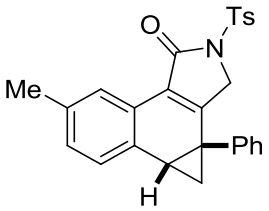
3b-(thiophen-2-yl)-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2p)



2p

Compound **2p** was prepared in 65% yield (56.3 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.46 (m, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.37 – 7.24 (m, 5H), 7.03 – 6.97 (m, 2H), 4.57 (d, *J* = 19.2 Hz, 1H), 4.35 (d, *J* = 19.2 Hz, 1H), 2.95 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.42 (s, 3H), 2.36 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.51 (dd, *J* = 5.6, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 155.3, 145.0, 143.2, 135.6, 134.4, 129.7, 128.7, 128.1, 127.7, 127.5, 127.2, 126.7, 126.0, 124.6, 124.1, 122.1, 50.6, 33.6, 26.0, 21.6, 19.1; IR (neat): 2923, 2852, 1719, 1493, 1362, 1169, 1118, 1091, 674, 580, 545; HRESIMS Calcd for $[C_{24}H_{19}NNaO_3S_2]^+$ (M + Na^+) 456.0699, found 456.0700.

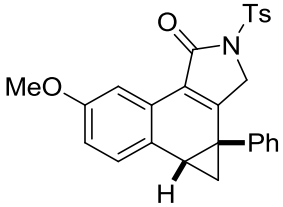
7-methyl-3b-phenyl-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2r)



2r

Compound **2r** was prepared in 76% yield (67.0 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.42 – 7.27 (m, 8H), 7.12 (d, *J* = 7.2 Hz, 1H), 4.47 (d, *J* = 19.2 Hz, 1H), 4.11 (d, *J* = 19.2 Hz, 1H), 2.82 (dd, *J* = 9.2, 6.0 Hz, 1H), 2.41 (s, 3H), 2.34 (s, 3H), 2.25 (dd, *J* = 9.2, 4.0 Hz, 1H), 0.45 – 0.33 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 156.7, 144.9, 139.7, 136.3, 135.7, 132.0, 129.7, 129.6, 129.4, 129.0, 128.2, 128.1, 127.5, 124.9, 124.1, 122.0, 50.8, 31.7, 31.5, 21.6, 21.2, 17.1; IR (neat): 3056, 2922, 1718, 1498, 1363, 1170, 1093, 814, 660, 593, 544; HRESIMS Calcd for $[C_{27}H_{23}NNaO_3S]^+$ (M + Na^+) 464.1291, found 464.1294.

7-methoxy-3b-phenyl-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2s)

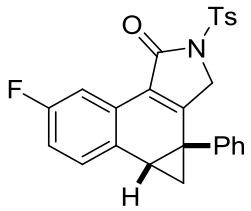


2s

Compound **2s** was prepared in 76% yield (69.5 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 2.5 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.40 – 7.29 (m, 8H), 6.89 (dd, *J* = 8.0, 2.5 Hz, 1H), 4.46 (d, *J* = 19.2 Hz, 1H), 4.11 (d, *J* = 19.2 Hz, 1H), 3.83 (s, 3H), 2.82 (dd, *J* = 9.5, 5.5 Hz, 1H), 2.42 (s, 3H), 2.24 (dd, *J* = 9.5, 4.5 Hz, 1H), 0.39 (dd, *J* = 5.5, 4.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.1, 158.4, 157.3, 145.0, 139.6, 135.6, 129.7, 129.6, 129.0, 128.5, 128.2, 128.0, 127.2, 125.2, 121.9, 116.0, 108.3, 55.5, 50.8, 31.6, 31.3, 21.6,

17.0; IR (neat): 2926, 1716, 1601, 1497, 1361, 1169, 1093, 1033, 662, 590, 545; HRESIMS Calcd for $[C_{27}H_{23}NNaO_4S]^+$ (M + Na^+) 480.1240, found 480.1240.

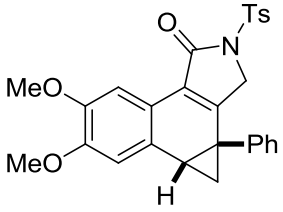
7-fluoro-3b-phenyl-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2t)



2t

Compound **2t** was prepared in 64% yield (56.9 mg) according to the general procedure. Pale yellow solid. (mp 202-203 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 10.0, 2.8 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.42 – 7.28 (m, 8H), 7.04 – 6.95 (m, 1H), 4.49 (d, *J* = 19.2 Hz, 1H), 4.12 (d, *J* = 19.2 Hz, 1H), 2.84 (dd, *J* = 9.6, 6.0 Hz, 1H), 2.42 (s, 3H), 2.29 (dd, *J* = 9.6, 4.4 Hz, 1H), 0.41 (dd, *J* = 6.0, 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 161.5 (d, *J* = 242.0 Hz), 157.8, 145.1, 139.3, 135.5, 130.6 (d, *J* = 3.0 Hz), 129.7, 129.6, 129.1, 128.9 (d, *J* =8.0 Hz), 128.3, 128.1, 125.7 (d, *J* = 9.0 Hz), 121.4 (d, *J* = 3.0 Hz), 115.5 (d, *J* = 22.0 Hz), 111.3 (d, *J* = 24.0 Hz), 50.8, 31.9, 31.2, 21.6, 17.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.9; IR (neat): 3064, 2923, 1718, 1496, 1435, 1362, 1170, 1092, 660, 594, 544; HRESIMS Calcd for $[C_{26}H_{20}FNNaO_3S]^+$ (M + Na^+) 468.1040, found 468.1042.

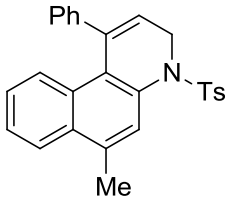
6,7-dimethyl-3b-phenyl-2-tosyl-2,3,4,4a-tetrahydrobenzo[*e*]cyclopropa[*g*]isoindol-1(3b*H*)-one (2u)



2u

Compound **2u** was prepared in 66% yield (60.0 mg) according to the general procedure. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.95 (d, *J* = 8.5 Hz, 2H), 7.41 – 7.30 (m, 7H), 6.93 (s, 1H), 4.45 (d, *J* = 19.0 Hz, 1H), 4.11 (d, *J* = 19.0 Hz, 1H), 3.92 (s, 6H), 2.78 (dd, *J* = 9.5, 5.5 Hz, 1H), 2.42 (s, 3H), 2.24 (dd, *J* = 9.5, 4.5 Hz, 1H), 0.43 – 0.33 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.3, 154.2, 149.3, 147.6, 144.9, 139.8, 135.7, 129.8, 129.6, 129.0, 128.1(4), 128.1(2), 128.0, 121.9, 117.1, 110.4, 107.3, 56.0, 55.9, 50.7, 31.8, 31.5, 21.6, 16.2; IR (neat): 2922, 2851, 1716, 1516, 1362, 1270, 1168, 1144, 1093, 664, 585, 544; HRESIMS Calcd for $[C_{28}H_{25}NNaO_5S]^+$ (M + Na^+) 510.1346, found 510.1350.

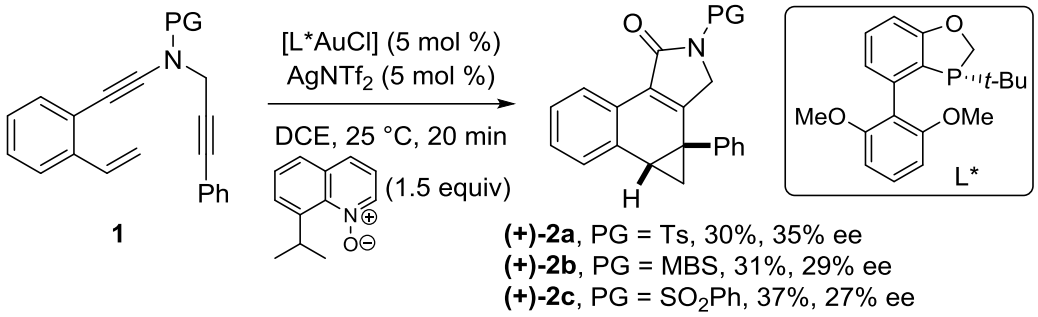
6-methyl-1-phenyl-4-tosyl-3,4-dihydrobenzo[*f*]quinolone (2v')



2v'

The product **2v'** was afforded as a pale yellow solid (81%, 68.9 mg; mp 194-195 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.90 (m, 2H), 7.42 – 7.30 (m, 3H), 7.21 – 7.04 (m, 4H), 7.04 – 6.96 (m, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.70 – 6.43 (m, 2H), 5.72 (t, *J* = 5.6 Hz, 1H), 4.46 (d, *J* = 5.6 Hz, 2H), 2.77 (s, 3H), 2.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 141.0, 138.6, 136.5, 135.8, 135.6, 132.0, 129.5, 129.1, 128.2, 127.8, 127.4, 127.1, 127.0, 125.7, 125.2(0), 125.1(7), 124.7, 124.3, 123.2, 45.5, 21.2, 19.9; IR (neat): 2924, 1597, 1351, 1164, 1089, 927, 738, 664, 580; HRESIMS Calcd for $[C_{27}H_{23}NNaO_2S]^+$ (M + Na^+) 448.1342, found 448.1340.

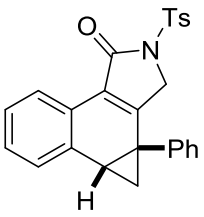
Synthesis of chiral γ-lactams (+)-2.



(+)-2a, PG = Ts, 30%, 35% ee
(+)-2b, PG = MBS, 31%, 29% ee
(+)-2c, PG = SO_2Ph, 37%, 27% ee

To a dry flask, the powdered L*AuCl (0.01 mmol, 5.6 mg), $AgNTf_2$ (0.01 mmol, 3.9 mg) was added. Then DCE (1.5 mL) was injected into the flask and the mixture was stirred at 25 ^oC for about 10 min. Then 8-isopropylquinoline *N*-oxide (0.3 mmol, 56.1 mg) and the diyne **1** (0.2 mmol) was dissolved in DCE (1.5 mL), the solution was added to the previous mixture. The reaction was stirred at 25 ^oC for about 20 min and the progress of the reaction was monitored by TLC. Upon completed, the mixture was evaporated in vacuum. The residue was purified by flash chromatography on silica gel (eluent: PE/EtOAc and PE/DCM) to afford the desired chiral (+)-**2**.

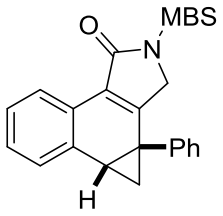
chiral γ-lactam (+)-2a



(+)-**2a**

Compound (+)-**2a** was prepared in 30% yield (26.0 mg) according to the above procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1 and PE:DCM = 2:1) as a pale yellow solid. [α]D 25 = +29.3 °(c = 1.0, $CHCl_3$). 35% ee (determined by HPLC (IC, *n*-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, I = 254 nm) tR = 20.13 min (minor), 22.05 min (major)).

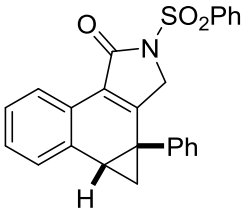
chiral γ-lactam (+)-2b



(+)-**2b**

Compound (+)-**2b** was prepared in 31% yield (27.5 mg) according to the above procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1 and PE:DCM = 2:1) as a pale yellow oil. [α]D 25 = +16.0 º(c = 1.0, $CHCl_3$). 29% ee (determined by HPLC (IC, *n*-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, I = 254 nm) tR = 35.23 min (minor), 40.56 min (major)).

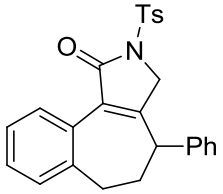
chiral γ-lactam (+)-2c



(+)-**2c**

Compound (+)-**2c** was prepared in 37% yield (30.5 mg) according to the above procedure. The product was isolated through silica gel column chromatography (PE:EA = 15:1 and PE:DCM = 2:1) as a pale yellow oil. [α]D 25 = +16.3 º(c = 1.0, $CHCl_3$). 27% ee (determined by HPLC (IC, *n*-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, I = 254 nm) tR = 32.47 min (minor), 34.74 min (major)).

4-phenyl-2-tosyl-2,3,5,6-tetrahydrobenzo[3,4]cyclohepta[1,2-*c*]pyrrol-1(4*H*)-one (3a)

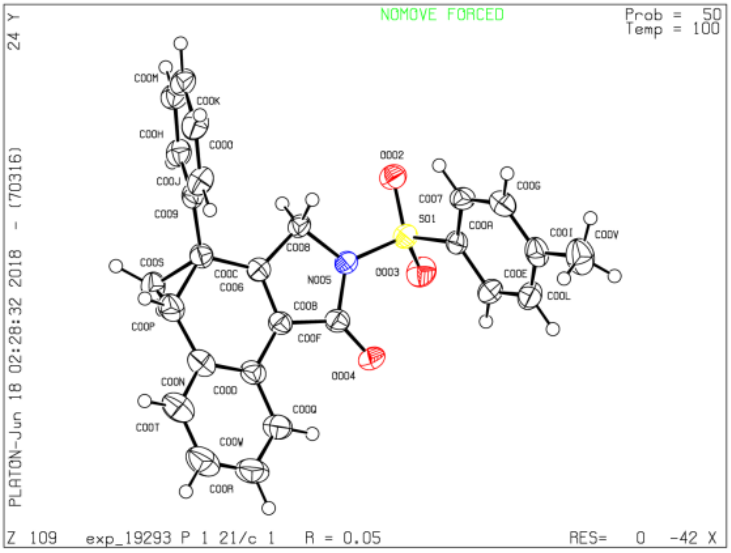


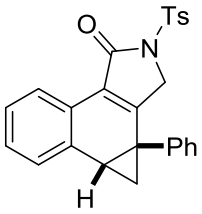
3a

Compound **3a** was prepared in 85% yield (54.2 mg) according to the known procedure (0.20 mmol scale). Pale yellow solid. (mp 196-197 ^{o}C). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.0 Hz, 1H), 7.95 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.19 (m, 7H), 7.15 – 7.07 (m, 3H), 4.24 – 4.12 (m, 2H), 3.97 – 3.89 (m, 1H), 2.86 – 2.69 (m, 2H), 2.53 – 2.42 (m, 1H), 2.40 (s, 3H), 2.08 – 1.93 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3, 157.7, 145.0, 143.1, 141.9, 135.2, 129.7, 129.5, 129.2(0), 129.1(7), 128.7, 128.5(2), 128.5(0), 128.2, 127.7, 127.5, 126.2, 51.8, 49.8, 37.9, 33.2, 21.6; IR (neat): 3059, 2929, 1720, 1597, 1450, 1361, 1170, 1129, 669, 592, 543; HRESIMS Calcd for $[C_{26}H_{23}NNaO_3S]^+$ (M + Na^+) 452.1291, found 452.1293.

Crystal data and structure refinement for 2a. CCDC Number = 2133059

ORTEP drawing of **2a** (thermal ellipsoids set at 50% probability). Recrystallization from *n*-hexane/DCM afforded single crystals suitable for X-ray diffraction analysis.





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Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:            a=13.7021(10)     b=15.1512(11)      c=11.1435(8)
                 alpha=90          beta=93.894(6)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           2308.1(3)                 2308.1(3)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C26 H21 N O3 S [+ solvent] C26 H21 N O3 S
Sum formula      C26 H21 N O3 S [+ solvent] C26 H21 N O3 S
Mr               427.50                    427.50
Dx,g cm-3        1.230                     1.230
Z                4                         4
Mu (mm-1)        0.167                     0.167
F000             896.0                     896.0
F000'            896.88
h,k,lmax         19,21,15                  17,21,15
Nref             6730                      5784
Tmin,Tmax        0.943,0.967               0.763,1.000
Tmin'            0.943

Correction method= # Reported T Limits: Tmin=0.763 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.859          Theta(max)= 29.983

R(reflections)= 0.0548( 4265)     wR2(reflections)= 0.1413( 5784)

S = 0.998                 Npar= 281
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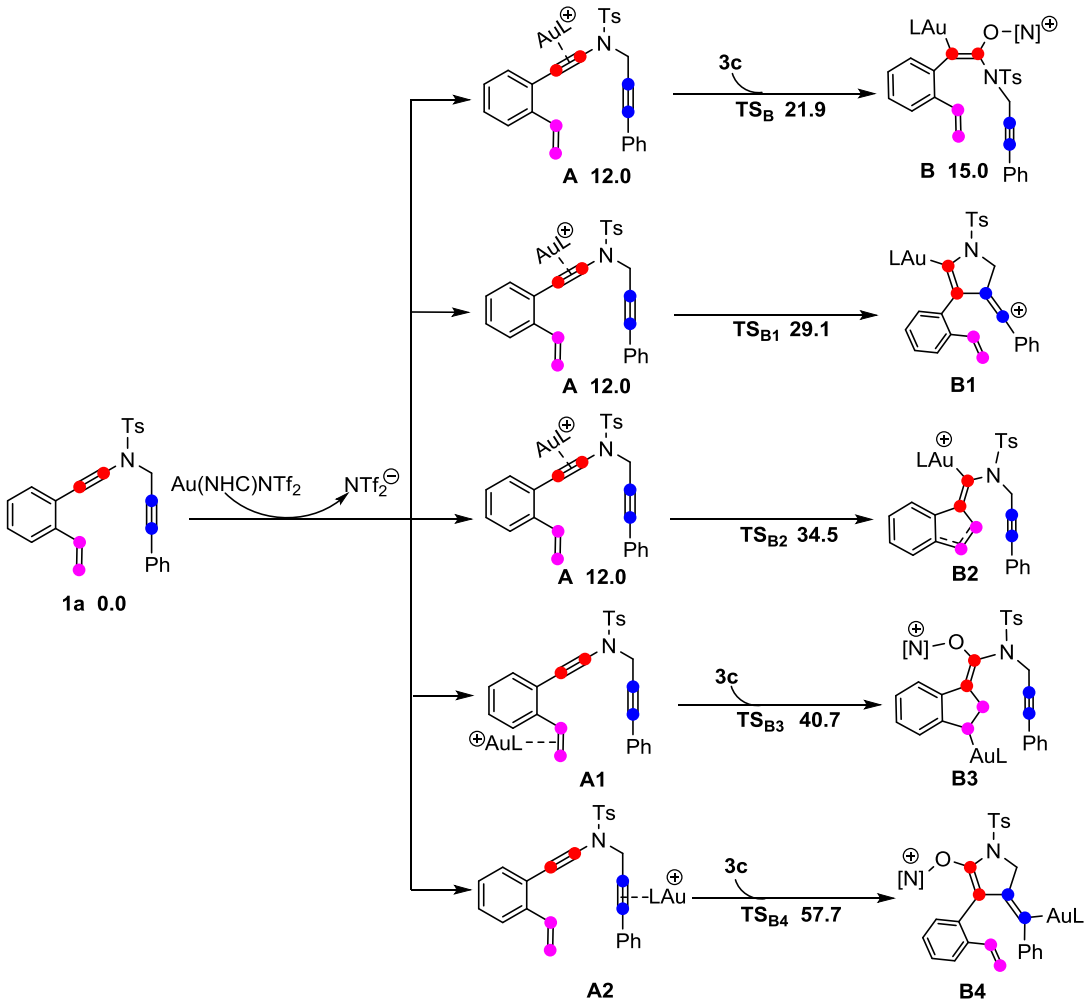
Computational Details

All calculations were carried out with the Gaussian 09 programs.[4] The geometries of all the species were fully optimized by using density functional theory (DFT) of the M06 method.[5] The 6-31G(d,p)[6] basis set was used for all atoms except for gold which were described by the Stuttgart/Dresden small-core RECP (relativistic effective core potential) plus valence double-ζ basis set (SDD).[7] Frequency calculations at the same level were performed to confirm each stationary point to be either a local minimum or a transition state (TS). The transition states were verified by intrinsic reaction coordinate (IRC) calculations.[8] The intermediates were characterized by all real frequencies. The solvent effect of chloroform (ε = 4.7113) was studied by performing the self-consistent reaction field (SCRF) of the SMD method of Truhlar and Cramer[9] at the same computational level.



Scheme S1. The possible coordination of Au catalyst with substrate **1a** and energies for the formation of metal carbene-like intermediates. Our calculations demonstrate that the catalytic Au^{I} species preferentially bound to the electron-richer amide-tethered C-C triple bond of the substrate **1a** to form the precursor **A** and subsequent nucleophilic attack of *N*-oxide **3c** on the gold-ligated ynamide **A** via $\mathbf{TS_B}$ to give a vinyl metal intermediate **B** is the most favored pathway.

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Cartesian Coordinates and Thermochemical Data (Energies in Hartree)

1a

Number of imaginary frequencies: 0

C	-1.04455200	-4.86063700	-0.06491800
C	-0.83209100	-3.54183800	-0.43663000
C	-0.42014900	-2.59198500	0.50986400
C	-0.21171300	-2.97763600	1.85605200
C	-0.44104100	-4.31338500	2.20222300
C	-0.84830100	-5.24768400	1.25974000
H	-1.37195000	-5.58565400	-0.80633900
H	-0.98249700	-3.22641200	-1.46683300
H	-0.31914800	-4.61544500	3.24088600
H	-1.02589400	-6.27768100	1.56041100
C	-0.19228700	-1.24597400	0.10655100
C	0.00950500	-0.09036700	-0.20601200
N	0.23302200	1.19283200	-0.54628900
C	0.48677300	1.47705300	-1.98061800
C	1.65706600	0.76990200	-2.48382400
C	2.65119900	0.13713300	-2.76767700
C	3.83599700	-0.60598900	-3.05084200
C	4.93918600	0.00594800	-3.66398200
C	3.91811400	-1.95355500	-2.66940800
C	6.09672700	-0.72441900	-3.90233400
H	4.87449600	1.05381700	-3.95020200
C	5.08116700	-2.67472400	-2.90709300
H	3.06383600	-2.41845600	-2.18102100
C	6.17016200	-2.06416900	-3.52646000
H	6.94684000	-0.24515300	-4.38271200
H	5.13724900	-3.71947600	-2.61023600
H	7.07777400	-2.63279800	-3.71614700

S	1.09940400	2.13138700	0.61928900
O	0.57252600	1.70750700	1.90507200
O	0.97504000	3.50449600	0.15615100
C	2.77378300	1.60883800	0.45837500
C	3.16072200	0.39260200	1.02390800
C	3.64093700	2.35467000	-0.33431000
C	4.44036500	-0.07742900	0.77389300
H	2.47171200	-0.17253400	1.64791100
C	4.92003900	1.86696300	-0.56525900
H	3.31436700	3.29882700	-0.76360000
C	5.33170400	0.64357100	-0.03107100
H	4.75798100	-1.02769500	1.20058600
H	5.61130300	2.44059500	-1.18074800
C	6.68754800	0.08860600	-0.33016500
H	7.30246200	0.80059400	-0.89023800
H	7.22139100	-0.18094900	0.58900300
H	6.60101200	-0.82560700	-0.93315800
H	-0.42210200	1.18653500	-2.52127100
H	0.58565000	2.56324900	-2.08728200
C	0.21832100	-1.98138600	2.84281600
C	0.85923100	-2.24125300	3.98585500
H	0.00053100	-0.94057000	2.59129900
H	1.12951100	-1.43866800	4.66758000
H	1.14622400	-3.24967700	4.28196600

Electronic Energy (0K) = -1605.723755

Electronic Energy (0K) + ZPE = -1605.325306

Enthalpy (298K) = -1605.297580

Free Energy (298K) = -1605.384319

Au(NHC)NTf$_2$

Number of imaginary frequencies: 0

C	-1.50232000	-2.21032400	0.87790100
F	-0.21952200	-2.49716800	1.04400700
F	-1.88544100	-1.36613900	1.81970400
F	-2.20898600	-3.32264400	0.96391700
S	-1.80932700	-1.48868900	-0.80584500
O	-3.25079900	-1.47512600	-0.95705900
O	-0.96874500	-2.27336400	-1.69476300
N	-1.15929000	0.01543400	-0.62811000
O	-3.15607800	1.32272800	-1.64189300
O	-1.01506500	2.47775900	-0.95810900
S	-1.99909100	1.42278400	-0.77601300
C	-2.65167000	1.69408600	0.92962200
F	-3.54213600	0.76691600	1.22928700
F	-1.65178400	1.64844400	1.79802400
F	-3.21795500	2.88692900	0.97360600
Au	0.94169900	0.13888700	-0.25907300
C	5.06123200	-0.48406200	0.34527800
C	5.03692700	0.86658400	0.44999700
H	5.87516700	-1.19188000	0.41505700
H	5.82574600	1.58497700	0.62248300
C	3.27412700	2.63785300	0.29126000
H	2.19673000	2.65845200	0.10803800
H	3.48553100	3.08682200	1.26580700
H	3.78432600	3.20549800	-0.49193500
C	3.34768600	-2.27412400	-0.04577400
H	3.19414700	-2.73491800	0.93501700
H	2.41382500	-2.30650500	-0.61427300
H	4.11902100	-2.82428800	-0.59010900
N	3.72345100	1.25560800	0.27237400

N	3.76311800	-0.88780100	0.10259900
C	2.93616500	0.17974600	0.06106400

Electronic Energy (0K) = -2267.1796324

Electronic Energy (0K) + ZPE = -2266.992654

Enthalpy (298K) = -2266.968023

Free Energy (298K) = -2267.047666

NTf_2^-

Number of imaginary frequencies: 0

C	-2.08301900	0.74971500	0.18406100
F	-2.38116700	0.83708100	1.47145700
F	-1.26505900	1.74303700	-0.13850800
F	-3.20050100	0.86749200	-0.52440600
S	-1.30847000	-0.87478200	-0.20139700
O	-1.05011900	-0.82819100	-1.63624700
O	-2.26844100	-1.84805500	0.30746200
N	-0.03037300	-0.79525000	0.76714400
O	1.74227400	-1.60981900	-0.93979500
O	2.32547400	-1.10171300	1.45296400
S	1.49295500	-0.85526300	0.28262600
C	1.89265500	0.88663800	-0.16683100
F	1.23023700	1.24958500	-1.25486800
F	1.57730800	1.70916000	0.82421700
F	3.19579700	0.98604200	-0.40546100

Electronic Energy (0K) = -1826.852068

Electronic Energy (0K) + ZPE = -1826.795769

Enthalpy (298K) = -1826.781250

Free Energy (298K) = -1826.836518

A

Number of imaginary frequencies: 0

C	0.67018200	-2.32399200	-2.72036800
C	0.46097100	-1.75739400	-1.47241600
C	1.45998400	-0.99739900	-0.84884000
C	2.69738800	-0.78669900	-1.50591900
C	2.88168000	-1.36305200	-2.76611100
C	1.88899800	-2.12828500	-3.36502000
H	-0.11480700	-2.90967800	-3.19157900
H	-0.48458800	-1.90407200	-0.95150400
H	3.81865900	-1.18145200	-3.28903800
H	2.06144000	-2.56090000	-4.34781600
C	1.23002800	-0.46256200	0.48077400
C	1.87130400	0.11732200	1.40858600
N	2.41998200	0.74856500	2.39743500
C	2.82321500	0.04698200	3.64528600
C	1.67456300	-0.29140600	4.47117400
C	0.70940500	-0.55182500	5.15835600
C	-0.41179300	-0.85928800	5.98790800
C	-1.64690900	-0.22574300	5.78073200
C	-0.28793000	-1.80754300	7.01523400
C	-2.73372600	-0.53710200	6.58886200
H	-1.74233800	0.50848400	4.98106300
C	-1.38109600	-2.11453000	7.81469100
H	0.67051100	-2.29614300	7.17619400
C	-2.60523700	-1.48249700	7.60371900
H	-3.68733000	-0.03899900	6.42504400
H	-1.27677800	-2.85013700	8.60868300
H	-3.45775900	-1.72462600	8.23396700
S	2.33387400	2.53136300	2.40827100
O	3.43308200	2.92479700	3.26908900

O	2.27135500	2.88136900	1.00267300
C	0.79627700	2.84898000	3.18945300
C	0.75911500	2.96077500	4.57799000
C	-0.36019300	2.88917100	2.40942100
C	-0.47358700	3.11269200	5.19565000
H	1.67664300	2.93056500	5.16091500
C	-1.57856900	3.05030400	3.05174600
H	-0.29965100	2.82102100	1.32541000
C	-1.65418600	3.14982200	4.44647300
H	-0.52653900	3.19286400	6.27970800
H	-2.49345700	3.10314000	2.46329000
C	-2.98615200	3.27971700	5.11280800
H	-2.91796400	3.10688000	6.19167300
H	-3.70575800	2.56549200	4.69061100
H	-3.40644000	4.28211000	4.96137300
H	3.52697000	0.70261100	4.17153400
H	3.38159500	-0.84512300	3.34003400
Au	-0.63951300	-0.67920500	1.54615000
C	-2.47371600	-1.02758500	2.40968700
C	-4.11251800	-1.90964800	3.66796600
C	-4.62698800	-0.83165300	3.02748700
H	-4.55326800	-2.60338400	4.37067400
H	-5.61778500	-0.39923400	3.03667600
N	-2.79412900	-2.01417900	3.27572500
N	-3.60768400	-0.30576800	2.25824000
C	-1.90100200	-3.06286000	3.73926000
H	-0.90889400	-2.89554700	3.31145400
H	-1.83413800	-3.04014900	4.83172500
H	-2.27566400	-4.03787500	3.41430500
C	-3.78774800	0.79911800	1.33166600

H	-2.81100100	1.09358000	0.93675400
H	-4.42976300	0.49010100	0.50119400
H	-4.25087900	1.64573000	1.84761500
C	3.75358800	0.03469500	-0.90528200
C	5.05856800	-0.22637100	-1.00642900
H	3.43205600	0.92512400	-0.35959500
H	5.80113000	0.43513000	-0.56745800
H	5.42984900	-1.11222600	-1.52050000

Electronic Energy (0K) = -2046.0350526

Electronic Energy (0K) + ZPE = -2045.505919

Enthalpy (298K) = -2045.468392

Free Energy (298K) = -2045.576284

3c

Number of imaginary frequencies: 0

O	-0.00075000	2.99895100	0.00002300
C	1.18003700	1.04384900	-0.00007500
C	-1.18036700	1.04330600	0.00002800
C	1.17706100	-0.33669300	0.00001300
C	-1.17674600	-0.33695600	-0.00003900
H	-2.07243600	1.65831100	0.00032500
C	0.00021100	-1.07435900	0.00000300
H	0.00025900	-2.15905400	0.00001300
N	-0.00047200	1.73473400	-0.00000300
H	2.07171200	1.65944900	-0.00031000
Cl	-2.70847000	-1.15705700	-0.00001200
Cl	2.70897600	-1.15637400	0.00002500

Electronic Energy (0K) = -1242.358683

Electronic Energy (0K) + ZPE = -1242.285077

Enthalpy (298K) = -1242.276717

Free Energy (298K) = -1242.318163

TS_B

Number of imaginary frequencies: 1

C	2.40793500	-3.77202700	-1.30151900
C	2.18725400	-3.02838500	-0.14971600
C	1.91433500	-1.65814700	-0.22862400
C	1.84096500	-1.01999200	-1.48359900
C	2.07945500	-1.79143900	-2.62969600
C	2.35680000	-3.14764700	-2.54758300
H	2.62911700	-4.83437400	-1.22805400
H	2.23364400	-3.49959200	0.83130500
H	2.05648900	-1.30893200	-3.60565100
H	2.53946600	-3.71912300	-3.45462300
C	1.67074900	-0.91657800	1.01839700
C	2.53063900	-0.41804500	1.85181700
N	2.74865700	0.17274100	3.01199700
C	2.82159400	-0.59384500	4.27375700
C	1.51569100	-0.75935900	4.89715900
C	0.43440800	-0.85939200	5.43758800
C	-0.82739100	-0.98309800	6.09400500
C	-1.92693200	-0.21808700	5.67550800
C	-0.97896700	-1.87884200	7.16362000
C	-3.15233500	-0.34997100	6.31759700
H	-1.80444300	0.47418600	4.84256700
C	-2.20778900	-2.00444800	7.79797500
H	-0.12563600	-2.47094700	7.48680600
C	-3.29636200	-1.24260000	7.37761200
H	-4.00122700	0.24539100	5.98705800
H	-2.31685900	-2.70063600	8.62614600

H	-4.25648600	-1.34337500	7.87837500
S	2.91724100	1.89746600	3.06049400
O	3.91412600	2.16484800	4.08225300
O	3.10755300	2.29519100	1.67411900
C	1.34050900	2.44659600	3.61383500
C	1.11183900	2.58931100	4.97997100
C	0.33012700	2.64778100	2.67331700
C	-0.16337600	2.93258300	5.40885900
H	1.91626500	2.43151500	5.69467300
C	-0.93084700	3.00469900	3.12562400
H	0.53580900	2.54381200	1.61000300
C	-1.19999500	3.13522400	4.49281800
H	-0.36355000	3.03399900	6.47401200
H	-1.72837600	3.18467700	2.40661700
C	-2.58432600	3.47160300	4.94743900
H	-2.71172900	3.29943200	6.02085300
H	-3.32845700	2.87061200	4.40697000
H	-2.81968700	4.52492200	4.74822100
H	3.51928100	-0.07584500	4.94326000
H	3.27987700	-1.55978300	4.03010100
Au	-0.34359800	-0.77502700	1.63094200
C	-2.34494400	-0.78631100	2.15282400
C	-4.30042400	-1.34084500	3.11794100
C	-4.50676100	-0.20738500	2.40520200
H	-4.96585500	-1.93169100	3.73235600
H	-5.39496100	0.38875100	2.24899300
N	-2.97267200	-1.67963700	2.95055800
N	-3.29709000	0.11658900	1.82043000
C	-2.36410100	-2.84975900	3.56047500
H	-1.29259900	-2.84283600	3.34363400

H	-2.51558500	-2.82126800	4.64433400
H	-2.81179300	-3.75966500	3.14984200
C	-3.12607500	1.20786500	0.87763400
H	-2.05718500	1.37610700	0.72251200
H	-3.59147300	0.95584300	-0.08033700
H	-3.59125300	2.11533400	1.27402900
C	1.56932800	0.42099500	-1.55586300
C	1.37562800	1.14136300	-2.66517800
H	1.53409800	0.94072300	-0.59539500
H	1.19245400	2.21140500	-2.60798700
H	1.39046400	0.70761900	-3.66408000
C	5.53542100	-1.62789900	-1.90249000
C	5.45571300	-0.42567100	-2.59694400
C	5.00784800	0.68403100	-1.89425700
C	4.63321200	0.59324500	-0.56449600
C	5.16243700	-1.71261300	-0.57562300
H	5.74140900	-0.35714900	-3.64244500
H	5.19258800	-2.61723600	0.02073200
N	4.70980100	-0.60537900	0.05891600
O	4.37652800	-0.70490200	1.32296800
H	4.27339700	1.42085400	0.04207300
Cl	6.09887600	-3.05742800	-2.69652100
Cl	4.89784000	2.22271100	-2.67563800

Electronic Energy (0K) = -3288.4018137

Electronic Energy (0K) + ZPE = -3287.798373

Enthalpy (298K) = -3287.752655

Free Energy (298K) = -3287.878653

B

Number of imaginary frequencies: 0

C	2.49800200	-3.83531500	-1.17977400
C	2.28361200	-3.04085400	-0.06031000
C	1.87982800	-1.70496300	-0.18893200
C	1.65433000	-1.16950500	-1.47654200
C	1.87486600	-1.99017200	-2.59203700
C	2.30375600	-3.30238400	-2.45364000
H	2.81927700	-4.86777400	-1.06032500
H	2.43879100	-3.44601100	0.93992100
H	1.68685100	-1.58972200	-3.58697000
H	2.47023500	-3.91573500	-3.33610800
C	1.68726600	-0.89999300	1.03446800
C	2.72557500	-0.41952300	1.71821700
N	2.74485500	0.17754500	2.97299300
C	2.71524500	-0.63706900	4.19677500
C	1.39646100	-0.76012700	4.81067900
C	0.33156800	-0.84927400	5.38513700
C	-0.91794400	-0.96848900	6.06551600
C	-2.01667600	-0.18057700	5.68966400
C	-1.06059500	-1.89022600	7.11457900
C	-3.23092100	-0.31594500	6.35192300
H	-1.90322200	0.52935400	4.87073100
C	-2.27888100	-2.02092900	7.76797300
H	-0.20781500	-2.49952700	7.40615100
C	-3.36658300	-1.23663700	7.38884500
H	-4.07835700	0.29924800	6.05600400
H	-2.38063500	-2.73862300	8.57872200
H	-4.31879000	-1.34094100	7.90387900
S	2.91920600	1.84851300	3.12079600
O	3.90069200	2.09608200	4.16795200
O	3.13632800	2.33966400	1.76192600

C	1.35085400	2.42931400	3.68208400
C	1.12506200	2.57292800	5.04733100
C	0.34168000	2.65467900	2.74661400
C	-0.14332400	2.93734600	5.48137000
H	1.92799100	2.39570400	5.75900000
C	-0.91142800	3.03591400	3.20103200
H	0.54349400	2.54415600	1.68279500
C	-1.17690200	3.16483500	4.56925600
H	-0.34061700	3.03445700	6.54760000
H	-1.70708700	3.23326100	2.48432100
C	-2.55404800	3.52283600	5.03058300
H	-2.67768500	3.35150900	6.10478200
H	-3.31018000	2.93121400	4.49672300
H	-2.77709100	4.57913500	4.83279900
H	3.42827000	-0.21276200	4.91665300
H	3.10604800	-1.62601400	3.92717100
Au	-0.29667300	-0.74001800	1.66020200
C	-2.31182000	-0.74010500	2.17408800
C	-4.28652300	-1.31223100	3.09697200
C	-4.47930300	-0.16201700	2.40844500
H	-4.96209300	-1.91484500	3.68851600
H	-5.36360700	0.44019700	2.25327200
N	-2.95683400	-1.64994800	2.94059600
N	-3.25956500	0.17178100	1.84935000
C	-2.35992900	-2.83560200	3.53056400
H	-1.29302600	-2.84626600	3.29265800
H	-2.48947500	-2.81585500	4.61769000
H	-2.83196400	-3.73337600	3.12026000
C	-3.07686600	1.27957300	0.92887900
H	-2.00613600	1.45604300	0.79549800

H	-3.52451400	1.04281700	-0.04163000
H	-3.55279500	2.17839800	1.33256800
C	1.23039600	0.22803600	-1.62046600
C	1.35929300	0.98187700	-2.71701000
H	0.77747200	0.67448900	-0.73019200
H	0.99673900	2.00641900	-2.74124900
H	1.82912100	0.61324200	-3.62915600
C	5.37245900	-1.44037900	-1.90190500
C	5.24984400	-0.22753100	-2.57476100
C	4.71660700	0.85656800	-1.88842700
C	4.29604500	0.72882100	-0.57439700
C	4.96755400	-1.55595900	-0.58530100
H	5.57181400	-0.13113300	-3.60835500
H	5.03216600	-2.45684200	0.01449100
N	4.43590500	-0.47316800	0.01023900
O	4.13688200	-0.60804100	1.33315000
H	3.87210200	1.52148300	0.04124100
Cl	6.03223300	-2.82137300	-2.69295000
Cl	4.55873900	2.38936400	-2.65906100

Electronic Energy (0K) = -3288.4146607

Electronic Energy (0K) + ZPE = -3287.809365

Enthalpy (298K) = -3287.763699

Free Energy (298K) = -3287.889657

TS_{B1}

Number of imaginary frequencies: 1

C	1.36287100	0.08147500	-0.56402900
C	0.21272600	0.52847500	-0.98844500
N	0.07714000	1.76639300	-1.58137800
C	1.24030000	2.66933400	-1.37971400

C	2.39445000	1.83678200	-1.06399000
C	3.57107800	1.51957100	-0.88391000
C	4.81486400	0.92692100	-0.59939700
C	5.54685300	0.29700600	-1.62508200
C	5.28835700	0.89673800	0.72631900
C	6.72828800	-0.35831200	-1.32174600
H	5.16708900	0.32809300	-2.64364900
C	6.46832100	0.23210400	1.01727500
H	4.71526800	1.39107600	1.50759800
C	7.18397400	-0.39411600	-0.00345800
H	7.29560700	-0.84772000	-2.10882400
H	6.83554900	0.19902100	2.03944900
S	-1.44494000	2.50968300	-1.70886300
O	-2.35579100	1.50367600	-2.23146300
O	-1.17456400	3.74311400	-2.43045800
C	-1.90652500	2.90197800	-0.04754800
C	-2.65783900	1.98635300	0.69070500
C	-1.45797500	4.09354000	0.51941900
C	-2.94254200	2.26878300	2.01779000
H	-3.02103200	1.07414400	0.22091900
C	-1.75418000	4.35573700	1.85147100
H	-0.90528700	4.81549000	-0.07733200
C	-2.48998900	3.44984700	2.61941600
H	-3.53329800	1.56584100	2.60352000
H	-1.41298000	5.28515700	2.30367300
C	-2.81366200	3.73594700	4.05144500
H	-2.54945500	2.88766400	4.69420400
H	-2.28470000	4.62166400	4.41625000
H	-3.88913700	3.90989200	4.18194700
H	1.40662100	3.26291600	-2.28352400

H	1.05122100	3.35761800	-0.53960400
H	8.10924300	-0.91537400	0.23107200
C	2.11900100	-0.85683600	0.20158400
C	3.00118000	-1.73628500	-0.44886600
C	1.98475100	-0.89358300	1.61456400
C	3.73712000	-2.66055000	0.27427700
H	3.08796600	-1.67688100	-1.53220100
C	2.72862600	-1.84639500	2.31838600
C	3.59095400	-2.71491200	1.66073300
H	4.42474600	-3.33153300	-0.23403000
H	2.65423000	-1.88271800	3.40313200
H	4.16749200	-3.43437500	2.23775300
C	1.09122100	0.04285400	2.30351400
H	0.91027400	0.99490100	1.79856900
C	0.48521000	-0.19414900	3.47066600
H	0.59488600	-1.13824000	4.00329100
H	-0.15017500	0.55622300	3.93426900
Au	-1.24292900	-0.95519700	-0.64072700
C	-2.61413000	-2.43085200	-0.22849500
C	-3.57479000	-4.26938200	0.63609900
C	-4.50538400	-3.64012800	-0.12224100
H	-3.62169300	-5.18138500	1.21432300
H	-5.53390700	-3.88772300	-0.34405800
N	-3.89625600	-2.51539000	-0.64336900
N	-2.42162500	-3.51393200	0.55697400
C	-1.18107800	-3.81399400	1.25545400
H	-0.33795500	-3.76034100	0.56067200
H	-1.02410300	-3.10322900	2.07343900
H	-1.24297800	-4.82508400	1.66313500
C	-4.56575100	-1.54605400	-1.49519800

H	-3.82310100	-0.84544100	-1.88654700
H	-5.05192900	-2.05969200	-2.32885800
H	-5.31777600	-0.99556300	-0.92158600

Electronic Energy (0K) = -2046.0079467

Electronic Energy (0K) + ZPE = -2045.479566

Enthalpy (298K) = -2045.442564

Free Energy (298K) = -2045.549140

TS_{B2}

Number of imaginary frequencies: 1

C	1.13636300	0.36643400	1.05938400
C	0.32801100	0.87760200	0.15308800
N	0.23300700	2.13145500	-0.36084400
C	1.34059900	3.11599000	-0.25962000
C	2.61500600	2.48829300	-0.55965900
C	3.63899600	1.86877600	-0.75787400
C	4.82550400	1.10257300	-0.96221900
C	5.55689500	1.20817800	-2.15366300
C	5.25090400	0.20966000	0.03369600
C	6.69165600	0.43064800	-2.34167000
H	5.22291400	1.89994800	-2.92353900
C	6.38168100	-0.56956300	-0.16640700
H	4.68027600	0.13134200	0.95886600
C	7.10415700	-0.45949700	-1.35251700
H	7.25603400	0.51646000	-3.26707700
H	6.70129300	-1.26406300	0.60733900
S	-1.18260200	2.57563800	-1.23599500
O	-1.39093700	1.64706700	-2.33950600
O	-1.00351800	3.99385600	-1.51026900
C	-2.45257300	2.33012500	-0.03191000

C	-3.59393400	1.62237000	-0.39246900
C	-2.30179700	2.87757800	1.24122900
C	-4.59737400	1.44810500	0.55286600
H	-3.68906200	1.21349000	-1.39542700
C	-3.31256200	2.68787500	2.17057600
H	-1.39858500	3.42674200	1.50668300
C	-4.47179500	1.97204600	1.84219500
H	-5.49556300	0.89353600	0.28665700
H	-3.20643100	3.10050200	3.17233600
C	-5.56343400	1.79933000	2.84956600
H	-5.15999500	1.66543100	3.85895400
H	-6.20776300	2.68770700	2.87565900
H	-6.19897700	0.94059700	2.61118800
H	1.12454400	3.92986000	-0.95804100
H	1.34133100	3.55505800	0.74835700
H	7.99148300	-1.06881600	-1.50723400
C	1.95703200	-0.73448100	1.39522100
C	2.20757500	-1.83000100	0.53561800
C	2.55586900	-0.70562200	2.68782100
C	2.94114600	-2.89818800	1.00341000
H	1.79539300	-1.82662300	-0.47161600
C	3.28378900	-1.81796100	3.14707900
C	3.47737900	-2.89448400	2.30803300
H	3.11308200	-3.75597100	0.35794300
H	3.71909100	-1.79912700	4.14360800
H	4.06283000	-3.74627500	2.64534100
C	2.32624600	0.51432100	3.38497100
H	2.25575100	0.53290800	4.47161500
C	2.03075100	1.60523000	2.61318700
H	1.56634100	2.49630700	3.03403600

H	2.58107700	1.76508500	1.68029200
Au	-0.99005500	-0.72790100	-0.30632500
C	-2.21880000	-2.30855300	-0.78538000
C	-3.68465700	-3.64169500	-1.84548700
C	-3.23152000	-4.31503000	-0.76062100
H	-4.39556200	-3.91597000	-2.61205400
H	-3.45992900	-5.30263100	-0.38528600
N	-3.05132100	-2.41461400	-1.84416600
N	-2.33597000	-3.48048600	-0.12196400
C	-1.57233800	-3.85097000	1.05773400
H	-0.73194400	-4.49575600	0.78146300
H	-1.18852200	-2.94165000	1.52801500
H	-2.22034600	-4.37775900	1.76262200
C	-3.26967100	-1.39066900	-2.85310800
H	-4.29413700	-1.01095300	-2.78869800
H	-2.56144700	-0.57322000	-2.69001000
H	-3.10621000	-1.81459200	-3.84780200

Electronic Energy (0K) = -2045.9953734

Electronic Energy (0K) + ZPE = -2045.468564

Enthalpy (298K) = -2045.431255

Free Energy (298K) = -2045.540560

TS_{B3}

Number of imaginary frequencies: 1

C	1.35253300	3.68421600	-1.87741200
C	0.72902900	2.52021800	-1.43866300
C	-0.62459800	2.58177400	-1.01953900
C	-1.33102900	3.78836500	-1.04210400
C	-0.68547100	4.93813900	-1.47868700
C	0.64628100	4.88455000	-1.89287500

H	2.39119400	3.65045800	-2.20181300
H	-2.37109600	3.80057200	-0.71997500
H	-1.22179800	5.88365900	-1.49896000
H	1.14119300	5.79240900	-2.23088700
C	-1.19178700	1.32879000	-0.60201100
C	-2.05550300	0.51862800	-0.22703400
N	-2.79779200	-0.47403900	0.21573700
C	-2.60278500	-0.97791200	1.60642800
C	-1.22521300	-1.36645500	1.86338600
C	-0.04746600	-1.61090000	2.02048900
C	1.35561200	-1.84711100	2.14900600
C	1.98034400	-2.81914100	1.35269200
C	2.13151000	-1.07011400	3.02405500
C	3.35508700	-3.00486500	1.42584300
H	1.37185200	-3.42263000	0.68127600
C	3.50595900	-1.26479700	3.09296300
H	1.64632300	-0.31781300	3.64261400
C	4.12070200	-2.22706300	2.29288100
H	3.82844100	-3.76455500	0.80718800
H	4.10295000	-0.66234600	3.77465300
H	5.19898600	-2.36885900	2.34650500
S	-3.45183700	-1.56526200	-0.99763400
O	-3.93180100	-0.70141500	-2.05898900
O	-4.33908800	-2.44259100	-0.25323600
C	-2.01774200	-2.43392700	-1.52900000
C	-1.22365500	-1.87532100	-2.53285400
C	-1.63390700	-3.58146000	-0.83971000
C	-0.00905600	-2.47709700	-2.82563100
H	-1.54867700	-0.98622000	-3.06816300
C	-0.41609500	-4.16847000	-1.15524100

H	-2.27392700	-4.00364500	-0.06825000
C	0.42180700	-3.61277300	-2.12757500
H	0.62649700	-2.05772400	-3.60421100
H	-0.09956200	-5.06580900	-0.62619600
C	1.76627700	-4.20216300	-2.41023600
H	2.55613100	-3.45701400	-2.24374400
H	1.97087800	-5.06714300	-1.77137000
H	1.84795500	-4.52113400	-3.45639000
H	-2.90570500	-0.16494200	2.27865200
H	-3.31266400	-1.80024300	1.75422900
O	-4.33002400	2.74386000	-0.69082800
C	1.27208300	1.13901900	-1.44706800
C	0.61300900	0.35652000	-0.45622100
H	1.29562700	0.69206300	-2.44864800
H	0.48598000	-0.72043500	-0.58022700
H	0.62099600	0.69550100	0.57908000
C	-4.81386500	1.88699700	1.37604000
C	-5.91874500	1.11410000	-0.56005500
C	-5.52873700	0.98295100	2.13854300
C	-6.62547100	0.20795900	0.20474400
H	-6.01299800	1.21883400	-1.63390700
C	-6.44671400	0.10479200	1.57904200
H	-6.99897200	-0.61083200	2.17944100
N	-5.00372700	1.93957500	0.02483900
Au	3.21961100	0.80175900	-0.55858900
C	5.06316100	0.50971100	0.33978800
N	5.99502100	-0.42711500	0.05533100
C	6.77616000	0.66712200	1.78986500
C	7.05698600	-0.34650000	0.93441200
H	7.32809800	1.07016600	2.62748300

H	7.90261400	-1.01721500	0.87187500
N	5.55117100	1.17759600	1.40983000
C	5.89470500	-1.41605200	-1.00351600
H	4.90364000	-1.33804700	-1.45824500
H	6.66142000	-1.23950600	-1.76339900
H	6.02428600	-2.41849200	-0.58412300
C	4.88980600	2.28555500	2.07847300
H	5.32257000	3.23926200	1.76164300
H	3.82640800	2.26640900	1.82406200
H	5.00597900	2.17692400	3.16012700
H	-4.07770100	2.58022500	1.76814800
Cl	-7.76196900	-0.82443400	-0.60271000
Cl	-5.23576400	0.95082800	3.85313000

Electronic Energy (0K) = -3288.3736749

Electronic Energy (0K) + ZPE = -3287.769472

Enthalpy (298K) = -3287.724122

Free Energy (298K) = -3287.848792

TS_{B4}

Number of imaginary frequencies: 1

C	-2.99307000	-0.14711000	2.39353700
C	-1.93193400	-0.02366100	1.49045600
C	-1.89098800	1.10949700	0.62860200
C	-2.96610600	2.02278800	0.67372500
C	-4.01704200	1.85912600	1.56270200
C	-4.03019700	0.77582900	2.44228800
H	-2.99628700	-0.99237700	3.08113200
H	-2.95717500	2.87036300	-0.01240200
H	-4.82724200	2.58630300	1.57692600
H	-4.84133500	0.65166100	3.15594900

C	-0.84953700	1.26443700	-0.33585300
C	0.24121000	1.89351700	-0.57883300
N	1.01821300	1.94503100	-1.76103600
C	0.21601600	1.52818000	-2.91108800
C	-0.39532300	0.20276500	-2.74472200
C	-0.80053300	-0.97946900	-2.76248300
C	-1.60380400	-2.01918500	-2.15771400
C	-1.23643700	-3.36737700	-2.25080500
C	-2.74092600	-1.65763400	-1.42222100
C	-1.99038500	-4.33936400	-1.60519800
H	-0.35034800	-3.63895000	-2.82500700
C	-3.49606900	-2.63646600	-0.79134100
H	-3.01155100	-0.60673700	-1.34080800
C	-3.12185500	-3.97571500	-0.87860500
H	-1.69759000	-5.38439700	-1.67365400
H	-4.37246800	-2.34840900	-0.21471600
H	-3.71346100	-4.73914300	-0.37848700
S	2.64328800	1.37888400	-1.70521800
O	3.45074600	2.45756000	-1.16016100
O	2.92222500	0.87695400	-3.05101100
C	2.68876200	0.02829000	-0.55638700
C	3.19661000	0.25079700	0.72130100
C	2.22873100	-1.22928400	-0.94130800
C	3.22535900	-0.80240500	1.62483000
H	3.57086800	1.23467300	0.99299700
C	2.25662600	-2.26782000	-0.01990600
H	1.85077100	-1.39729300	-1.94940600
C	2.74625600	-2.06940200	1.27528000
H	3.62564100	-0.64239200	2.62563000
H	1.89039200	-3.25239600	-0.30873400

C	2.75016300	-3.17656500	2.28117200
H	3.73683800	-3.28793900	2.74619400
H	2.03843100	-2.96484400	3.08980900
H	2.47292400	-4.13559900	1.83176600
H	-0.57449900	2.27912300	-3.03196400
H	0.83180100	1.55315100	-3.81541200
O	0.99978200	2.92985800	0.38890600
C	-0.88325000	-1.04304400	1.38453400
C	-0.95924900	-2.30910400	1.80854300
H	0.02306200	-0.73310500	0.85832900
H	-1.84472200	-2.71613500	2.29664600
H	-0.13057300	-2.99778000	1.65101000
C	-0.60217400	4.54820800	0.84895000
C	-0.00520900	2.94531600	2.49398000
C	-1.52436700	5.11157700	1.70464500
C	-0.92419400	3.48322500	3.37302600
C	-1.69475200	4.56469100	2.97070600
H	-1.02719000	3.03994700	4.35760700
H	-2.42610500	4.99033800	3.65102300
N	0.14743700	3.47507100	1.24474500
Au	0.57940100	-1.38862100	-4.41121600
C	1.81735500	-2.02997800	-5.91333200
N	1.49056100	-2.31731000	-7.19136600
C	3.64391300	-2.70556200	-7.02754300
C	2.60157000	-2.73603000	-7.89439700
H	4.68936600	-2.94534100	-7.16058000
H	2.54831000	-3.00658800	-8.93944300
N	3.14373700	-2.26928000	-5.81852400
C	3.93240000	-2.11016800	-4.60370000
H	3.71898400	-1.14095400	-4.14273800

H	3.70574800	-2.91424600	-3.89661300
H	4.99104500	-2.15530900	-4.86720800
C	0.15874900	-2.21049600	-7.76319300
H	-0.22483000	-3.20376200	-8.01361400
H	-0.49909300	-1.74110000	-7.02741100
H	0.19245200	-1.59491900	-8.66610200
H	-2.10233400	5.96447400	1.36500100
Cl	-0.34583600	5.13782100	-0.72776100
Cl	0.97813700	1.62563100	2.91682300

Electronic Energy (0K) = -3288.3407044

Electronic Energy (0K) + ZPE = -3287.739855

Enthalpy (298K) = -3287.693633

Free Energy (298K) = -3287.821611

TS_C

Number of imaginary frequencies: 1

C	-0.45212900	-3.81134300	-1.67630400
C	-0.30609100	-3.04219600	-0.53049900
C	0.30868300	-1.78362600	-0.58674800
C	0.73062100	-1.26648400	-1.83236600
C	0.53148300	-2.04473400	-2.98216300
C	-0.03434200	-3.30911900	-2.90854900
H	-0.90776700	-4.79659100	-1.61071500
H	-0.64657600	-3.41959800	0.43301500
H	0.80774800	-1.63214300	-3.95108200
H	-0.17388900	-3.89445300	-3.81419800
C	0.50031800	-1.03112700	0.66418100
C	1.76516700	-0.97950100	1.20778700
N	2.17589300	-0.12769100	2.25824000
C	2.36415100	-0.67676000	3.60816100

C	1.18334700	-0.52510200	4.45405500
C	0.22819600	-0.34608000	5.18064300
C	-0.88237400	-0.12587600	6.05155500
C	-1.80566000	0.89808500	5.78697100
C	-1.05953800	-0.93460800	7.18457600
C	-2.87863400	1.10760400	6.64523600
H	-1.66844900	1.52358800	4.90446300
C	-2.13680900	-0.72000100	8.03423100
H	-0.34305500	-1.72731100	7.38839000
C	-3.04845400	0.30014700	7.76787400
H	-3.58520900	1.90889400	6.43802100
H	-2.26433200	-1.35014700	8.91122400
H	-3.88706100	0.46916300	8.43936400
S	2.55617500	1.48688800	1.98100600
O	3.82998400	1.72191700	2.65623100
O	2.45289100	1.67291500	0.53852600
C	1.32281000	2.45563600	2.78688500
C	1.47442300	2.76947600	4.13456900
C	0.19730500	2.85151700	2.06639100
C	0.46427400	3.47461200	4.77531300
H	2.36853000	2.46748000	4.67482300
C	-0.78946000	3.57318300	2.72200100
H	0.11203500	2.61485400	1.00743100
C	-0.68169600	3.87659400	4.08367400
H	0.55893100	3.70964000	5.83406200
H	-1.66677300	3.90879700	2.17141100
C	-1.78956800	4.60293700	4.77856800
H	-1.70613800	4.51921400	5.86715000
H	-2.76735500	4.20763100	4.47294000
H	-1.78447800	5.67115900	4.52662200

H	3.23252600	-0.19242100	4.07456400
H	2.63330000	-1.73412100	3.49331300
Au	-1.21136200	-0.34392800	1.59182900
C	-3.02879200	0.20284500	2.45060600
C	-4.83727500	0.24989200	3.79089200
C	-4.92213200	1.31433200	2.95702800
H	-5.48478800	-0.08743300	4.58847800
H	-5.66750900	2.09179200	2.86204100
N	-3.67294900	-0.41690600	3.46586100
N	-3.80734700	1.26574700	2.14166400
C	-3.25210800	-1.65826000	4.09346000
H	-2.17976500	-1.79537700	3.93181800
H	-3.45356000	-1.61108800	5.16730600
H	-3.79483600	-2.50349400	3.65825800
C	-3.58324900	2.17334800	1.03060100
H	-2.56227800	2.03711800	0.66377200
H	-4.28621100	1.95652900	0.22028500
H	-3.72450000	3.20701200	1.36018600
C	1.33238300	0.06998300	-1.90189700
C	2.18486400	0.49758700	-2.83809400
H	1.07978300	0.75400400	-1.09025700
H	2.58520900	1.50845300	-2.80359000
H	2.51527800	-0.13199600	-3.66489400
C	4.72007900	-1.78501500	-2.34287100
C	5.65673700	-0.78358500	-2.11003100
C	5.65023900	-0.14474600	-0.87418000
C	4.72780800	-0.51354300	0.09925500
C	3.79497900	-2.11779700	-1.36104300
H	6.37602100	-0.50461000	-2.87576200
H	3.01405800	-2.86761900	-1.48078600

N	3.85811100	-1.46376900	-0.21239600
O	2.63177500	-1.92412200	0.87362200
H	4.69633200	-0.07395200	1.09469500
Cl	4.66035600	-2.60353300	-3.86350900
Cl	6.78213700	1.11061100	-0.52535000

Electronic Energy (0K) = -3288.3956552

Electronic Energy (0K) + ZPE = -3287.791655

Enthalpy (298K) = -3287.746615

Free Energy (298K) = -3287.869655

[N]

Number of imaginary frequencies: 0

C	1.14641700	1.38029400	0.00018900
C	-1.14661900	1.38001400	-0.00024100
C	1.18077700	-0.01123300	0.00014900
C	-1.18067100	-0.01118500	-0.00010300
H	-2.07375300	1.95202800	-0.00038800
C	0.00002100	-0.73970200	0.00002000
H	-0.00002900	-1.82604300	-0.00005000
N	-0.00018800	2.05624200	0.00001000
H	2.07348300	1.95236000	0.00046300
Cl	-2.71498900	-0.83714100	0.00006500
Cl	2.71511100	-0.83704500	-0.00007600

Electronic Energy (0K) = -1167.2318682

Electronic Energy (0K) + ZPE = -1167.162383

Enthalpy (298K) = -1167.154891

Free Energy (298K) = -1167.194318

C

Number of imaginary frequencies: 0

C	-1.09663900	-2.74916100	3.14778500
C	-0.33879700	-2.06251400	2.19981000
C	-0.96302000	-0.99037300	1.47699500
C	-2.33863100	-0.72765000	1.70997000
C	-3.06569500	-1.42736200	2.65024100
C	-2.43050400	-2.43176500	3.38192700
H	-0.63918400	-3.57670600	3.68483400
H	-2.80362800	0.07893000	1.14544400
H	-4.11414000	-1.19952000	2.81954200
H	-2.98707000	-2.99172000	4.13005800
C	-0.28283100	-0.13024400	0.57296200
C	1.18667300	0.04189200	0.63114200
N	1.98286600	-0.26408500	-0.45323500
C	1.47574000	-0.82075100	-1.72389700
C	0.21776600	-1.51537700	-1.52448000
C	-0.83401100	-2.11513800	-1.40701300
C	-2.09884500	-2.69803700	-1.13370000
C	-2.18730300	-3.85001800	-0.33697300
C	-3.27139600	-2.07267200	-1.59256000
C	-3.43310100	-4.35662900	0.00668700
H	-1.27455800	-4.32863400	0.01289100
C	-4.51067900	-2.59439300	-1.25198600
H	-3.19045900	-1.17992500	-2.21118000
C	-4.59217400	-3.73194200	-0.44926400
H	-3.50062700	-5.24389600	0.63126300
H	-5.41794700	-2.11413200	-1.61039200
H	-5.56548400	-4.13555000	-0.18043400
S	3.62676700	0.28715000	-0.43529800
O	3.63200000	1.70705600	-0.13426500
O	4.14733600	-0.19516100	-1.70654700

C	4.35415300	-0.63720100	0.87708200
C	4.48990800	-0.07104500	2.14035800
C	4.79116500	-1.93296200	0.59917500
C	5.07882500	-0.82757300	3.14502600
H	4.14222800	0.94003200	2.32875600
C	5.37682200	-2.66853300	1.61787700
H	4.69113300	-2.34651300	-0.40206200
C	5.52509900	-2.12963000	2.90275000
H	5.19943200	-0.39852300	4.13794800
H	5.73446500	-3.67726100	1.41765100
C	6.12141700	-2.95313400	3.99902200
H	6.42817800	-2.33449800	4.84805800
H	5.39232500	-3.68571400	4.37120000
H	6.99193000	-3.51865700	3.64844600
H	1.34680500	-0.01525600	-2.46142800
H	2.23251600	-1.50636300	-2.12175600
O	1.61541600	0.58839300	1.63862000
C	1.03593600	-2.49574700	1.93762300
C	1.87557900	-2.93603500	2.87839700
H	1.37842100	-2.46322700	0.90214500
H	1.60244200	-2.96015800	3.93231900
H	2.88340300	-3.25556600	2.61896000
Au	-1.11858000	1.39955100	-0.54564200
C	-3.28607900	4.28449700	-2.83001900
C	-2.02254700	4.70252900	-3.08647000
H	-4.24356400	4.65904100	-3.16385200
H	-1.64977800	5.52167300	-3.68530000
C	-4.31695900	2.43211700	-1.50394000
H	-3.95863800	1.68756200	-0.78734900
H	-5.02318700	3.10220100	-1.00639000

H	-4.81983200	1.92493900	-2.33291000
C	0.27140900	3.98347100	-2.39565200
H	0.56750500	4.86646600	-1.82203100
H	0.70394100	3.09252700	-1.93107200
H	0.64006700	4.07366000	-3.42069500
C	-1.88210000	2.91744200	-1.72756300
N	-1.17708300	3.85145400	-2.40517000
N	-3.17903900	3.19073500	-1.99532600

Electronic Energy (0K) = -2121.2356099

Electronic Energy (0K) + ZPE = -2120.701940

Enthalpy (298K) = -2120.663201

Free Energy (298K) = -2120.774683

TS_D

Number of imaginary frequencies: 1

C	-1.80384500	-1.66433900	1.97040800
C	-1.05715300	-1.01033700	0.98850300
C	-1.68773800	0.02165100	0.22921900
C	-3.05237900	0.29474600	0.46334200
C	-3.77167700	-0.36592800	1.44380700
C	-3.13519800	-1.34127900	2.20800000
H	-1.33596900	-2.46803300	2.53477700
H	-3.52503800	1.07725200	-0.12875800
H	-4.81846200	-0.12745900	1.61152900
H	-3.68433300	-1.87135200	2.98285800
C	-0.99791800	0.82898200	-0.74919500
C	0.44963100	1.11889500	-0.57475800
N	1.28550200	0.85160200	-1.63983400
C	0.78374000	0.13864100	-2.81867100
C	-0.54622700	-0.38413200	-2.51392300

C	-1.58987800	-1.03179100	-2.56151700
C	-2.86270900	-1.59805600	-2.36215800
C	-2.99549000	-2.73880500	-1.54884300
C	-4.00874200	-0.96116900	-2.87924500
C	-4.25897900	-3.21862000	-1.24198300
H	-2.10198800	-3.22567800	-1.16394500
C	-5.26477700	-1.45660300	-2.57145000
H	-3.89045800	-0.08410100	-3.51310200
C	-5.38878700	-2.57893300	-1.75030800
H	-4.36673900	-4.09269600	-0.60543000
H	-6.15276600	-0.97027500	-2.96711600
H	-6.37777900	-2.96058700	-1.50802100
S	2.91057000	1.41276600	-1.62217200
O	2.89567900	2.82886400	-1.30714400
O	3.43382400	0.94106400	-2.89611200
C	3.64166100	0.49287600	-0.30915000
C	3.69111400	1.02860300	0.97449400
C	4.15174100	-0.77350900	-0.59765500
C	4.26632000	0.27238400	1.98680400
H	3.28215200	2.01487300	1.17156300
C	4.72183800	-1.50994400	0.42980900
H	4.12406800	-1.16138000	-1.61359400
C	4.78320800	-1.00167700	1.73368100
H	4.31833500	0.67887300	2.99505000
H	5.13663100	-2.49479900	0.22133400
C	5.35723900	-1.82834200	2.83939400
H	5.66921200	-1.20972900	3.68664700
H	4.61037200	-2.54220000	3.21326200
H	6.21876500	-2.41365000	2.50016100
H	0.73511100	0.81423600	-3.68326700

H	1.45875500	-0.68804900	-3.07351600
O	0.81213200	1.69184500	0.43981500
C	0.32066200	-1.44300900	0.72958900
C	1.17178800	-1.86721400	1.66672500
H	0.65956000	-1.42553800	-0.30822900
H	0.91036500	-1.87776700	2.72393900
H	2.17543900	-2.19430300	1.40116800
Au	-1.86020900	2.41043000	-1.81565100
C	-4.07502200	5.37236800	-3.94826200
C	-2.81723600	5.80316900	-4.21025200
H	-5.03903000	5.75713200	-4.25016100
H	-2.45636900	6.64645600	-4.78228600
C	-5.07769200	3.46141800	-2.68306200
H	-4.71065400	2.72046100	-1.96695100
H	-5.80127900	4.11412700	-2.18755600
H	-5.56396700	2.94872100	-3.51885400
C	-0.51003600	5.06082600	-3.58606400
H	-0.20328800	5.91118200	-2.97025600
H	-0.07052500	4.14510900	-3.18005800
H	-0.15999800	5.20772500	-4.61119900
C	-2.64936100	3.96643200	-2.92464900
N	-1.95833100	4.92765000	-3.57757900
N	-3.95137400	4.24645400	-3.15889000

Electronic Energy (0K) = -2121.2338429

Electronic Energy (0K) + ZPE = -2120.700924

Enthalpy (298K) = -2120.662849

Free Energy (298K) = -2120.774108

D

Number of imaginary frequencies: 0

C	0.38669800	3.51241800	2.94372400
C	-0.01557800	2.72182300	1.86033600
C	0.70034700	1.53295800	1.57914400
C	1.80310300	1.21227700	2.37392100
C	2.20039800	2.01786500	3.43608200
C	1.48340500	3.17244100	3.72447200
H	-0.19545700	4.39937700	3.18746400
H	2.36194100	0.30374500	2.14714100
H	3.05963500	1.73568400	4.04008700
H	1.76814200	3.80233000	4.56416200
C	0.30903500	0.66461600	0.41651600
C	-1.06861200	0.10658100	0.41041200
N	-1.52620000	0.07383500	-0.92836900
C	-0.54203500	0.57832100	-1.88040100
C	0.46649700	1.23629200	-0.95388400
C	1.27934000	2.18423700	-1.29509800
C	2.13498600	3.20519500	-1.59322200
C	1.69598300	4.55460200	-1.44202900
C	3.46289400	2.93318300	-2.03928300
C	2.56011200	5.58705600	-1.72879300
H	0.67970600	4.73198800	-1.09487900
C	4.31099800	3.97934900	-2.32211200
H	3.77773700	1.89815300	-2.14540300
C	3.85751000	5.29565100	-2.16677800
H	2.24343100	6.61973400	-1.61841200
H	5.32512800	3.79243300	-2.66204100
H	4.53461700	6.11618100	-2.39299400
S	-2.63875500	-1.10411400	-1.44456300
O	-2.21789500	-2.41157000	-0.95489200
O	-2.73745400	-0.86992400	-2.88044800

C	-4.13311800	-0.62135800	-0.64896800
C	-4.64416300	-1.39293200	0.38712000
C	-4.78237300	0.52711700	-1.10201000
C	-5.84218900	-1.00537200	0.97395600
H	-4.10797700	-2.27472100	0.72674500
C	-5.97130100	0.89892600	-0.49769700
H	-4.36449400	1.11080000	-1.91946100
C	-6.51852500	0.13887200	0.54511300
H	-6.25974500	-1.59936500	1.78465500
H	-6.49581700	1.79035800	-0.83807900
C	-7.80241700	0.56344100	1.18383600
H	-7.68424400	1.52649700	1.69609100
H	-8.59060700	0.69796700	0.43335900
H	-8.15069600	-0.16874400	1.91844800
H	-0.05580400	-0.23005300	-2.44514500
H	-0.98575000	1.28673400	-2.58470200
O	-1.72753900	-0.27945000	1.35465200
C	-1.16489700	3.15413500	1.04770200
C	-1.47120300	4.42907700	0.79111000
H	-1.82045000	2.38122400	0.64162500
H	-0.85778400	5.25399200	1.15341300
H	-2.35368000	4.69204500	0.21291600
Au	1.32784000	-1.27815700	0.25798600
C	3.38608600	-5.00496300	0.47499700
C	2.68838800	-5.19728800	-0.67066400
H	4.06704500	-5.64845600	1.01392900
H	2.63645200	-6.04432500	-1.33987300
C	3.61526200	-3.14674200	2.13211400
H	4.68046100	-2.93355400	2.00180100
H	3.07843700	-2.21727100	2.33924600

H	3.48216000	-3.83406600	2.97178500
C	1.07485000	-3.82640100	-2.02453500
H	0.09913900	-3.47503300	-1.67485600
H	1.50532200	-3.09081400	-2.71131500
H	0.94399900	-4.77297400	-2.55237400
N	3.06846500	-3.73813700	0.92325600
N	1.96363400	-4.04337400	-0.89224700
C	2.19414000	-3.13943600	0.08588200

Electronic Energy (0K) = -2121.2597237

Electronic Energy (0K) + ZPE = -2120.726281

Enthalpy (298K) = -2120.687613

Free Energy (298K) = -2120.801262

E

Number of imaginary frequencies: 0

C	-2.16317100	-3.25589400	2.77434200
C	-1.47050000	-2.16474800	2.23197000
C	-0.15944300	-2.38777300	1.75223500
C	0.43526600	-3.64296400	1.92486400
C	-0.26141100	-4.69838100	2.49765700
C	-1.57677700	-4.50694400	2.90726800
H	-3.18216300	-3.09832000	3.12474100
H	1.45336800	-3.79238400	1.57124100
H	0.21805100	-5.66737700	2.61147100
H	-2.14201800	-5.32683400	3.34367800
C	0.62086000	-1.39531200	1.00363600
C	1.98606600	-0.99675000	1.45348000
N	2.38992700	0.00798100	0.57880600
C	1.39477000	0.30019200	-0.43557400
C	0.30623000	-0.68873600	-0.11823300

C	-0.97385600	-0.62601000	-0.77373000
C	-1.64179500	-1.82608600	-1.14367200
C	-0.97299100	-3.07632800	-1.20492600
C	-3.03130900	-1.78880700	-1.42642800
C	-1.67095300	-4.23176000	-1.49284200
H	0.10056400	-3.11482900	-1.03979800
C	-3.72867600	-2.95065800	-1.69076100
H	-3.54093900	-0.82602900	-1.39508900
C	-3.04766800	-4.17042400	-1.72311400
H	-1.15317500	-5.18546400	-1.54406100
H	-4.79757900	-2.91849000	-1.88172600
H	-3.59513700	-5.08385700	-1.94436500
S	3.91917300	0.76440600	0.61853200
O	4.12384100	1.27073500	1.96247300
O	3.87605100	1.66598800	-0.52345400
C	5.04469300	-0.55183600	0.29739100
C	5.63371500	-1.22719300	1.36171100
C	5.31013200	-0.89479300	-1.02890600
C	6.51409900	-2.26455300	1.08247200
H	5.40213600	-0.94671700	2.38526700
C	6.18958400	-1.93450700	-1.28224500
H	4.84618100	-0.34315900	-1.84364200
C	6.80395900	-2.63218400	-0.23383800
H	6.98988700	-2.79934000	1.90224300
H	6.41628600	-2.21045800	-2.31096200
C	7.75296500	-3.74915400	-0.53193000
H	8.58442400	-3.40238700	-1.15737200
H	8.17162000	-4.17842900	0.38339000
H	7.25296500	-4.55298800	-1.08627700
H	1.01916400	1.33041300	-0.34808200

H	1.79720700	0.17238500	-1.44955700
O	2.63931300	-1.46055500	2.36340400
C	-2.17407000	-0.87562500	2.23503000
C	-1.65564900	0.35651400	2.28936800
H	-3.26263300	-0.96779700	2.26188500
H	-2.31023000	1.22293700	2.35858900
H	-0.58378100	0.55326000	2.31441700
Au	-1.76554800	1.26999500	-0.99219500
C	-2.69461200	5.43384000	-0.96325400
C	-3.66397400	5.01184400	-1.81282900
H	-2.45253900	6.41860300	-0.58934100
H	-4.44349600	5.55187500	-2.33129100
N	-1.98530800	4.31285500	-0.58544300
N	-3.51933600	3.64520900	-1.93034500
C	-2.48445500	3.20571800	-1.18026800
C	-0.81971800	4.33284700	0.28593500
H	-0.86291900	5.22075400	0.92015500
H	-0.82087100	3.44092100	0.91895800
H	0.10046600	4.35769100	-0.30616700
C	-4.34176600	2.79686900	-2.77985800
H	-3.78391100	2.49715100	-3.67197900
H	-4.65128500	1.90647200	-2.22641800
H	-5.23076200	3.35447100	-3.08165000

Electronic Energy (0K) = -2121.298672

Electronic Energy (0K) + ZPE = -2120.763179

Enthalpy (298K) = -2120.725397

Free Energy (298K) = -2120.834074

TS_F

Number of imaginary frequencies: 1

C	-1.82183800	-3.94958400	3.66552800
C	-1.34912000	-2.77254900	3.06862600
C	0.03426300	-2.46783500	3.11753500
C	0.86584200	-3.33288000	3.84550300
C	0.36589400	-4.45946500	4.48625100
C	-0.98216900	-4.78364000	4.38702500
H	-2.88250700	-4.18143300	3.58348400
H	1.92701200	-3.11803300	3.89970600
H	1.04360500	-5.09703700	5.04872400
H	-1.37583600	-5.67825900	4.86255200
C	0.65045700	-1.41287500	2.30229600
C	2.07522600	-0.99368700	2.47372900
N	2.36742300	-0.16804800	1.39059800
C	1.23327100	0.02888900	0.51831100
C	0.16265300	-0.78512800	1.19891500
C	-1.15608000	-0.71851600	0.57221000
C	-1.54371600	-1.77792400	-0.34523300
C	-0.75620900	-2.93740100	-0.49737200
C	-2.71132500	-1.64608800	-1.12602600
C	-1.11212800	-3.91395100	-1.41456000
H	0.13893700	-3.05812700	0.11069200
C	-3.07527300	-2.63350400	-2.02405200
H	-3.32439400	-0.75211400	-1.00441800
C	-2.27148700	-3.76556900	-2.17349100
H	-0.49233500	-4.79869000	-1.53359900
H	-3.97912500	-2.52542300	-2.61780600
H	-2.55286200	-4.53686100	-2.88639300
S	3.87990100	0.55824300	1.11602800
O	4.27658200	1.26895300	2.31713800
O	3.68041500	1.27206500	-0.13778600

C	4.95385000	-0.81301000	0.85048000
C	5.80364300	-1.23449600	1.86646300
C	4.91643500	-1.45331900	-0.38898900
C	6.64236100	-2.31582100	1.62499700
H	5.80703900	-0.72273400	2.82454200
C	5.75717700	-2.53173900	-0.60551200
H	4.24738400	-1.10179900	-1.17191300
C	6.63294300	-2.97644300	0.39442200
H	7.31866900	-2.65516900	2.40726900
H	5.74614400	-3.04067200	-1.56814000
C	7.54098300	-4.13524400	0.13054700
H	8.23405800	-3.90984700	-0.68930500
H	8.13383700	-4.39530200	1.01265700
H	6.97100100	-5.02232800	-0.17144900
H	0.95691300	1.08902300	0.44639200
H	1.42281700	-0.33781300	-0.50276900
O	2.87396100	-1.28028500	3.34247300
C	-2.36823900	-1.93220800	2.46379900
C	-2.44230700	-0.57794400	2.48489700
H	-3.20029800	-2.47100000	2.00410900
H	-3.34853200	-0.08383300	2.14375900
H	-1.72190500	0.03261100	3.02491800
Au	-1.82992700	1.25515700	0.21353700
C	-2.29068700	5.41672900	-0.56014300
C	-3.41169400	4.95903700	-1.17017300
H	-1.89291500	6.41599800	-0.45360100
H	-4.19705900	5.47685800	-1.70213800
N	-1.65631900	4.31609600	-0.02100600
N	-3.43062800	3.59119700	-0.98856900
C	-2.35098000	3.18765300	-0.28355000

C	-0.38108100	4.36289400	0.67813100
H	-0.23906800	5.36351300	1.09195400
H	-0.38558900	3.63814900	1.49575400
H	0.44086600	4.13656600	-0.00817600
C	-4.45446700	2.70068700	-1.51279900
H	-4.04912200	2.09276800	-2.32733300
H	-4.82579100	2.04811800	-0.71801800
H	-5.28258800	3.30246400	-1.89254100

Electronic Energy (0K) = -2121.2870888

Electronic Energy (0K) + ZPE = -2120.752906

Enthalpy (298K) = -2120.715454

Free Energy (298K) = -2120.825255

F

Number of imaginary frequencies: 0

C	-1.25369100	-3.89391300	3.44024800
C	-1.32609400	-2.76445400	2.54395000
C	-0.28171300	-1.74296200	2.62650400
C	0.54210300	-1.75792800	3.80016000
C	0.48173700	-2.79145600	4.68673500
C	-0.39556200	-3.90099000	4.48976400
H	-1.97530500	-4.69591200	3.29515600
H	1.26097400	-0.95732800	3.93566600
H	1.14031600	-2.78685200	5.55247600
H	-0.38630800	-4.72877300	5.19365100
C	0.04207800	-0.93570200	1.52982500
C	1.30287800	-0.16211900	1.42935400
N	1.56179900	-0.02702200	0.05527200
C	0.66006200	-0.84052900	-0.76224000
C	-0.50318600	-1.01870100	0.19480900

C	-1.82773300	-1.30223100	-0.13665500
C	-2.26192800	-1.74816600	-1.48182200
C	-1.46732400	-2.59311500	-2.26567700
C	-3.50231400	-1.33095500	-1.99087300
C	-1.88895200	-2.99244000	-3.52920300
H	-0.52538300	-2.97067700	-1.87444200
C	-3.92006500	-1.72738700	-3.25337500
H	-4.13894600	-0.67868600	-1.39333100
C	-3.11202600	-2.55677200	-4.02839800
H	-1.26168600	-3.65396100	-4.12181000
H	-4.87975000	-1.38772900	-3.63562300
H	-3.44114800	-2.87003900	-5.01626000
S	2.98660900	0.64842800	-0.57403300
O	3.20245300	1.91111800	0.10839800
O	2.77511000	0.60619100	-2.01471900
C	4.26142400	-0.48869200	-0.13892000
C	4.93538300	-0.33726400	1.07040800
C	4.55426300	-1.53276000	-1.01620300
C	5.92537100	-1.25421900	1.39636800
H	4.68769400	0.48248000	1.73830900
C	5.54664700	-2.43611900	-0.66828600
H	4.02665900	-1.61853700	-1.96317700
C	6.24652800	-2.30973700	0.53776800
H	6.46491000	-1.14831600	2.33574500
H	5.79327900	-3.25303500	-1.34447100
C	7.33766300	-3.27301800	0.88125600
H	7.06113500	-4.30122600	0.62253800
H	8.25165000	-3.03706800	0.32099600
H	7.58630200	-3.23824400	1.94662900
H	0.40309600	-0.33990800	-1.70043300

H	1.13044900	-1.80951400	-0.99272900
O	2.01941700	0.28628700	2.30276400
C	-2.42609900	-2.66683900	1.73580700
C	-2.80029300	-1.41975500	1.03296500
H	-3.07780200	-3.53592700	1.64558800
H	-3.83337100	-1.45232400	0.67990900
H	-2.69222500	-0.56301400	1.71213100
Au	-1.59568500	1.07340500	-0.27551100
C	-1.28395500	5.23486200	-0.86545400
C	-2.63066700	5.12222900	-0.97549900
H	-0.63127600	6.09382500	-0.93199000
H	-3.39799900	5.86140500	-1.15613000
N	-0.79670200	3.96831200	-0.61698300
N	-2.93373200	3.78733600	-0.79357100
C	-1.80873800	3.07721800	-0.57530800
C	0.61139600	3.62698900	-0.45489000
H	1.17998100	4.54207400	-0.27865300
H	0.73473300	2.96332500	0.40515900
H	0.99069700	3.13342000	-1.35537500
C	-4.28012200	3.24330700	-0.83900100
H	-4.70053600	3.36243100	-1.84152000
H	-4.23273800	2.18031000	-0.58735300
H	-4.91403900	3.75969300	-0.11318300

Electronic Energy (0K) = -2121.3379493

Electronic Energy (0K) + ZPE = -2120.799270

Enthalpy (298K) = -2120.762688

Free Energy (298K) = -2120.868336

TS_G

Number of imaginary frequencies: 1

C	-1.30896700	-3.87694400	3.26219400
C	-1.30477400	-2.84629700	2.27038500
C	-0.28892200	-1.81872200	2.35400400
C	0.46481200	-1.72549200	3.56074800
C	0.33544200	-2.66976900	4.54272300
C	-0.53201700	-3.77978100	4.37976400
H	-2.02138700	-4.69164900	3.14533800
H	1.18688100	-0.92214400	3.65977700
H	0.93352600	-2.58806200	5.44714700
H	-0.59160200	-4.53902500	5.15539400
C	0.12622800	-1.15175200	1.17691200
C	1.47070400	-0.52573300	1.02232800
N	1.76481400	-0.58895300	-0.34352300
C	0.75475200	-1.30229300	-1.12437100
C	-0.39998400	-1.35774800	-0.13925500
C	-1.70667400	-1.76670700	-0.44854300
C	-2.07867300	-2.26905100	-1.78341400
C	-1.36061000	-3.29712600	-2.40497600
C	-3.16954800	-1.69951500	-2.45505900
C	-1.71932700	-3.73932800	-3.67263100
H	-0.53630000	-3.77264400	-1.87632400
C	-3.51584600	-2.13089700	-3.72867200
H	-3.73399700	-0.89917200	-1.97619700
C	-2.79180000	-3.15287400	-4.33876600
H	-1.16269600	-4.54720000	-4.14120000
H	-4.35377000	-1.67033000	-4.24648800
H	-3.06828700	-3.49561300	-5.33297500
S	3.14751100	0.10914100	-1.04410000
O	3.27115600	1.45846200	-0.52049000
O	2.96286900	-0.12265500	-2.46945400

C	4.48376200	-0.87913000	-0.45892400
C	5.19204200	-0.48201700	0.67228000
C	4.79699400	-2.04963300	-1.14808200
C	6.23808700	-1.28028200	1.11309500
H	4.93022100	0.43672700	1.18945000
C	5.84475200	-2.83216800	-0.68730800
H	4.24199200	-2.32786000	-2.04146200
C	6.57665600	-2.46268500	0.44706700
H	6.80915400	-0.98069400	1.99005000
H	6.11043800	-3.74304300	-1.22097600
C	7.68821000	-3.32974600	0.94670700
H	7.30761200	-4.07507500	1.65736500
H	8.16890400	-3.87730200	0.12927100
H	8.45259000	-2.74525300	1.46898900
H	0.51343500	-0.77644600	-2.05344200
H	1.11920900	-2.30820200	-1.37694300
O	2.20896500	-0.05521500	1.86431300
C	-2.31990500	-2.86216300	1.32021800
C	-2.76271600	-1.65020800	0.61032000
H	-2.86430500	-3.79144900	1.15391300
H	-3.76883400	-1.74535000	0.19783600
H	-2.69117200	-0.74407900	1.22564400
Au	-1.03054200	0.92147400	-0.12581800
C	-1.16704600	5.12171900	-0.47977000
C	-2.49173300	4.86298900	-0.60647700
H	-0.61609300	6.05137700	-0.49531700
H	-3.33787400	5.52032900	-0.74769500
N	-0.53754200	3.90620500	-0.30523500
N	-2.63999400	3.49338100	-0.51243100
C	-1.44045000	2.90444500	-0.32773100

C	0.90241900	3.72669400	-0.18314900
H	1.33152100	4.60033600	0.31203400
H	1.10502900	2.83619100	0.41726100
H	1.35740000	3.60341400	-1.17016400
C	-3.91949800	2.80771900	-0.57163300
H	-4.45553600	3.10223400	-1.47776600
H	-3.73733100	1.72948600	-0.59372400
H	-4.52223700	3.05707300	0.30645900

Electronic Energy (0K) = -2121.3330851

Electronic Energy (0K) + ZPE = -2120.795459

Enthalpy (298K) = -2120.759202

Free Energy (298K) = -2120.864659

2a

Number of imaginary frequencies: 0

C	-2.15366500	-3.33346900	3.38623200
C	-1.68955200	-2.52552500	2.34855500
C	-0.51449300	-1.76742100	2.54295600
C	0.12854400	-1.79307200	3.78635200
C	-0.37058200	-2.57547800	4.81907300
C	-1.50645300	-3.35614600	4.61667400
H	-3.04802900	-3.93480700	3.22721800
H	1.03167600	-1.20399700	3.92195600
H	0.13516300	-2.58556800	5.78195700
H	-1.89312000	-3.97933000	5.42009200
C	0.03331700	-1.07488900	1.38679200
C	1.30862800	-0.34146300	1.30913100
N	1.44296800	0.02558400	-0.04182300
C	0.35512500	-0.48537100	-0.86716100
C	-0.51276700	-1.14187200	0.15082200

C	-1.80521400	-1.76552000	-0.14538500
C	-1.97578400	-2.34505900	-1.51397700
C	-1.40919900	-3.58601100	-1.81884600
C	-2.64251300	-1.63774600	-2.51537900
C	-1.51809200	-4.11489000	-3.10019900
H	-0.88526800	-4.13633800	-1.03725700
C	-2.74995600	-2.16461700	-3.79920500
H	-3.07973400	-0.66721500	-2.28238400
C	-2.18928500	-3.40433500	-4.09272200
H	-1.07943700	-5.08465800	-3.32532300
H	-3.27278700	-1.60578600	-4.57232000
H	-2.27633100	-3.81824300	-5.09493700
S	2.81215400	0.77898900	-0.68609600
O	3.06643600	1.99729400	0.06203500
O	2.53956500	0.83095000	-2.11636900
C	4.11735900	-0.37261400	-0.38711100
C	4.97127700	-0.18798900	0.69449000
C	4.25459900	-1.46010500	-1.24934700
C	5.98458600	-1.11417500	0.90879200
H	4.84213200	0.66529700	1.35364500
C	5.26919100	-2.37435900	-1.01459600
H	3.58265900	-1.57753800	-2.09694900
C	6.14791600	-2.21474300	0.06443600
H	6.66321100	-0.98272000	1.74963200
H	5.39076800	-3.22748600	-1.68031100
C	7.24989200	-3.20200900	0.28770000
H	6.88253400	-4.23190200	0.21087800
H	8.03611500	-3.08670200	-0.46944900
H	7.71385900	-3.07453600	1.27088100
H	-0.16451800	0.32304100	-1.39976500

H	0.71819800	-1.19919500	-1.62115700
O	2.12364700	-0.08906700	2.17569500
C	-2.43254900	-2.47074100	1.06968700
C	-2.99734000	-1.17920800	0.56563300
H	-3.02076000	-3.35785300	0.83345600
H	-3.94646000	-1.23280900	0.03737300
H	-2.84047100	-0.28362800	1.16285400

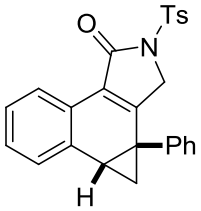
Electronic Energy (0K) = -1681.0820912

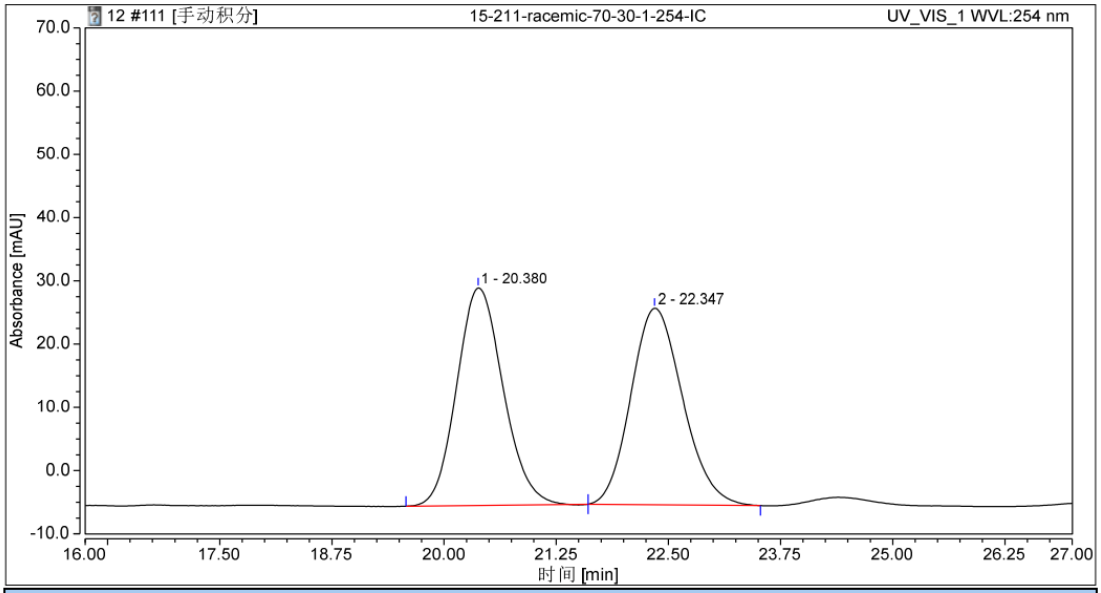
Electronic Energy (0K) + ZPE = -1680.674455

Enthalpy (298K) = -1680.647984

Free Energy (298K) = -1680.731092

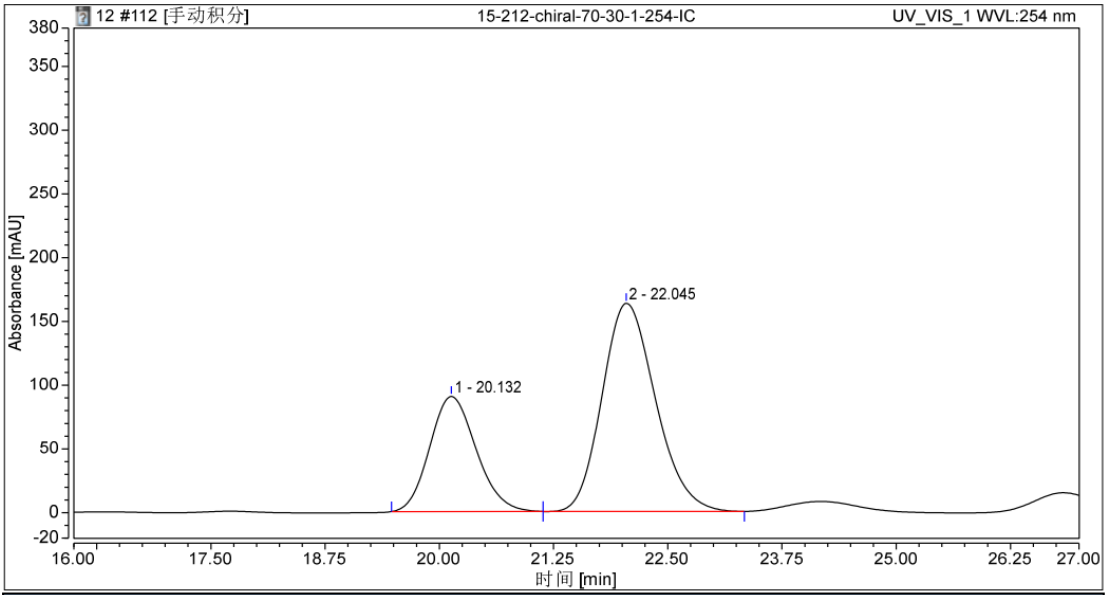
(+)-**2a**: HPLC (IC, *n*-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, I = 254 nm)





Integration Results

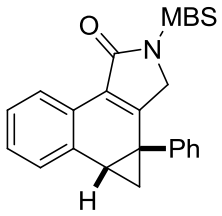
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		20.380	20.569	34.411	49.79	52.55	n.a.
2		22.347	20.744	31.069	50.21	47.45	n.a.
Total:			**41.313**	**65.480**	**100.00**	**100.00**	

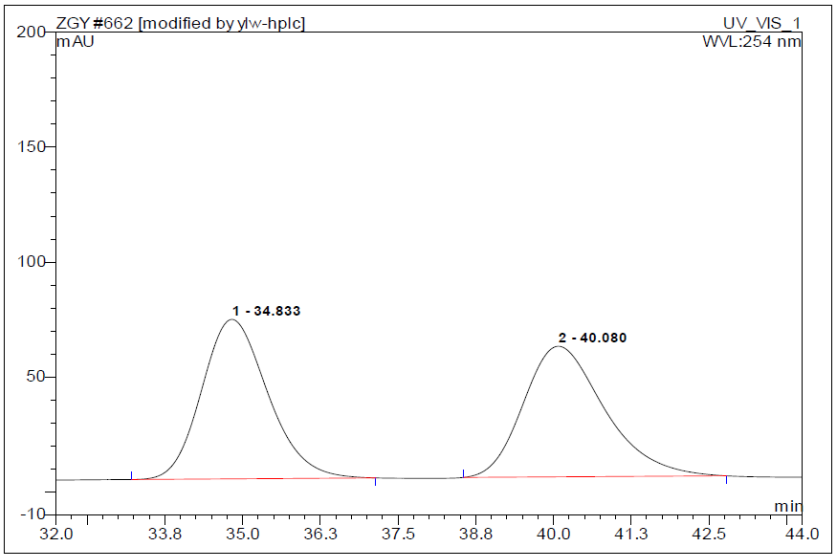


Integration Results

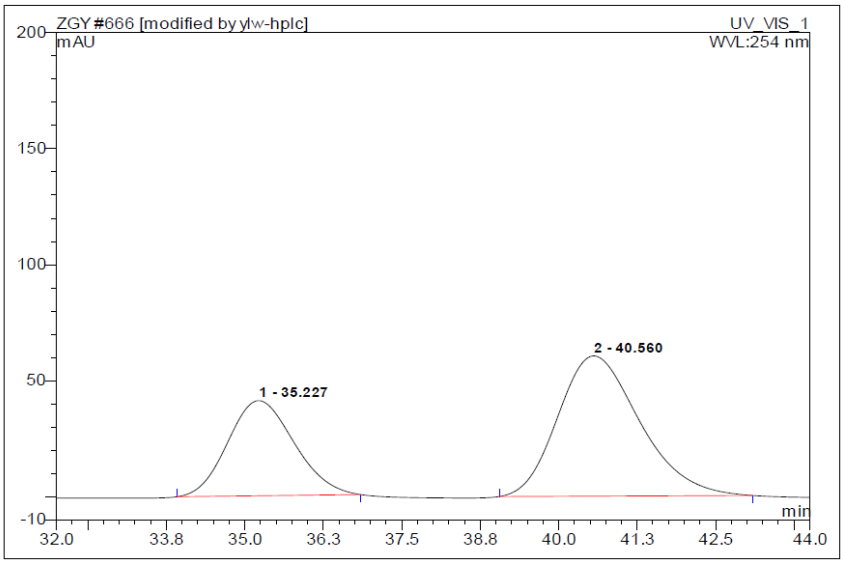
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		20.132	53.204	90.240	32.48	35.60	n.a.
2		22.045	110.579	163.223	67.52	64.40	n.a.
Total:			**163.783**	**253.462**	**100.00**	**100.00**	

(+)-**2b**: HPLC (IC, *n*-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, I = 254 nm)



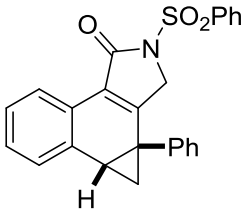


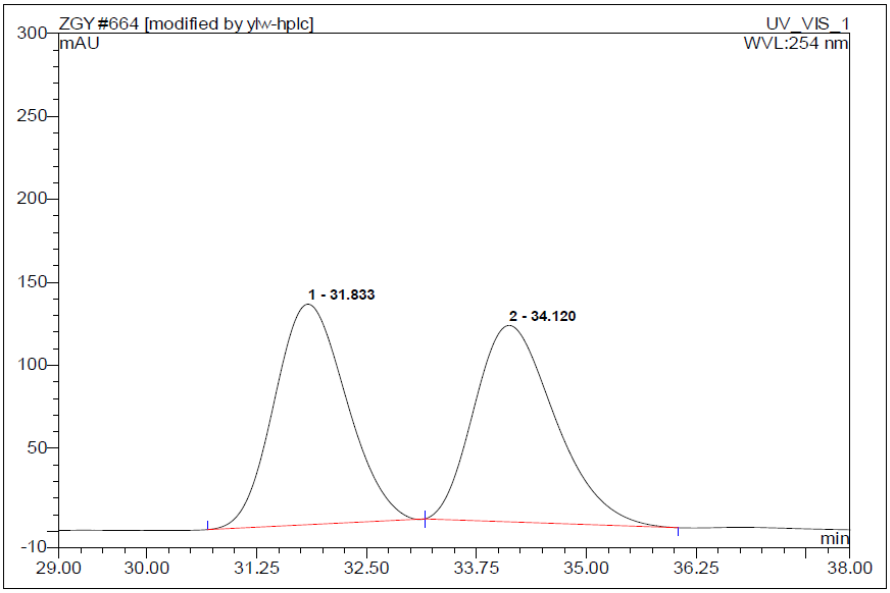
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	34.83	n.a.	69.408	85.781	50.00	n.a.	BMB*
2	40.08	n.a.	56.844	85.767	50.00	n.a.	BMB*
Total:			126.252	171.547	100.00	0.000	



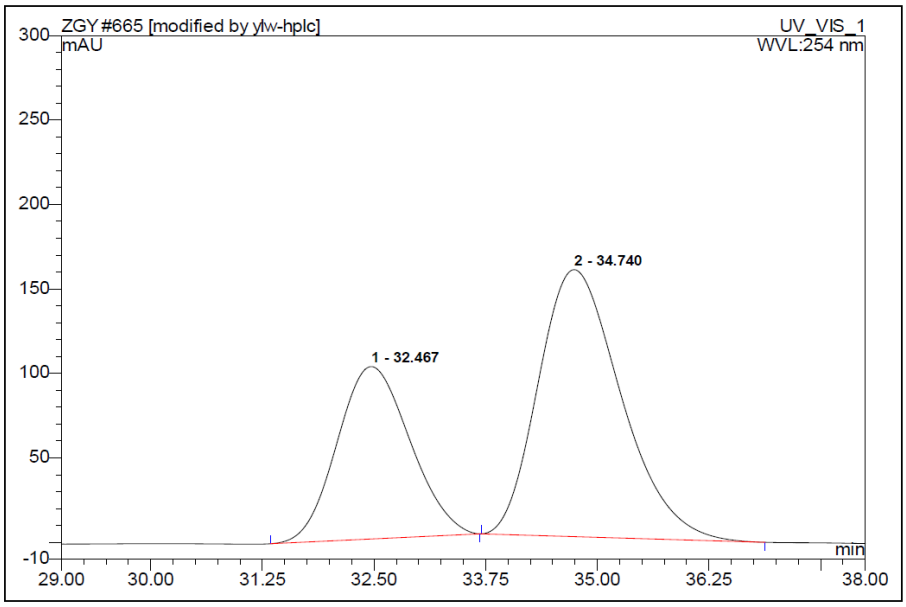
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	35.23	n.a.	41.002	50.224	35.48	n.a.	BMB*
2	40.56	n.a.	60.447	91.335	64.52	n.a.	BMB*
Total:			101.449	141.559	100.00	0.000	

(+)-**2c**: HPLC (IC, *n*-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, I = 254 nm)

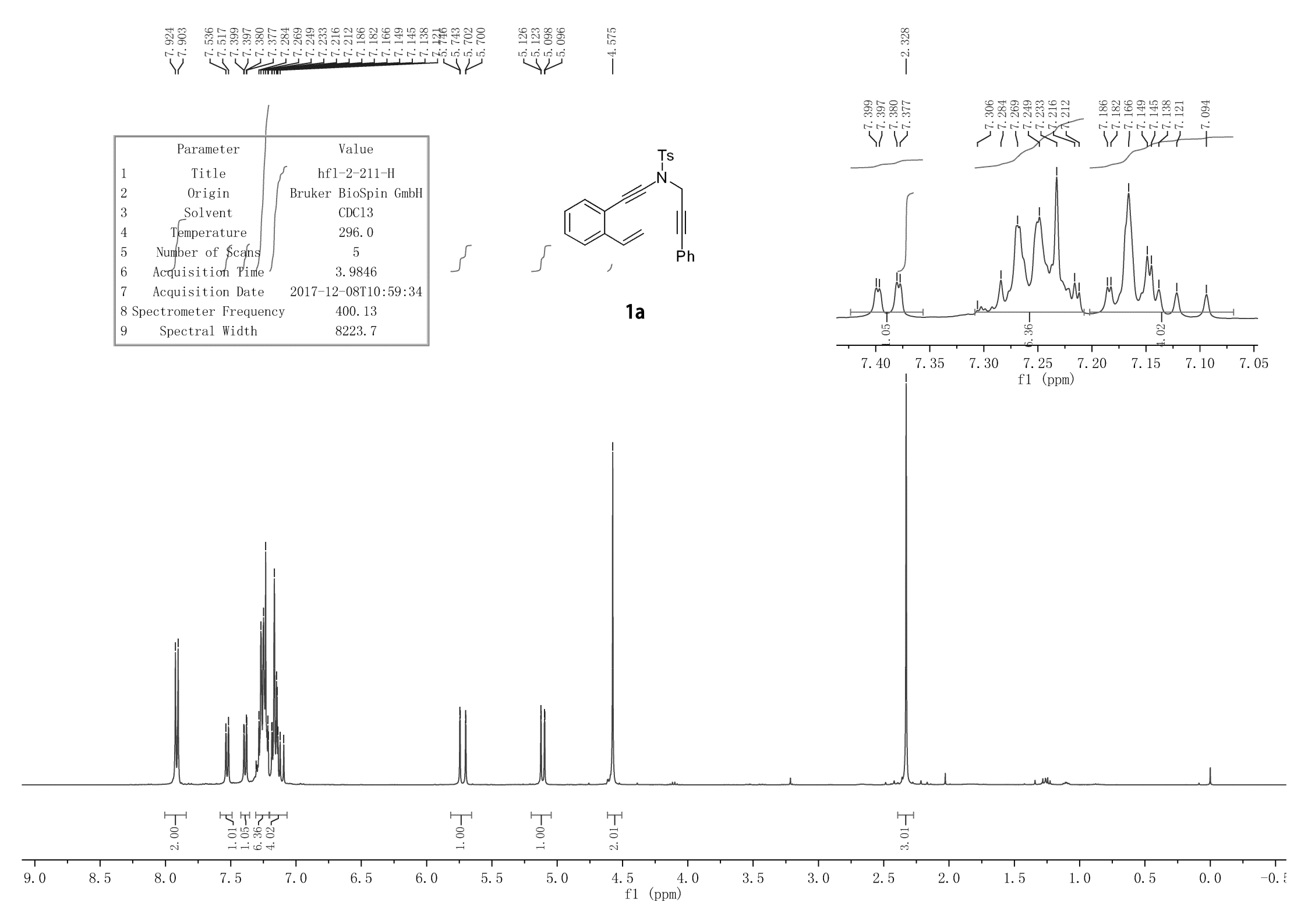


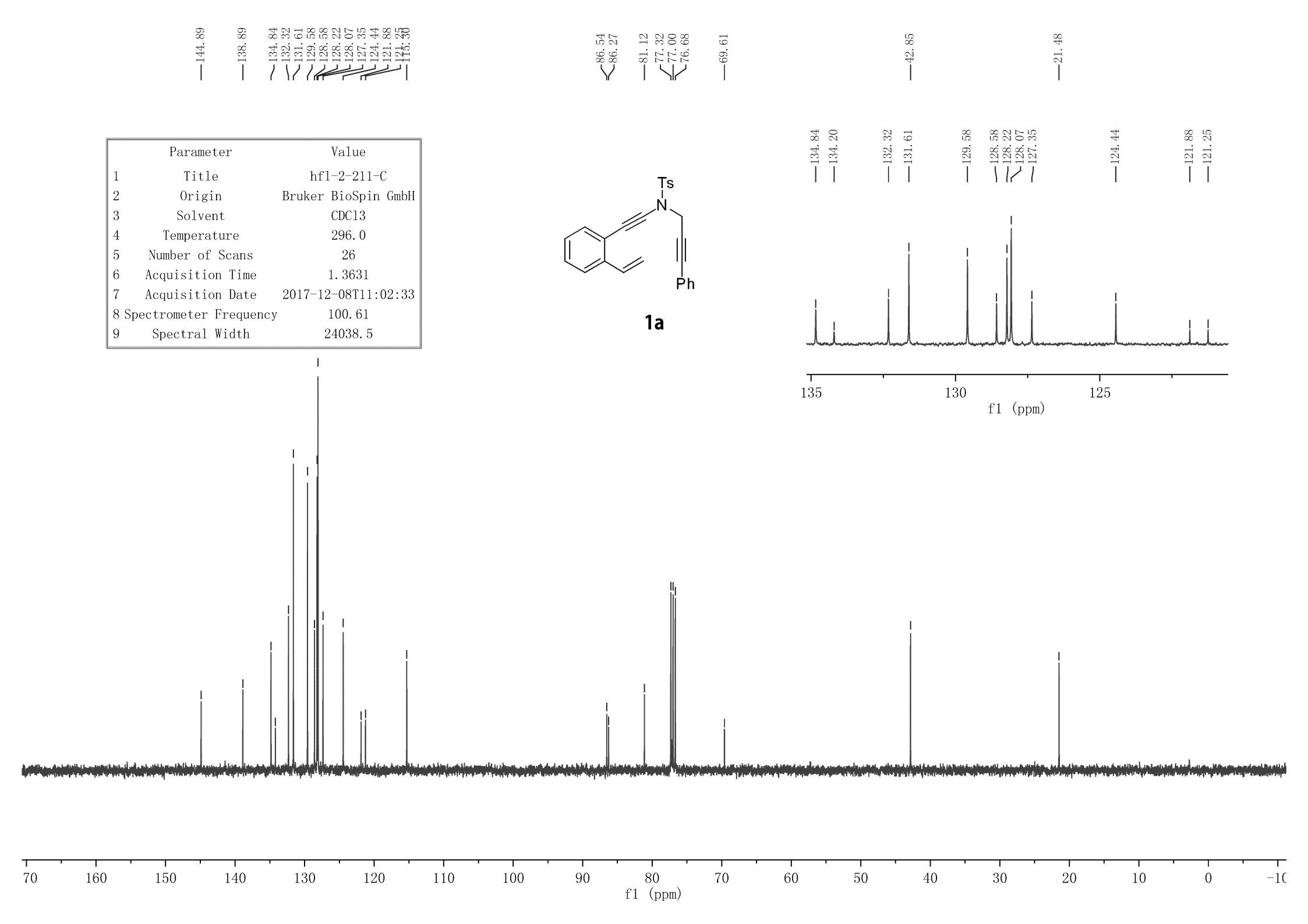


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	31.83	n.a.	132.891	126.242	50.05	n.a.	BMb*
2	34.12	n.a.	118.379	126.011	49.95	n.a.	bMB*
Total:			251.270	252.253	100.00	0.000	

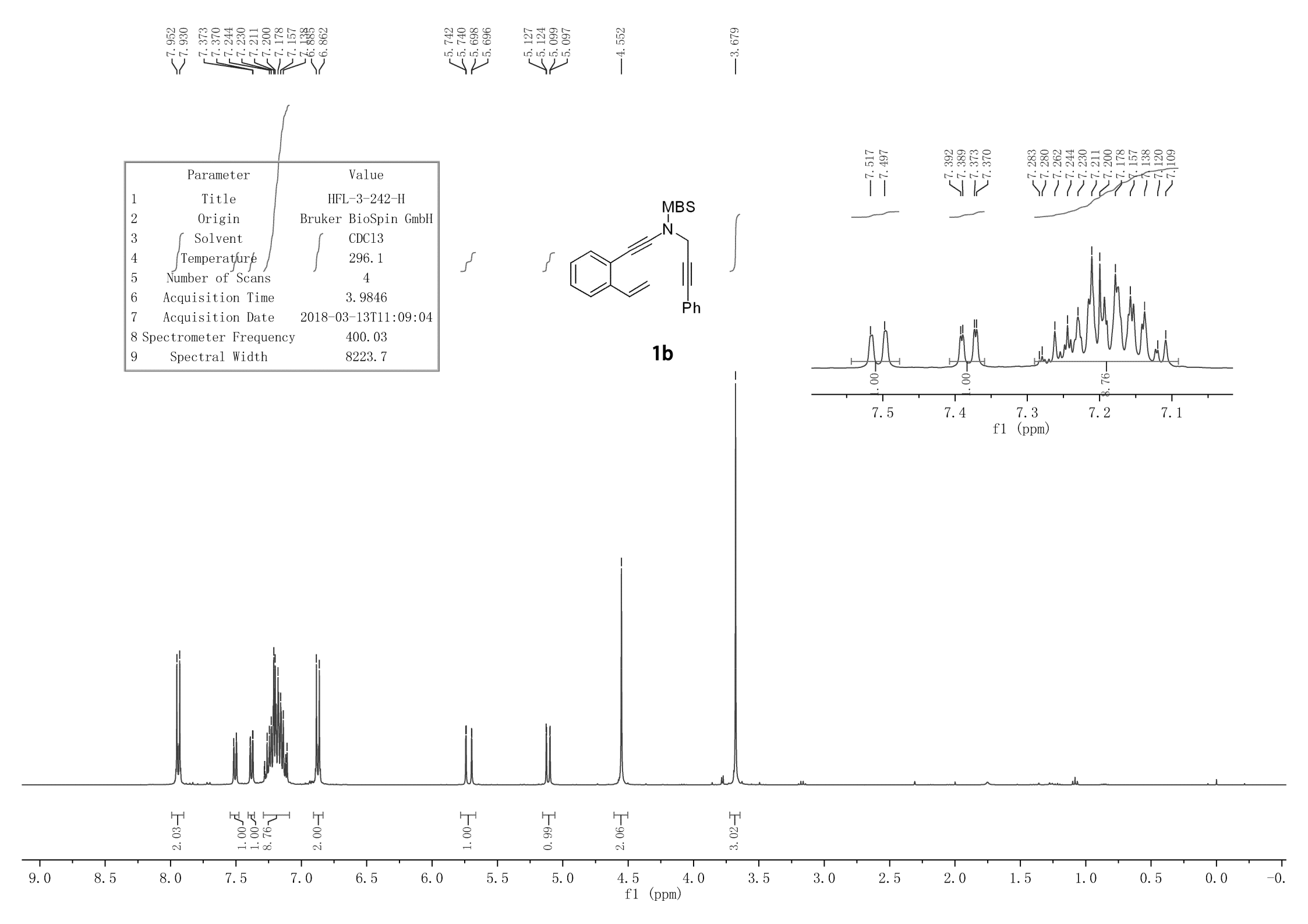


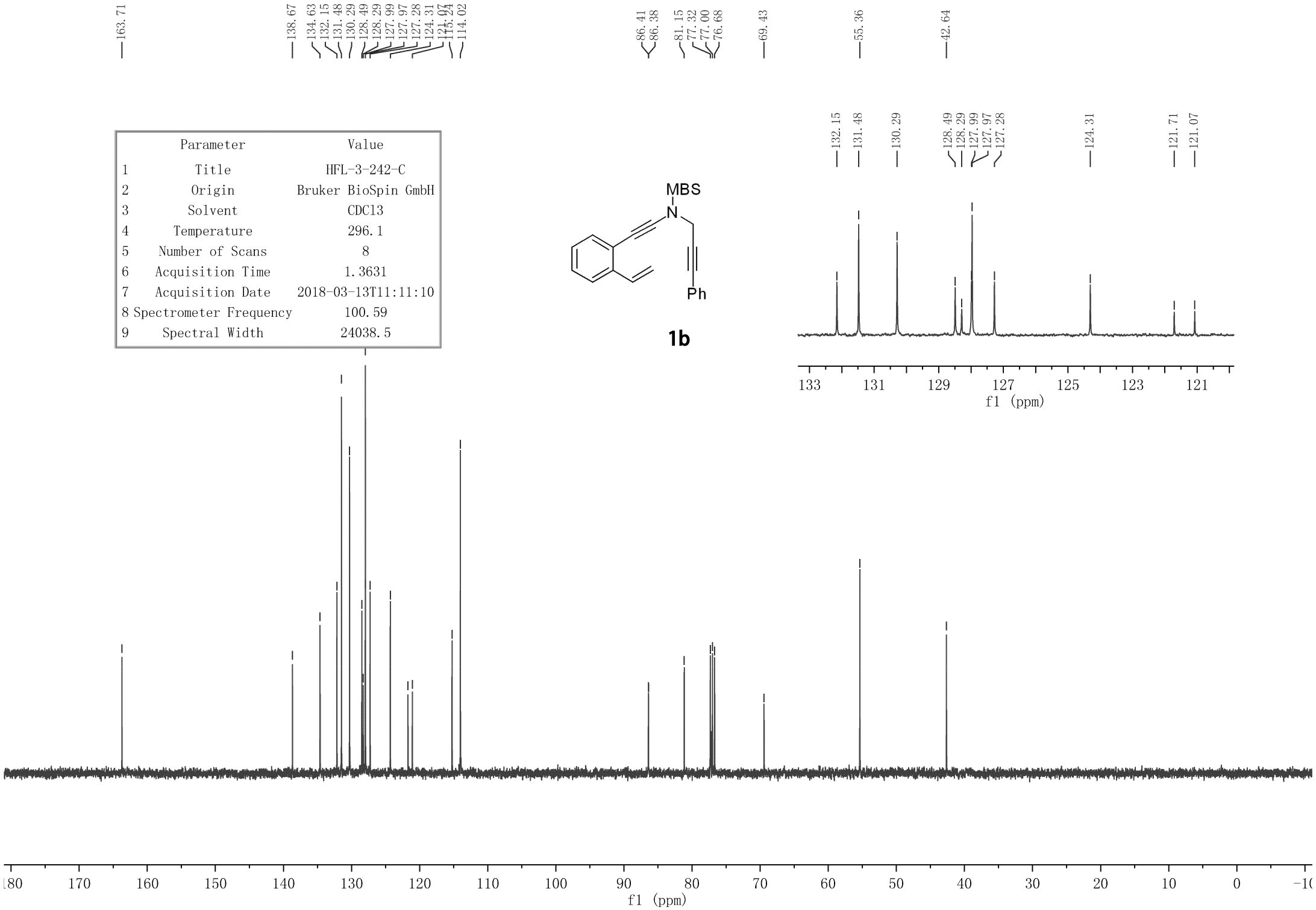
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	32.47	n.a.	102.038	96.417	36.29	n.a.	BMB*
2	34.74	n.a.	158.016	169.274	63.71	n.a.	BMB*
Total:			260.054	265.691	100.00	0.000	

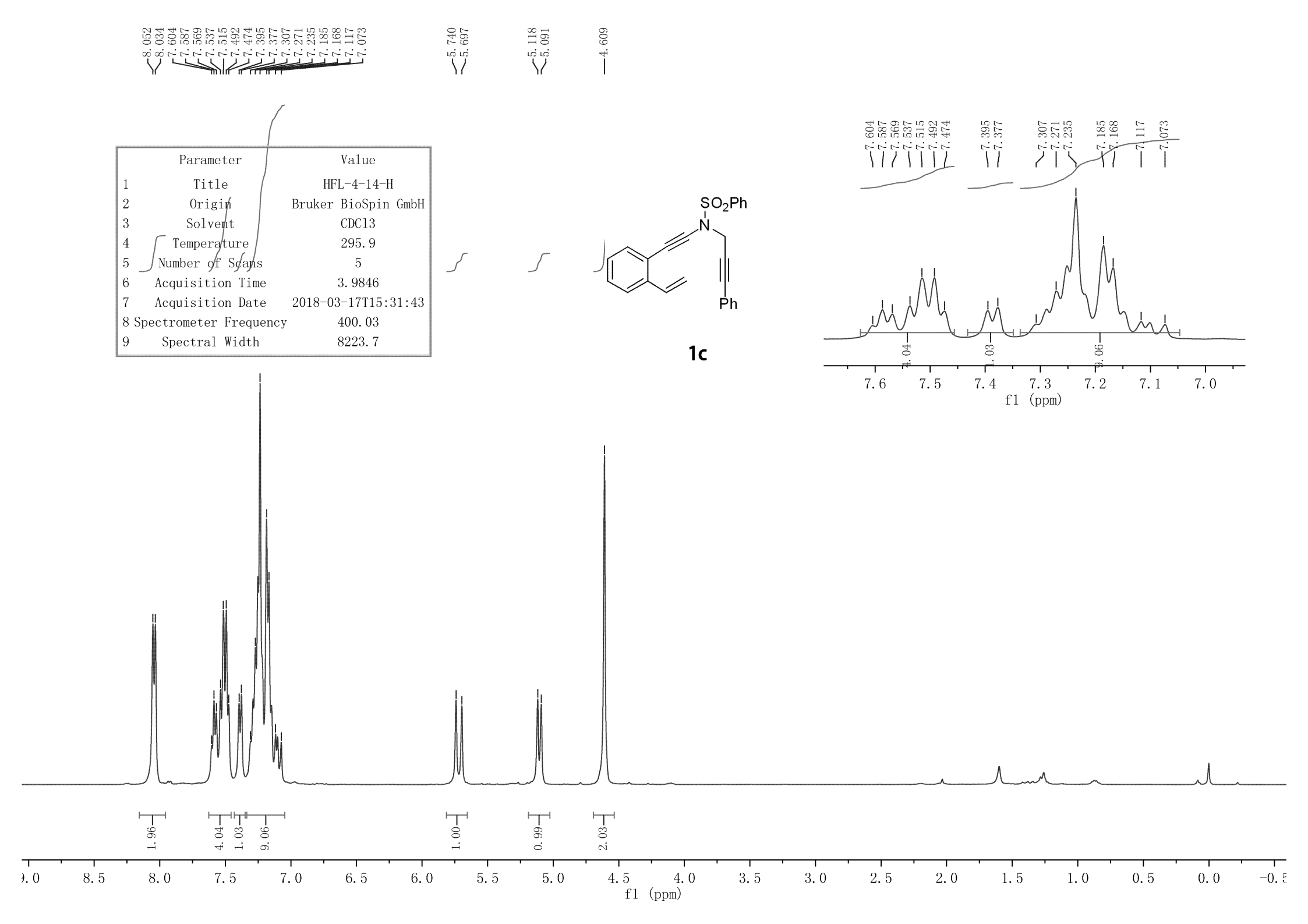

7.924
7.903
7.536
7.517
7.399
7.397
7.380
7.377
7.284
7.269
7.249
7.233
7.216
7.212
7.186
7.182
7.166
7.149
7.145
7.138
7.121
5.743
5.702
5.700
5.126
5.123
5.098
5.096
4.575
2.328
Parameter Value
1 Title hfl-2-211-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.0
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2017-12-08T10:59:34
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ts
N
Ph
1a
7.399
7.397
7.380
7.377
7.306
7.284
7.269
7.249
7.233
7.216
7.212
7.186
7.182
7.166
7.149
7.145
7.138
7.121
7.094
1.05
6.36
4.02
7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
2.00
1.01
1.05
6.36
4.02
1.00
1.00
2.01
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

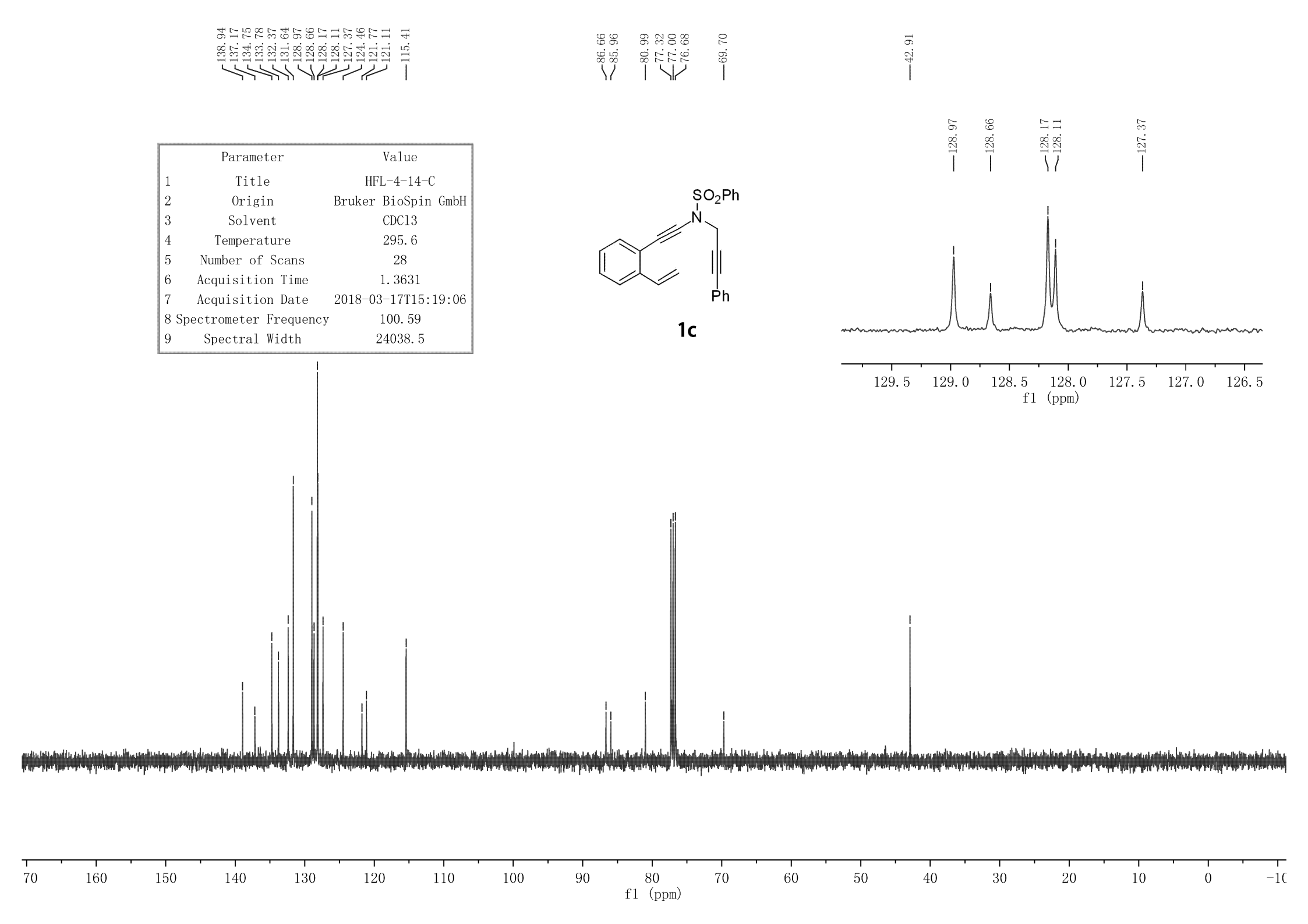


	Parameter	Value
1	Title	hf1-2-211-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.0
5	Number of Scans	26
6	Acquisition Time	1.3631
7	Acquisition Date	2017-12-08T11:02:33
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

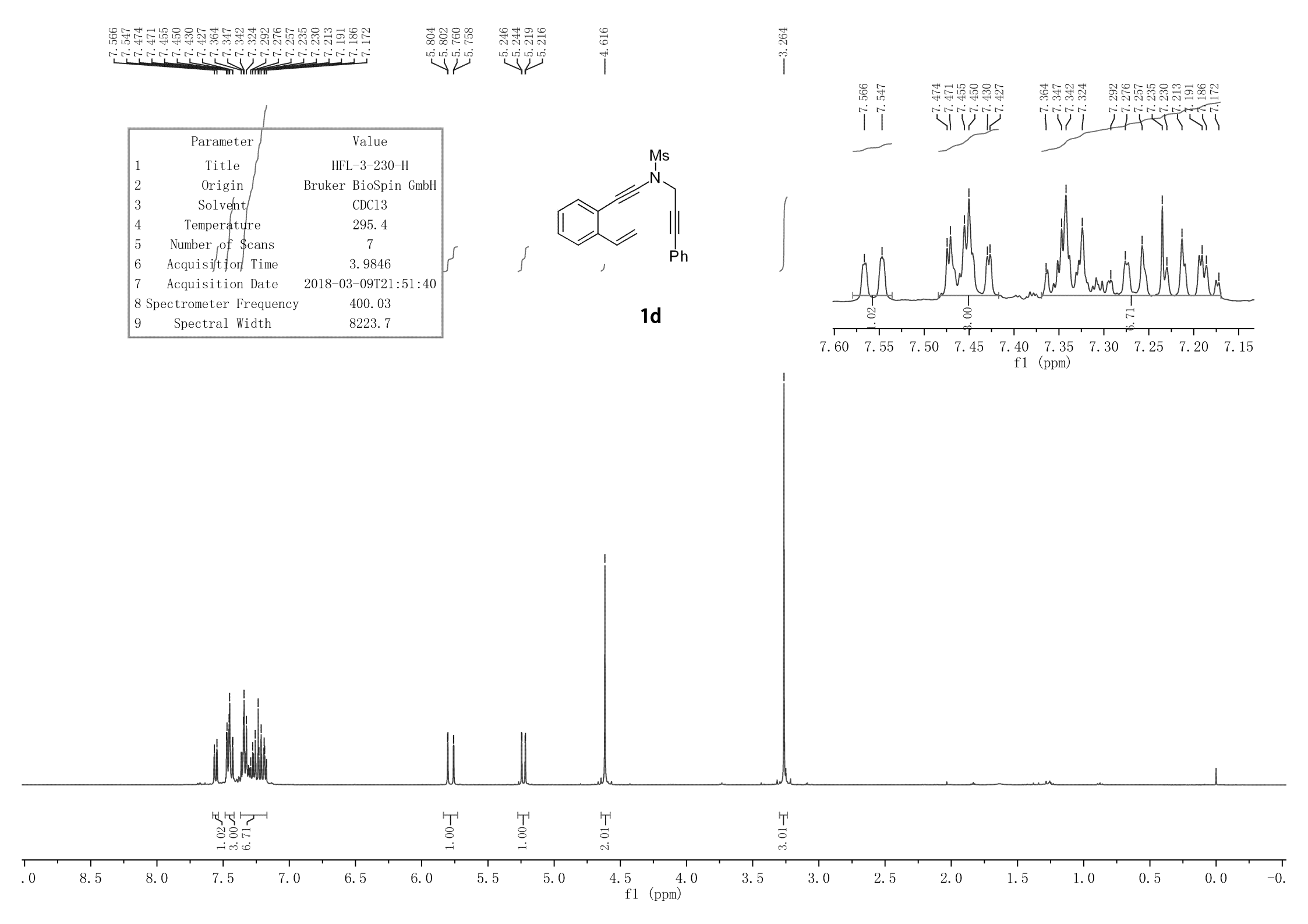

7.952
7.930
7.373
7.370
7.244
7.230
7.211
7.200
7.178
7.157
6.885
6.862
5.742
5.740
5.698
5.696
5.127
5.124
5.099
5.097
4.552
3.679
Parameter Value
1 Title HFL-3-242-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.1
5 Number of Scans 4
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-13T11:09:04
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
MBS
N
Ph
1b
7.517
7.497
7.392
7.389
7.373
7.370
7.283
7.280
7.262
7.244
7.230
7.211
7.200
7.178
7.157
7.138
7.120
7.109
1.00
1.00
8.76
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
2.03
1.00
1.00
8.76
2.00
1.00
0.99
2.06
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


163.71
138.67
134.63
132.15
131.48
130.29
128.49
128.29
127.99
127.97
127.28
124.31
121.71
121.07
114.02
86.41
86.38
81.15
77.32
77.00
76.68
69.43
55.36
42.64
Parameter Value
1 Title HFL-3-242-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.1
5 Number of Scans 8
6 Acquisition Time 1.3631
7 Acquisition Date 2018-03-13T11:11:10
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
MBS
N
Ph
1b
f1 (ppm)
f1 (ppm)


8.052
8.034
7.604
7.587
7.569
7.537
7.515
7.492
7.474
7.395
7.377
7.307
7.271
7.235
7.185
7.168
7.117
7.073
5.740
5.697
5.118
5.091
4.609
Parameter Value
1 Title HFL-4-14-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.9
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-17T15:31:43
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
SO2Ph
N
Ph
1c
1.04
1.03
9.06
f1 (ppm)
1.96
4.04
1.03
9.06
1.00
0.99
2.03
f1 (ppm)

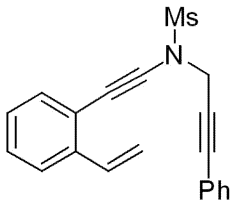


	Parameter	Value
1	Title	HFL-4-14-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.6
5	Number of Scans	28
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-17T15:19:06
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5

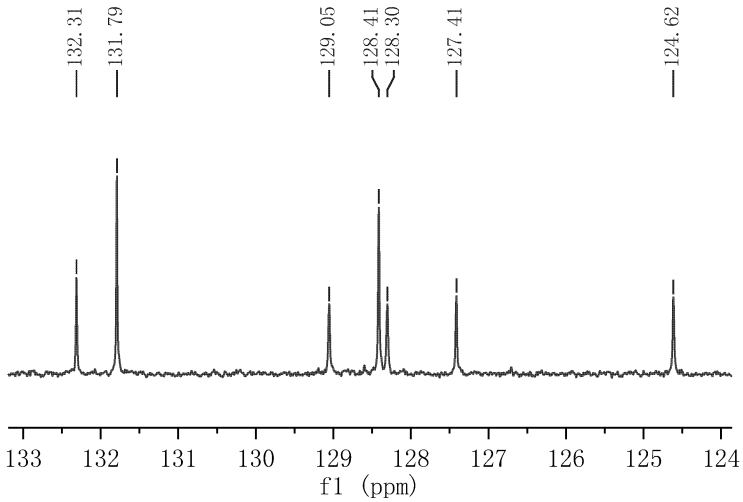

7.566
7.547
7.474
7.471
7.455
7.450
7.430
7.427
7.364
7.347
7.342
7.324
7.292
7.276
7.257
7.235
7.230
7.213
7.191
7.186
7.172
5.804
5.802
5.760
5.758
5.246
5.244
5.219
5.216
4.616
3.264
Parameter Value
1 Title HFL-3-230-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.4
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-09T21:51:40
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ms
N
Ph
1d
1.02
3.00
6.71
f1 (ppm)
1.00
1.00
2.01
3.01
f1 (ppm)

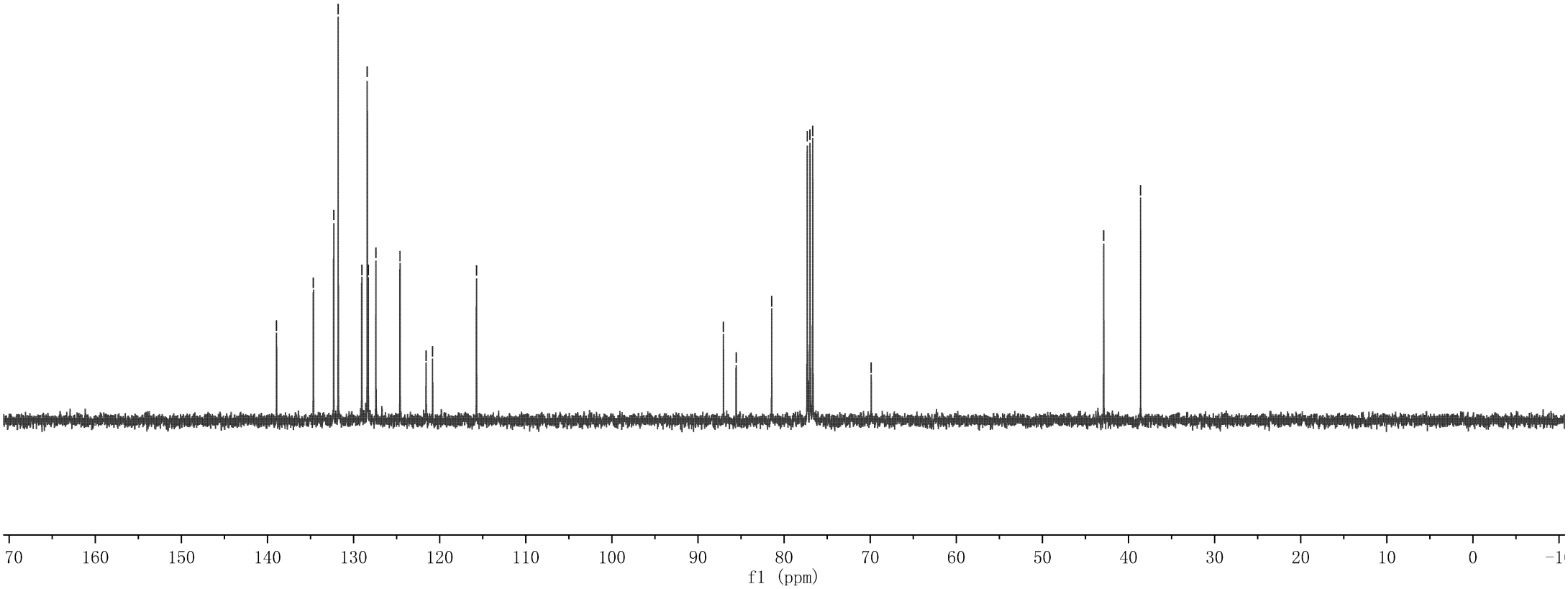
138.95
134.67
132.31
131.79
129.05
128.41
128.30
127.41
124.62
121.58
120.83
115.73
87.05
85.58
81.45
77.32
77.00
76.68
69.89
42.89
38.60

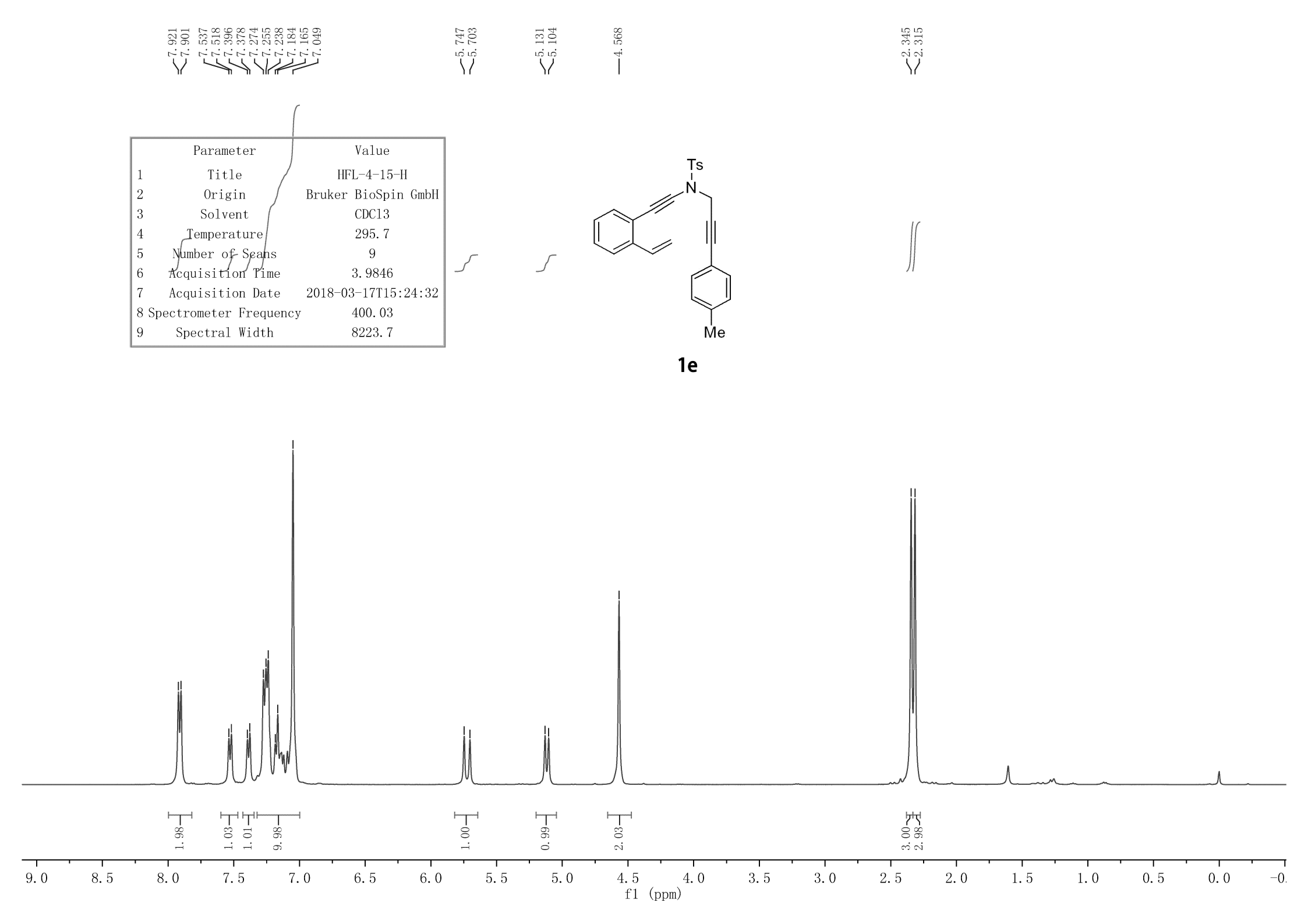
	Parameter	Value
1	Title	HFL-3-230-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.2
5	Number of Scans	45
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-09T21:56:09
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5

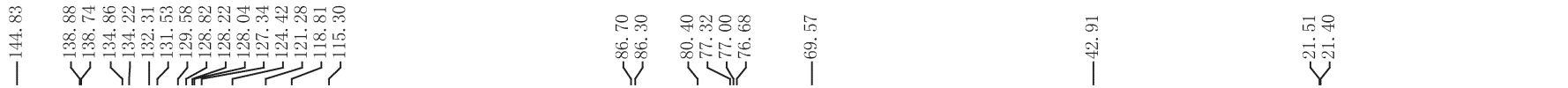


1d

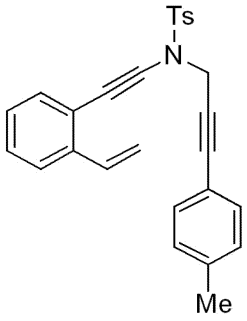




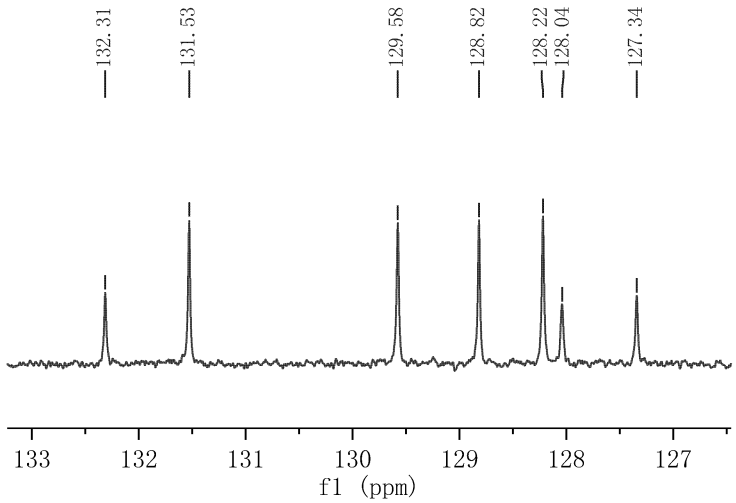

7.921
7.901
7.537
7.518
7.396
7.378
7.274
7.255
7.238
7.184
7.165
7.049
5.747
5.703
5.131
5.104
4.568
2.345
2.315
Parameter Value
1 Title HFL-4-15-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.7
5 Number of Scans 9
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-17T15:24:32
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ts
N
Me
1e
1.98
1.03
1.01
9.98
1.00
0.99
2.03
3.00
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

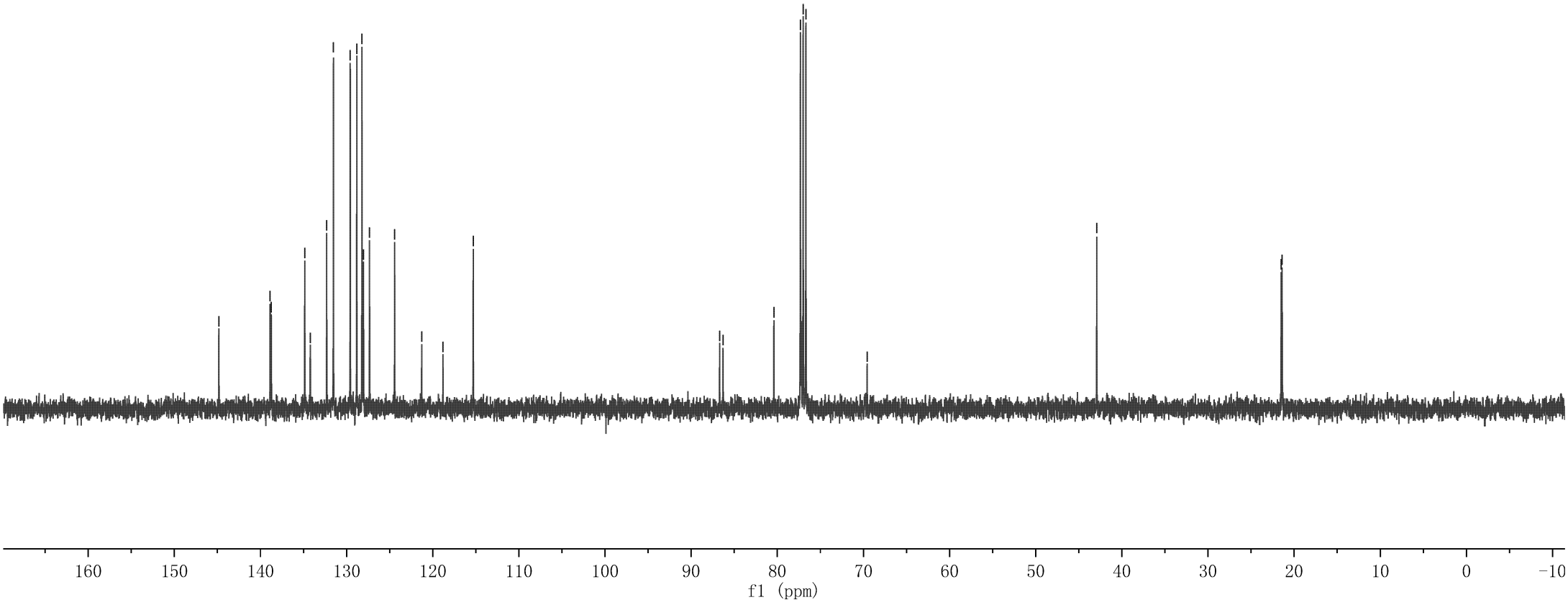


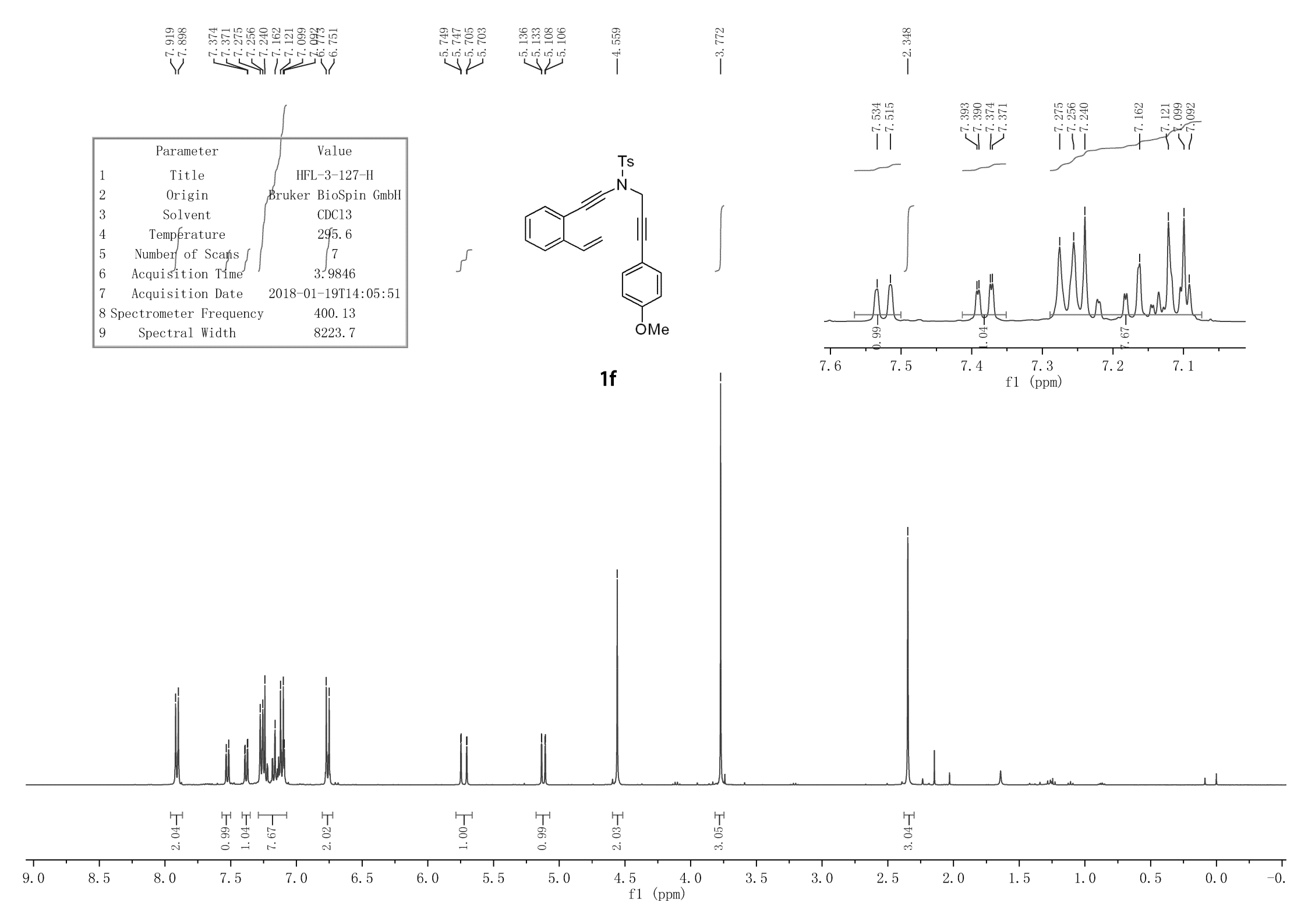
	Parameter	Value
1	Title	HFL-4-15-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.7
5	Number of Scans	34
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-17T15:27:04
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5

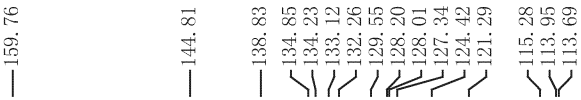


1e

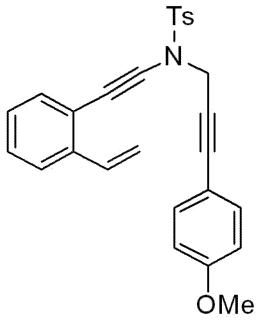




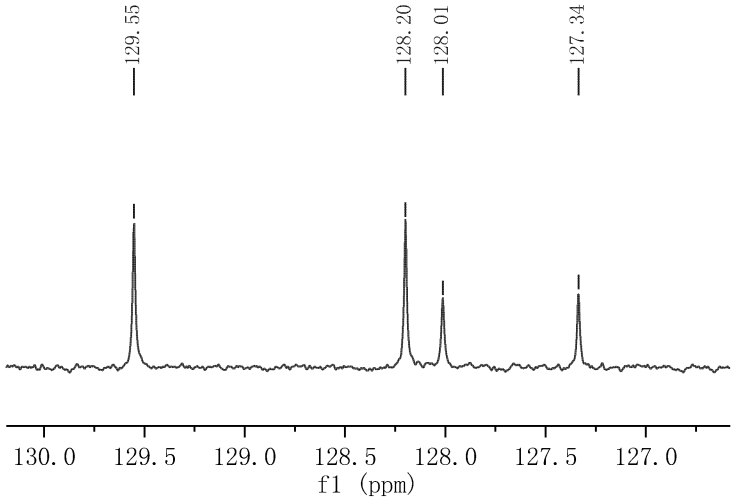

7.919
7.898
7.374
7.371
7.275
7.256
7.240
7.162
7.121
7.099
7.092
6.773
6.751
5.749
5.747
5.705
5.703
5.136
5.133
5.108
5.106
4.559
3.772
2.348
Parameter Value
1 Title HFL-3-127-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-01-19T14:05:51
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ts
N
OMe
1f
7.534
7.515
7.393
7.390
7.374
7.371
7.275
7.256
7.240
7.162
7.121
7.099
7.092
0.99
1.04
7.67
f1 (ppm)
2.04
0.99
1.04
7.67
2.02
1.00
0.99
2.03
3.05
3.04
f1 (ppm)

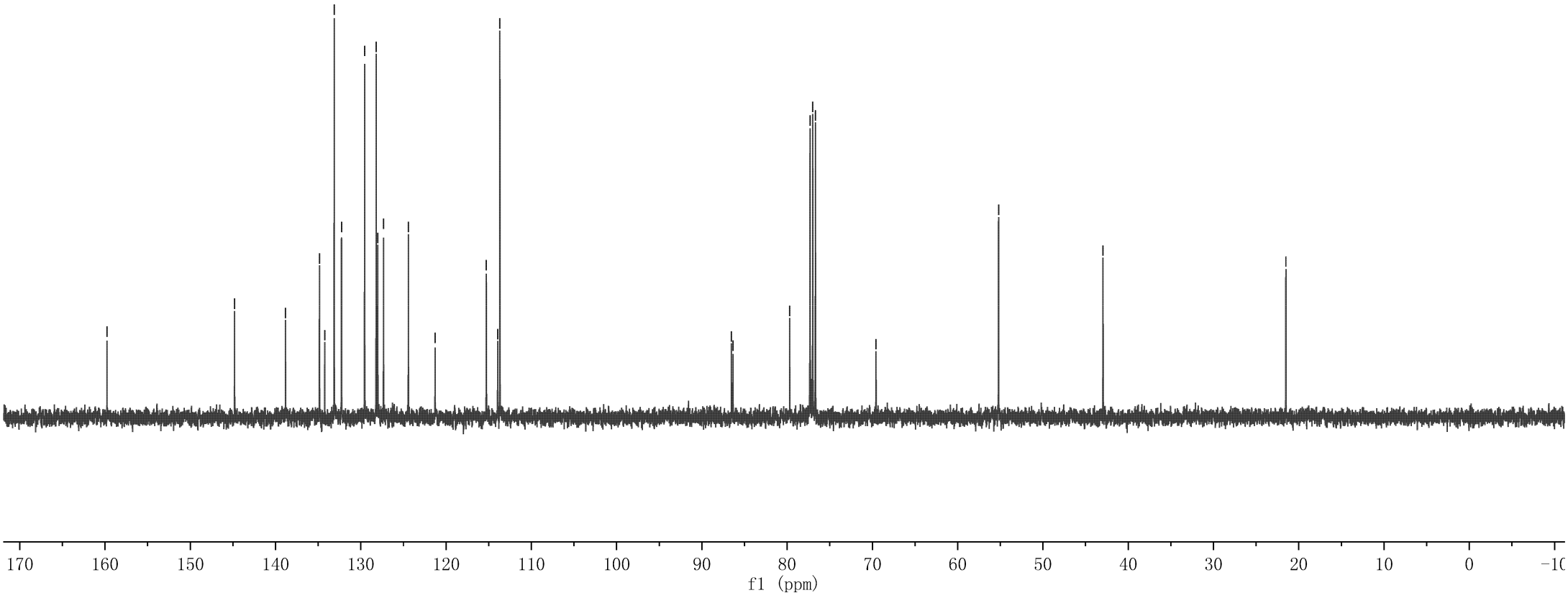


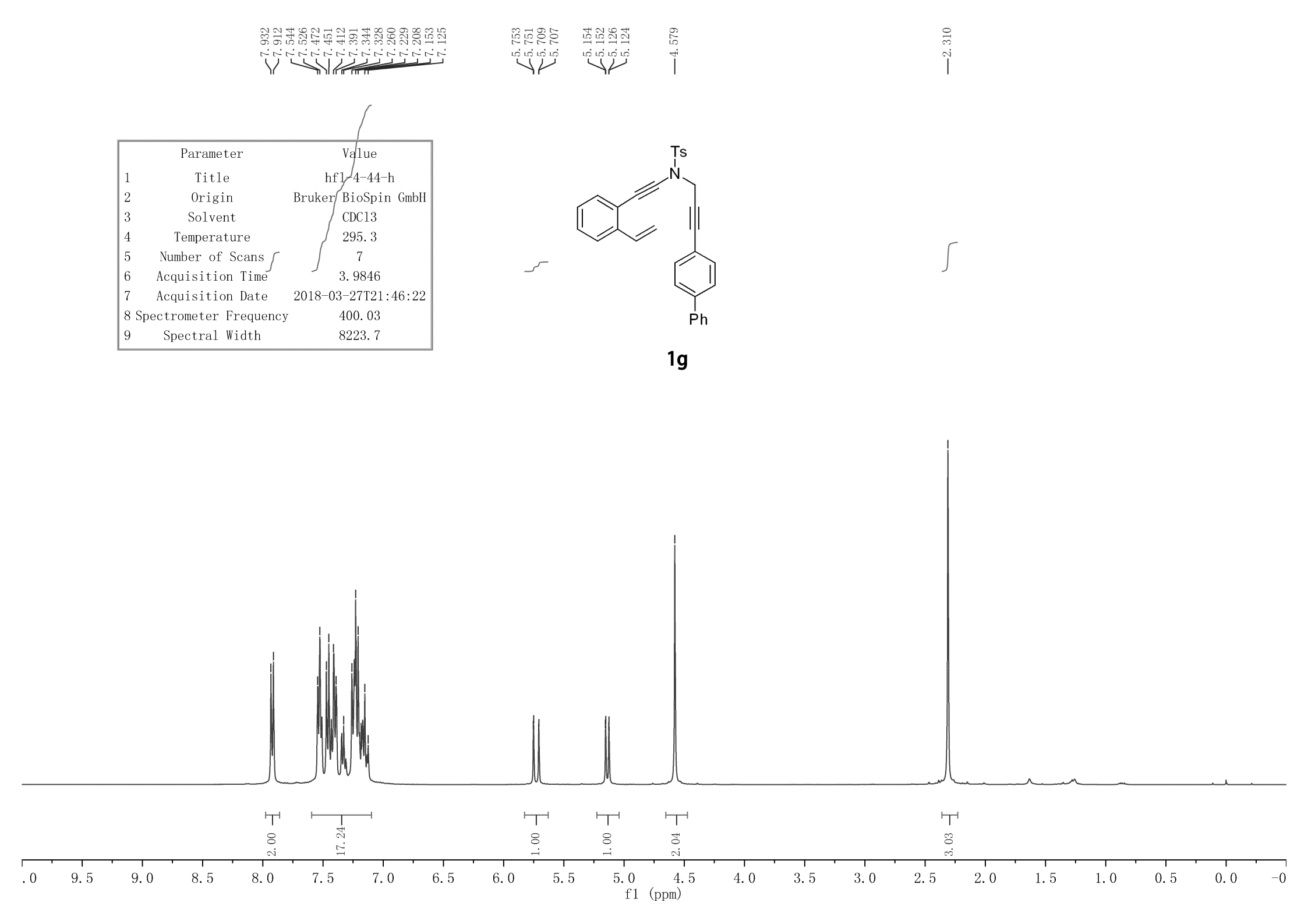
	Parameter	Value
1	Title	HFL-3-127-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.6
5	Number of Scans	12
6	Acquisition Time	1.3631
7	Acquisition Date	2018-01-19T14:08:05
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

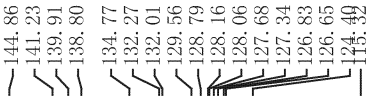


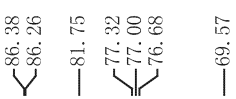
1f



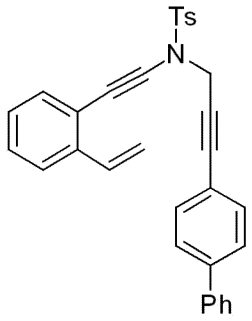



7.932
7.912
7.544
7.526
7.472
7.451
7.412
7.391
7.344
7.328
7.260
7.229
7.208
7.153
7.125
5.753
5.751
5.709
5.707
5.154
5.152
5.126
5.124
4.579
2.310
Parameter Value
1 Title hfl-4-44-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.3
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-27T21:46:22
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ts
N
Ph
1g
2.00
17.24
1.00
1.00
2.04
3.03
f1 (ppm)

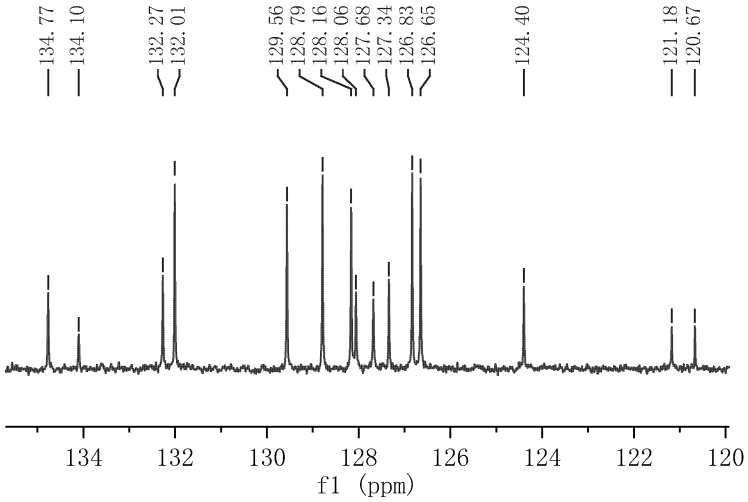


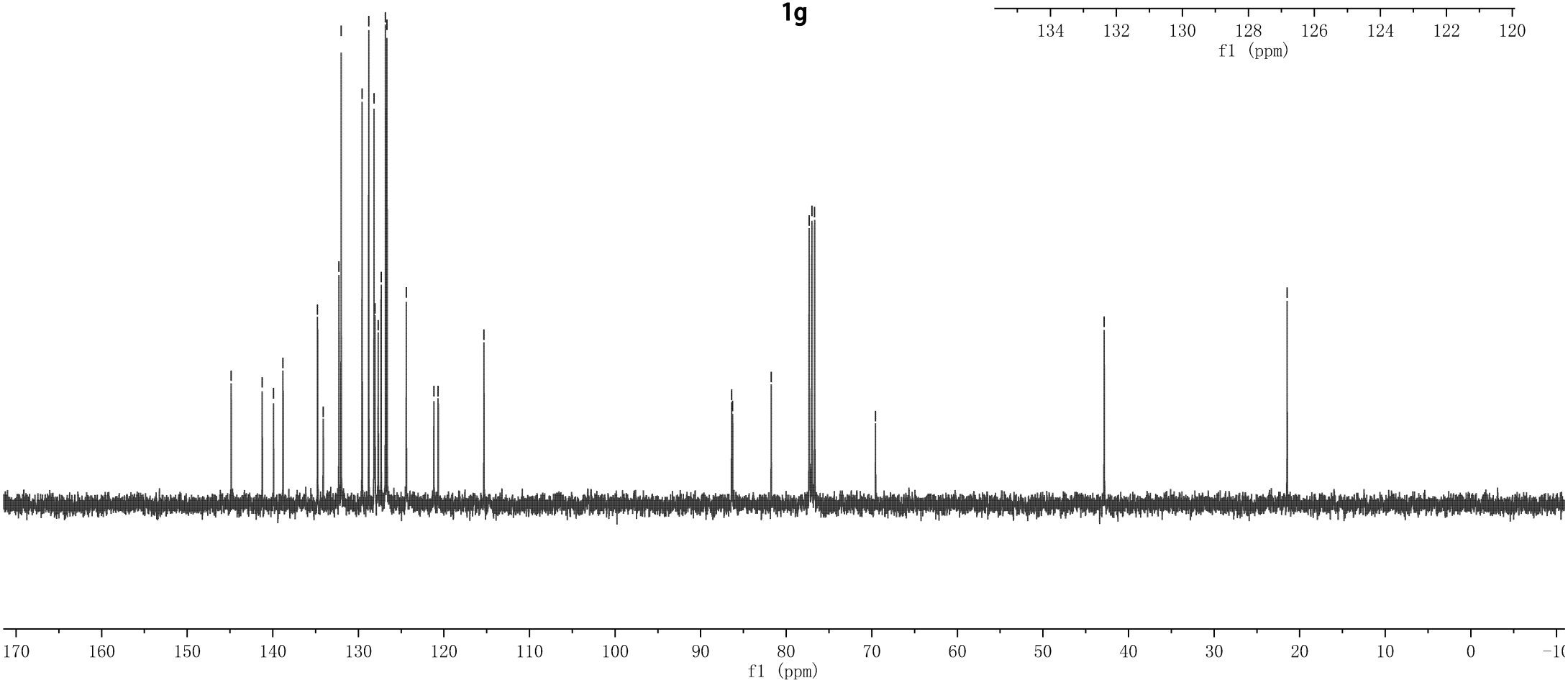


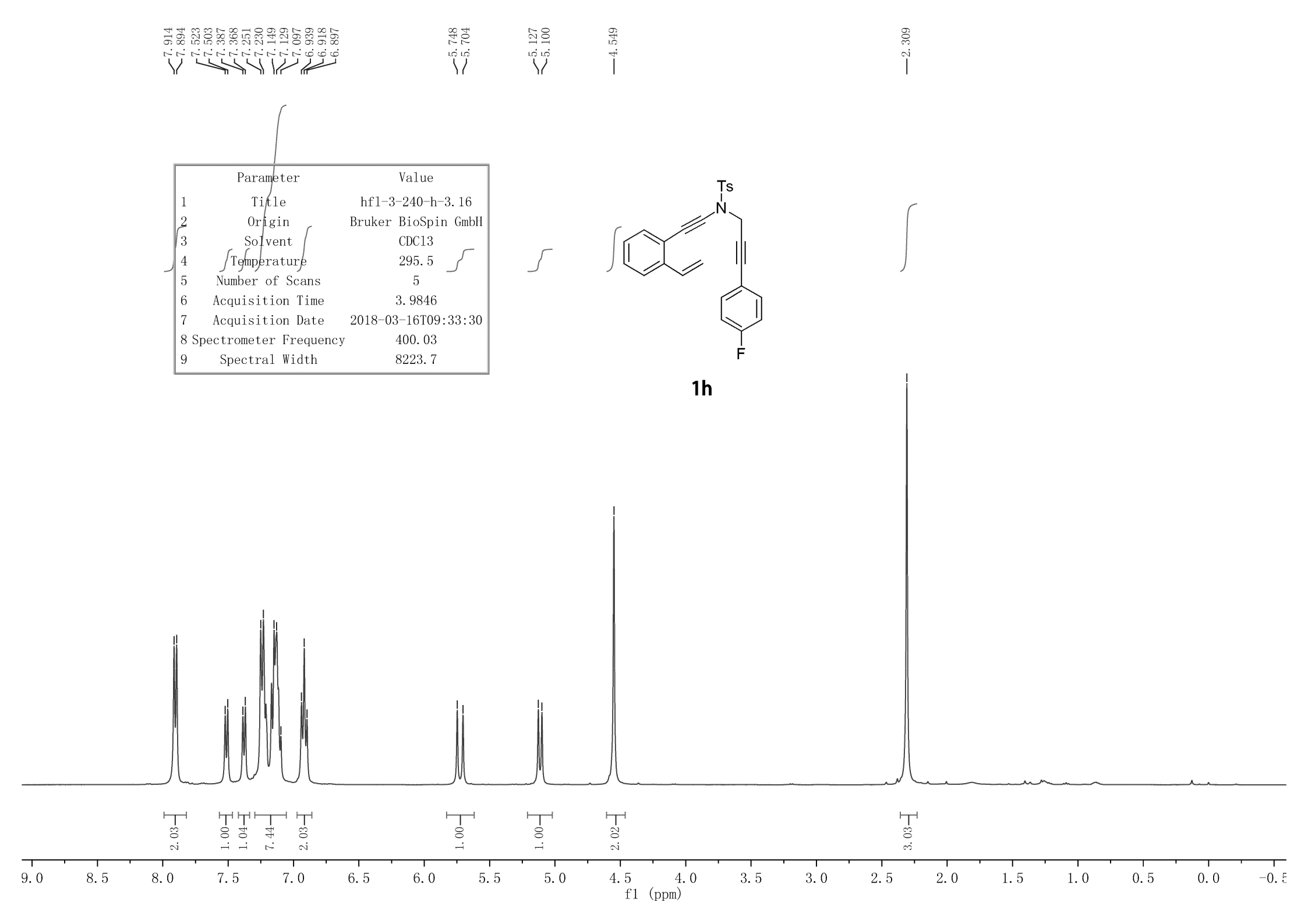
	Parameter	Value
1	Title	hfl-4-44-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.5
5	Number of Scans	14
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-27T21:48:58
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5



1g

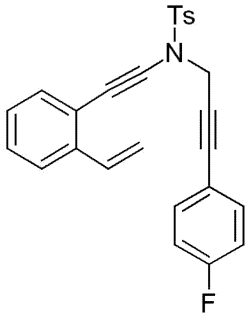





7.914
7.894
7.523
7.503
7.387
7.368
7.251
7.230
7.149
7.129
7.097
6.939
6.918
6.897
5.748
5.704
5.127
5.100
4.549
2.309
Parameter Value
1 Title hfl-3-240-h-3.16
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.5
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-16T09:33:30
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ts
N
F
1h
2.03
1.00
1.04
7.44
2.03
1.00
1.00
2.02
3.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

163.64
161.15
144.84
138.66
134.64
134.00
133.50
133.42
132.13
129.48
128.05
127.30
124.34
121.03
117.85
117.82
115.36
115.22
115.14
86.16
85.33
80.86
77.32
77.00
76.68
69.50
42.62
21.32

	Parameter	Value
1	Title	hfl-3-240-C-3.16
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.6
5	Number of Scans	25
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-16T09:36:13
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5



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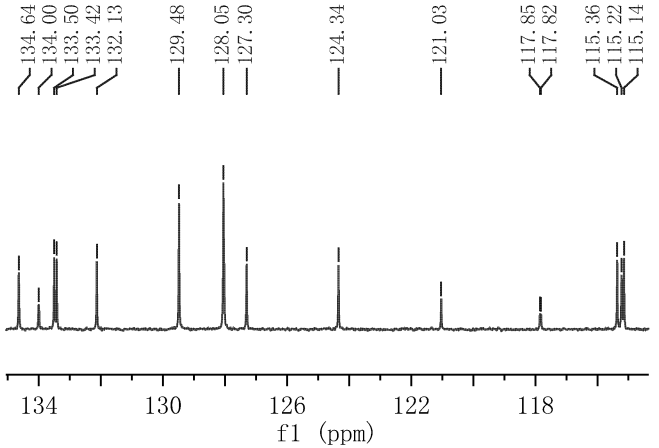
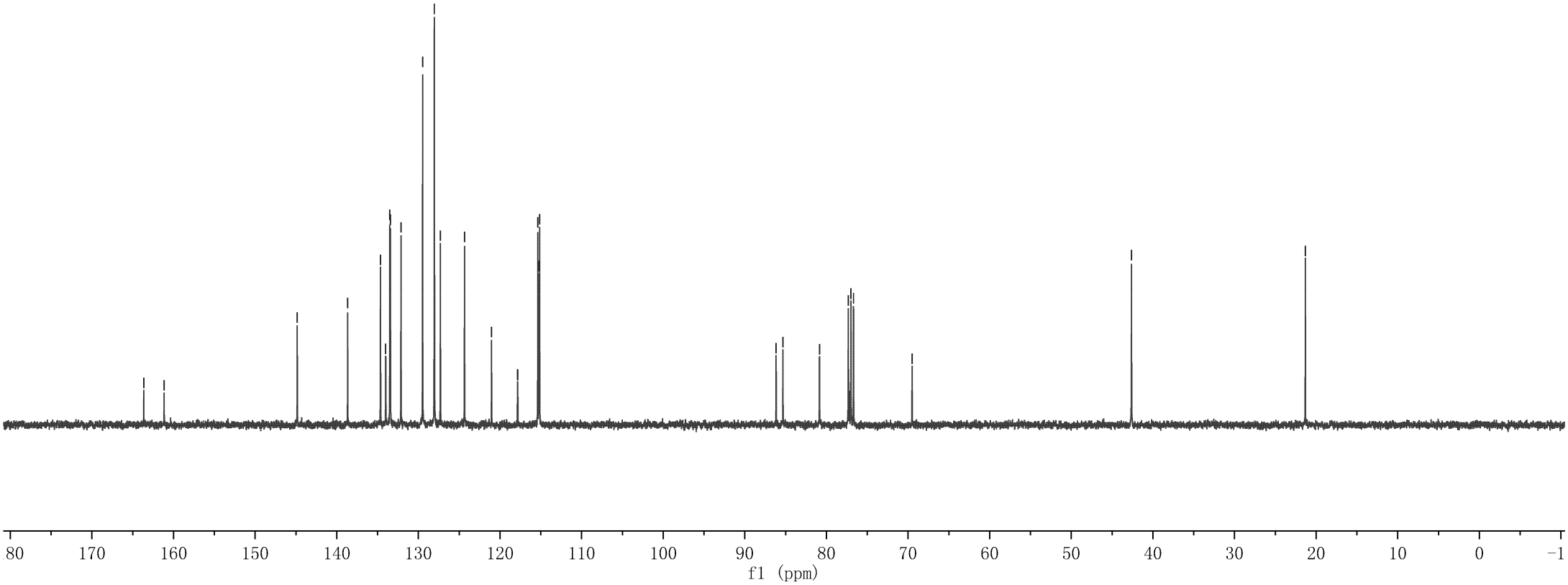
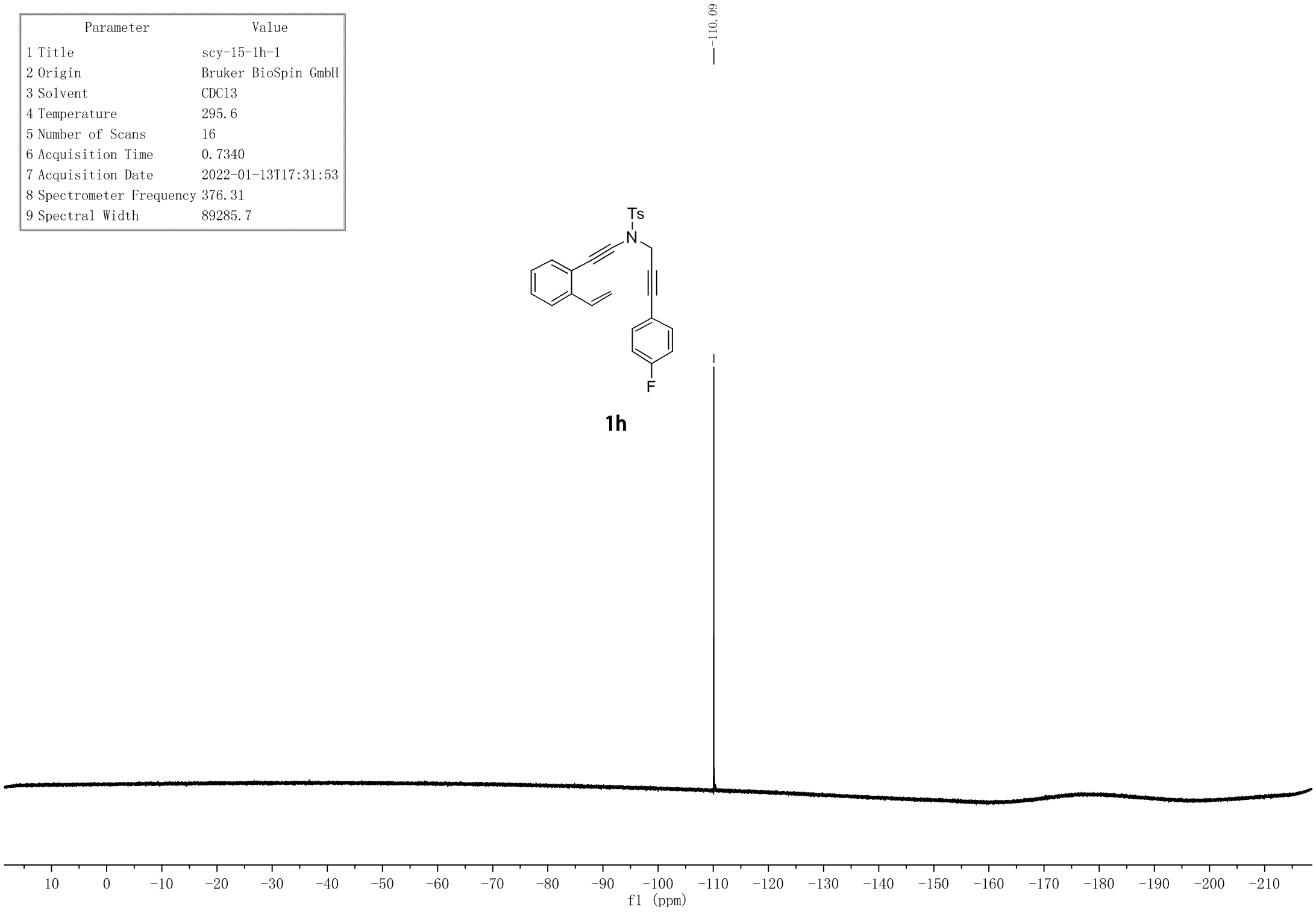
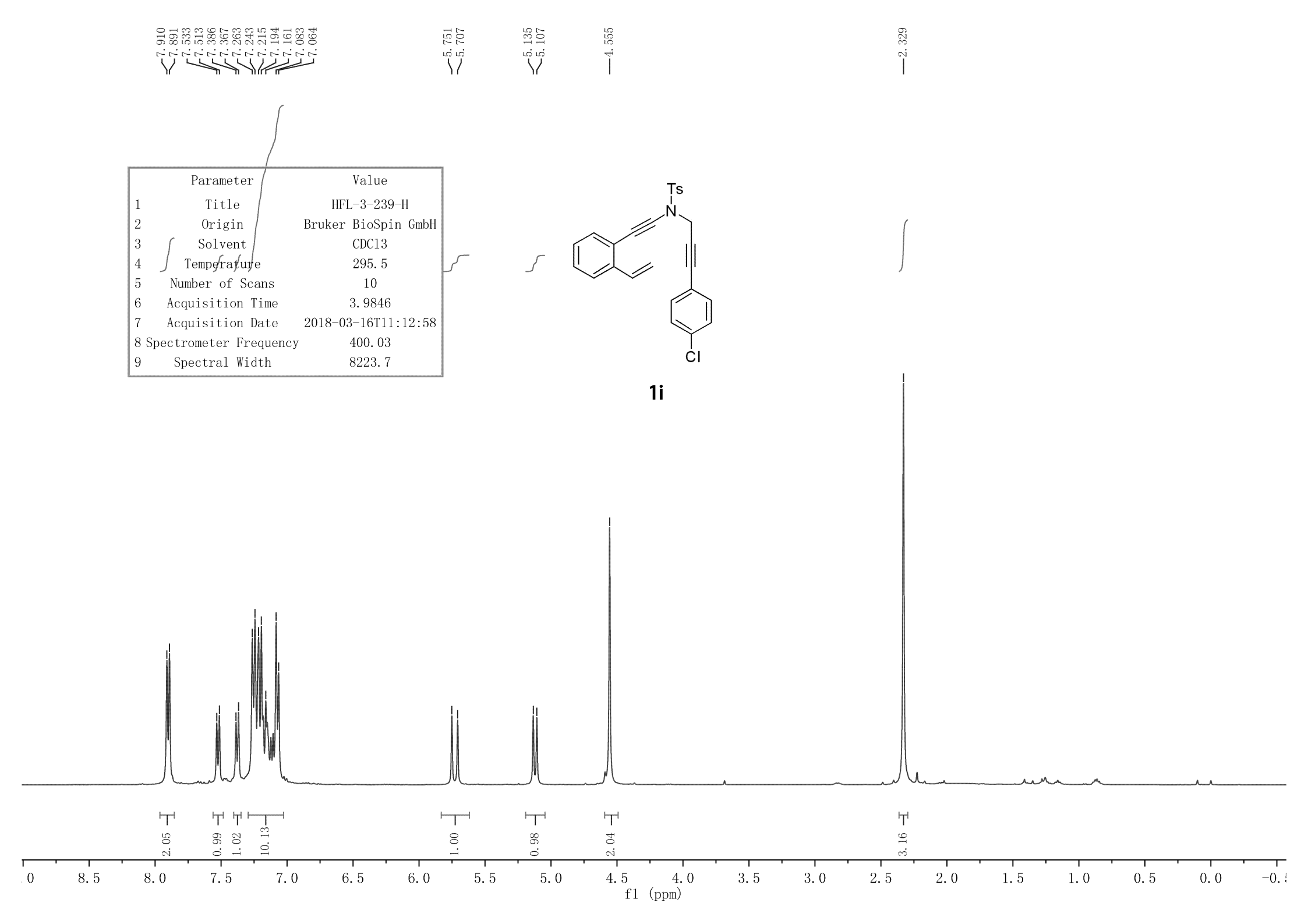


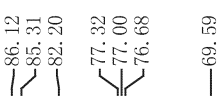


Parameter	Value
1 Title	scy-15-1h-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-13T17:31:53
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

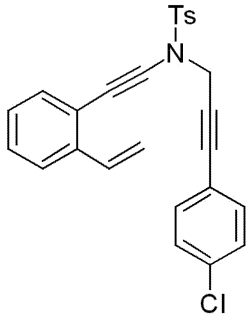
1h



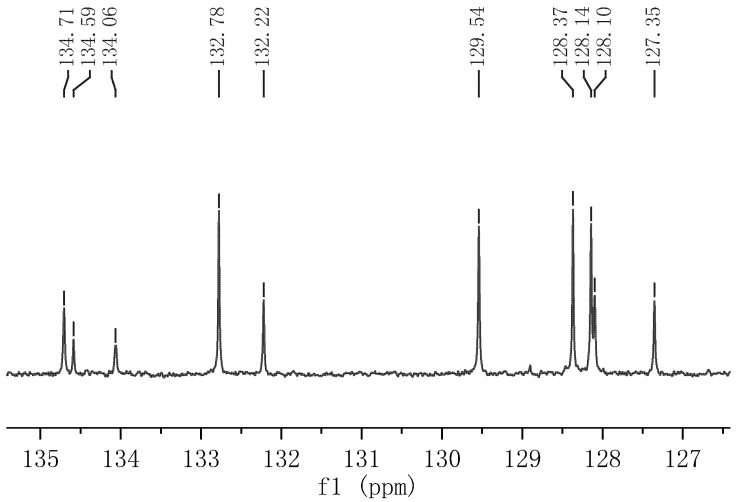

7.910
7.891
7.533
7.513
7.386
7.367
7.263
7.243
7.215
7.194
7.161
7.083
7.064
5.751
5.707
5.135
5.107
4.555
2.329
Parameter Value
1 Title HFL-3-239-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.5
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-16T11:12:58
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ts
N
Cl
1i
2.05
0.99
1.02
10.13
1.00
0.98
2.04
3.16
f1 (ppm)

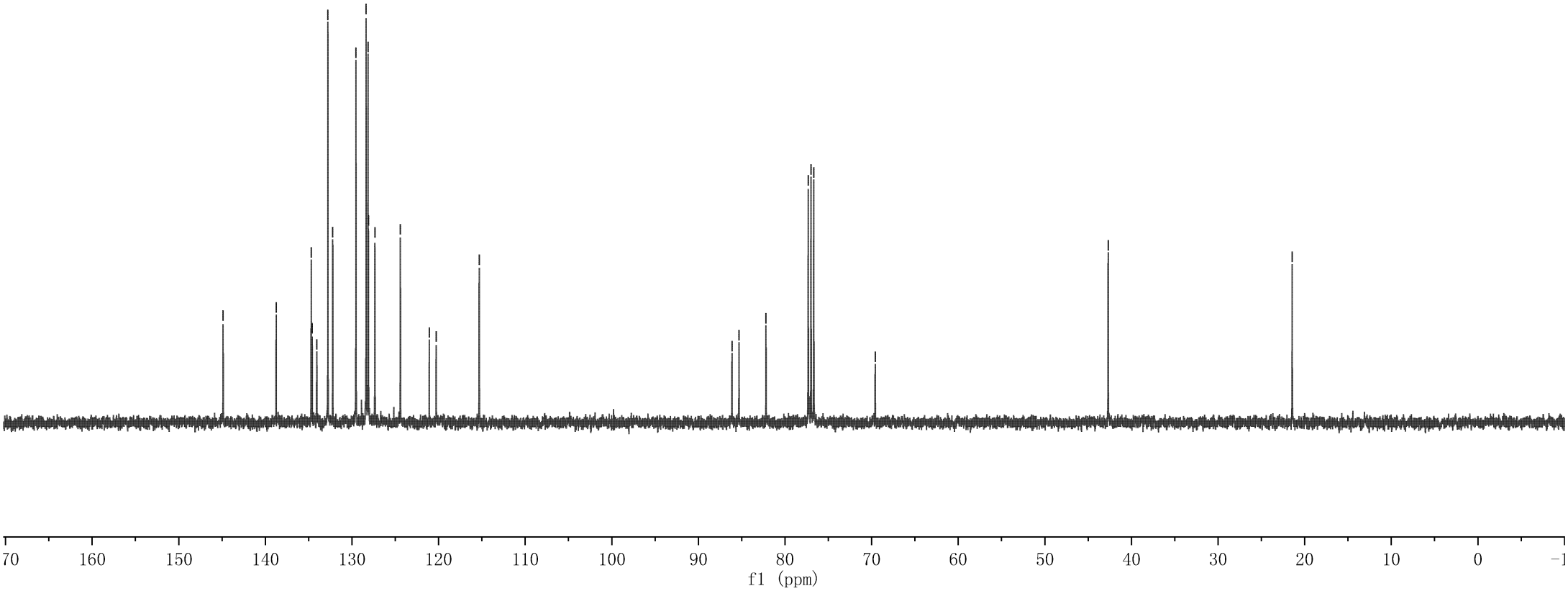


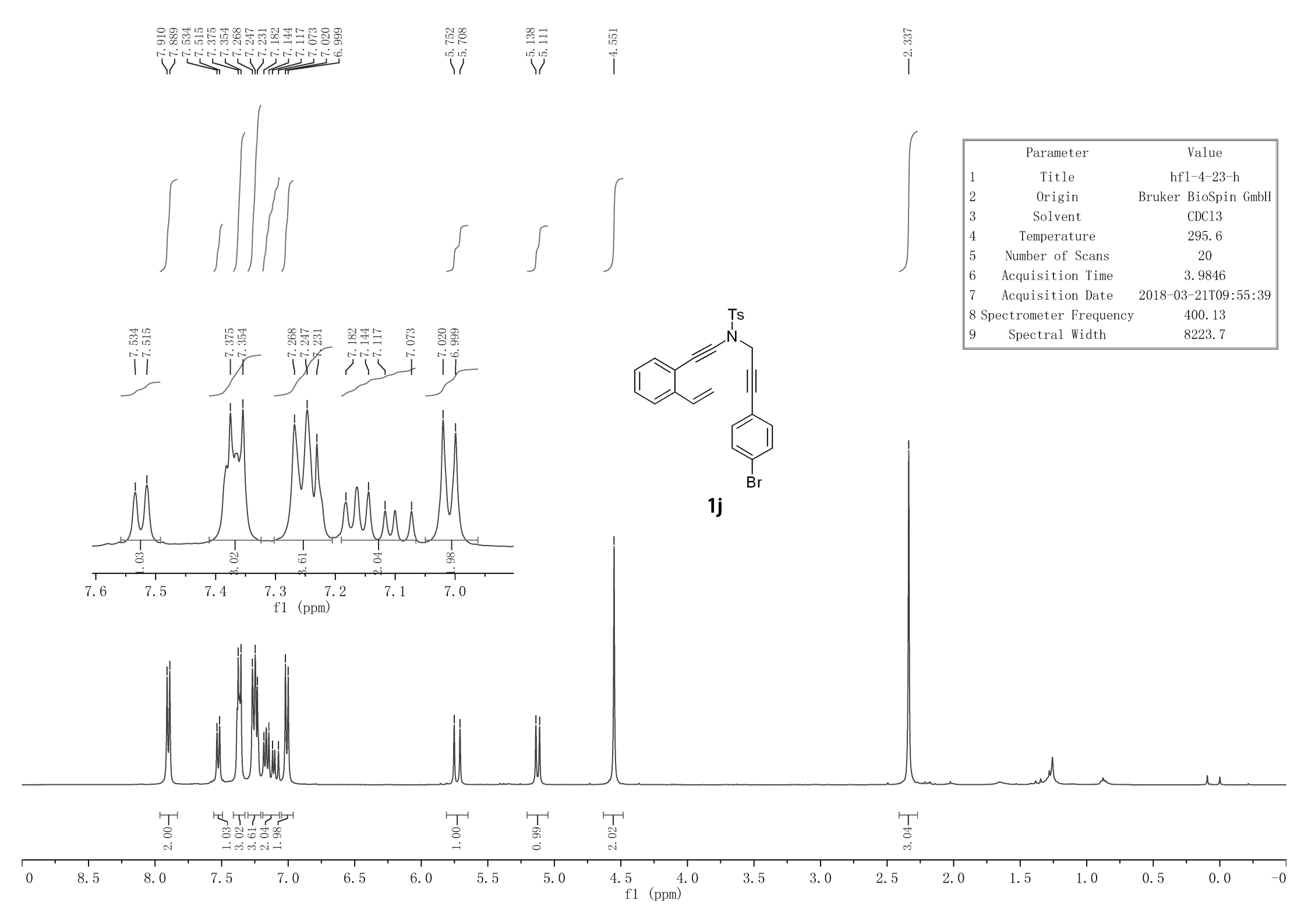
	Parameter	Value
1	Title	HFL-3-239-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.6
5	Number of Scans	22
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-16T11:16:03
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5

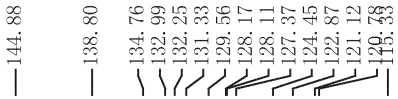


1i

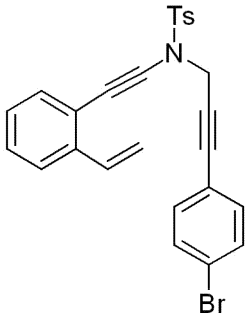




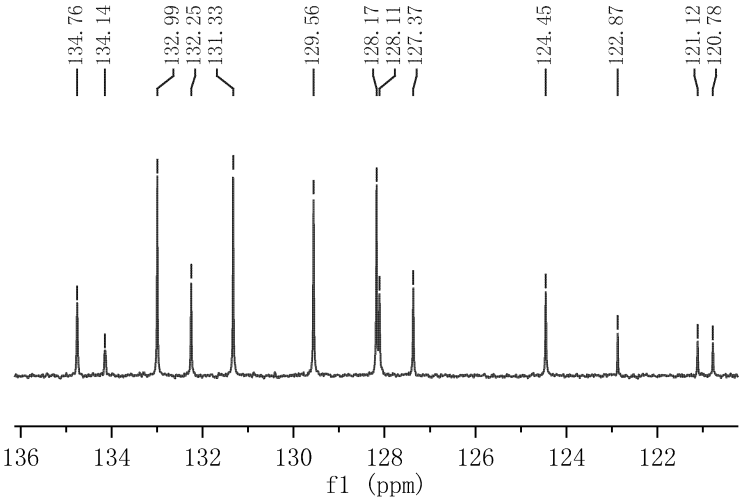

7.910
7.889
7.534
7.515
7.375
7.354
7.268
7.247
7.231
7.182
7.144
7.117
7.073
7.020
6.999
5.752
5.708
5.138
5.111
4.551
2.337
Parameter Value
1 Title hfl-4-23-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 20
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-21T09:55:39
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ts
N
Br
1j
1.03
3.02
3.61
2.04
1.98
f1 (ppm)
2.00
1.00
0.99
2.02
3.04
f1 (ppm)

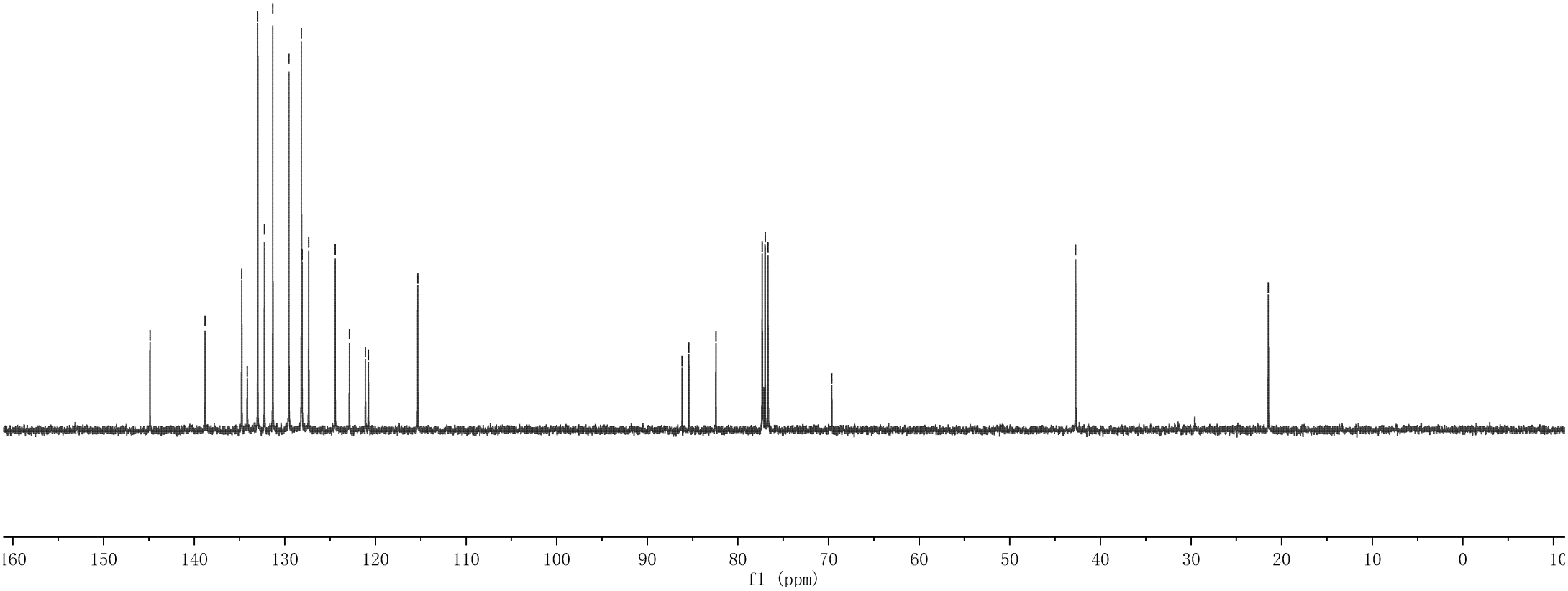


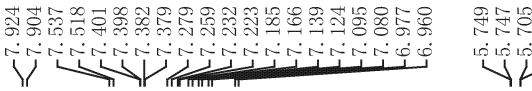
	Parameter	Value
1	Title	hfl-4-23-c
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.3
5	Number of Scans	45
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-21T10:01:06
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



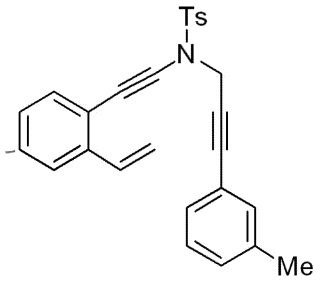
1j



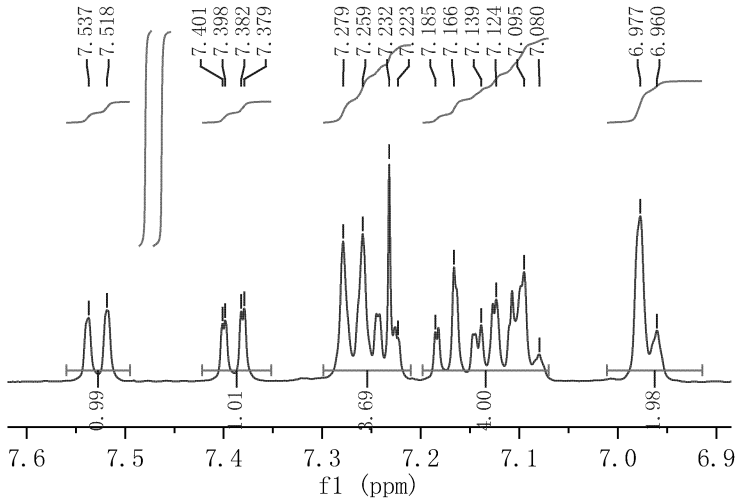


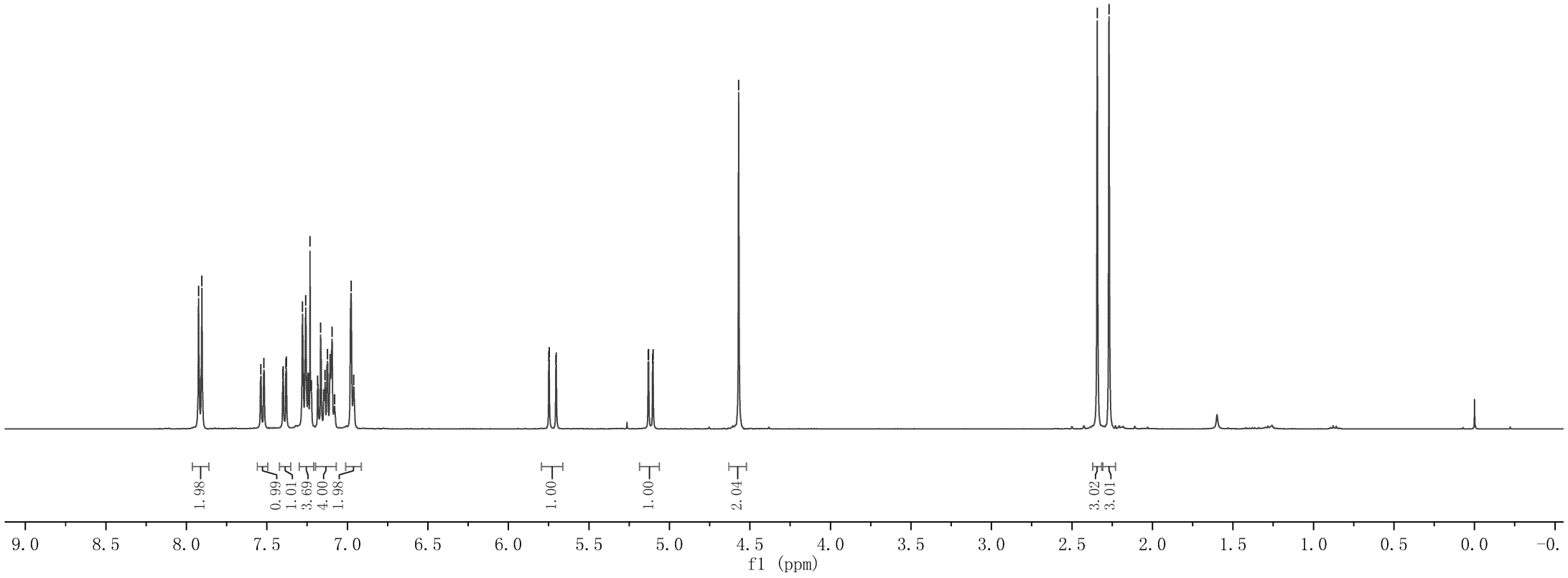


	Parameter	Value
1	Title	hf1-4-31-h
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.8
5	Number of Scans	3
6	Acquisition Time	3.9846
7	Acquisition Date	2018-03-21T16:02:49
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7



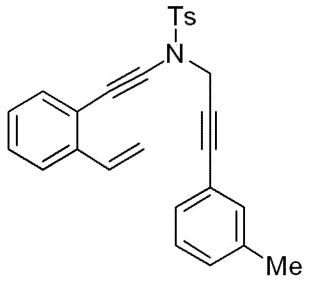
1k



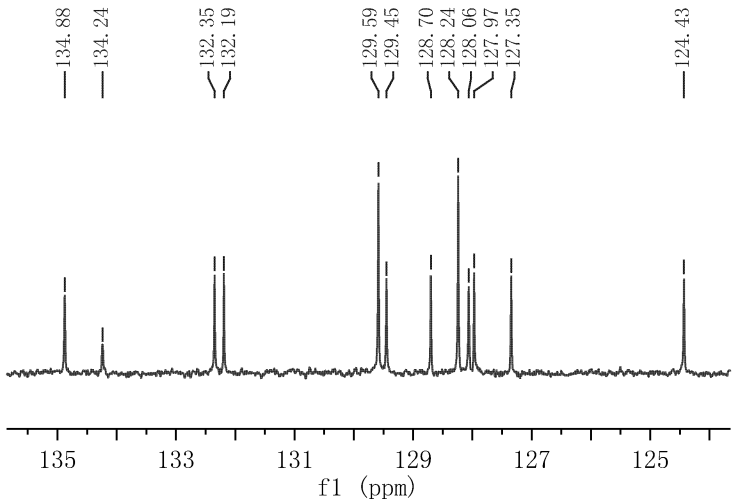


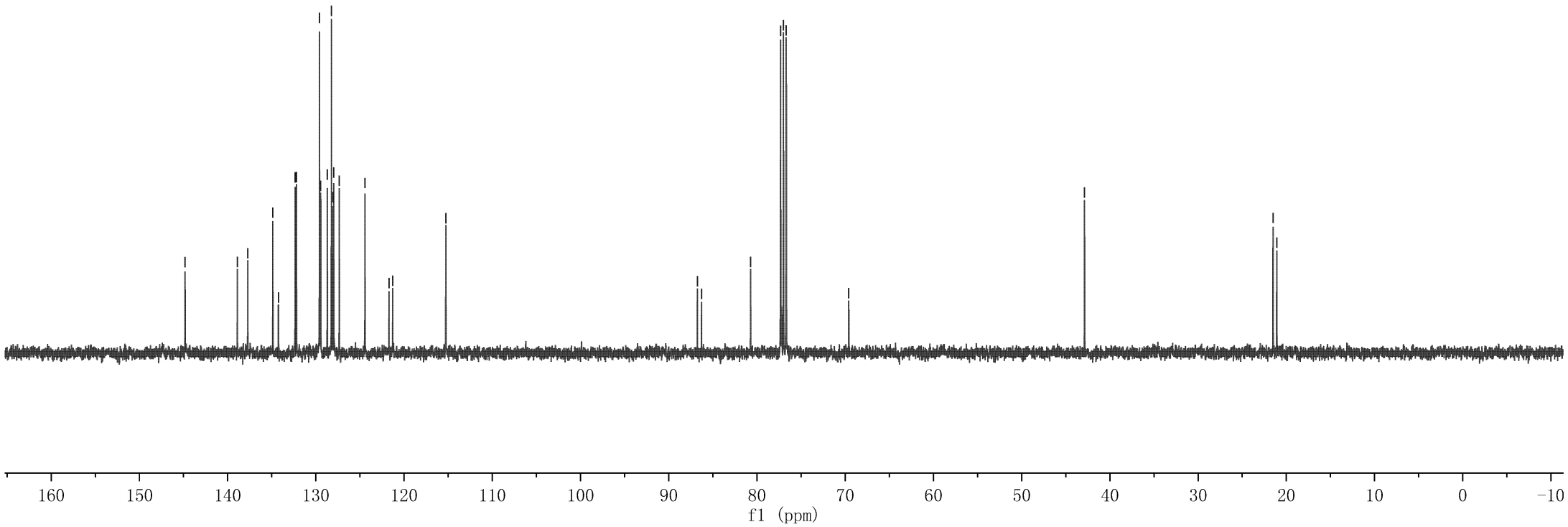
144.82
138.89
137.72
134.88
132.35
132.19
129.59
129.45
128.70
128.24
128.06
127.97
127.35
124.43
121.70
121.29
115.27
86.75
86.28
80.72
77.32
77.00
76.68
69.60
42.87
21.51
21.09

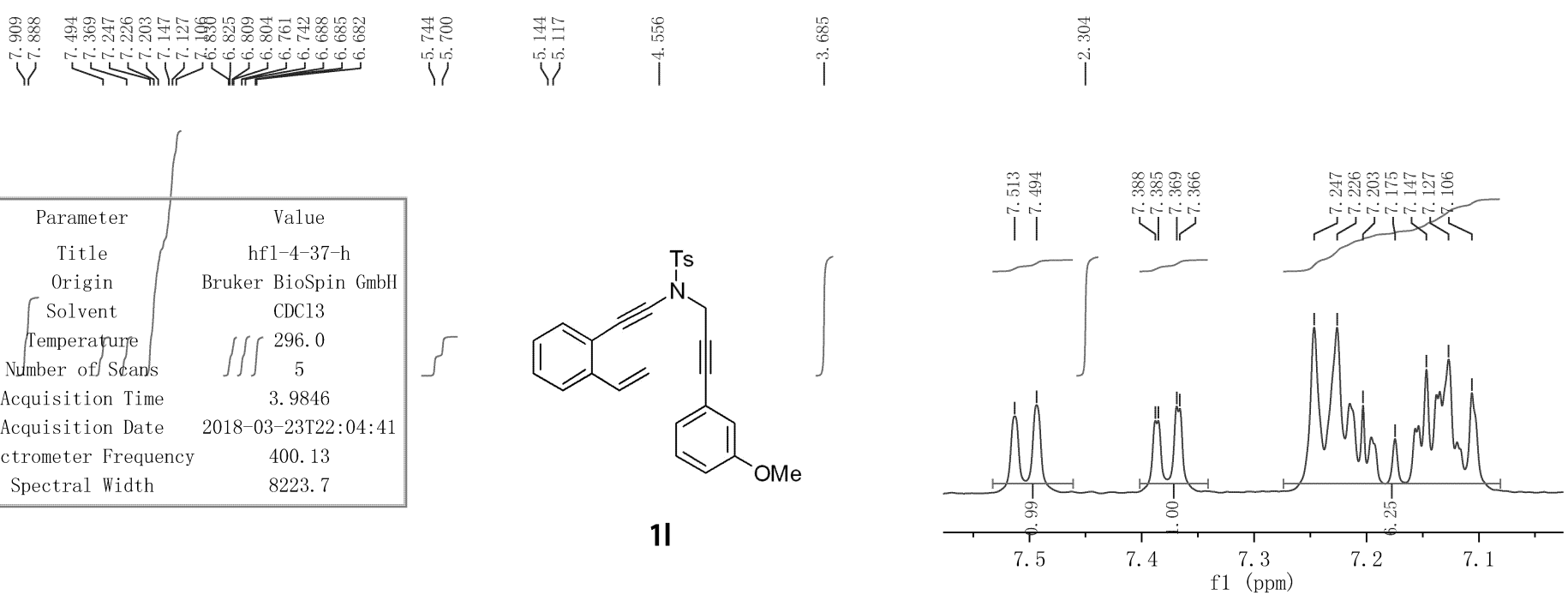
	Parameter	Value
1	Title	hfl-4-31-c
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.8
5	Number of Scans	22
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-21T16:04:43
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



1k

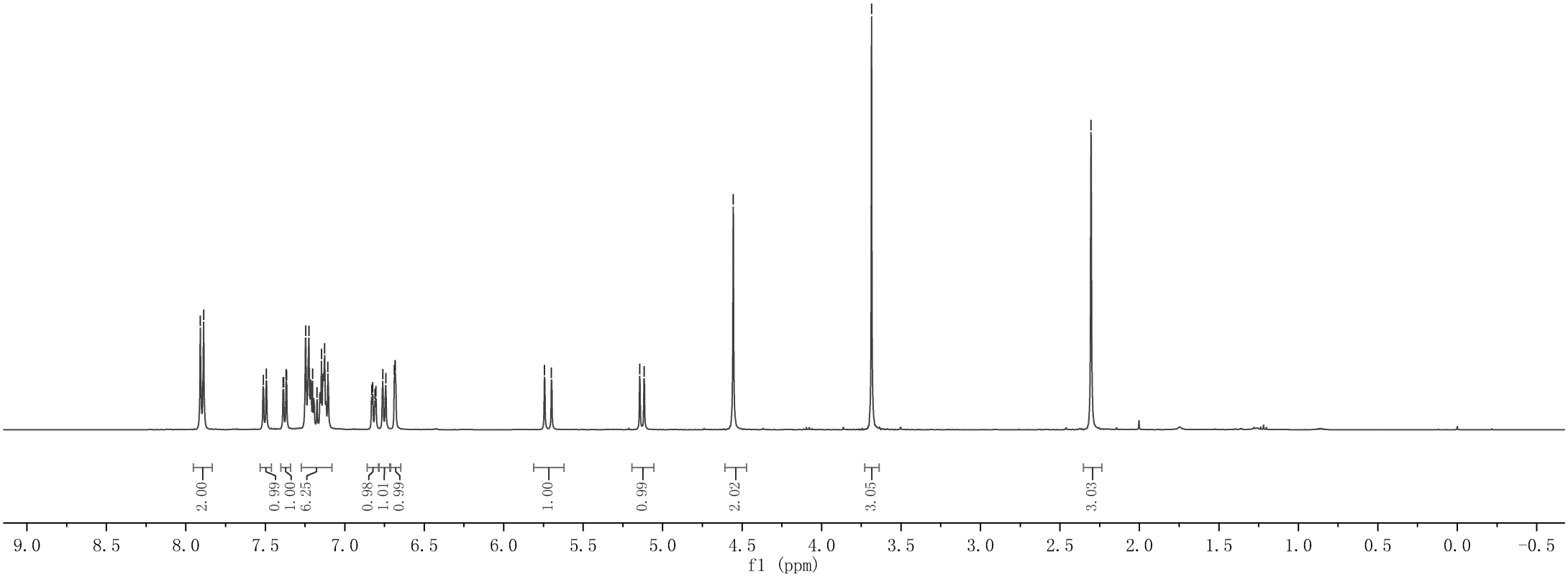






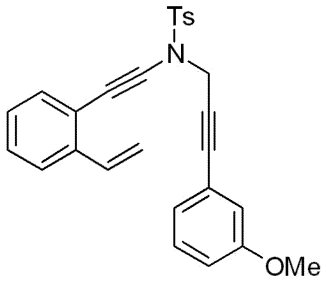
	Parameter	Value
1	Title	hfl-4-37-h
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.0
5	Number of Scans	5
6	Acquisition Time	3.9846
7	Acquisition Date	2018-03-23T22:04:41
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

1l

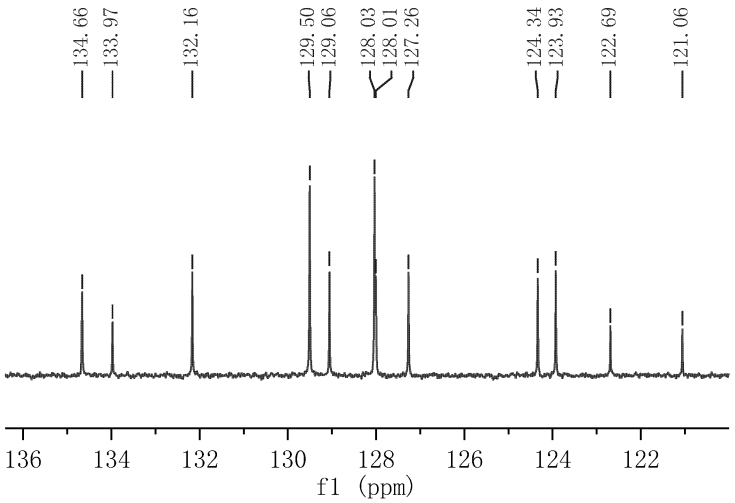


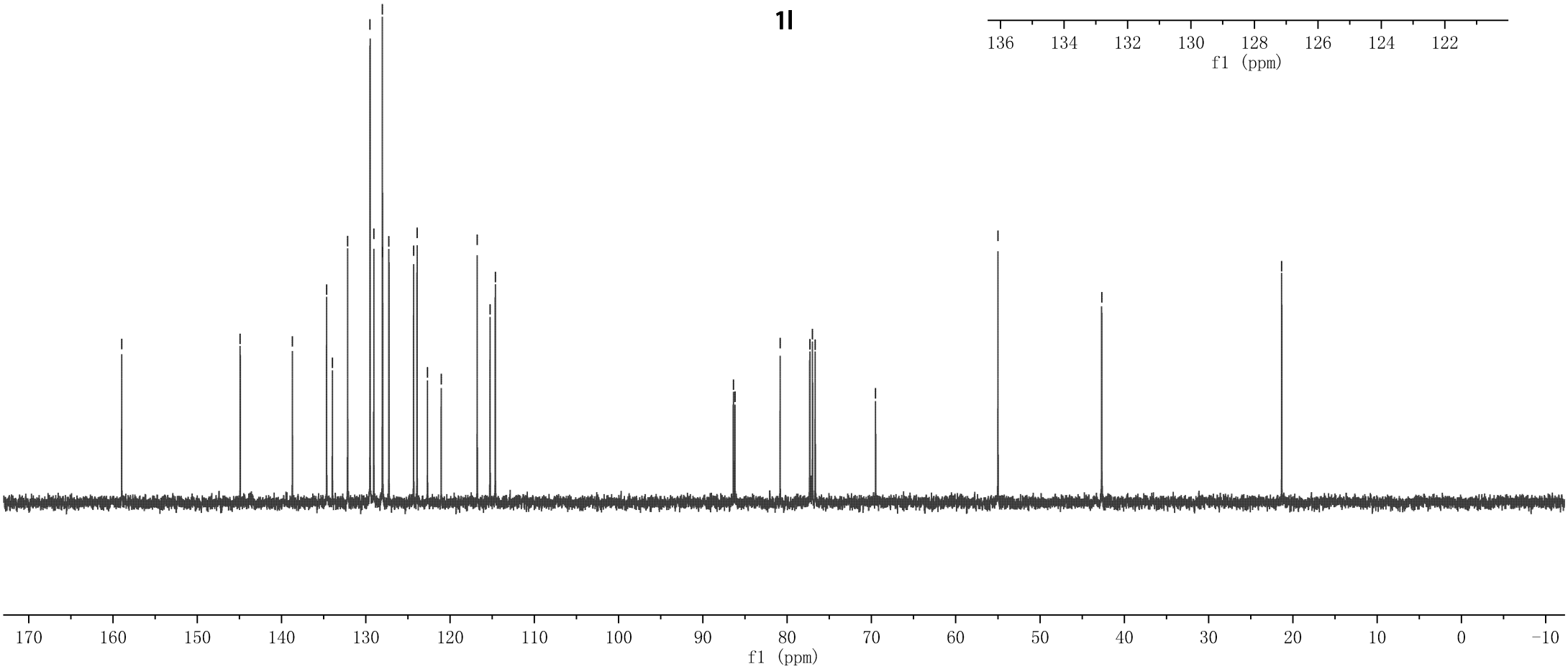
158.98
144.91
138.72
134.66
133.97
132.16
129.50
129.06
128.03
128.01
127.26
124.34
123.93
116.79
115.26
114.64
86.39
86.19
80.84
77.32
77.00
76.68
69.51
54.99
42.68
21.32

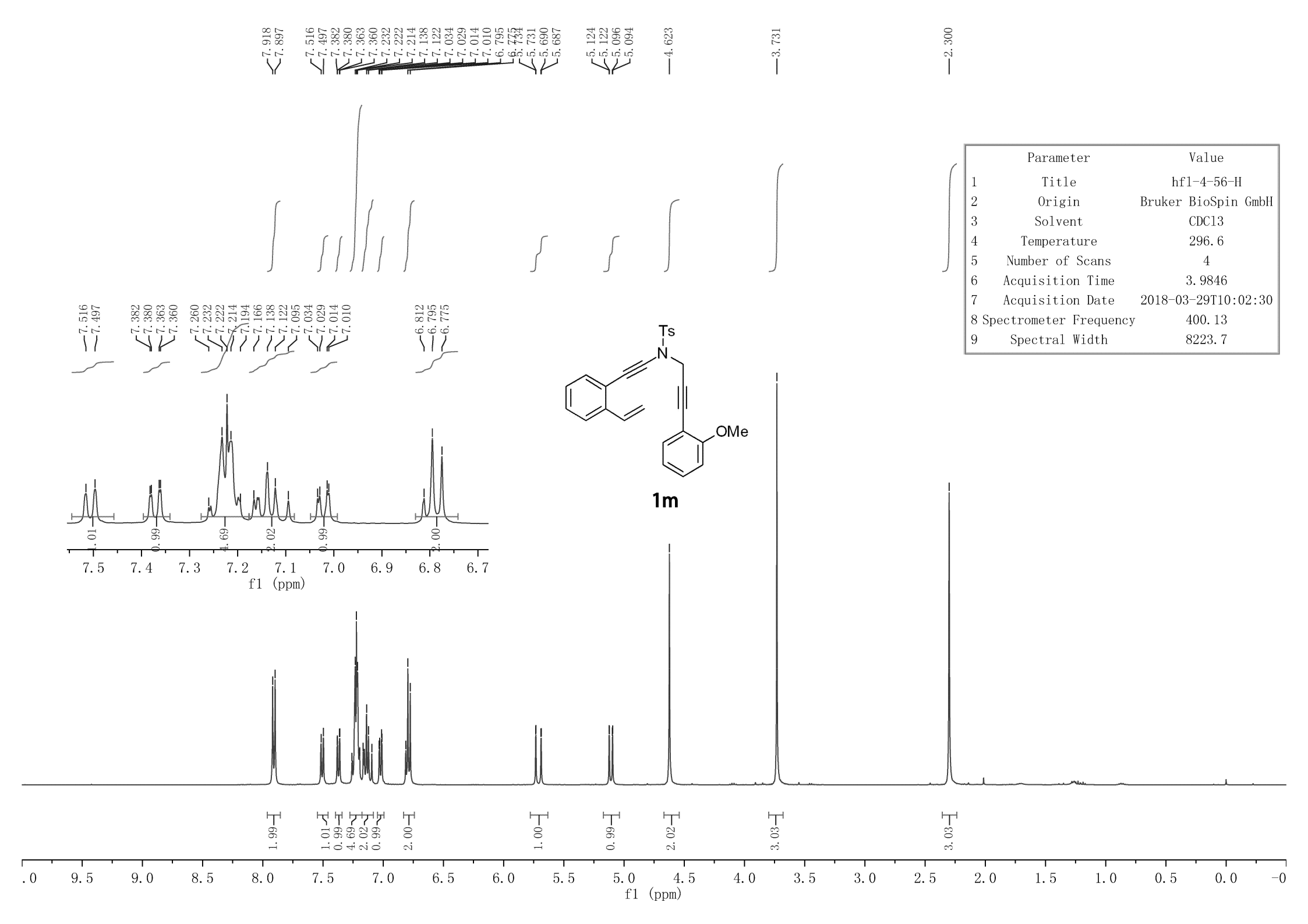
	Parameter	Value
1	Title	hfl-4-37-c
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.1
5	Number of Scans	8
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-23T22:06:48
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



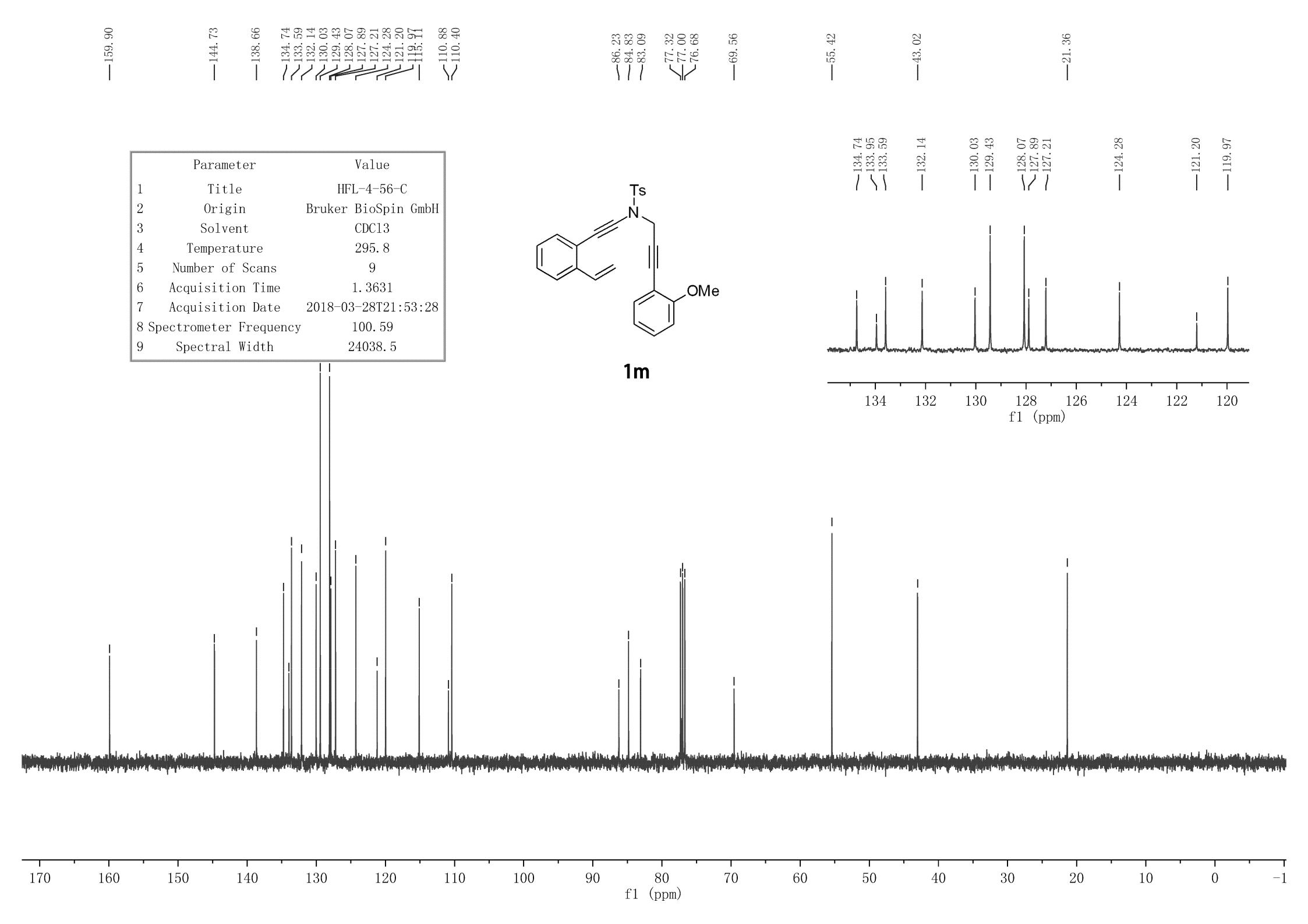
1l



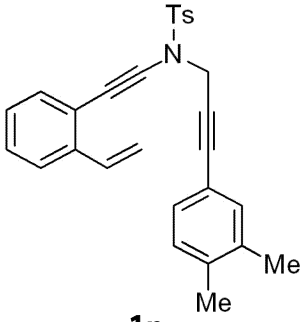




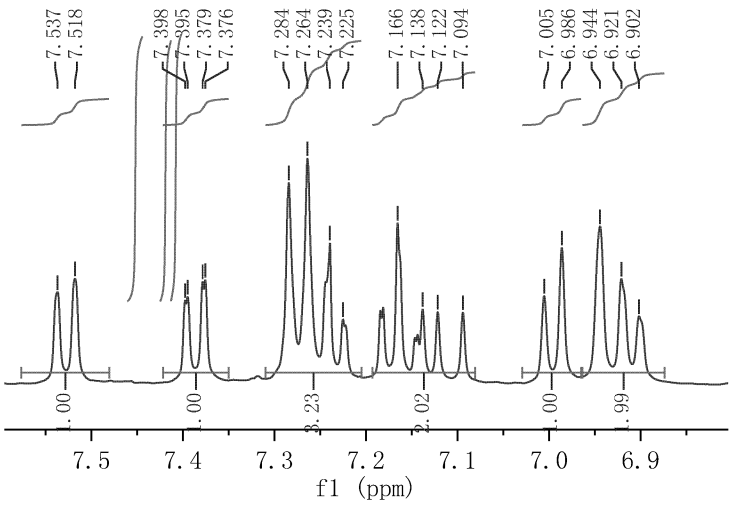
	Parameter	Value
1	Title	hf1-4-56-H
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.6
5	Number of Scans	4
6	Acquisition Time	3.9846
7	Acquisition Date	2018-03-29T10:02:30
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

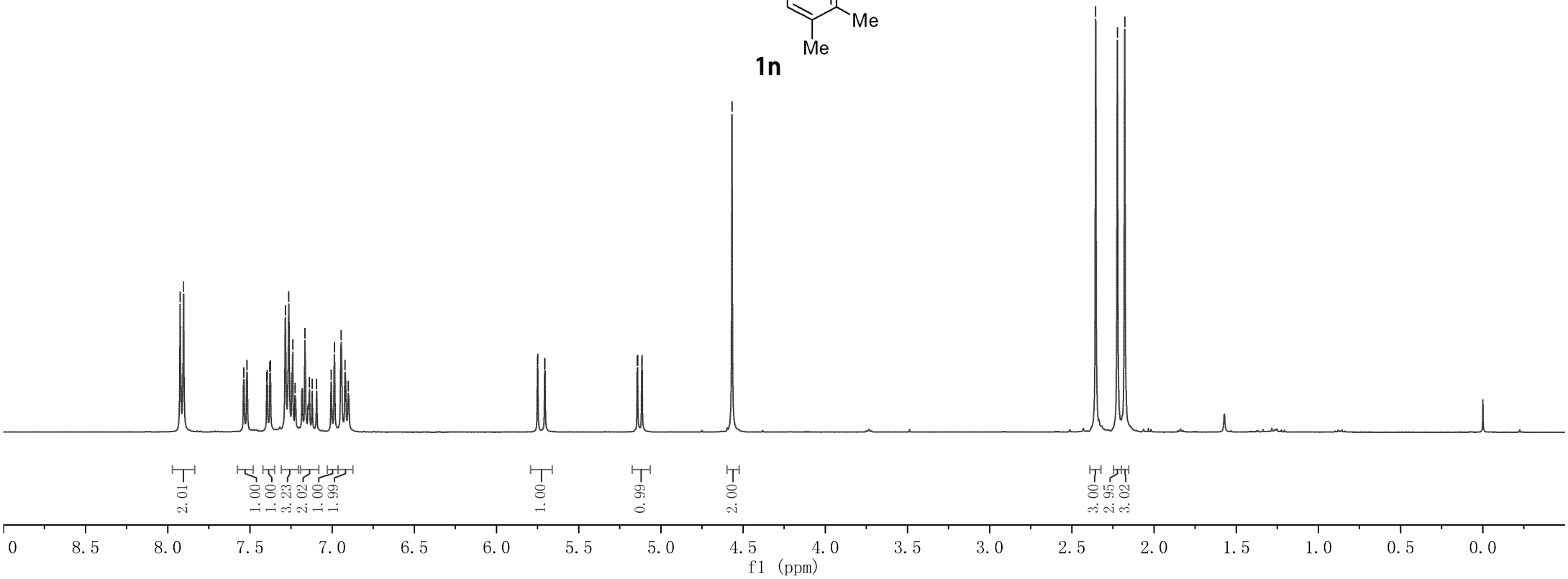

159.90
144.73
138.66
134.74
133.59
132.14
130.03
129.43
128.07
127.89
127.21
124.28
121.20
119.97
110.88
110.40
86.23
84.83
83.09
77.32
77.00
76.68
69.56
55.42
43.02
21.36
Parameter Value
1 Title HFL-4-56-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.8
5 Number of Scans 9
6 Acquisition Time 1.3631
7 Acquisition Date 2018-03-28T21:53:28
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
Ts
N
OMe
1m
f1 (ppm)

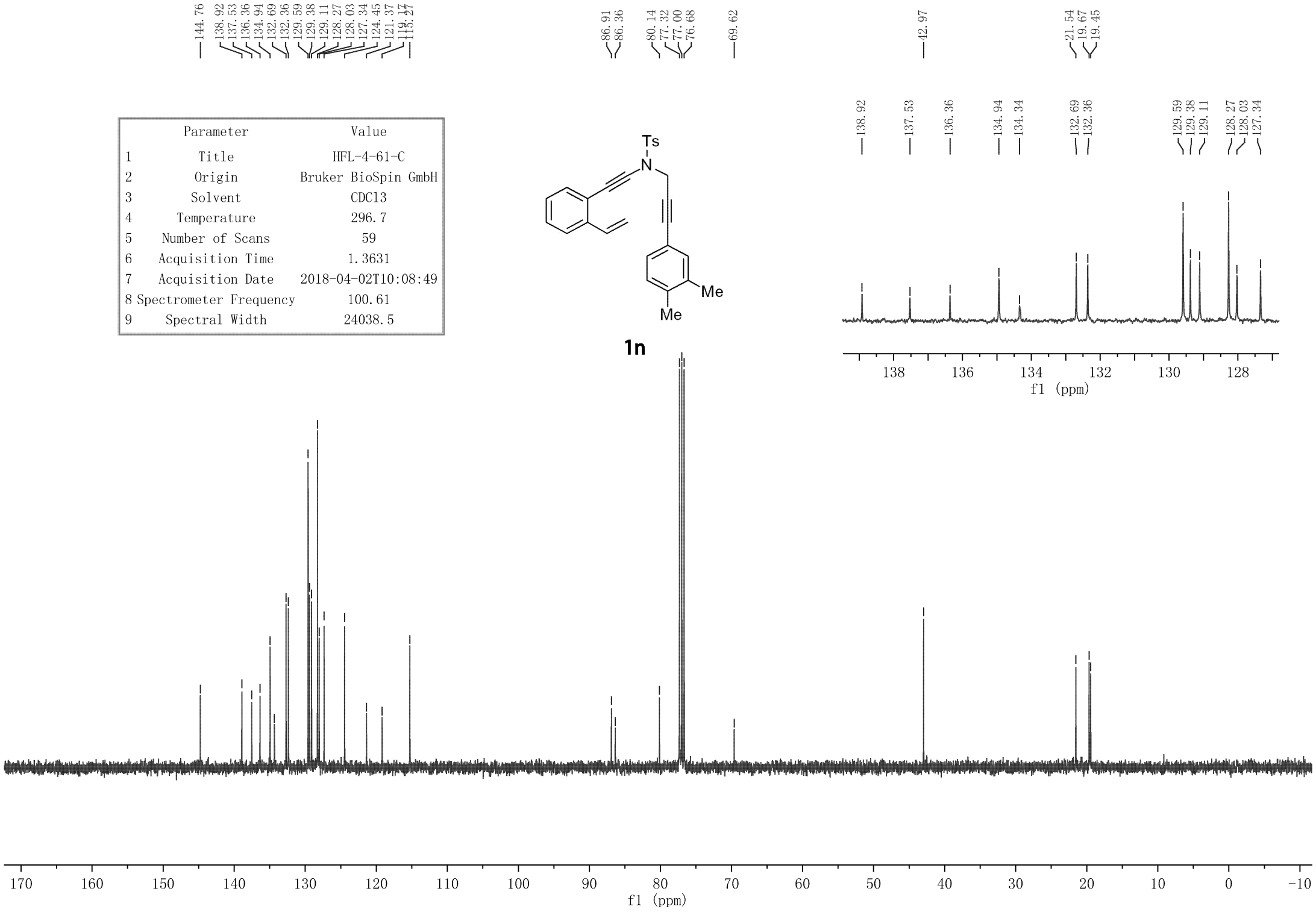
Parameter	Value
1 Title	HFL-4-61-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.6
5 Number of Scans	7
6 Acquisition Time	3.9846
7 Acquisition Date	2018-04-02T10:05:36
8 Spectrometer Frequency	400.13
9 Spectral Width	8223.7



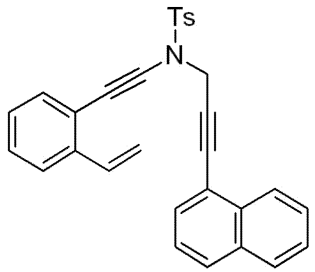
1n



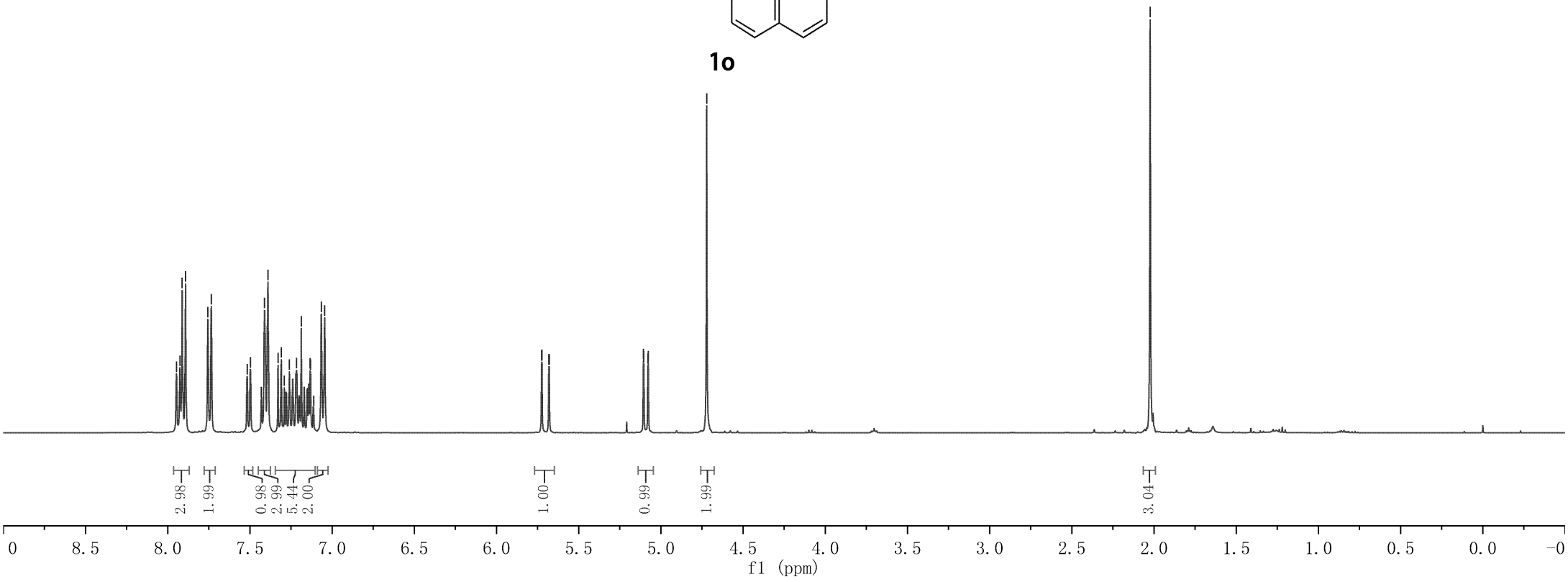


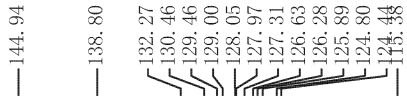

144.76
138.92
137.53
136.36
134.94
132.69
132.36
129.59
129.38
129.11
128.27
128.03
127.34
124.45
121.37
86.91
86.36
80.14
77.32
77.00
76.68
69.62
42.97
21.54
19.67
19.45
Parameter Value
1 Title HFL-4-61-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.7
5 Number of Scans 59
6 Acquisition Time 1.3631
7 Acquisition Date 2018-04-02T10:08:49
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ts
N
Me
Me
1n
f1 (ppm)
f1 (ppm)

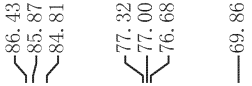
	Parameter	Value
1	Title	HFL-4-43-H
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	297.0
5	Number of Scans	6
6	Acquisition Time	3.9846
7	Acquisition Date	2018-03-26T16:04:53
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7



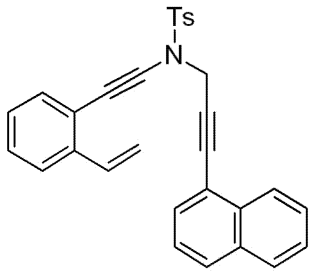
1o



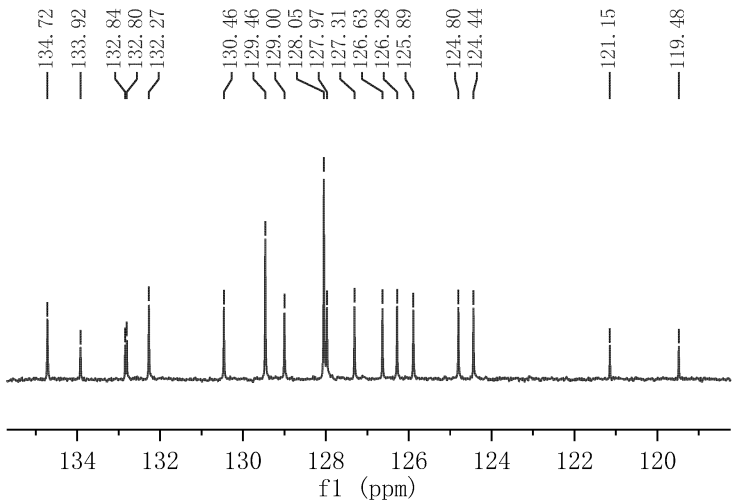


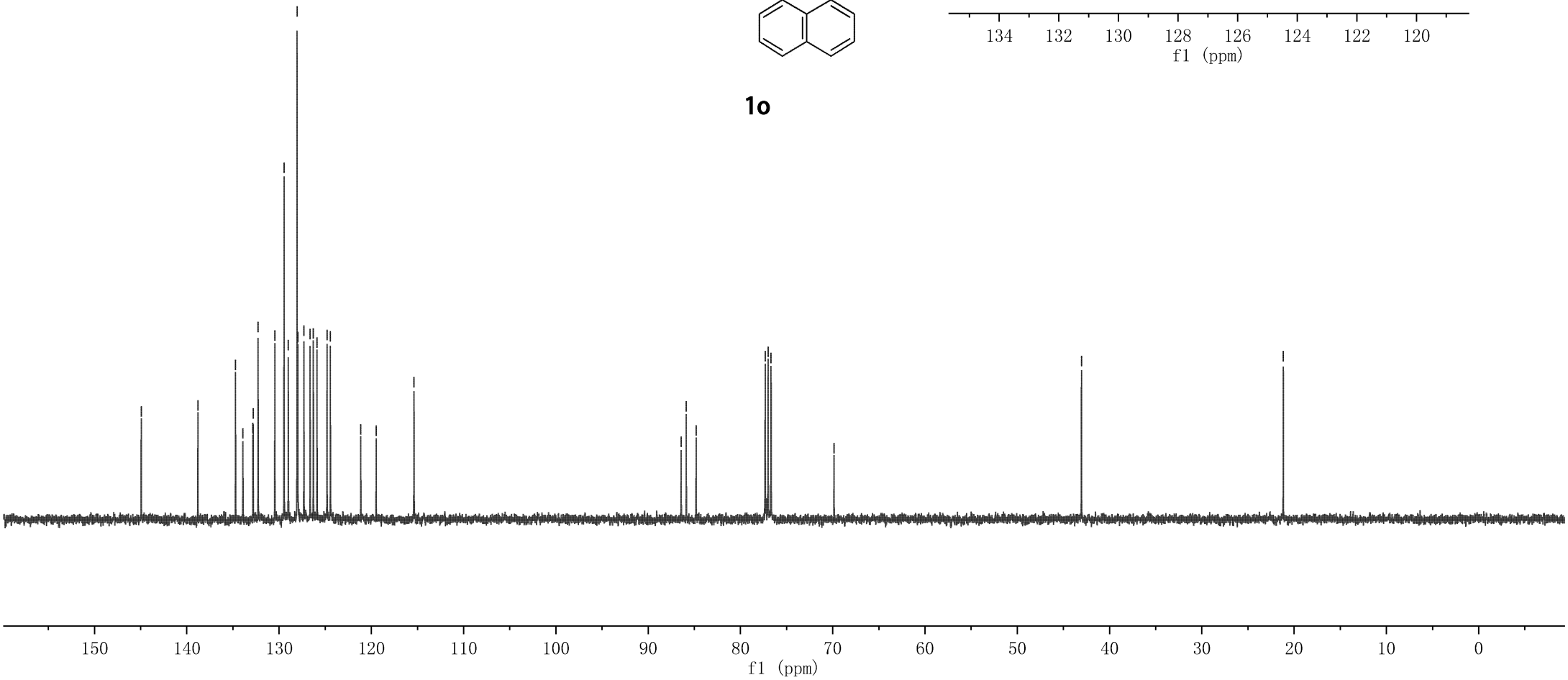


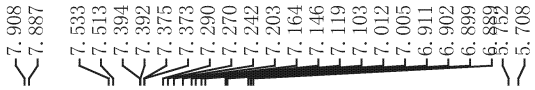
	Parameter	Value
1	Title	HFL-4-43-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	297.0
5	Number of Scans	12
6	Acquisition Time	1.3631
7	Acquisition Date	2018-03-26T16:07:24
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



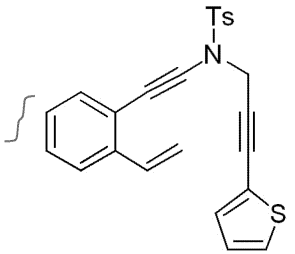
1o



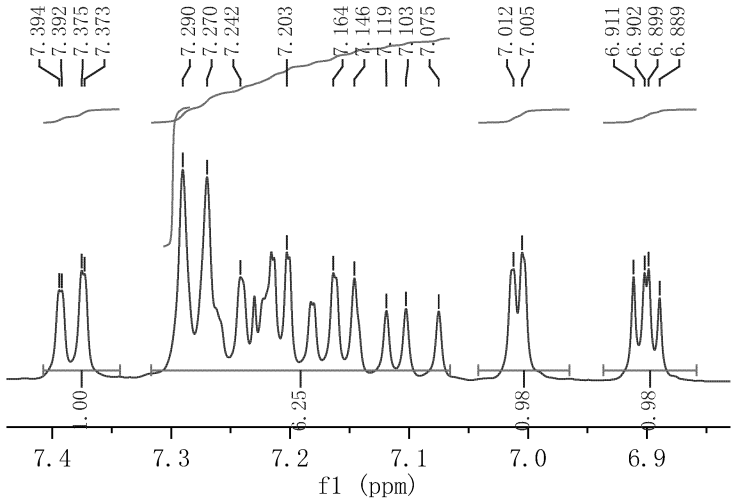


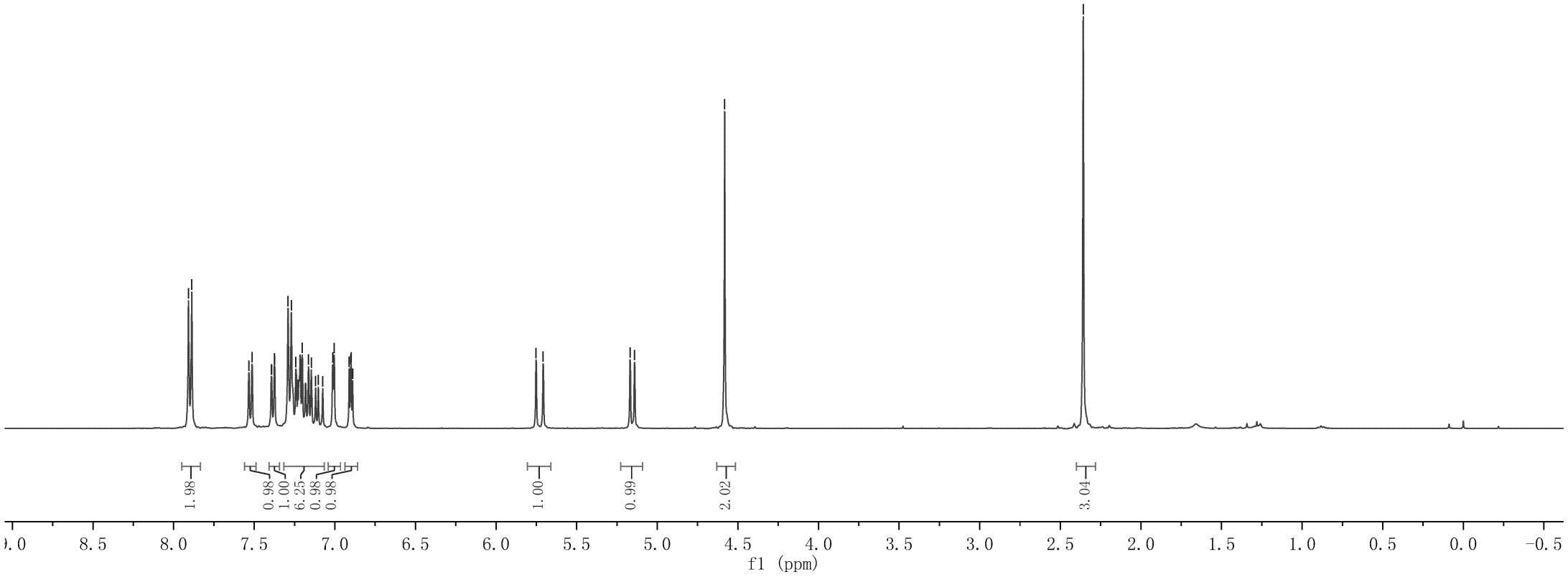


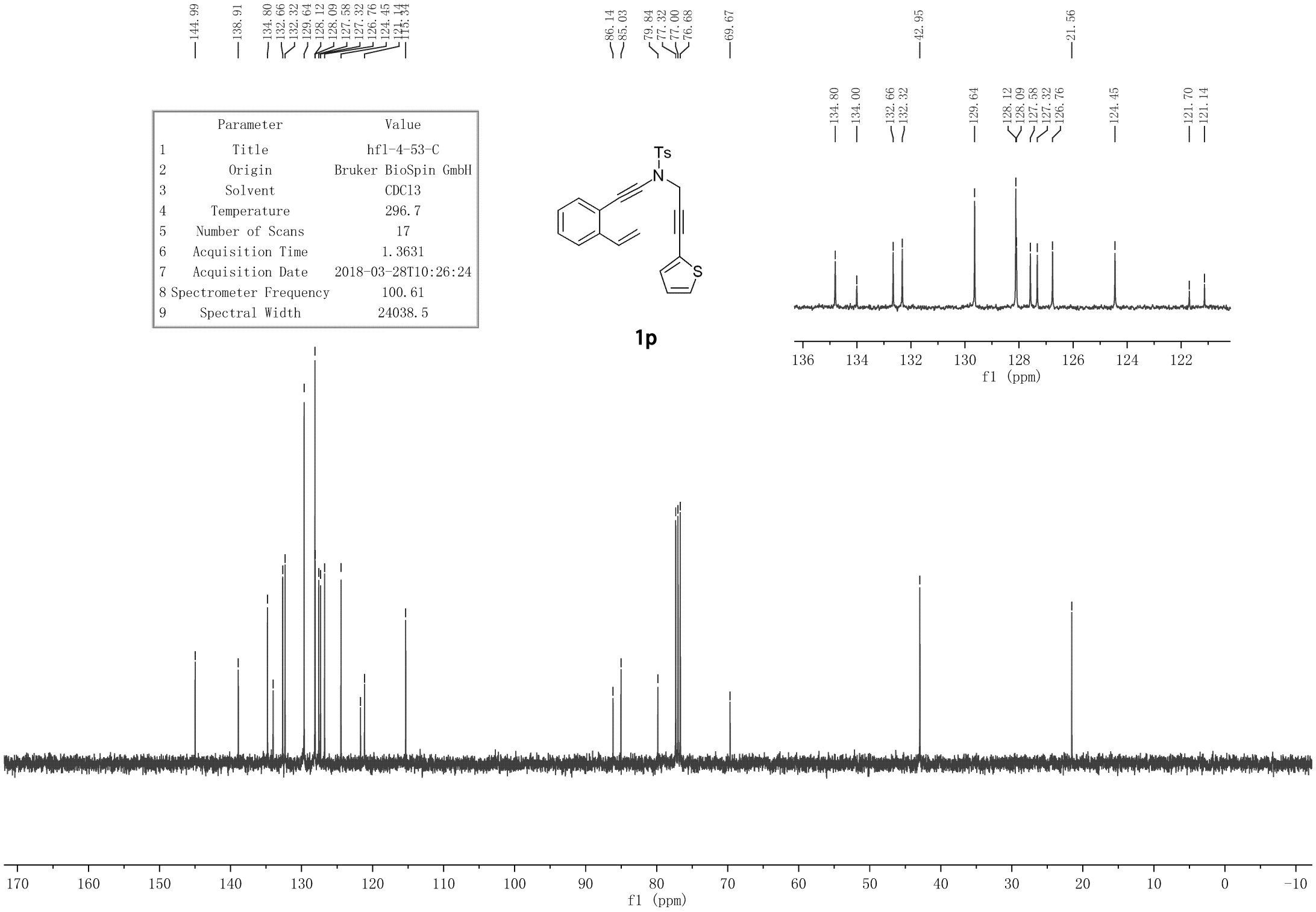
	Parameter	Value
1	Title	HFL-4-53-H
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.7
5	Number of Scans	4
6	Acquisition Time	3.9846
7	Acquisition Date	2018-03-28T10:22:14
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

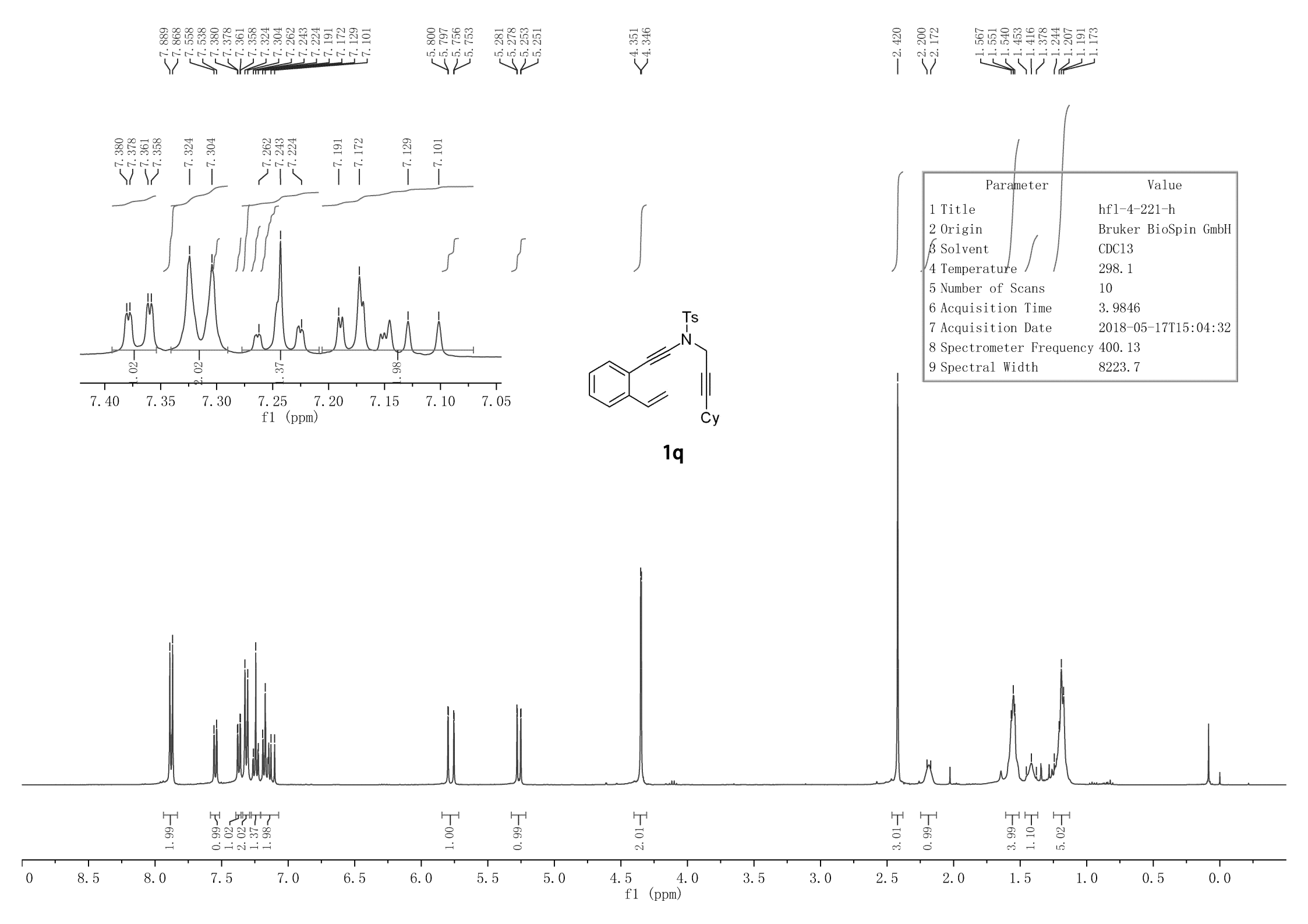


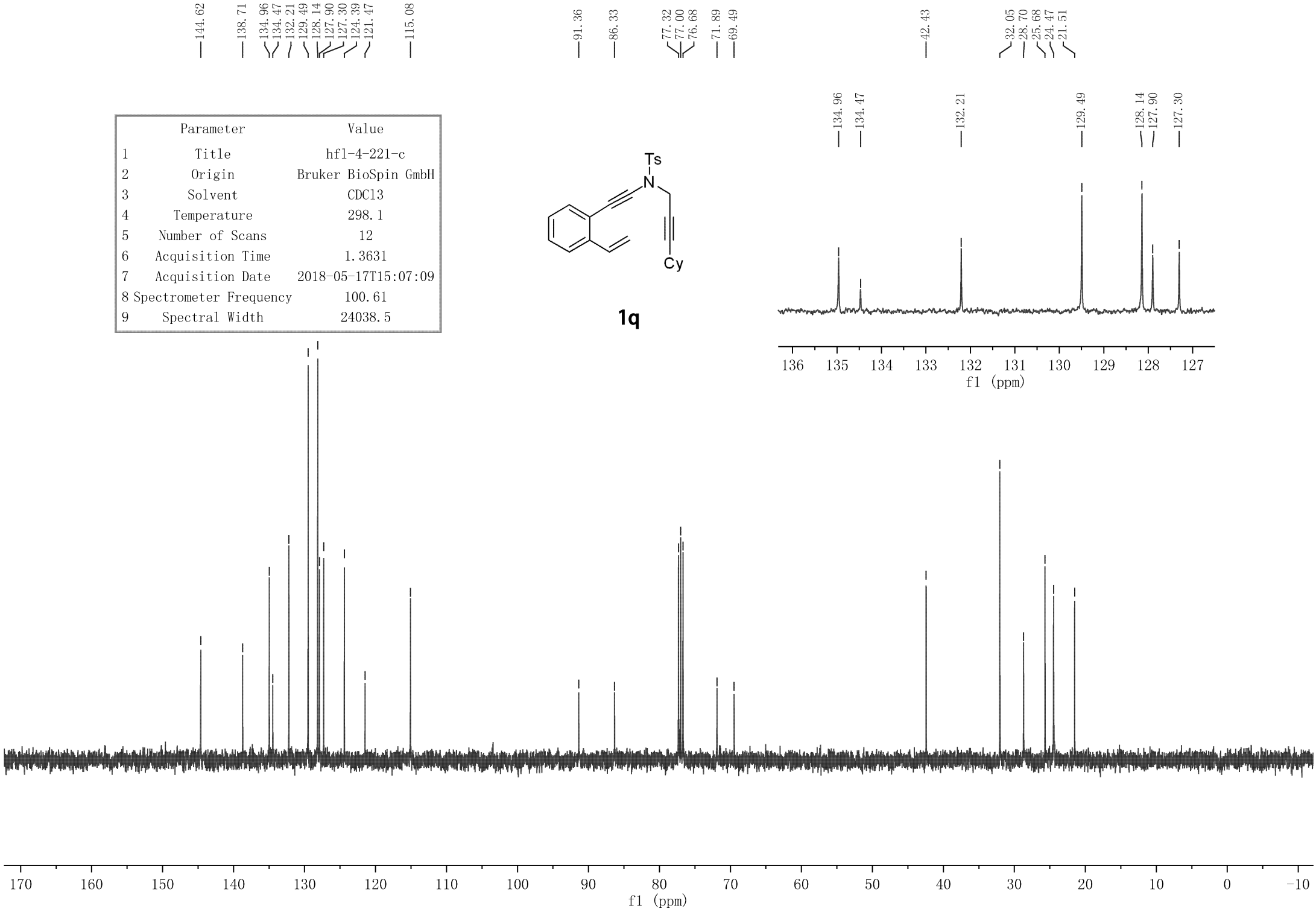
1p

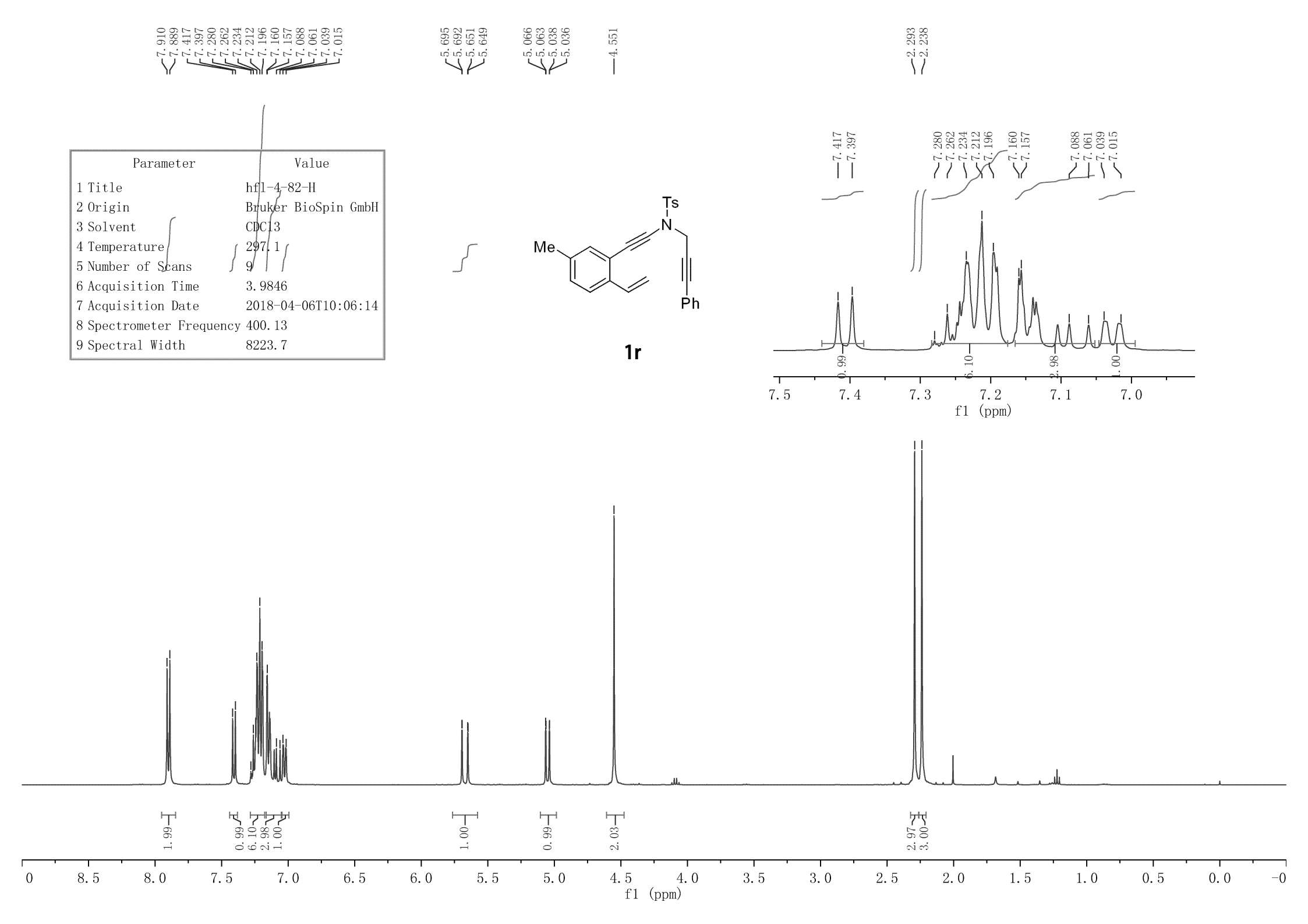


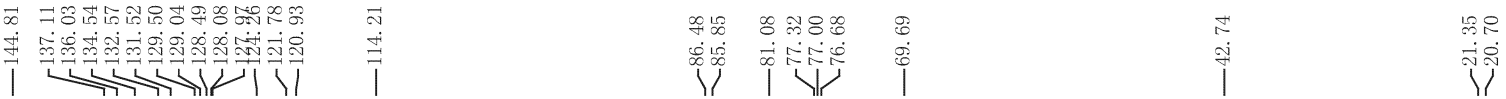



144.99
138.91
134.80
132.66
132.32
129.64
128.12
128.09
127.58
127.32
126.76
124.45
86.14
85.03
79.84
77.32
77.00
76.68
69.67
42.95
21.56
Parameter Value
1 Title hf1-4-53-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.7
5 Number of Scans 17
6 Acquisition Time 1.3631
7 Acquisition Date 2018-03-28T10:26:24
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ts
N
S
1p
134.80
134.00
132.66
132.32
129.64
128.12
128.09
127.58
127.32
126.76
124.45
121.70
121.14
136
134
132
130
128
126
124
122
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

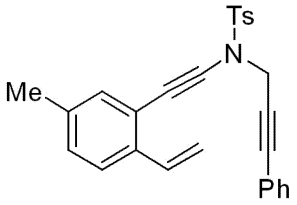

7.889
7.868
7.558
7.538
7.380
7.378
7.361
7.358
7.324
7.304
7.262
7.243
7.224
7.191
7.172
7.129
7.101
5.800
5.797
5.756
5.753
5.281
5.278
5.253
5.251
4.351
4.346
2.420
2.200
2.172
1.567
1.551
1.540
1.453
1.416
1.378
1.244
1.207
1.191
1.173
Parameter
Value
1 Title
hfl-4-221-h
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
298.1
5 Number of Scans
10
6 Acquisition Time
3.9846
7 Acquisition Date
2018-05-17T15:04:32
8 Spectrometer Frequency
400.13
9 Spectral Width
8223.7
Ts
N
Cy
1q
f1 (ppm)


144.62
138.71
134.96
134.47
132.21
129.49
128.14
127.90
127.30
124.39
121.47
115.08
91.36
86.33
77.32
77.00
76.68
71.89
69.49
42.43
32.05
28.70
25.68
24.47
21.51
Parameter Value
1 Title hfl-4-221-c
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.1
5 Number of Scans 12
6 Acquisition Time 1.3631
7 Acquisition Date 2018-05-17T15:07:09
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ts
N
Cy
1q
134.96
134.47
132.21
129.49
128.14
127.90
127.30
136 135 134 133 132 131 130 129 128 127
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

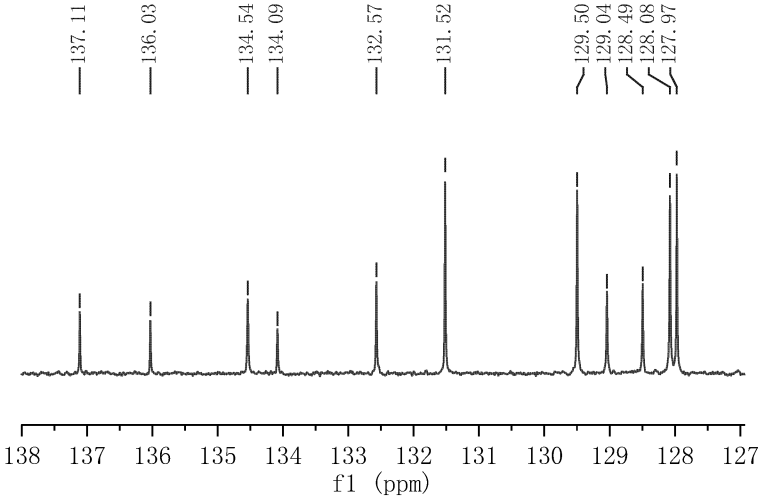

7.910
7.889
7.417
7.397
7.280
7.262
7.234
7.212
7.196
7.160
7.157
7.088
7.061
7.039
7.015
5.695
5.692
5.651
5.649
5.066
5.063
5.038
5.036
4.551
2.293
2.238
Parameter Value
1 Title hfl-4-82-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.1
5 Number of Scans 9
6 Acquisition Time 3.9846
7 Acquisition Date 2018-04-06T10:06:14
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ts
N
Me
Ph
1r
0.99
6.10
2.98
1.00
f1 (ppm)
1.99
0.99
6.10
2.98
1.00
1.00
0.99
2.03
2.97
3.00
f1 (ppm)

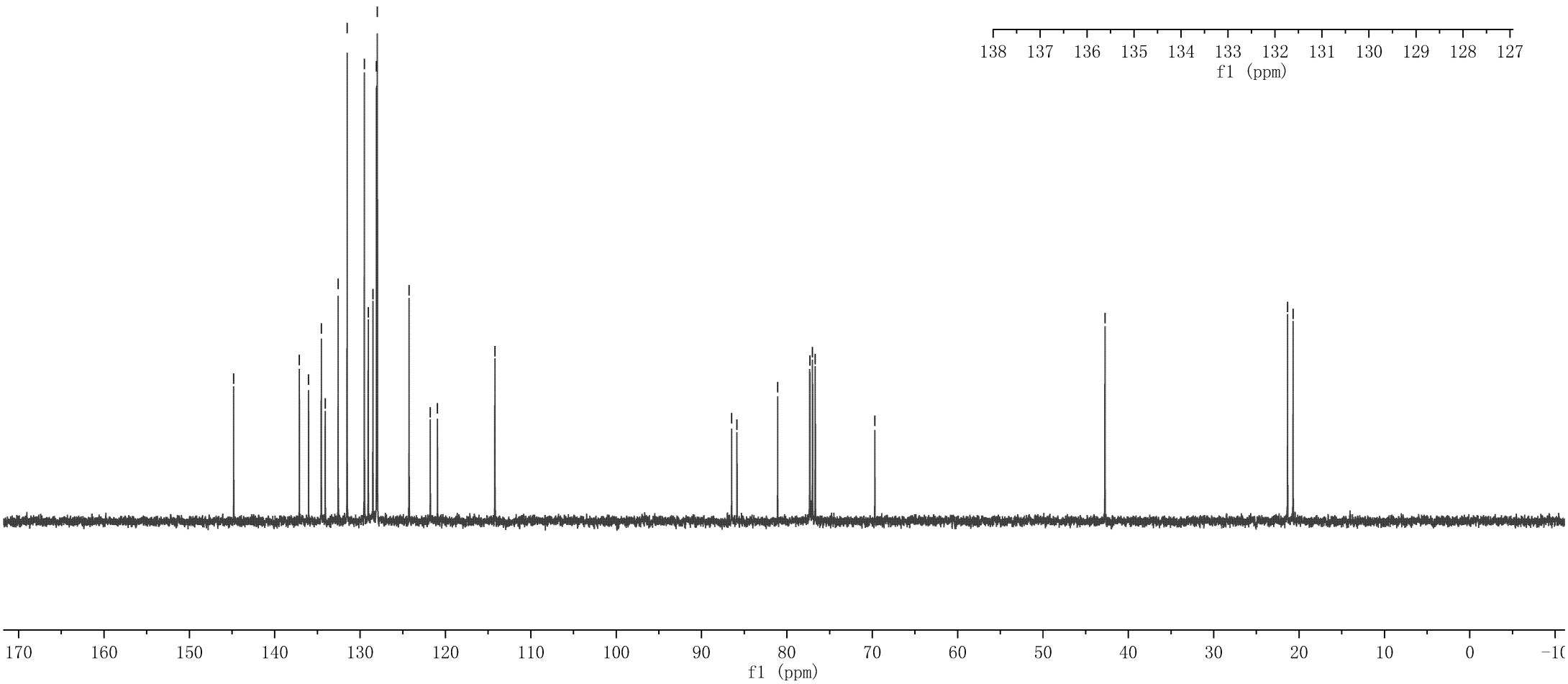


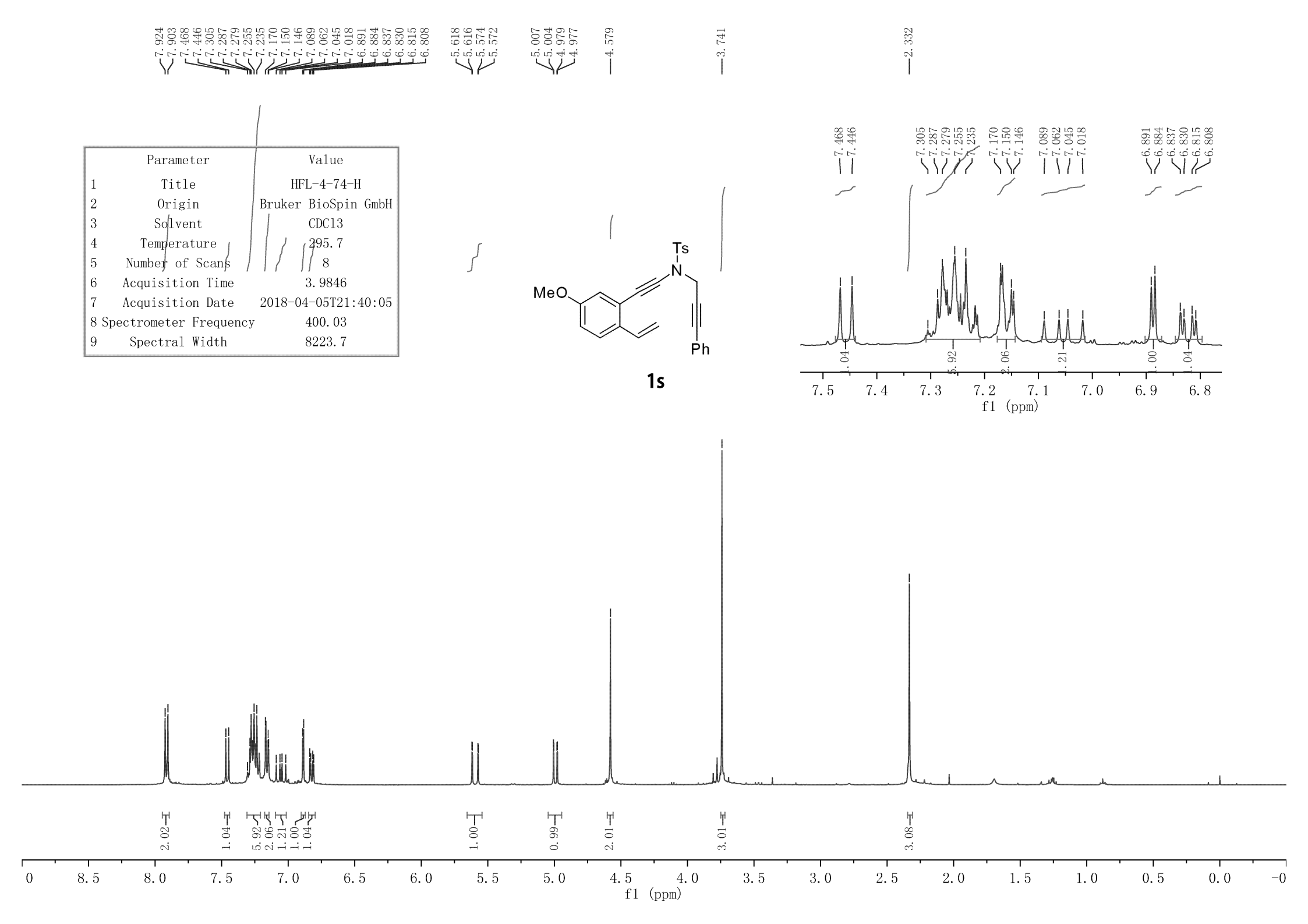
	Parameter	Value
1	Title	hfl-4-82-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	297.1
5	Number of Scans	10
6	Acquisition Time	1.3631
7	Acquisition Date	2018-04-06T10:08:44
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



1r

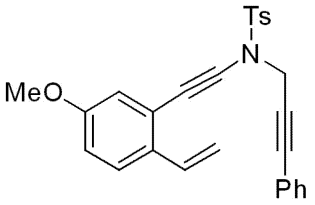




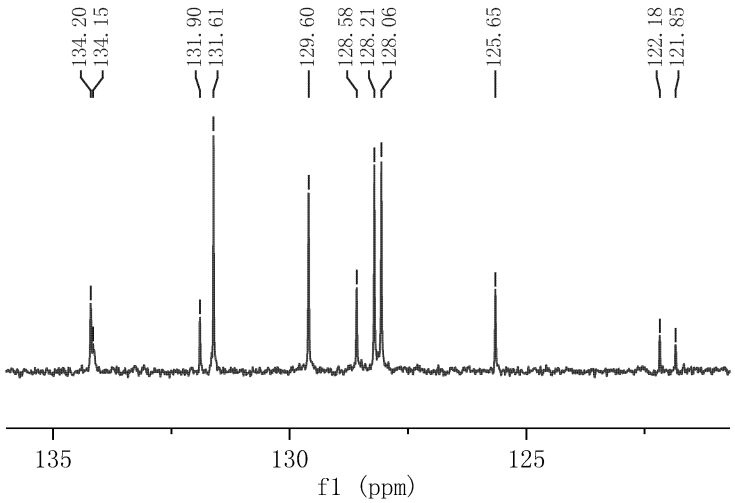

7.924
7.903
7.468
7.446
7.305
7.287
7.279
7.255
7.235
7.170
7.150
7.146
7.089
7.062
7.045
7.018
6.891
6.884
6.837
6.830
6.815
6.808
5.618
5.616
5.574
5.572
5.007
5.004
4.979
4.977
4.579
3.741
2.332
Parameter Value
1 Title HFL-4-74-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.7
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2018-04-05T21:40:05
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ts
N
MeO
Ph
1s
1.04
5.92
2.06
1.21
1.00
1.04
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)
2.02
1.04
5.92
2.06
1.21
1.00
1.04
1.00
0.99
2.01
3.01
3.08
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)

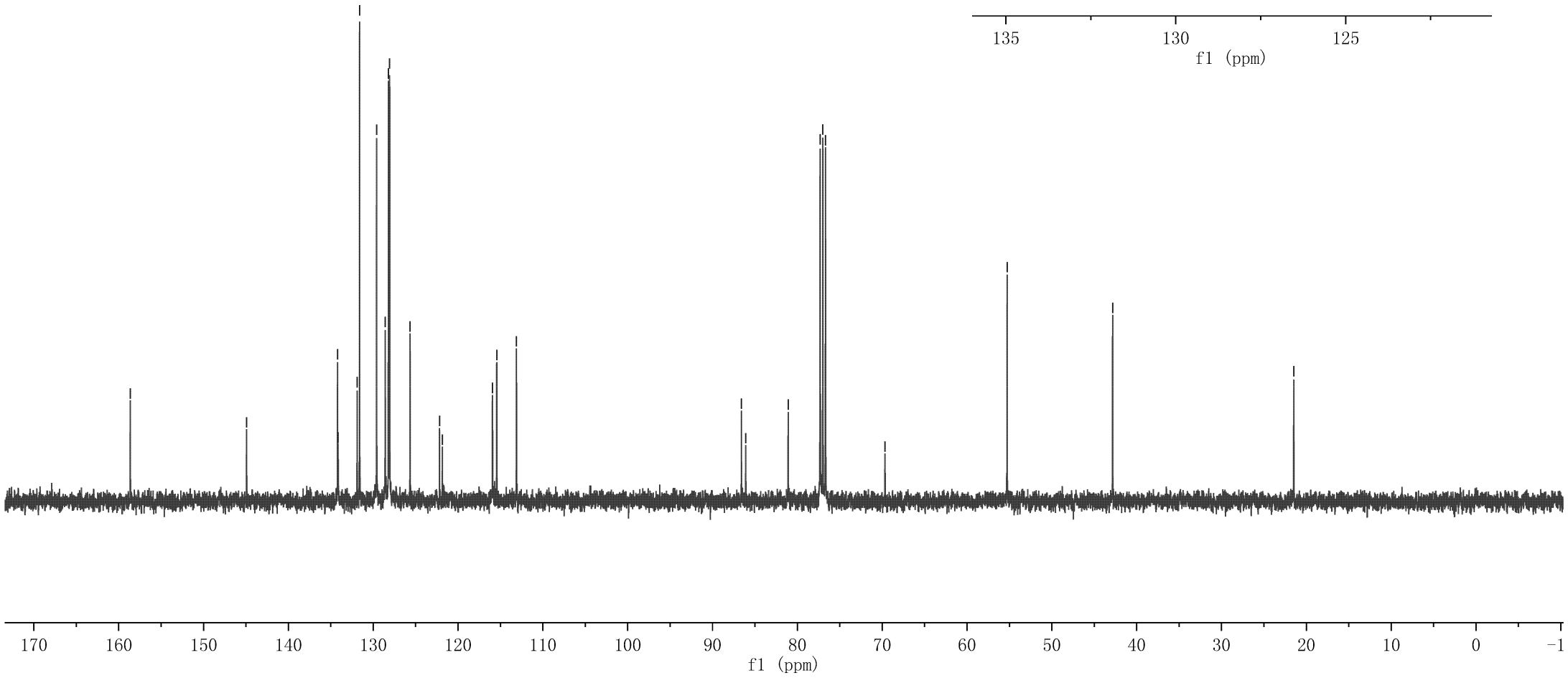
158.64
144.92
134.20
134.15
131.90
131.61
129.60
128.58
128.21
128.06
125.65
122.18
121.85
115.95
115.44
113.11
86.60
86.09
81.08
77.32
77.00
76.68
69.67
55.27
42.83
21.47

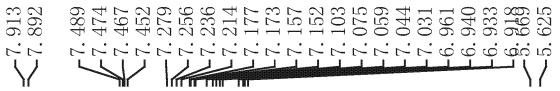
	Parameter	Value
1	Title	HFL-4-74-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	295.8
5	Number of Scans	52
6	Acquisition Time	1.3631
7	Acquisition Date	2018-04-05T21:42:41
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5



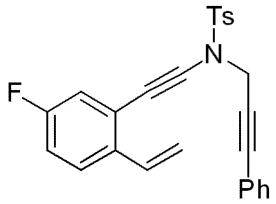
1s



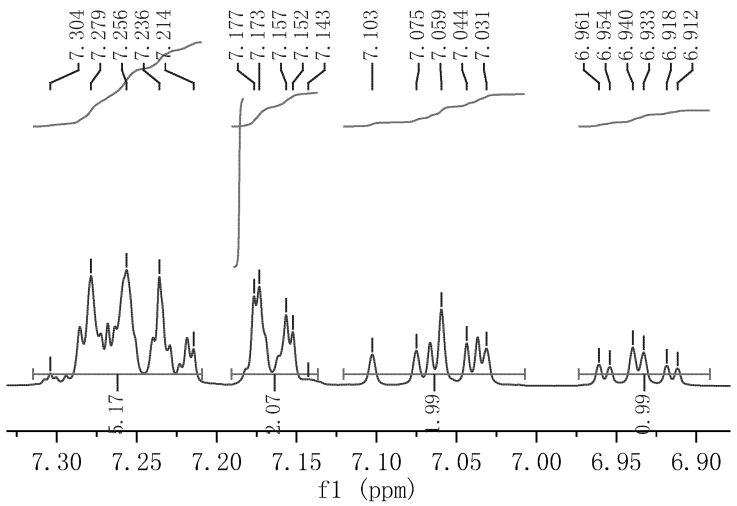


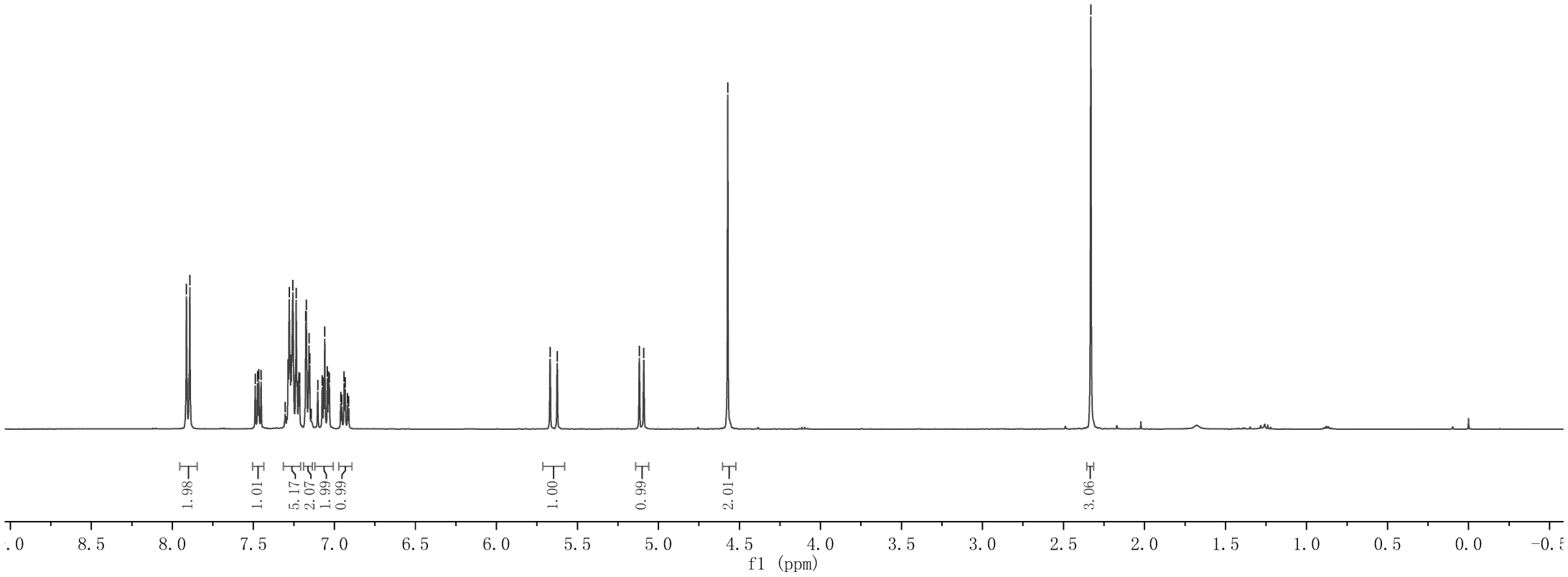


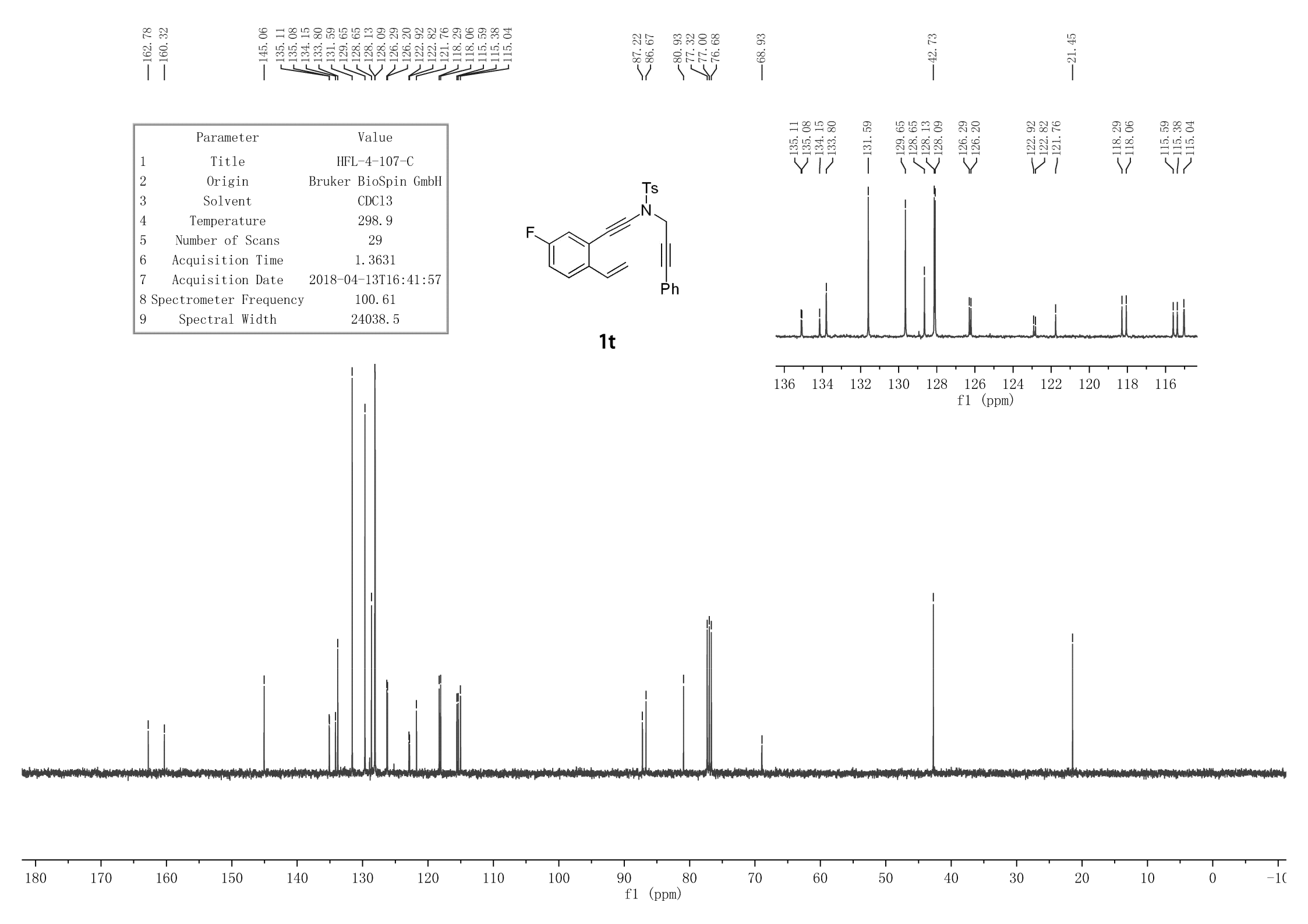
	Parameter	Value
1	Title	HFL-4-107-H
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	298.8
5	Number of Scans	4
6	Acquisition Time	3.9846
7	Acquisition Date	2018-04-13T16:40:03
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7



1t

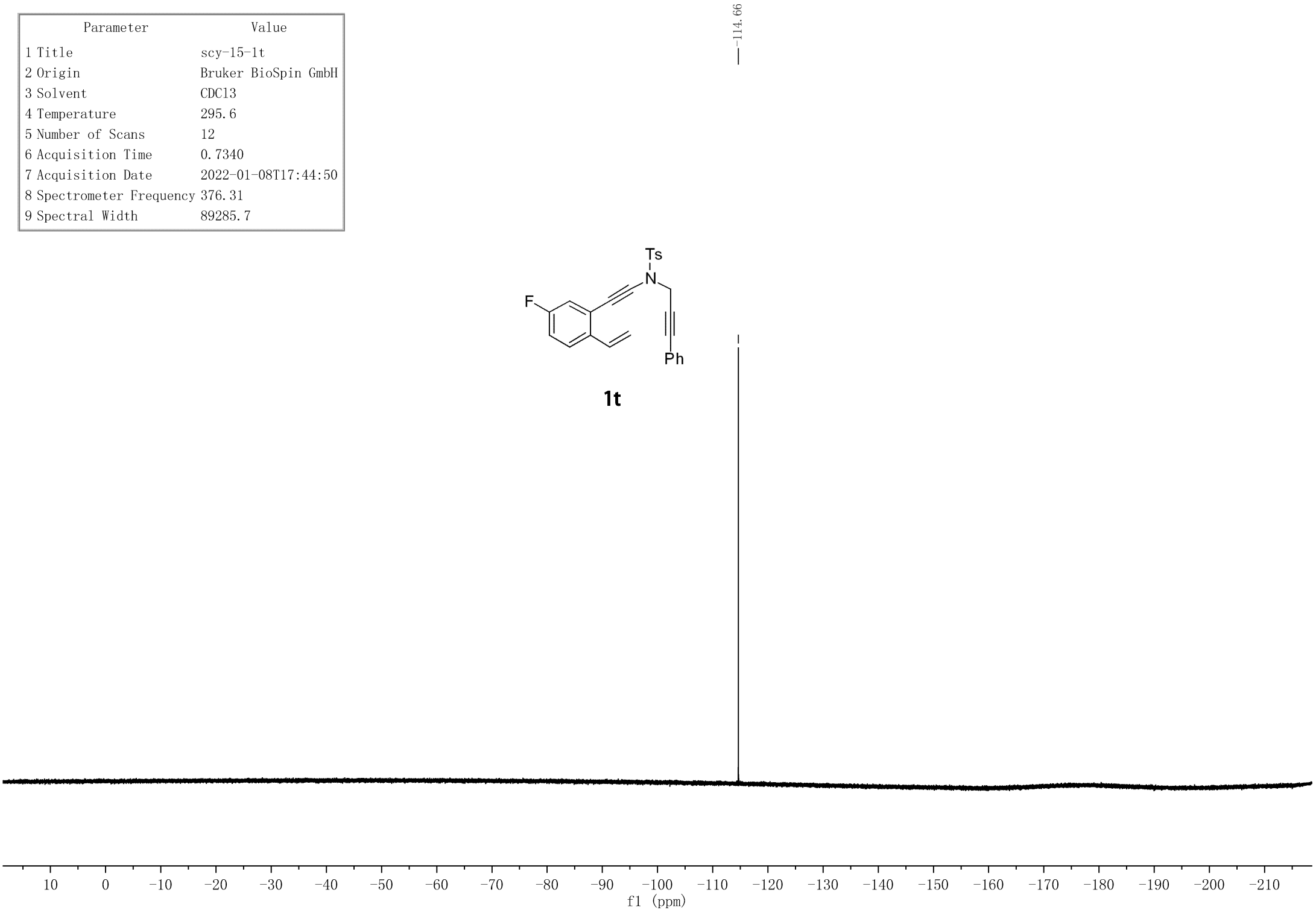


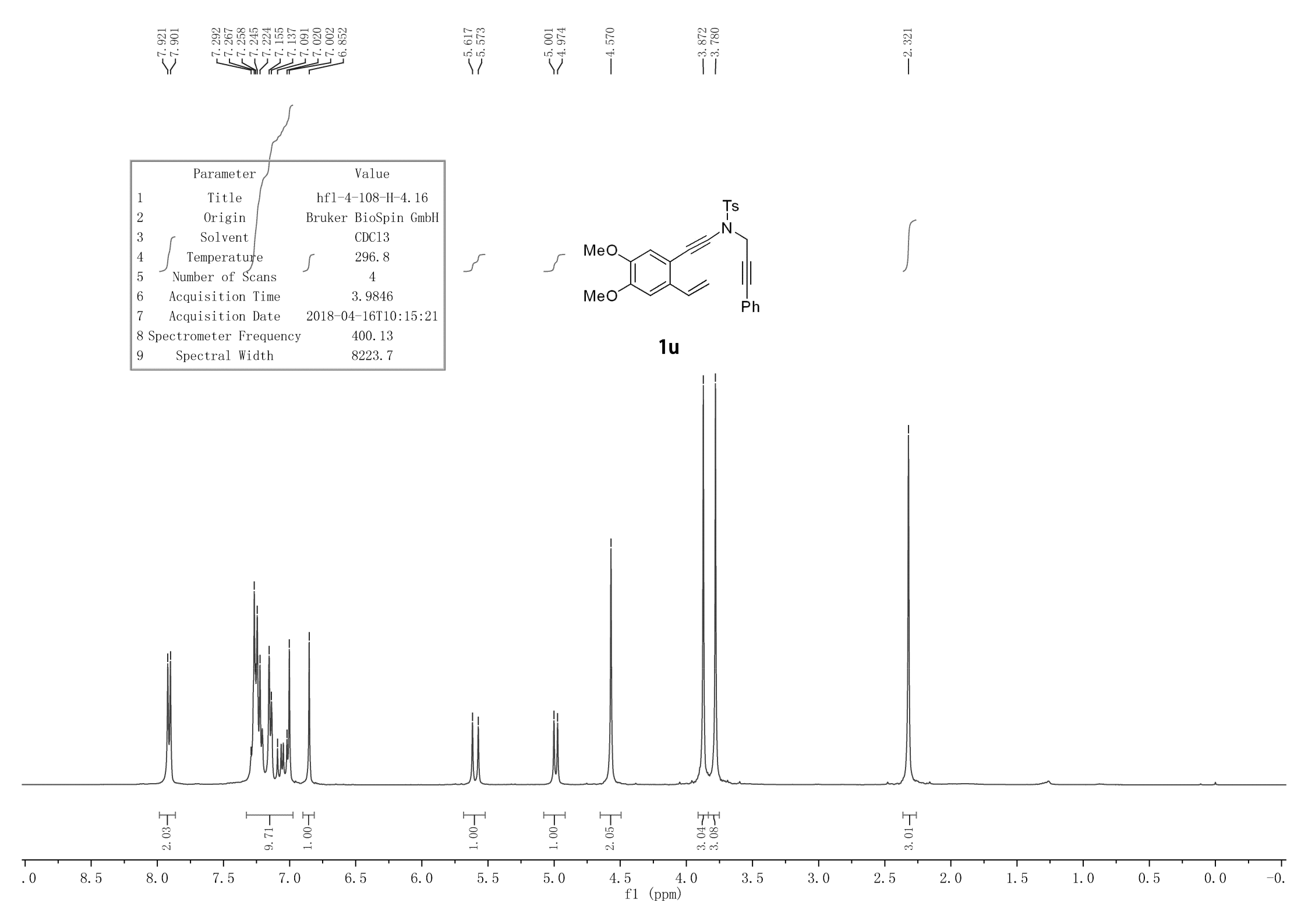


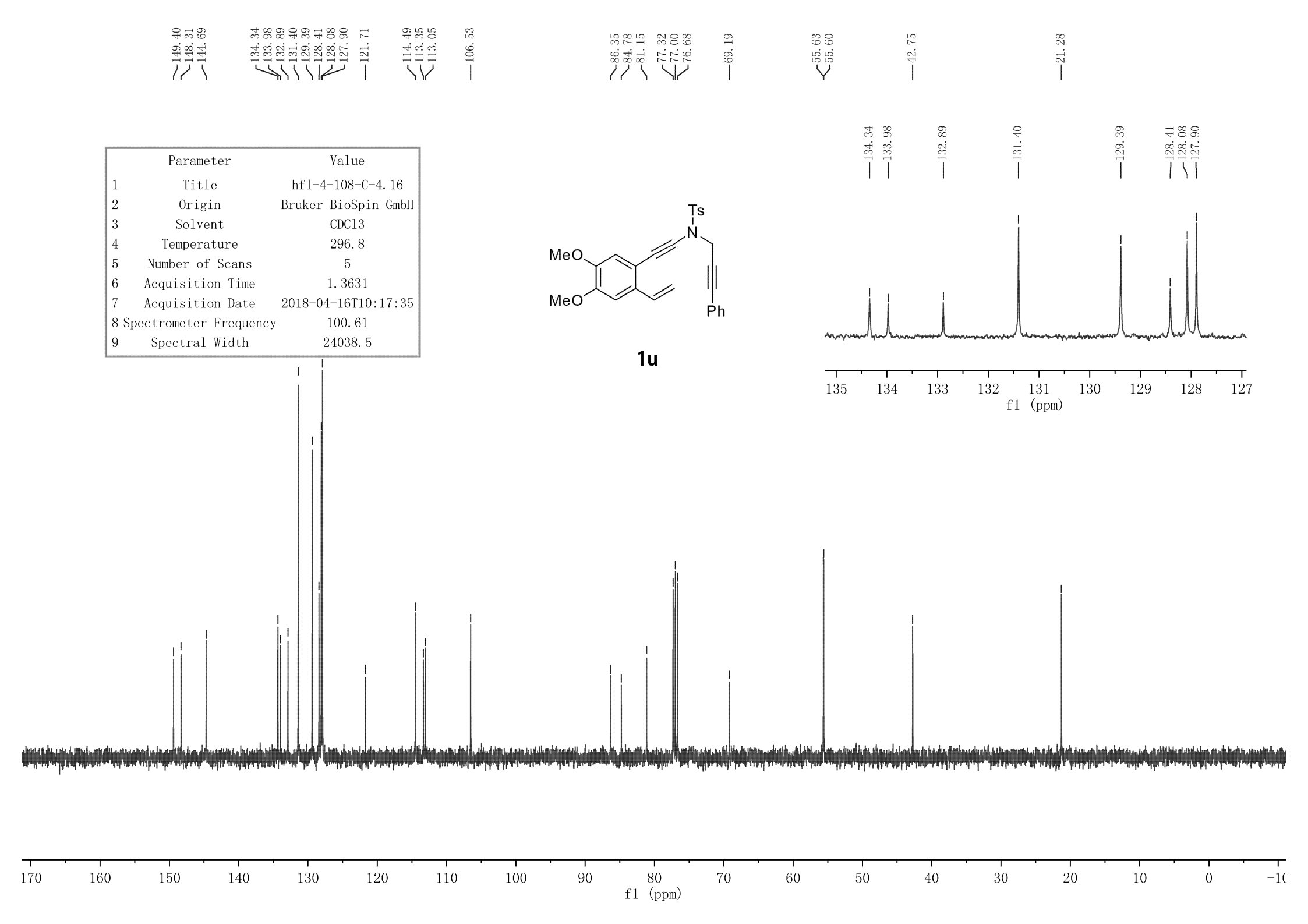

162.78
160.32
145.06
135.11
135.08
134.15
133.80
131.59
129.65
128.65
128.13
128.09
126.29
126.20
122.92
122.82
121.76
118.29
118.06
115.59
115.38
115.04
87.22
86.67
80.93
77.32
77.00
76.68
68.93
42.73
21.45
Parameter Value
1 Title HFL-4-107-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 29
6 Acquisition Time 1.3631
7 Acquisition Date 2018-04-13T16:41:57
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ts
N
F
Ph
1t
f1 (ppm)
f1 (ppm)

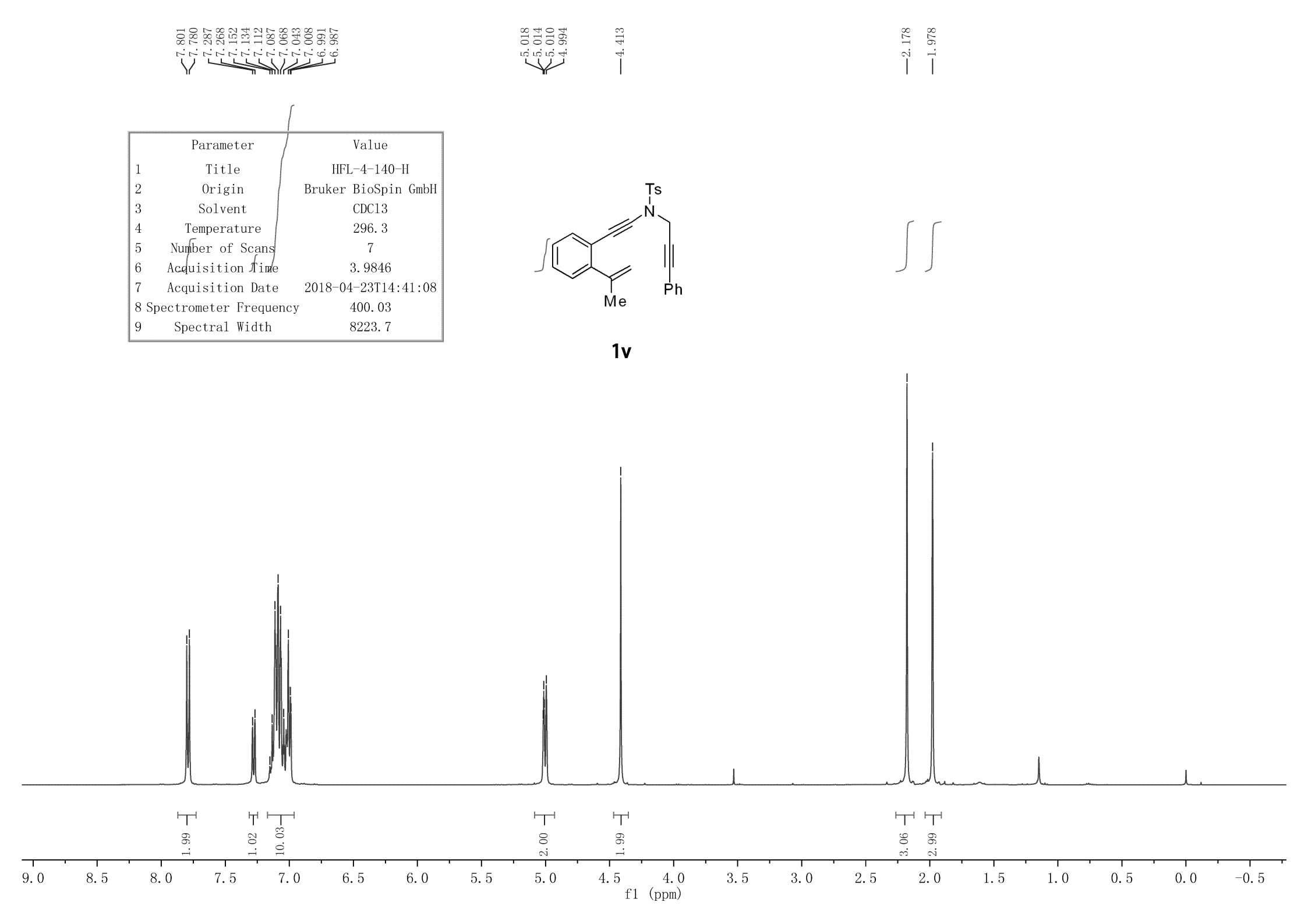
Parameter	Value
1 Title	scy-15-1t
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	12
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-08T17:44:50
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

1t



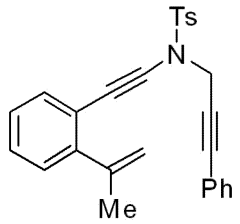

7.921
7.901
7.292
7.267
7.258
7.245
7.224
7.155
7.137
7.091
7.020
7.002
6.852
5.617
5.573
5.001
4.974
4.570
3.872
3.780
2.321
Parameter Value
1 Title hfl-4-108-H-4.16
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 4
6 Acquisition Time 3.9846
7 Acquisition Date 2018-04-16T10:15:21
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ts
N
MeO
MeO
Ph
1u
2.03
9.71
1.00
1.00
1.00
2.05
3.04
3.08
3.01
f1 (ppm)


149.40
148.31
144.69
134.34
133.98
132.89
131.40
129.39
128.41
128.08
127.90
121.71
114.49
113.35
113.05
106.53
86.35
84.78
81.15
77.32
77.00
76.68
69.19
55.63
55.60
42.75
21.28
Parameter Value
1 Title hfl-4-108-C-4.16
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 5
6 Acquisition Time 1.3631
7 Acquisition Date 2018-04-16T10:17:35
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ts
N
MeO
MeO
Ph
1u
f1 (ppm)
f1 (ppm)

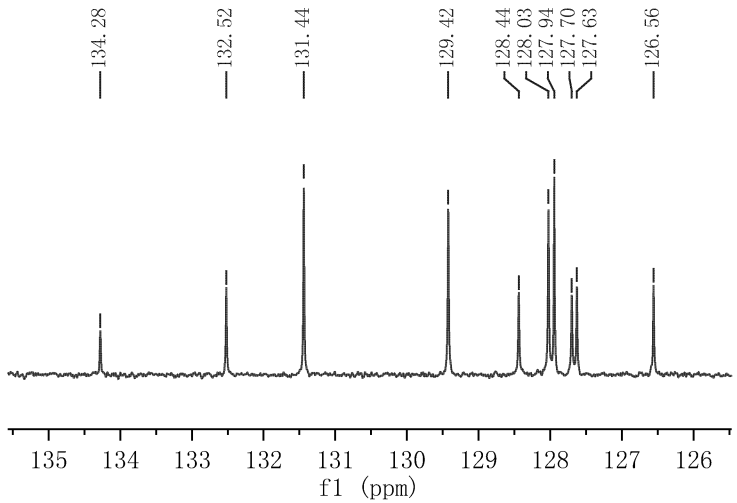

7.801
7.780
7.287
7.268
7.152
7.134
7.112
7.087
7.068
7.043
7.008
6.991
6.987
5.018
5.014
5.010
4.994
4.413
2.178
1.978
Parameter Value
1 Title HFL-4-140-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.3
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-04-23T14:41:08
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ts
N
Me
Ph
1v
1.99
1.02
10.03
2.00
1.99
3.06
2.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

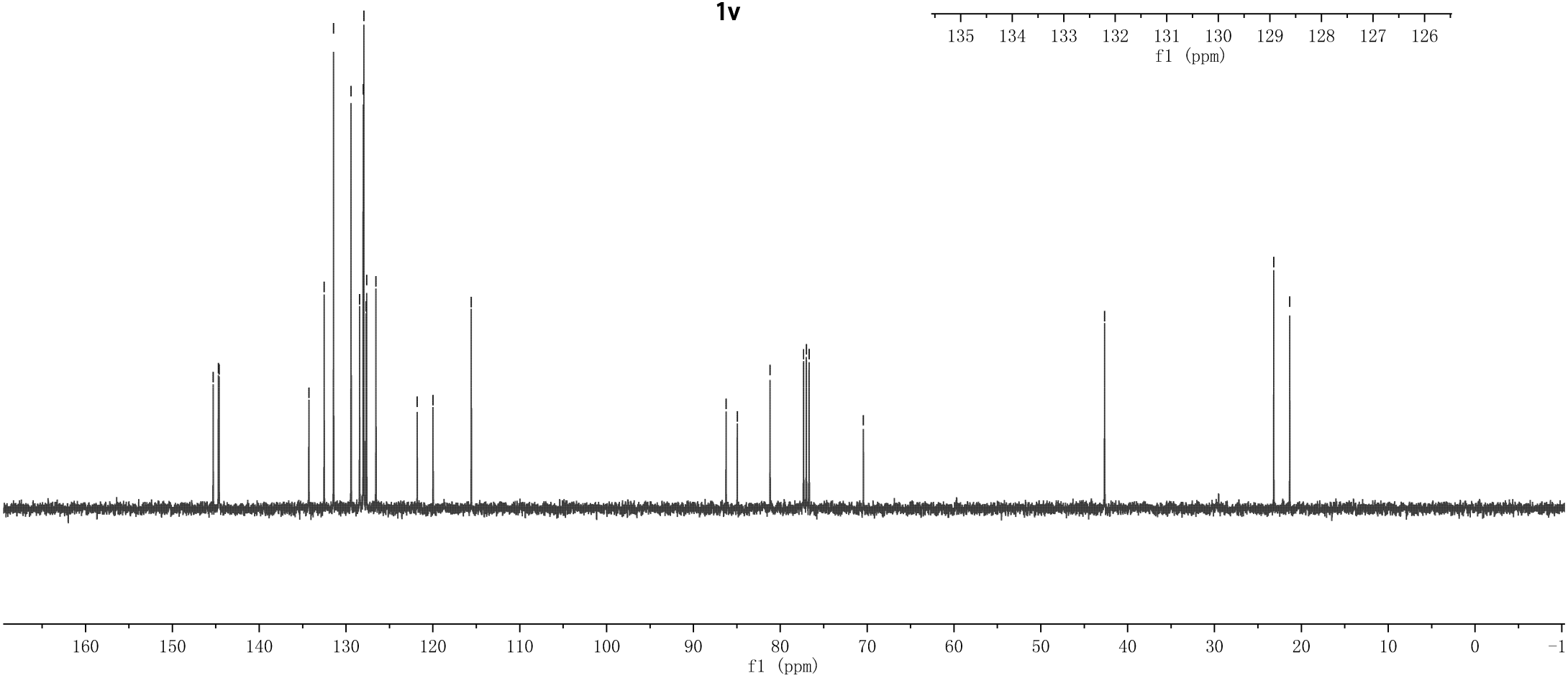
145.30
144.70
144.62
134.28
132.52
131.44
129.42
128.44
128.03
127.94
127.70
127.63
126.56
121.81
119.98
115.58
86.24
84.95
81.18
77.32
77.00
76.68
70.43
42.66
23.18
21.34

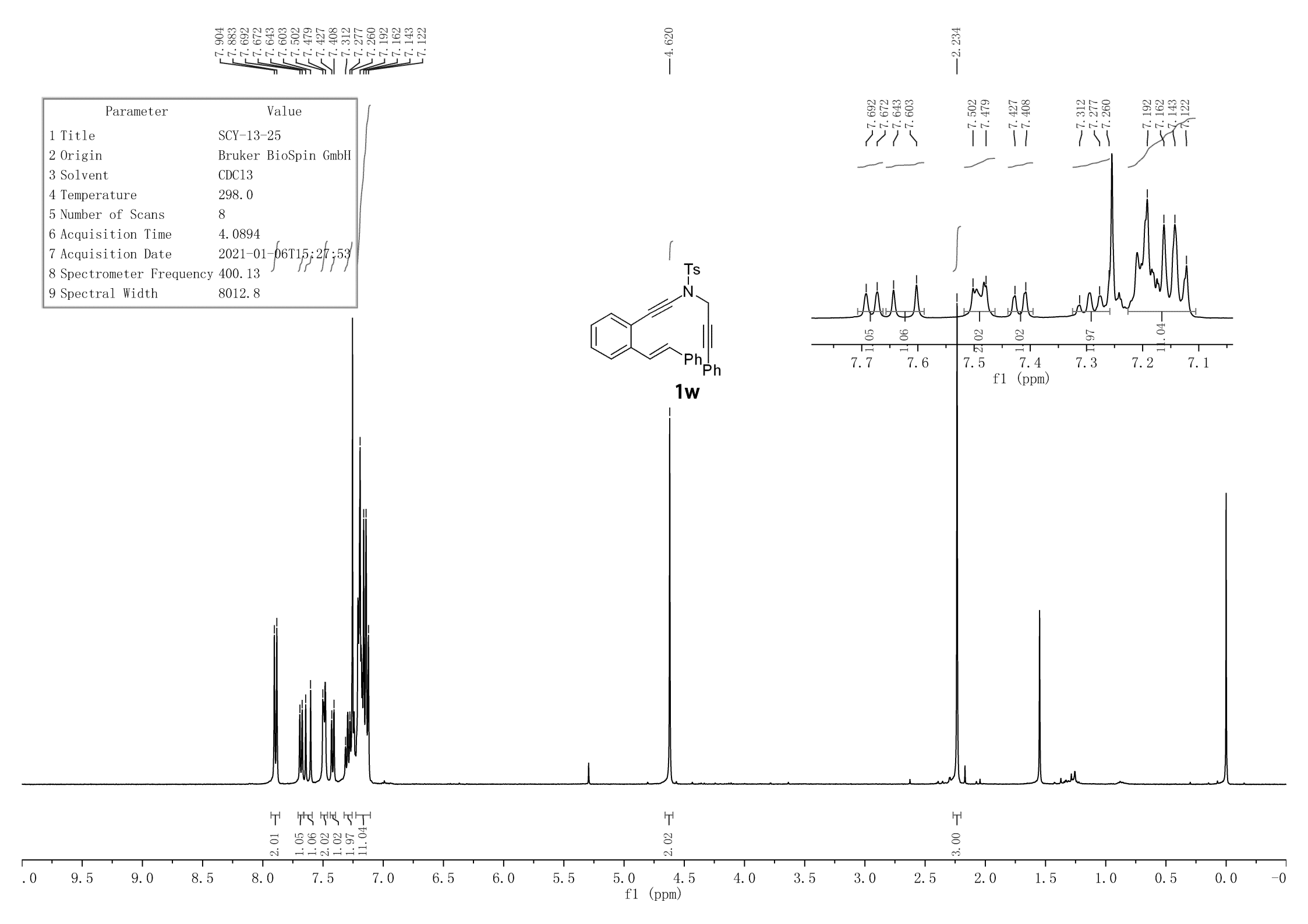
	Parameter	Value
1	Title	HFL-4-140-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	296.4
5	Number of Scans	8
6	Acquisition Time	1.3631
7	Acquisition Date	2018-04-23T14:43:19
8	Spectrometer Frequency	100.59
9	Spectral Width	24038.5

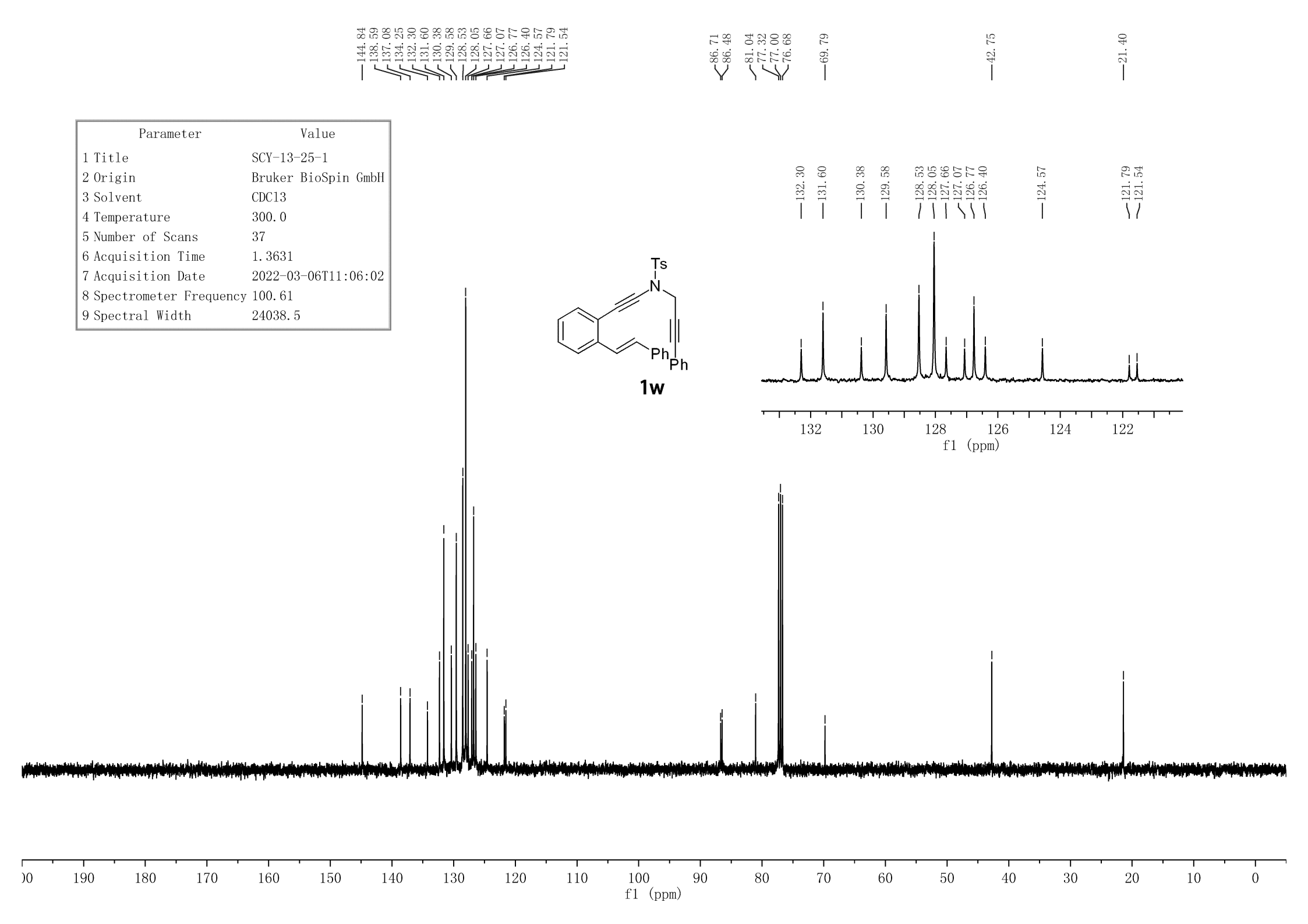


1v



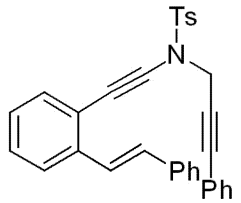



7.904
7.883
7.692
7.672
7.643
7.603
7.502
7.479
7.427
7.408
7.312
7.277
7.260
7.192
7.162
7.143
7.122
4.620
2.234
Parameter Value
1 Title SCY-13-25
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2021-01-06T15:27:53
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ts
N
Ph
Ph
1w
2.01
1.05
1.06
2.02
1.02
1.97
11.04
2.02
3.00
f1 (ppm)

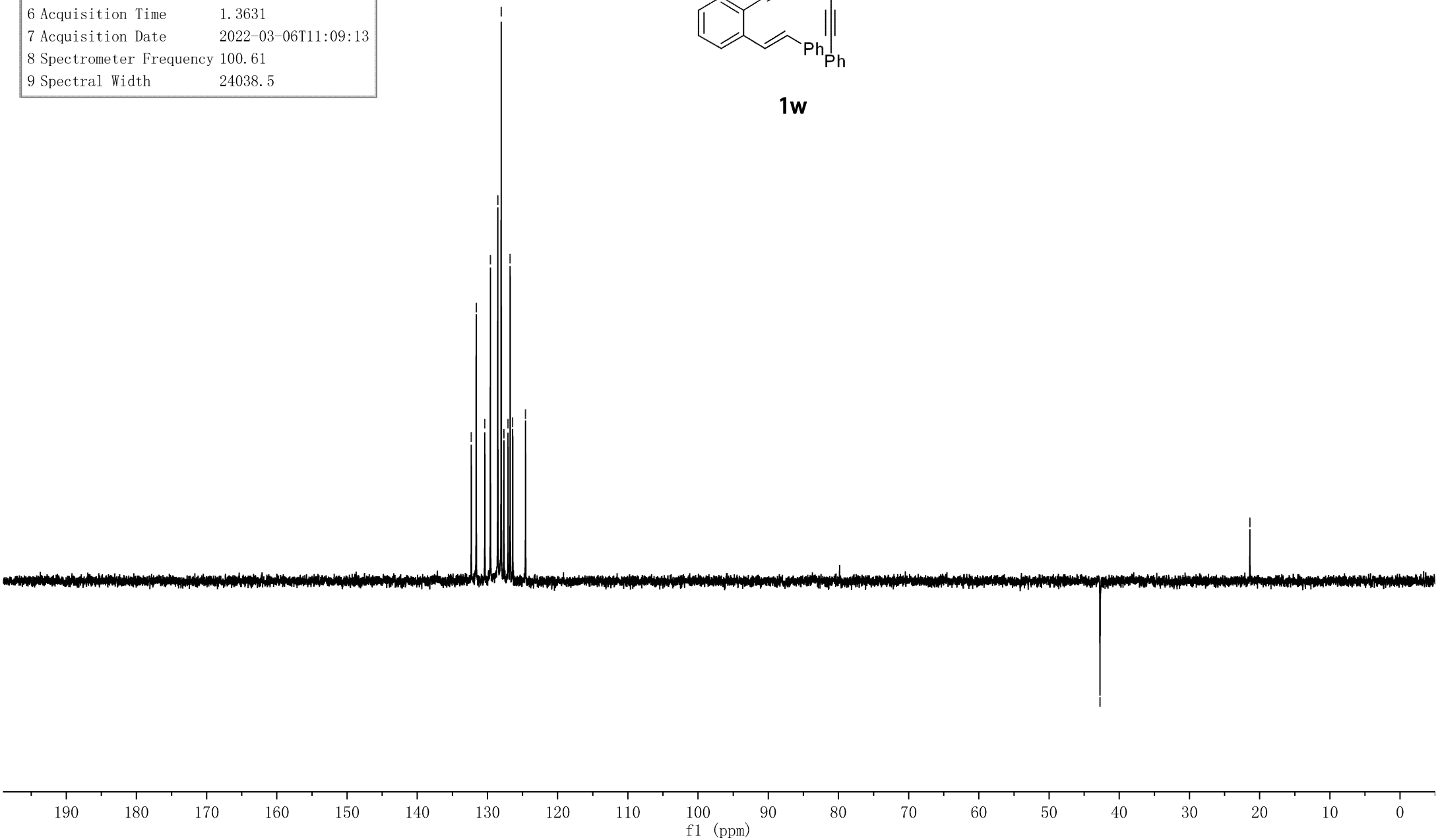

144.84
138.59
137.08
134.25
132.30
131.60
130.38
129.58
128.53
128.05
127.66
127.07
126.77
126.40
124.57
121.79
121.54
86.71
86.48
81.04
77.32
77.00
76.68
69.79
42.75
21.40
Parameter Value
1 Title SCY-13-25-1
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 37
6 Acquisition Time 1.3631
7 Acquisition Date 2022-03-06T11:06:02
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ts
N
Ph
Ph
1w
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	SCY-13-25-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	17
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-06T11:09:13
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

132.30
131.60
130.38
129.58
128.53
128.05
127.66
127.07
126.77
126.40
124.57
42.75
21.40

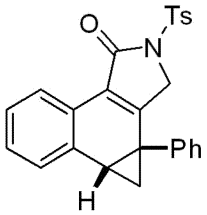


1w

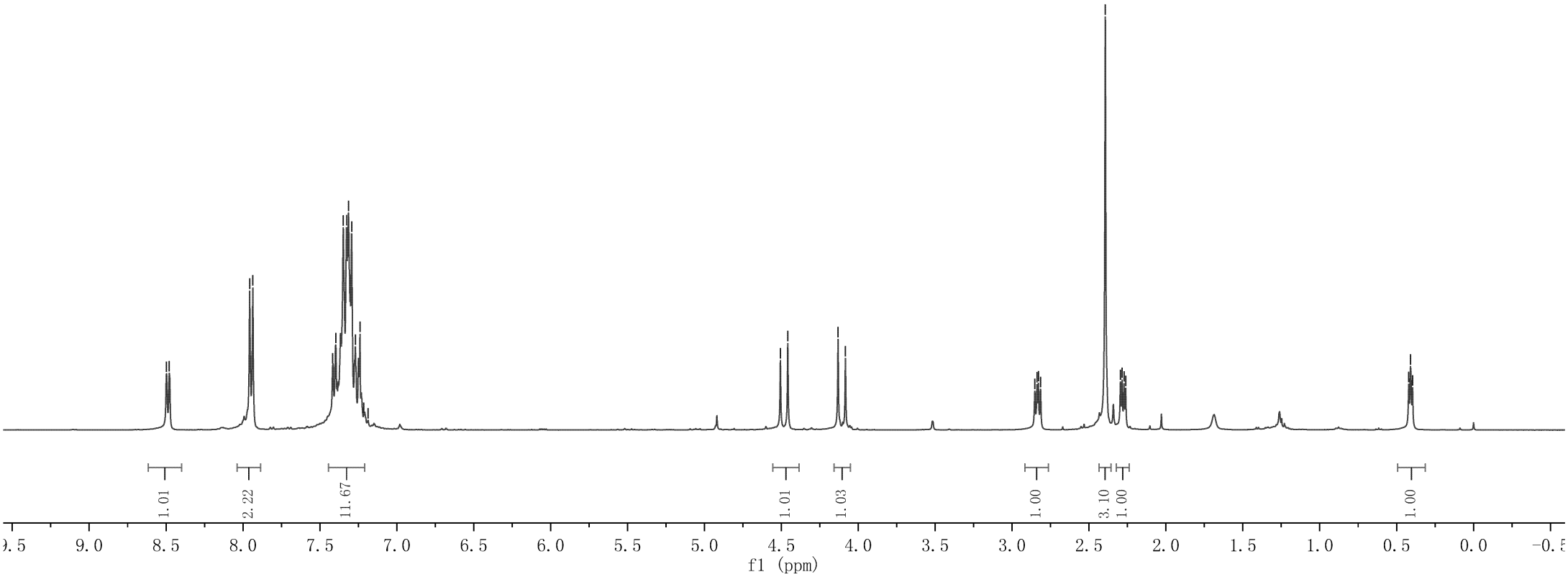


8.498
8.479
7.957
7.936
7.417
7.397
7.348
7.327
7.314
7.294
7.270
7.239
7.215
7.187
4.506
4.458
4.131
4.083
2.852
2.838
2.829
2.815
2.394
2.296
2.285
2.272
2.262
0.421
0.410
0.396

	Parameter	Value
1	Title	hfl-5-53-h
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	297.6
5	Number of Scans	7
6	Acquisition Time	3.9846
7	Acquisition Date	2018-06-07T21:14:25
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

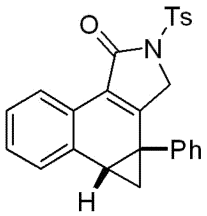


2a

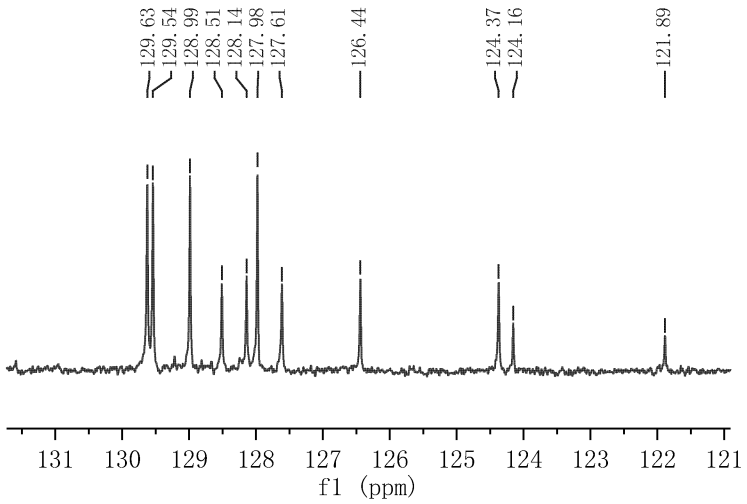


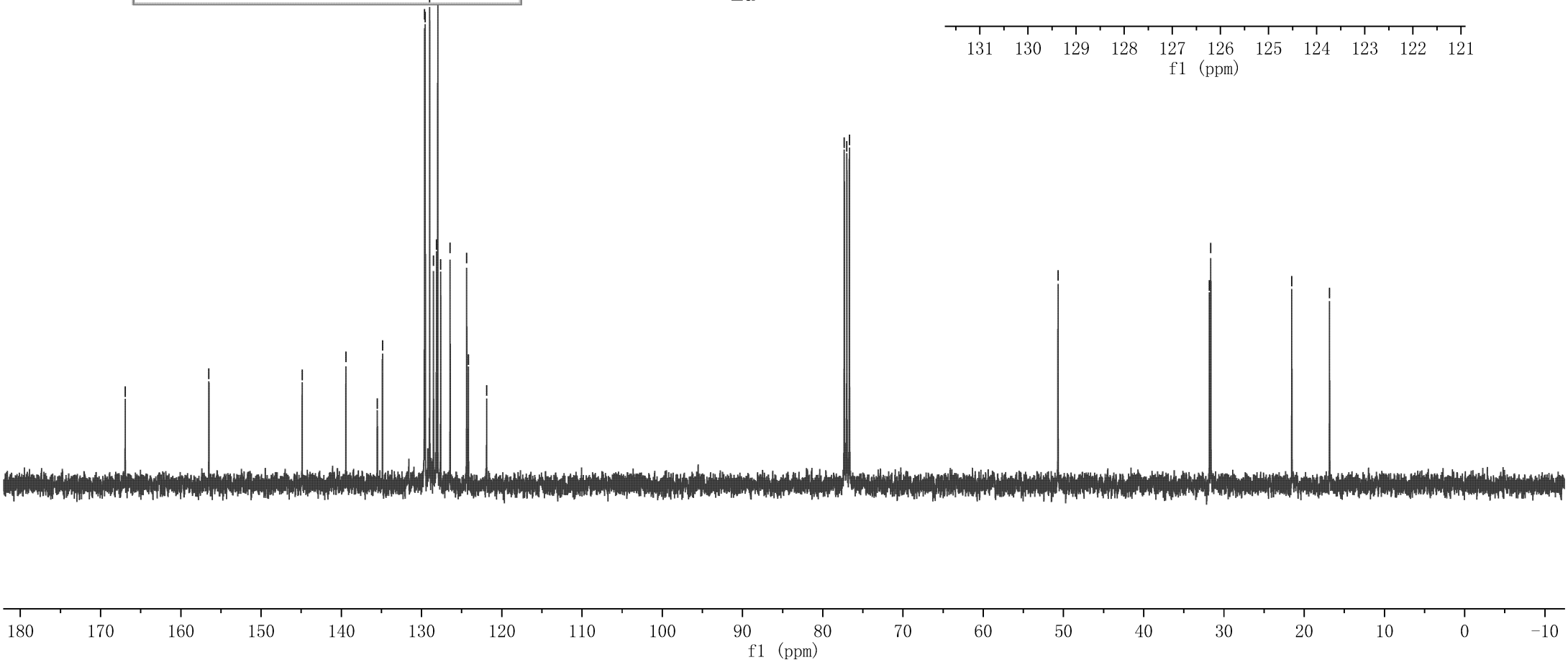
166.93
156.50
144.88
139.43
135.51
134.87
129.63
129.54
128.99
128.51
128.14
127.98
127.61
126.44
124.37
124.16
121.89
77.32
77.00
76.68
50.68
31.81
31.64
21.55
16.84

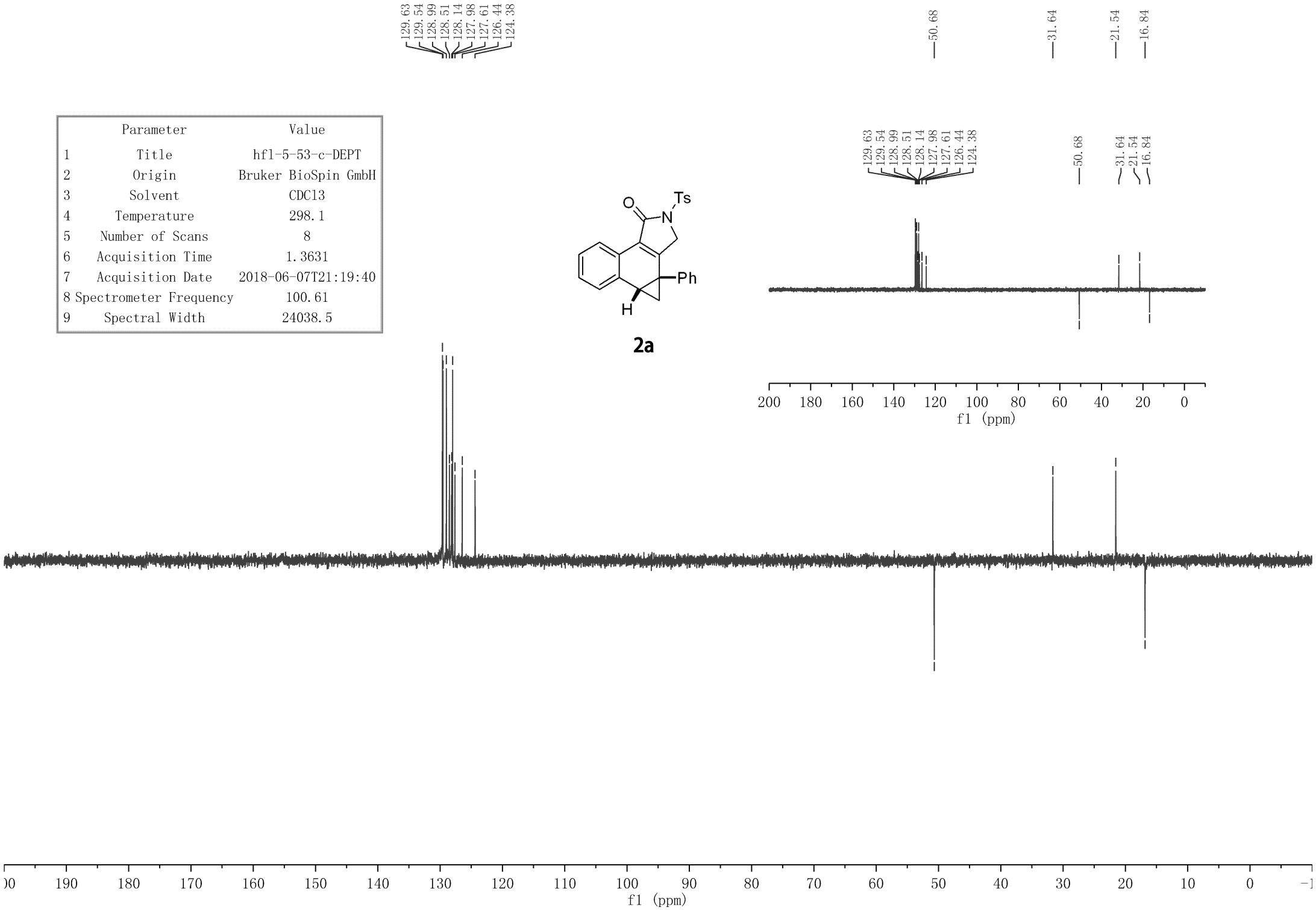
	Parameter	Value
1	Title	hf1-5-53-c
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	297.7
5	Number of Scans	34
6	Acquisition Time	1.3631
7	Acquisition Date	2018-06-07T21:17:04
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

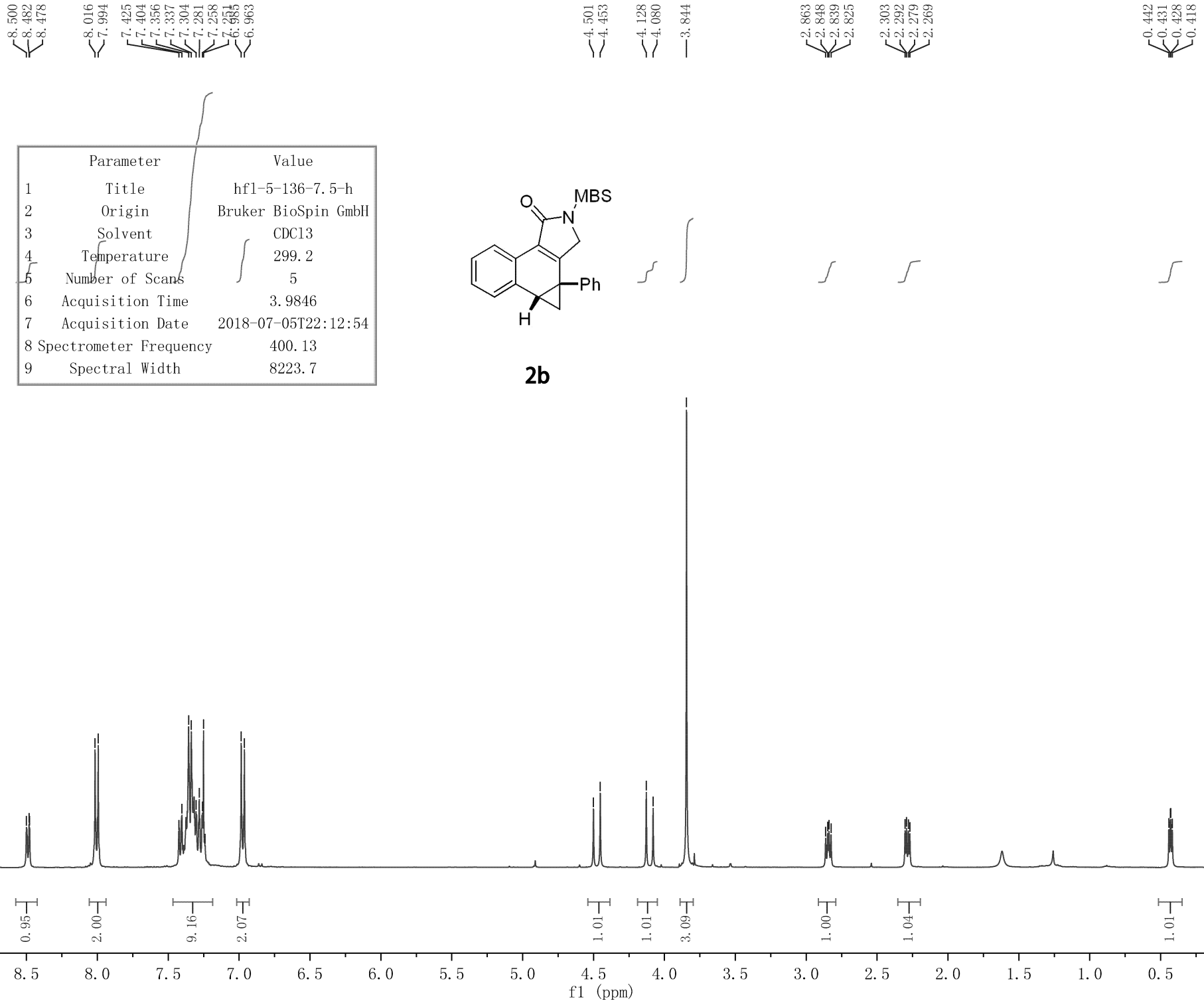


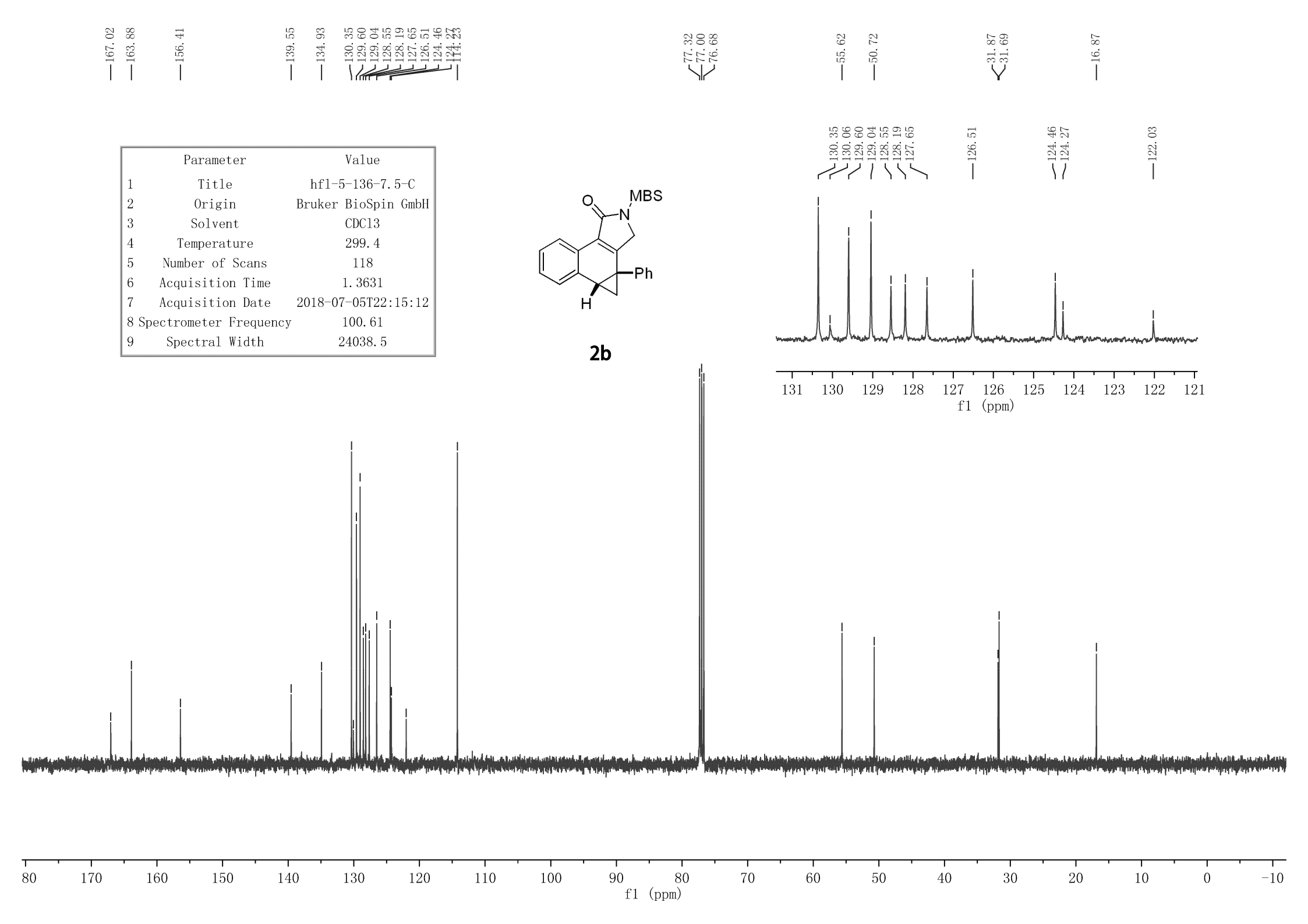
2a



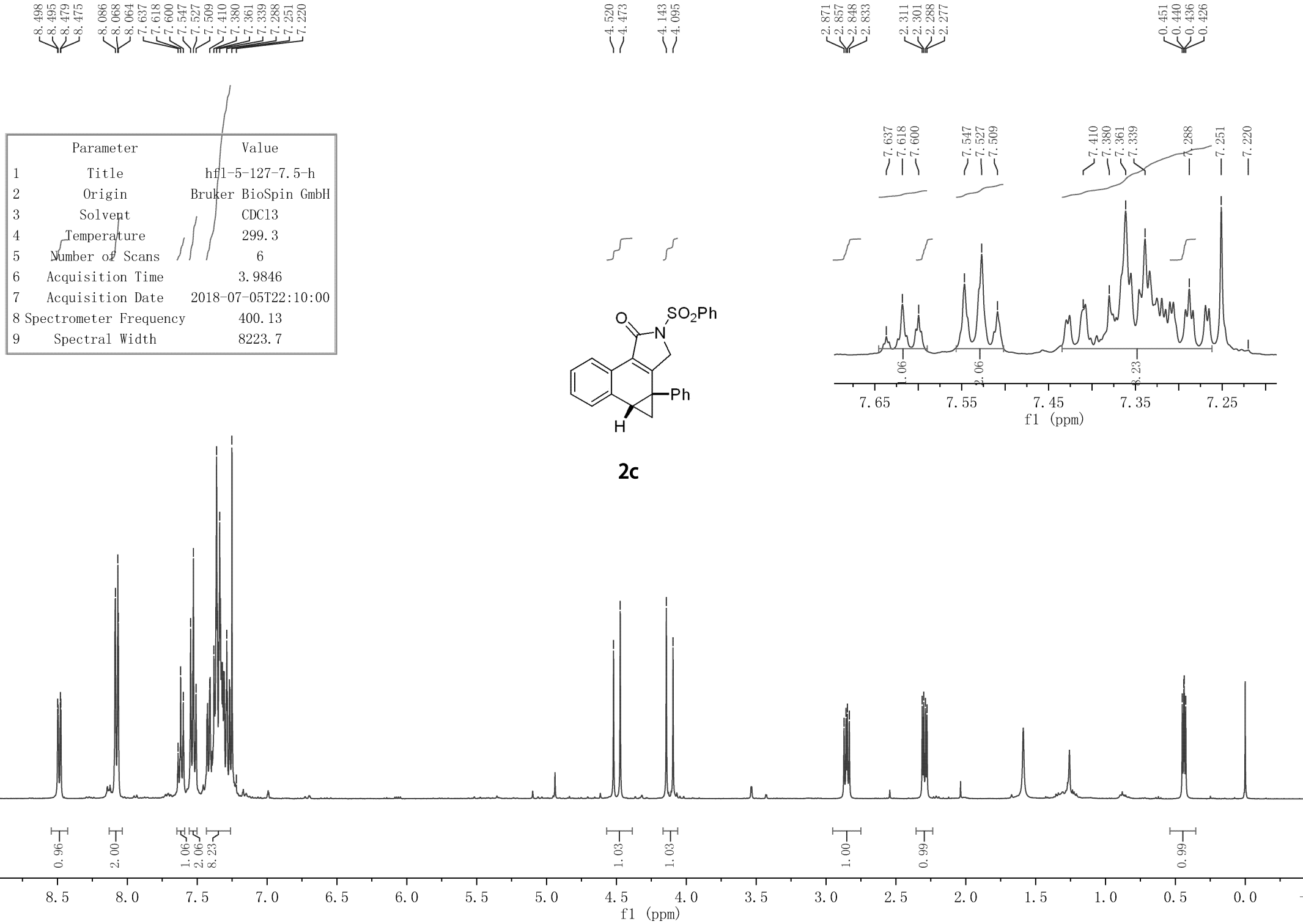



129.63
129.54
128.99
128.51
128.14
127.98
127.61
126.44
124.38
50.68
31.64
21.54
16.84
Parameter Value
1 Title hfl-5-53-c-DEPT
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.1
5 Number of Scans 8
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-07T21:19:40
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
Ph
H
2a
f1 (ppm)


8.500
8.482
8.478
8.016
7.994
7.425
7.404
7.356
7.337
7.304
7.281
7.258
7.251
6.985
6.963
4.501
4.453
4.128
4.080
3.844
2.863
2.848
2.839
2.825
2.303
2.292
2.279
2.269
0.442
0.431
0.428
0.418
Parameter Value
1 Title hfl-5-136-7.5-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.2
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-05T22:12:54
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
MBS
Ph
H
2b
0.95
2.00
9.16
2.07
1.01
1.01
3.09
1.00
1.04
1.01
f1 (ppm)

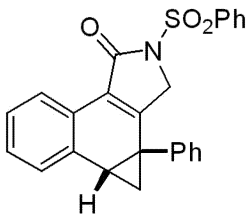


	Parameter	Value
1	Title	hfl-5-136-7.5-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.4
5	Number of Scans	118
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-05T22:15:12
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

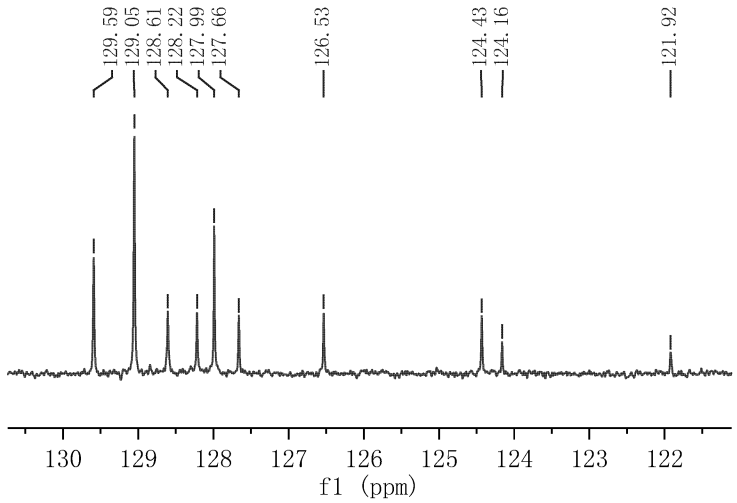

8.498
8.495
8.479
8.475
8.086
8.068
8.064
7.637
7.618
7.600
7.547
7.527
7.509
7.410
7.380
7.361
7.339
7.288
7.251
7.220
4.520
4.473
4.143
4.095
2.871
2.857
2.848
2.833
2.311
2.301
2.288
2.277
0.451
0.440
0.436
0.426
Parameter Value
1 Title hfl-5-127-7.5-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.3
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-05T22:10:00
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
SO2Ph
Ph
H
2c
1.06
2.06
8.23
7.65
7.55
7.45
7.35
7.25
f1 (ppm)
0.96
2.00
1.06
2.06
8.23
1.03
1.03
1.00
0.99
0.99
f1 (ppm)

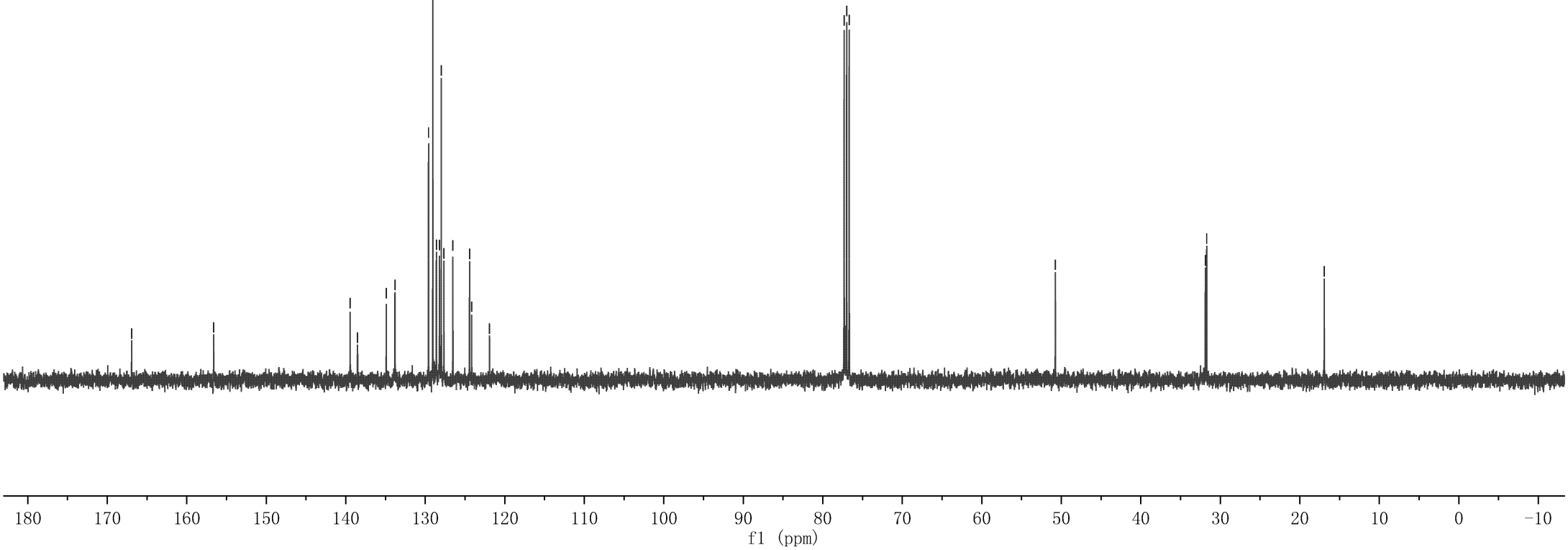
166.94
156.62
139.45
138.53
134.91
133.82
129.59
129.05
128.61
128.22
127.99
127.66
126.53
124.43
124.16
121.92
77.32
77.00
76.68
50.75
31.89
31.72
16.93

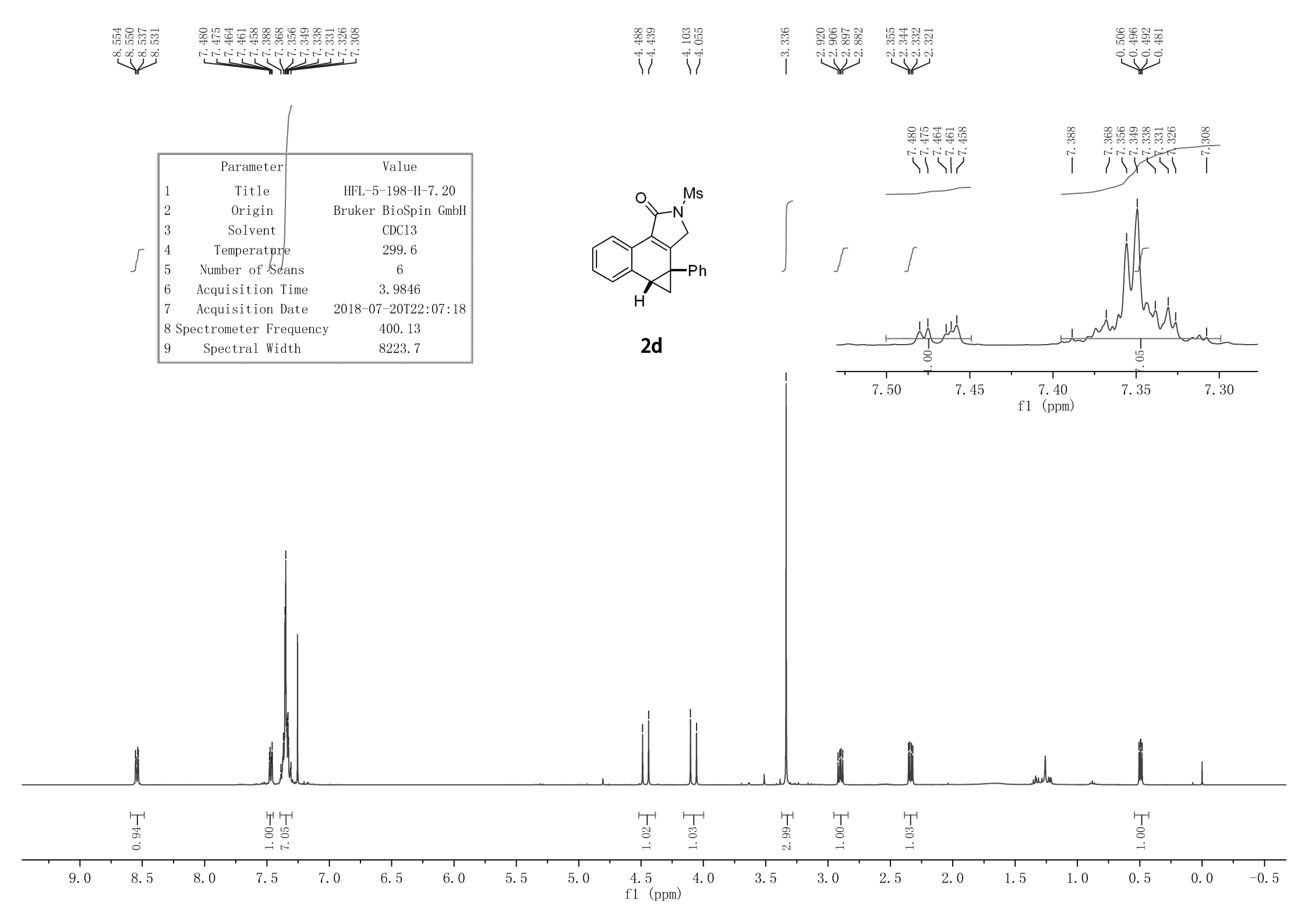
	Parameter	Value
1	Title	hfl-5-127-c
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.0
5	Number of Scans	37
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-04T15:50:25
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



2c

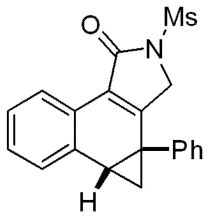




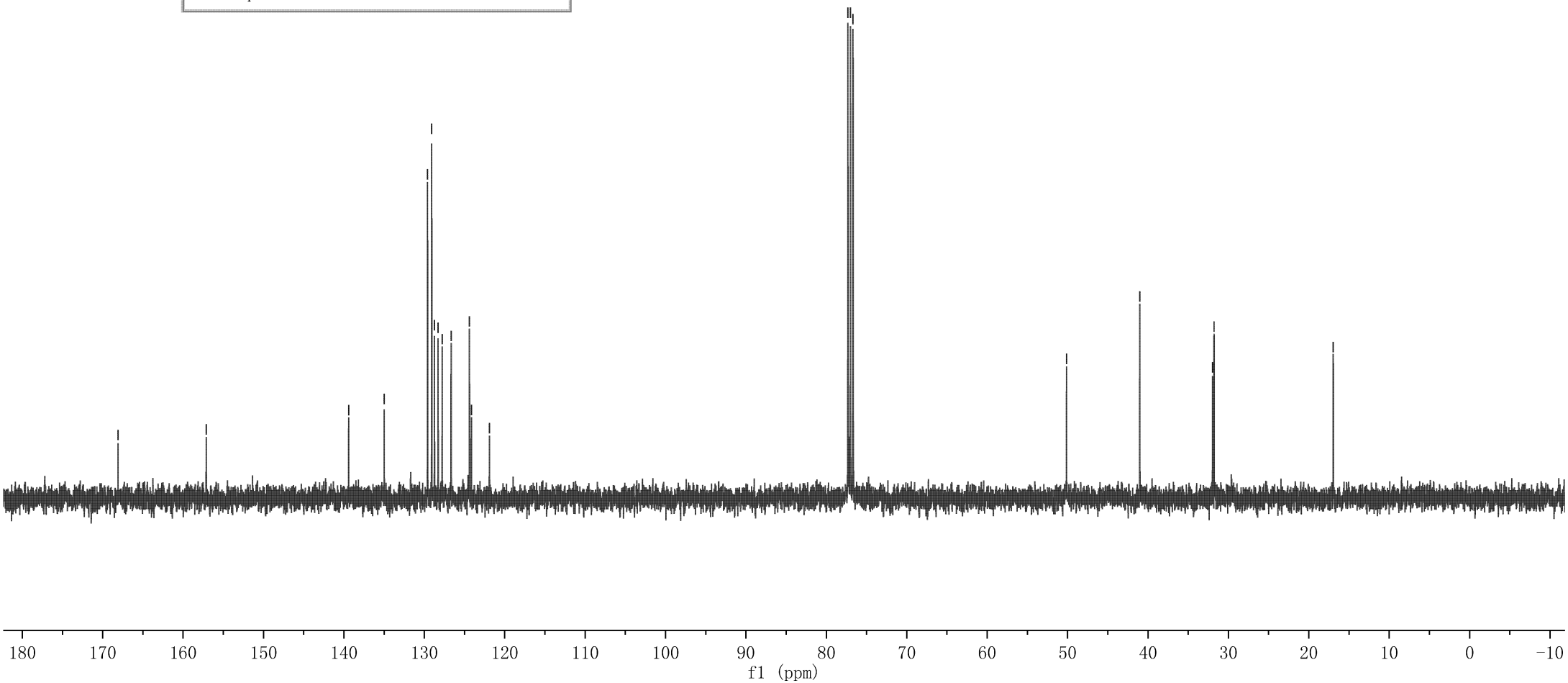

8.554
8.550
8.537
8.531
7.480
7.475
7.464
7.461
7.458
7.388
7.368
7.356
7.349
7.338
7.331
7.326
7.308
4.488
4.439
4.103
4.055
3.336
2.920
2.906
2.897
2.882
2.355
2.344
2.332
2.321
0.506
0.496
0.492
0.481
Parameter Value
1 Title HFL-5-198-H-7.20
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-20T22:07:18
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ms
Ph
H
2d
1.00
7.05
7.50
7.45
7.40
7.35
7.30
f1 (ppm)
0.94
1.00
7.05
1.02
1.03
2.99
1.00
1.03
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

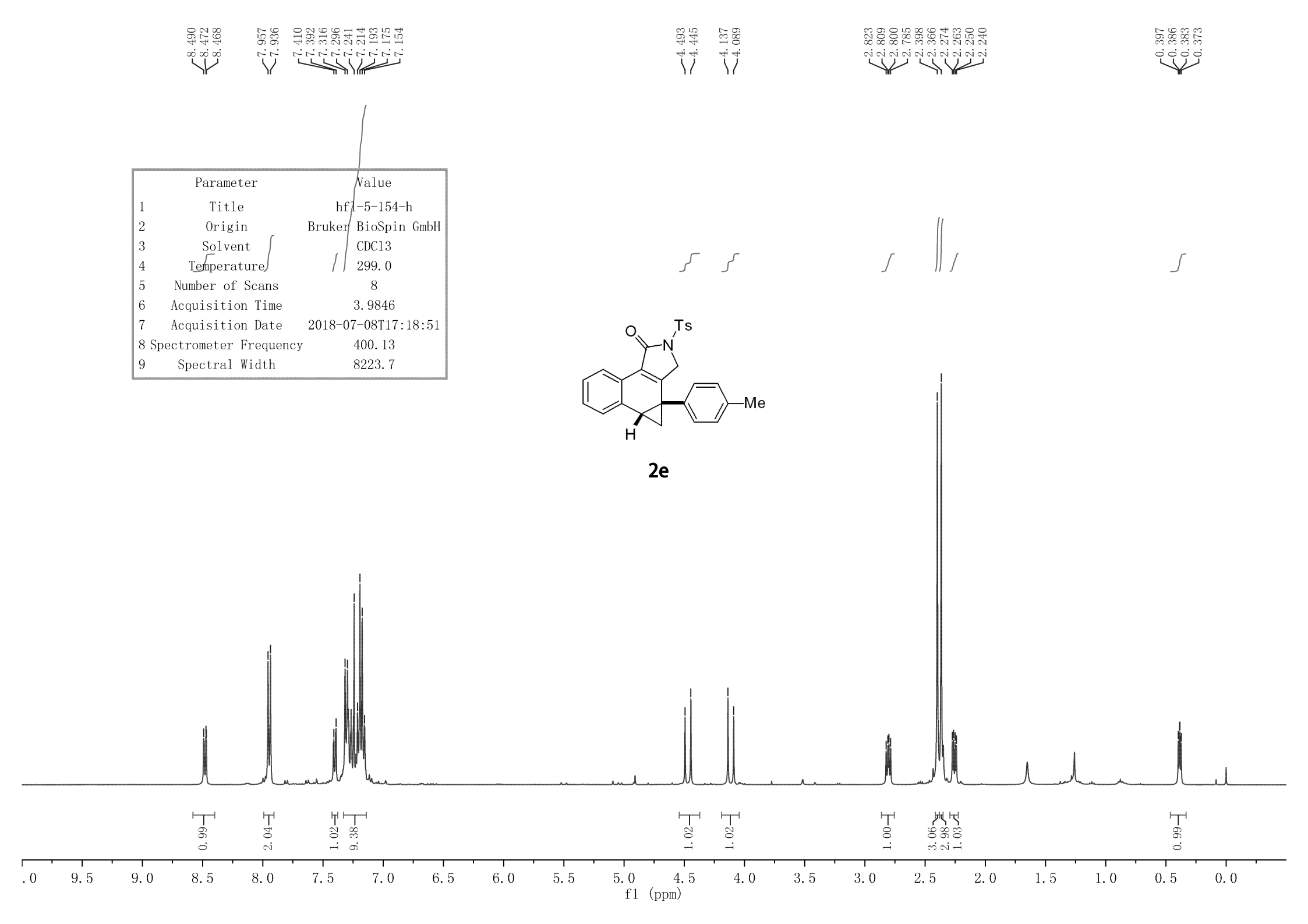
168.09
157.12
139.41
134.99
129.59
129.08
128.74
128.28
127.78
126.67
124.38
124.15
121.90
77.32
77.00
76.68
50.13
41.03
31.97
31.78
16.95

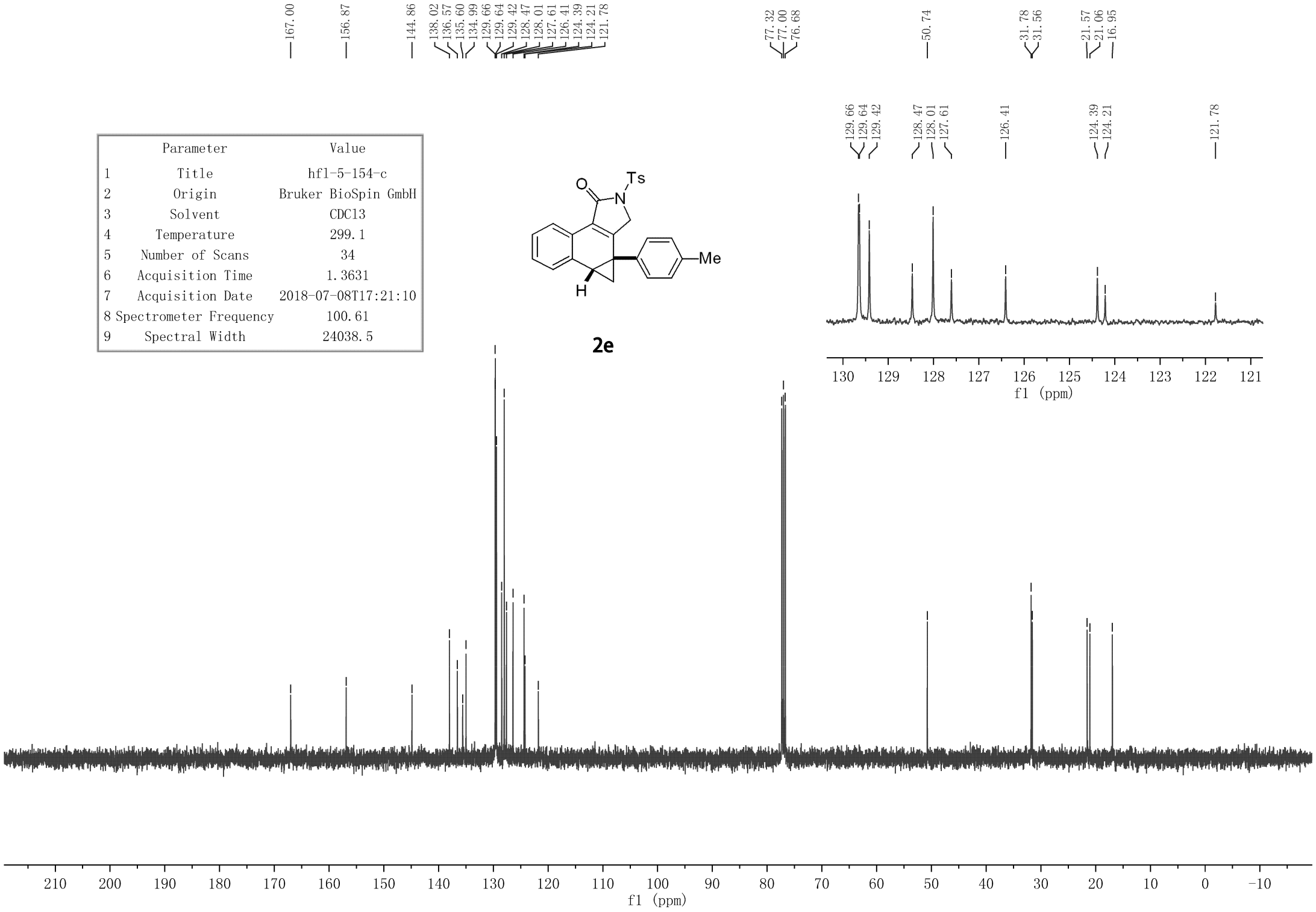
	Parameter	Value
1	Title	HFL-5-198-C-7.20
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.6
5	Number of Scans	32
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-20T22:09:37
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

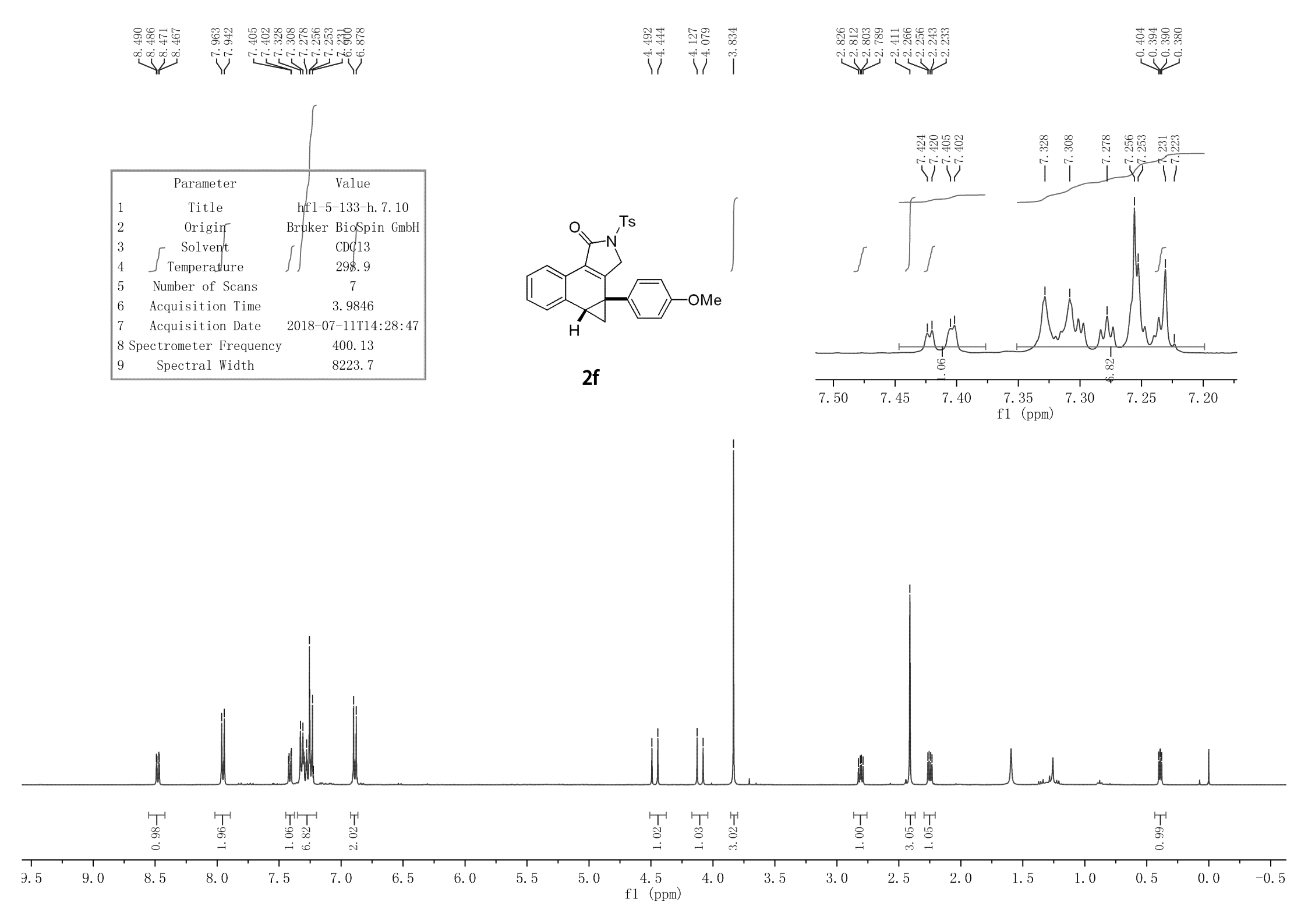


2d



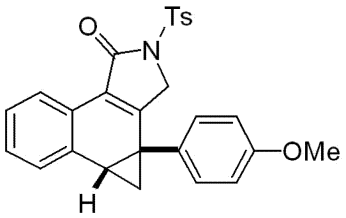

8.490
8.472
8.468
7.957
7.936
7.410
7.392
7.316
7.296
7.241
7.214
7.193
7.175
7.154
4.493
4.445
4.137
4.089
2.823
2.809
2.800
2.785
2.398
2.366
2.274
2.263
2.250
2.240
0.397
0.386
0.383
0.373
Parameter Value
1 Title hf1-5-154-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.0
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-08T17:18:51
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
Me
H
2e
0.99
2.04
1.02
9.38
1.02
1.02
1.00
3.06
2.98
1.03
0.99
f1 (ppm)


167.00
156.87
144.86
138.02
136.57
135.60
134.99
129.66
129.64
129.42
128.47
128.01
127.61
126.41
124.39
124.21
121.78
77.32
77.00
76.68
50.74
31.78
31.56
21.57
21.06
16.95
Parameter Value
1 Title hfl-5-154-c
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.1
5 Number of Scans 34
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-08T17:21:10
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
Me
H
2e
f1 (ppm)
f1 (ppm)

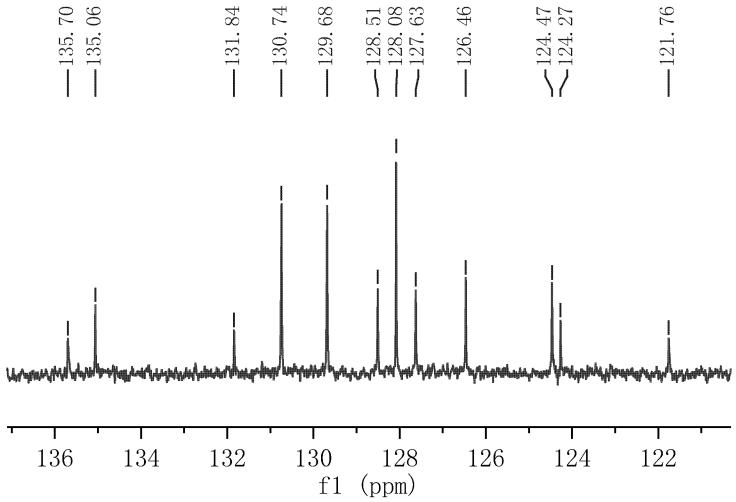

8.490
8.486
8.471
8.467
7.963
7.942
7.405
7.402
7.328
7.308
7.278
7.256
7.253
7.231
6.900
6.878
4.492
4.444
4.127
4.079
3.834
2.826
2.812
2.803
2.789
2.411
2.266
2.256
2.243
2.233
0.404
0.394
0.390
0.380
Parameter Value
1 Title hfl-5-133-h.7.10
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-11T14:28:47
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
OMe
H
2f
7.424
7.420
7.405
7.402
7.328
7.308
7.278
7.256
7.253
7.231
7.223
1.06
6.82
7.50
7.45
7.40
7.35
7.30
7.25
7.20
f1 (ppm)
0.98
1.96
1.06
6.82
2.02
1.02
1.03
3.02
1.00
3.05
1.05
0.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

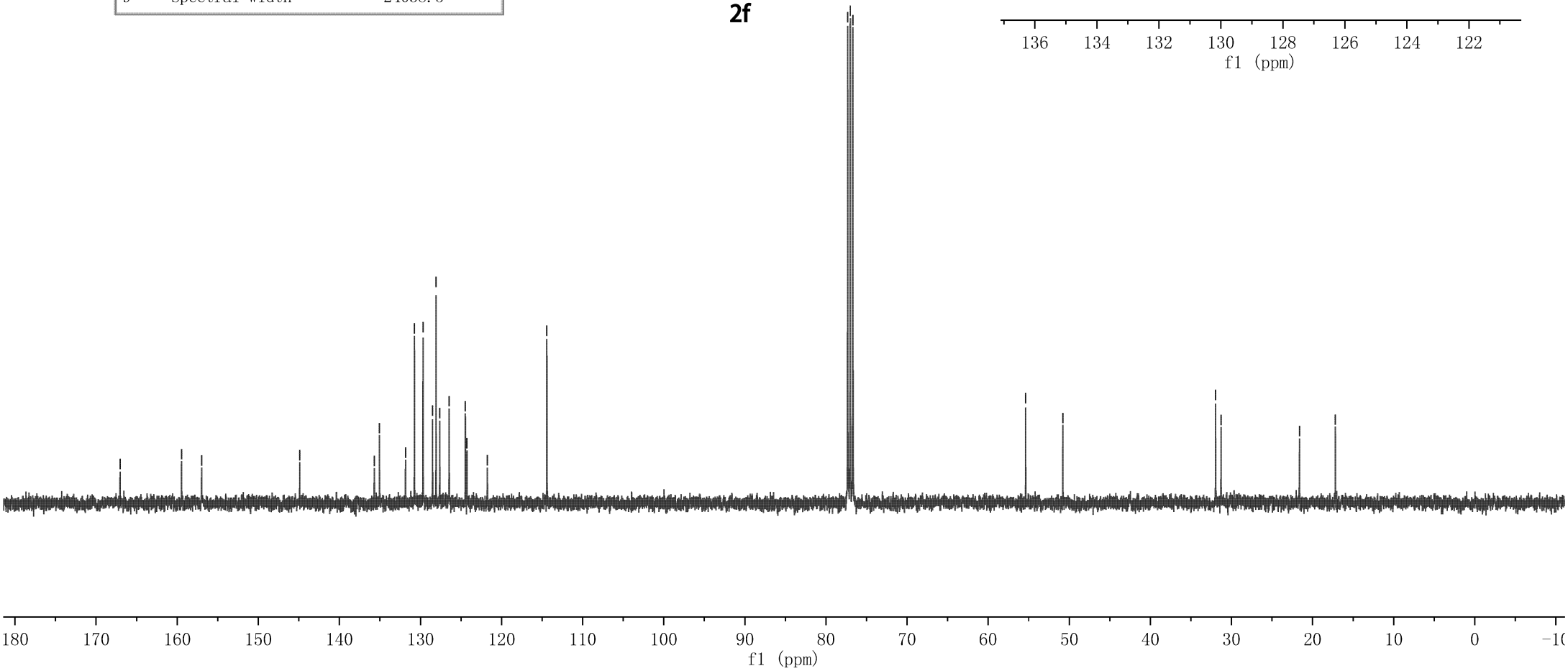
167.04
159.46
156.99
144.89
135.70
135.06
131.84
130.74
129.68
128.51
128.08
127.63
126.46
124.47
124.27
121.76
114.42
77.32
77.00
76.68
55.38
50.79
31.96
31.28
21.61
17.19

	Parameter	Value
1	Title	hfl-5-133-c.7.10
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.3
5	Number of Scans	155
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-11T14:32:06
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

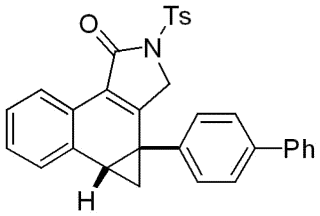


2f

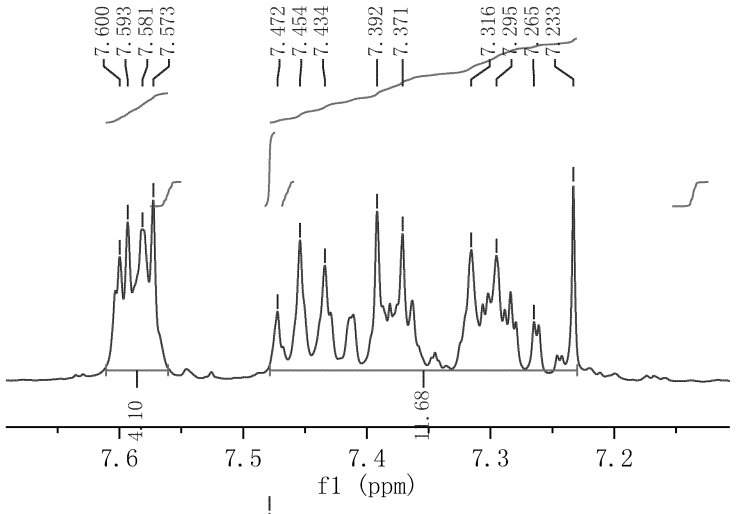


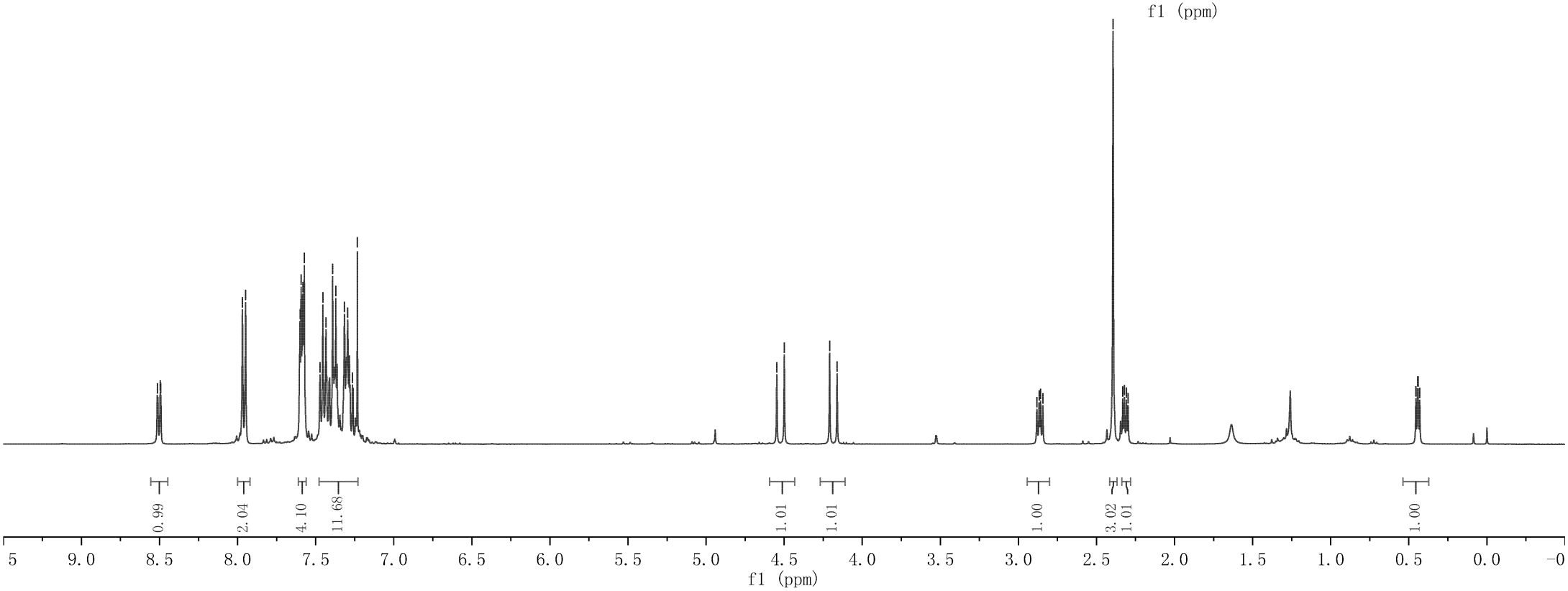


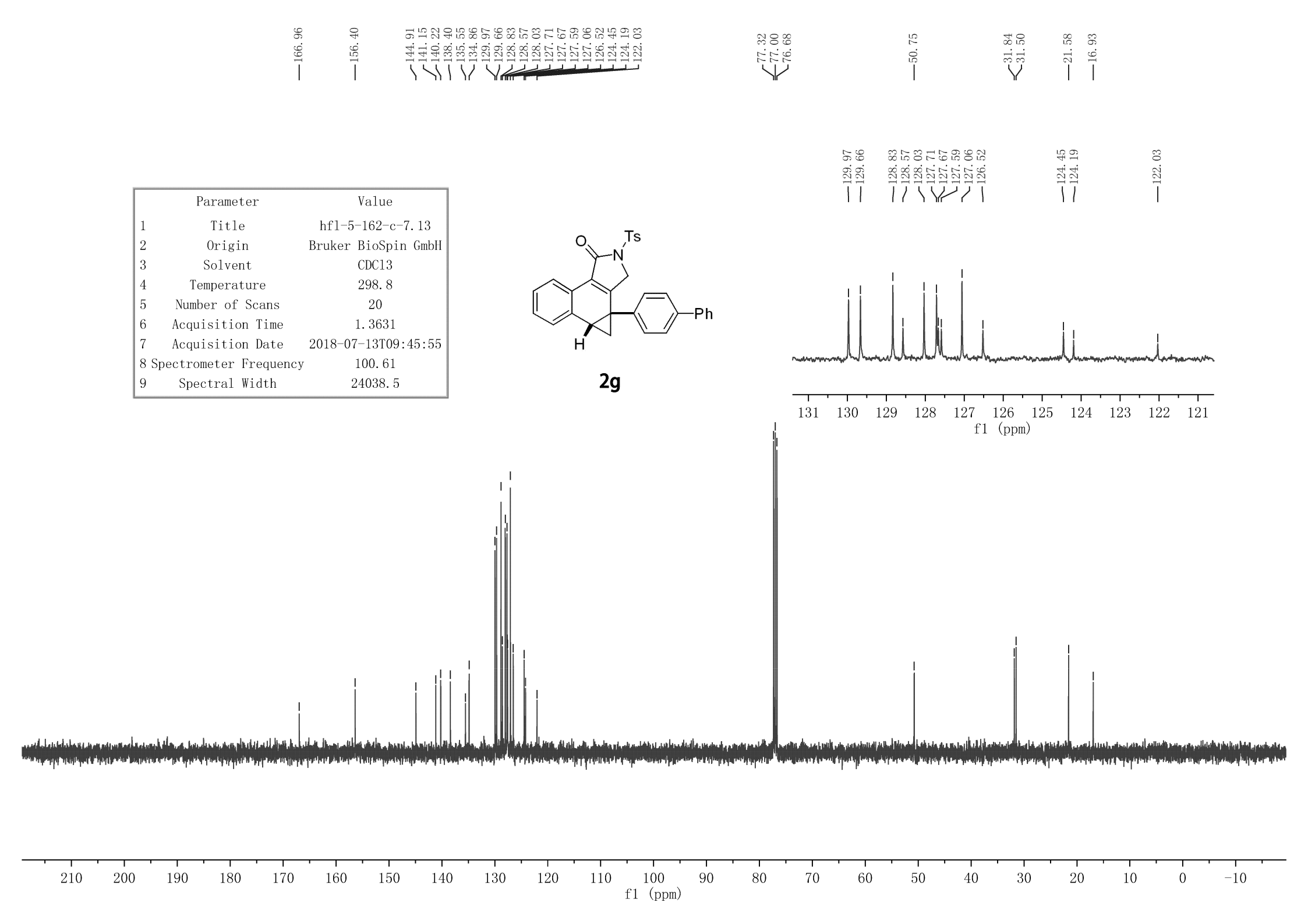
	Parameter	Value
1	Title	hfl-5-162-h
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.1
5	Number of Scans	7
6	Acquisition Time	3.9846
7	Acquisition Date	2018-07-12T21:44:58
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

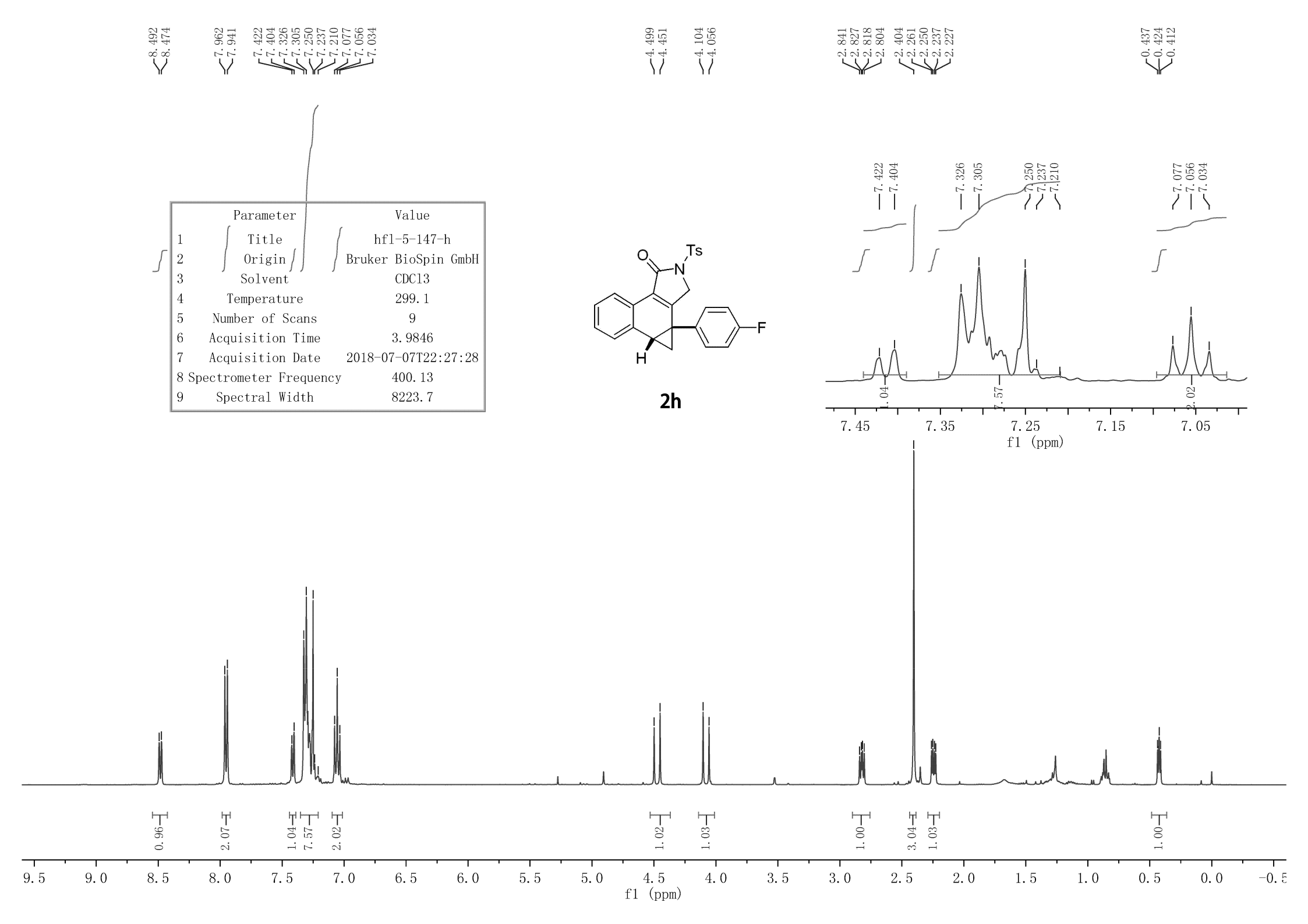


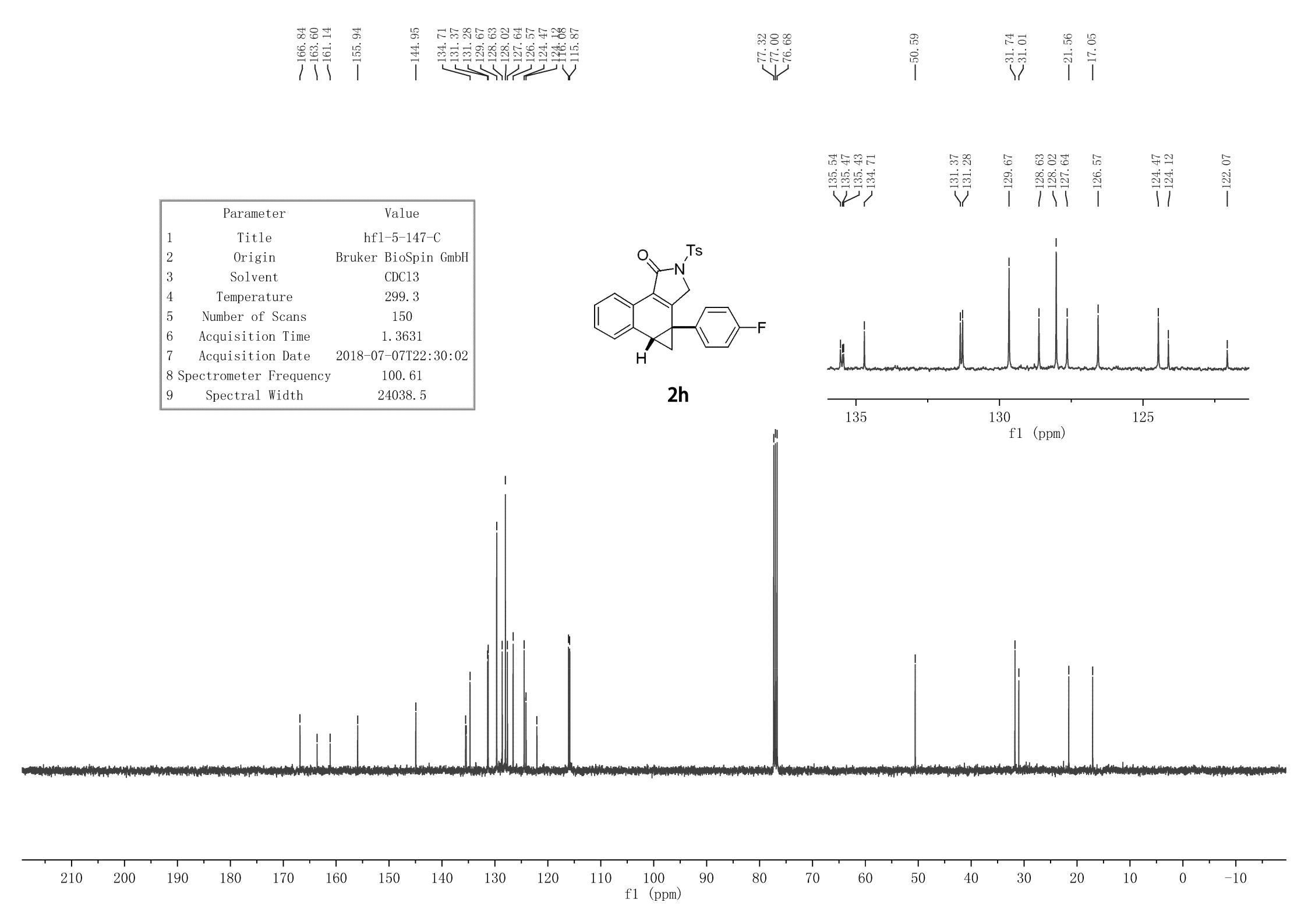
2g






166.96
156.40
144.91
141.15
140.22
138.40
135.55
134.86
129.97
129.66
128.83
128.57
128.03
127.71
127.67
127.59
127.06
126.52
124.45
124.19
122.03
77.32
77.00
76.68
50.75
31.84
31.50
21.58
16.93
Parameter Value
1 Title hfl-5-162-c-7.13
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.8
5 Number of Scans 20
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-13T09:45:55
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
Ph
H
2g
f1 (ppm)
f1 (ppm)

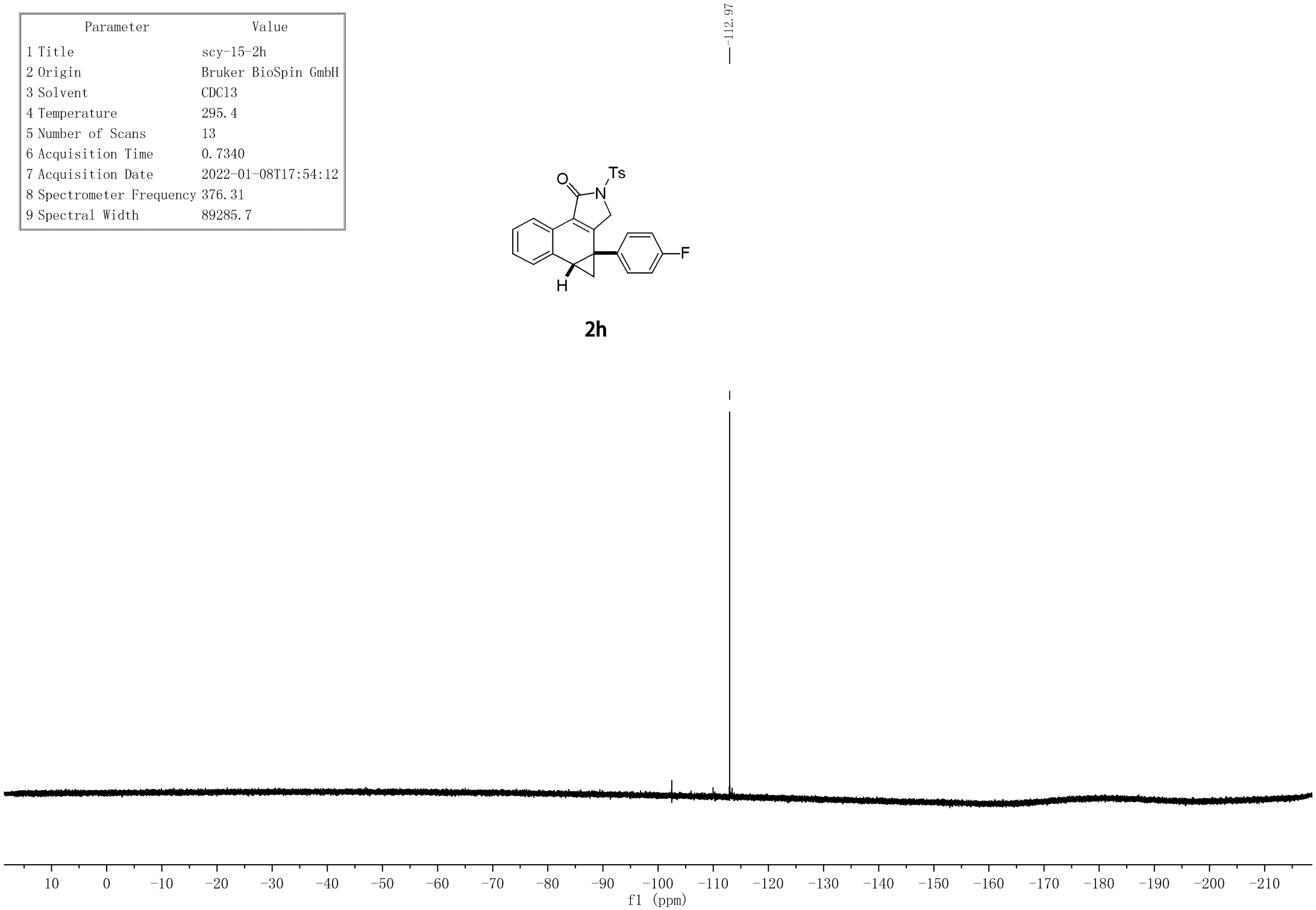

8.492
8.474
7.962
7.941
7.422
7.404
7.326
7.305
7.250
7.237
7.210
7.077
7.056
7.034
4.499
4.451
4.104
4.056
2.841
2.827
2.818
2.804
2.404
2.261
2.250
2.237
2.227
0.437
0.424
0.412
Parameter Value
1 Title hfl-5-147-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.1
5 Number of Scans 9
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-07T22:27:28
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
F
H
2h
1.04
7.57
2.02
7.45
7.35
7.25
7.15
7.05
f1 (ppm)
0.96
2.07
1.04
7.57
2.02
1.02
1.03
1.00
3.04
1.03
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



	Parameter	Value
1	Title	hfl-5-147-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.3
5	Number of Scans	150
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-07T22:30:02
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

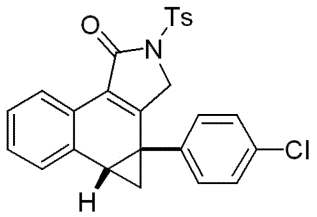
Parameter	Value
1 Title	scy-15-2h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	13
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-08T17:54:12
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

2h



8.493
8.475
8.472
7.964
7.944
7.419
7.401
7.362
7.341
7.331
7.310
7.280
7.259
7.254
4.493
4.445
4.109
4.061
2.839
2.825
2.815
2.801
2.411
2.260
2.249
2.236
2.226
0.455
0.444
0.442
0.430

	Parameter	Value
1	Title	HFL-5-148-H-7.16-1
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.0
5	Number of Scans	6
6	Acquisition Time	3.9846
7	Acquisition Date	2018-07-16T11:45:02
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7



2i

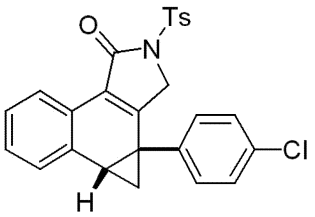
0.96
1.95
9.70
1.02
1.02
1.00
3.00
1.04
1.01

.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

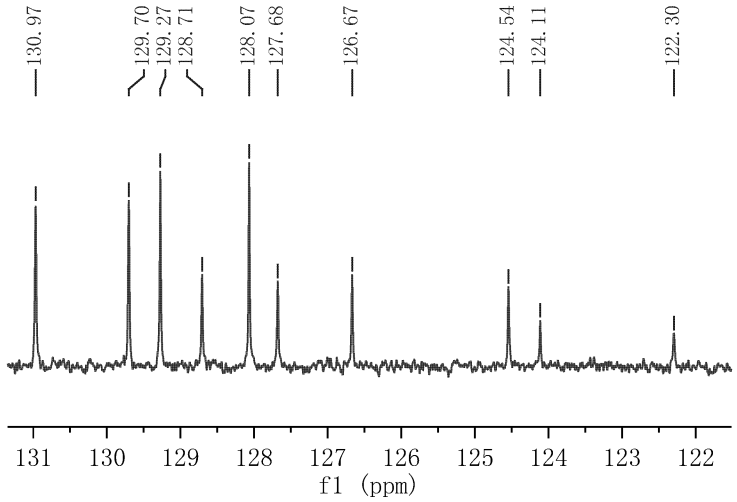
f1 (ppm)

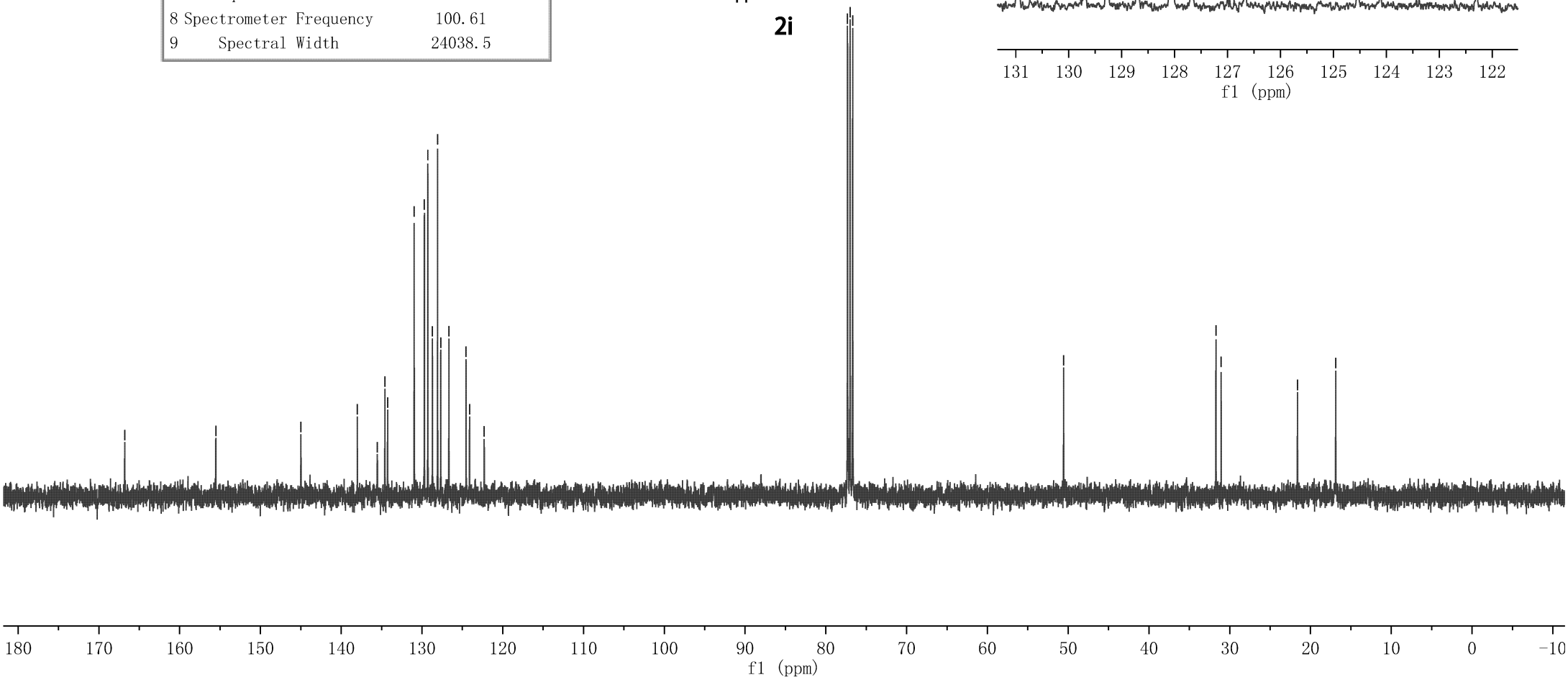
166.80
155.52
144.99
138.00
135.52
134.59
134.25
130.97
129.70
129.27
128.71
128.07
127.68
126.67
124.54
124.11
122.30
77.32
77.00
76.68
50.57
31.71
31.06
21.61
16.88

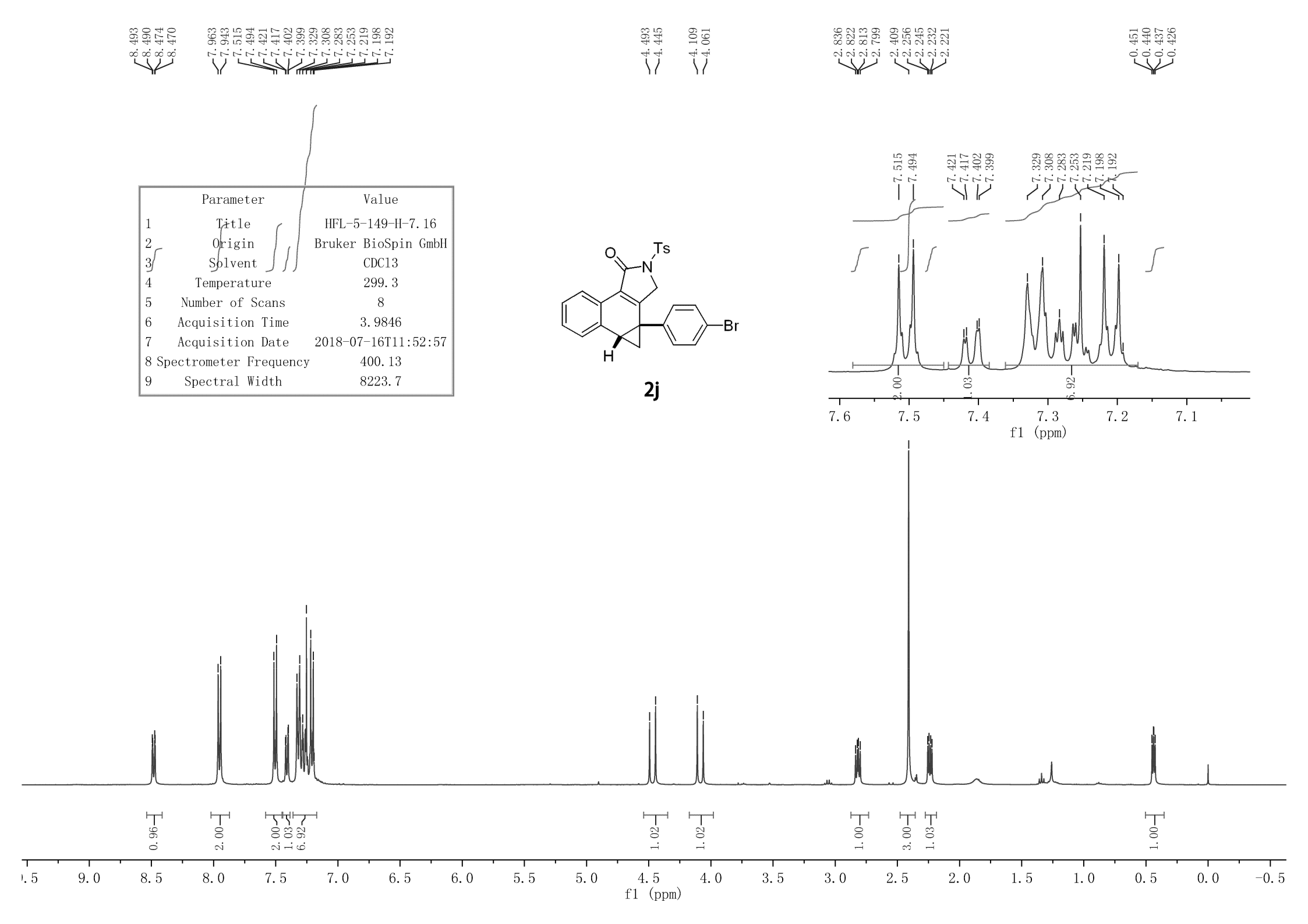
	Parameter	Value
1	Title	HFL-5-148-C-7.16-1
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.4
5	Number of Scans	53
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-16T11:48:37
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



2i

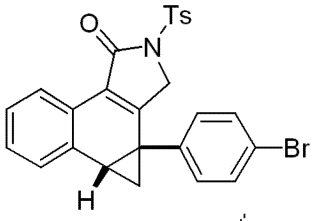




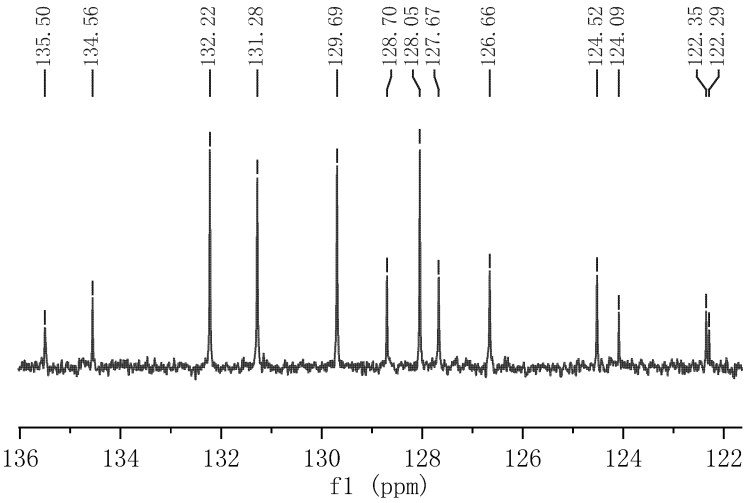

8.493
8.490
8.474
8.470
7.963
7.943
7.515
7.494
7.421
7.417
7.402
7.399
7.329
7.308
7.283
7.253
7.219
7.198
7.192
4.493
4.445
4.109
4.061
2.836
2.822
2.813
2.799
2.409
2.256
2.245
2.232
2.221
0.451
0.440
0.437
0.426
Parameter Value
1 Title HFL-5-149-H-7.16
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.3
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-16T11:52:57
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
Br
H
2j
2.00
1.03
6.92
f1 (ppm)
0.96
2.00
2.00
1.03
6.92
1.02
1.02
1.00
3.00
1.03
1.00
f1 (ppm)

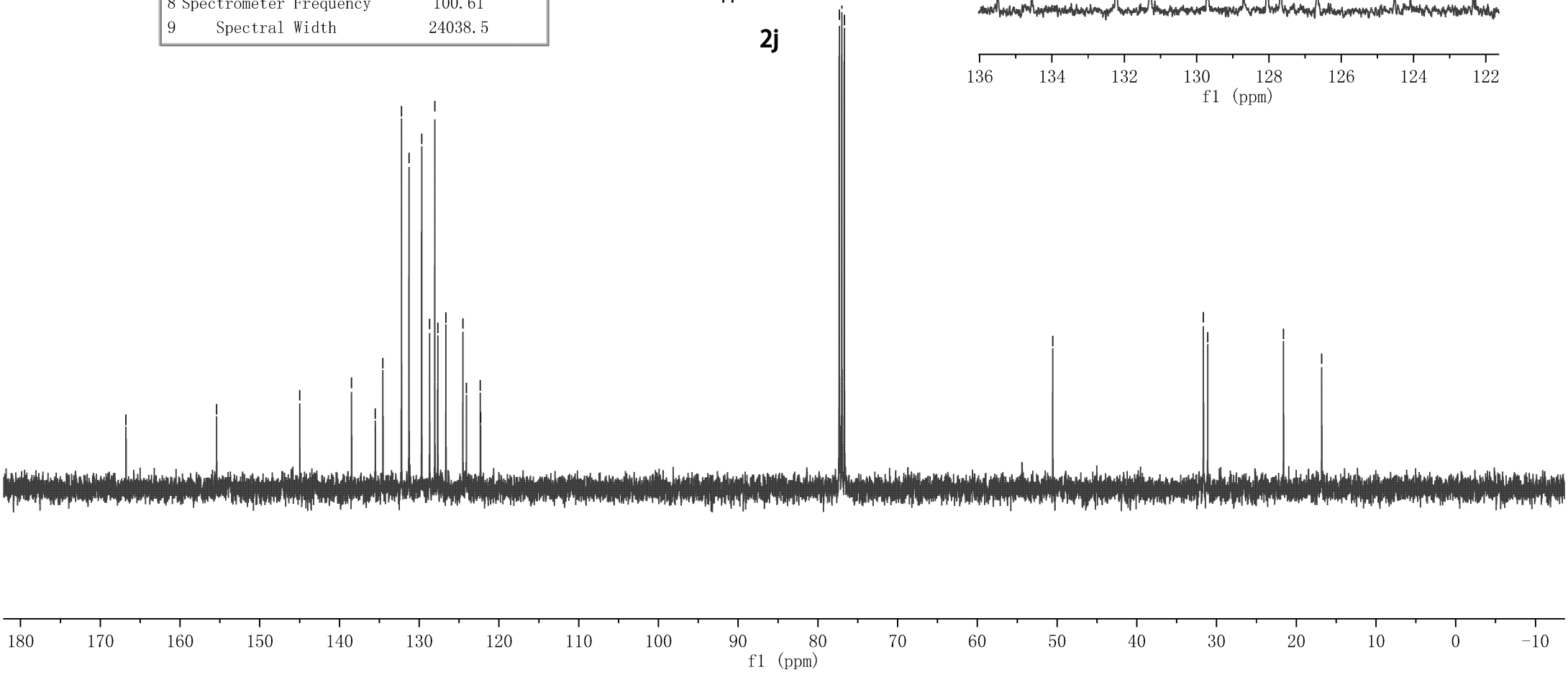
166.78
155.41
144.98
138.48
135.50
134.56
132.22
131.28
129.69
128.70
128.05
127.67
126.66
124.52
124.09
122.35
122.29
77.32
77.00
76.68
50.55
31.65
31.11
21.60
16.81

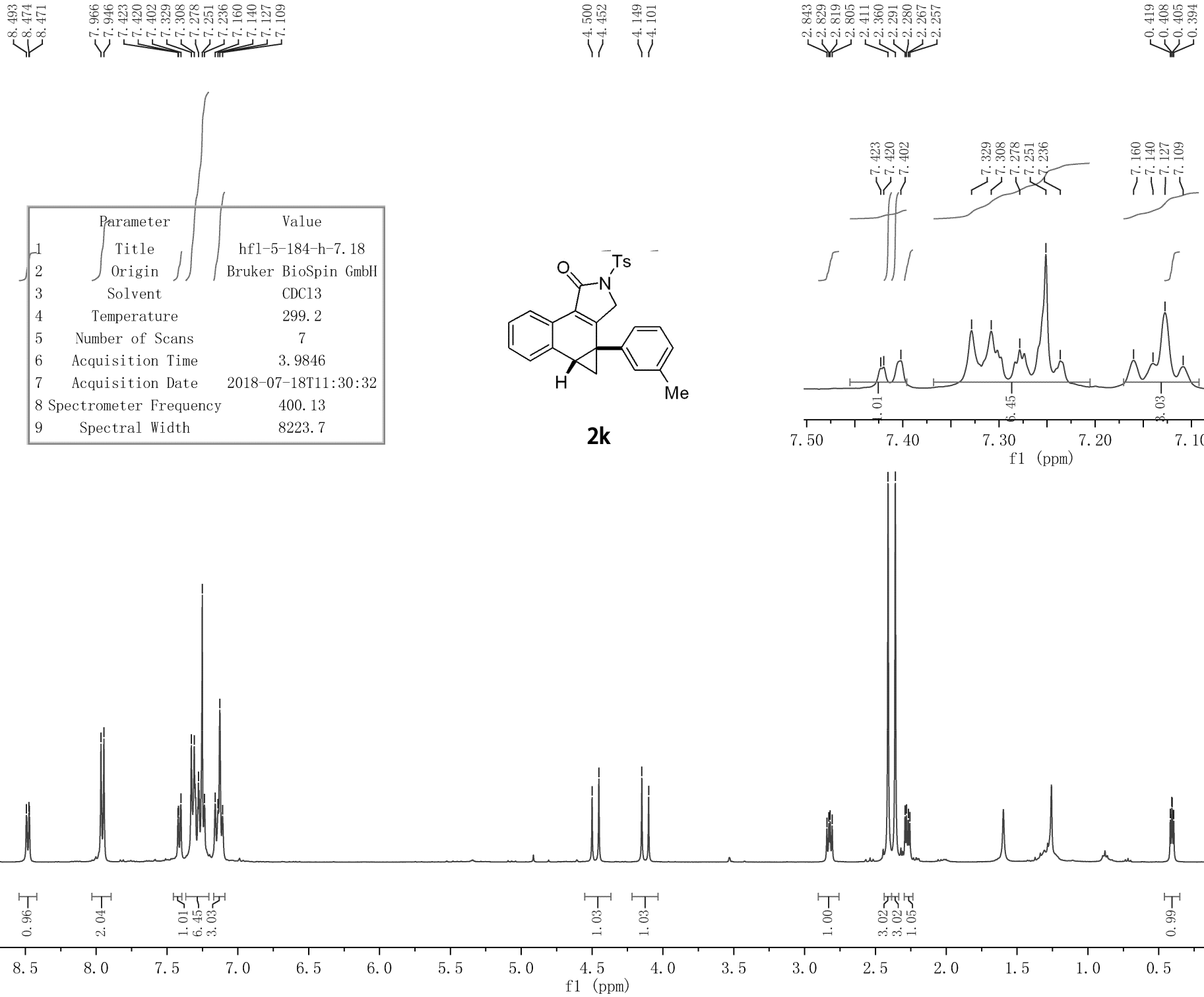
	Parameter	Value
1	Title	HFL-5-149-C-7.16
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.2
5	Number of Scans	28
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-16T11:54:43
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



2j

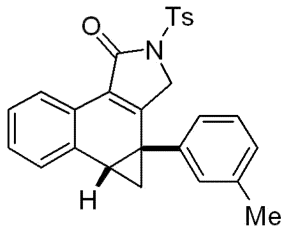




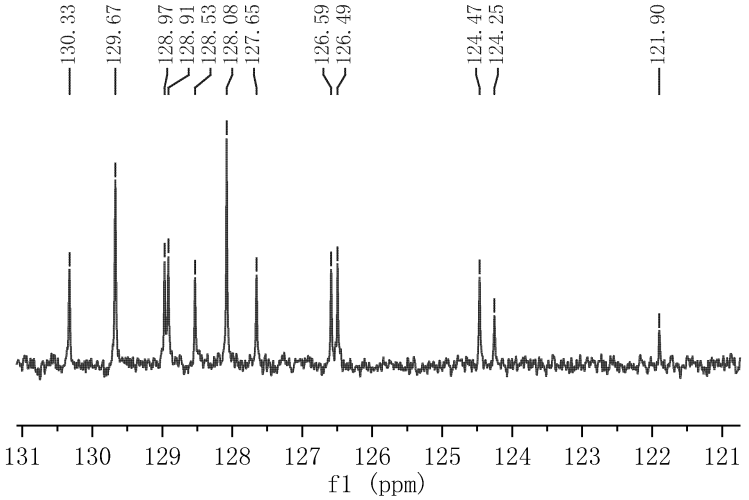

8.493
8.474
8.471
7.966
7.946
7.423
7.420
7.402
7.329
7.308
7.278
7.251
7.236
7.160
7.140
7.127
7.109
4.500
4.452
4.149
4.101
2.843
2.829
2.819
2.805
2.411
2.360
2.291
2.280
2.267
2.257
0.419
0.408
0.405
0.394
Parameter Value
1 Title hfl-5-184-h-7.18
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.2
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-18T11:30:32
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
H
Me
2k
1.01
6.45
3.03
7.50
7.40
7.30
7.20
7.10
f1 (ppm)
0.96
2.04
1.01
6.45
3.03
1.03
1.03
1.00
3.02
3.02
1.05
0.99
f1 (ppm)

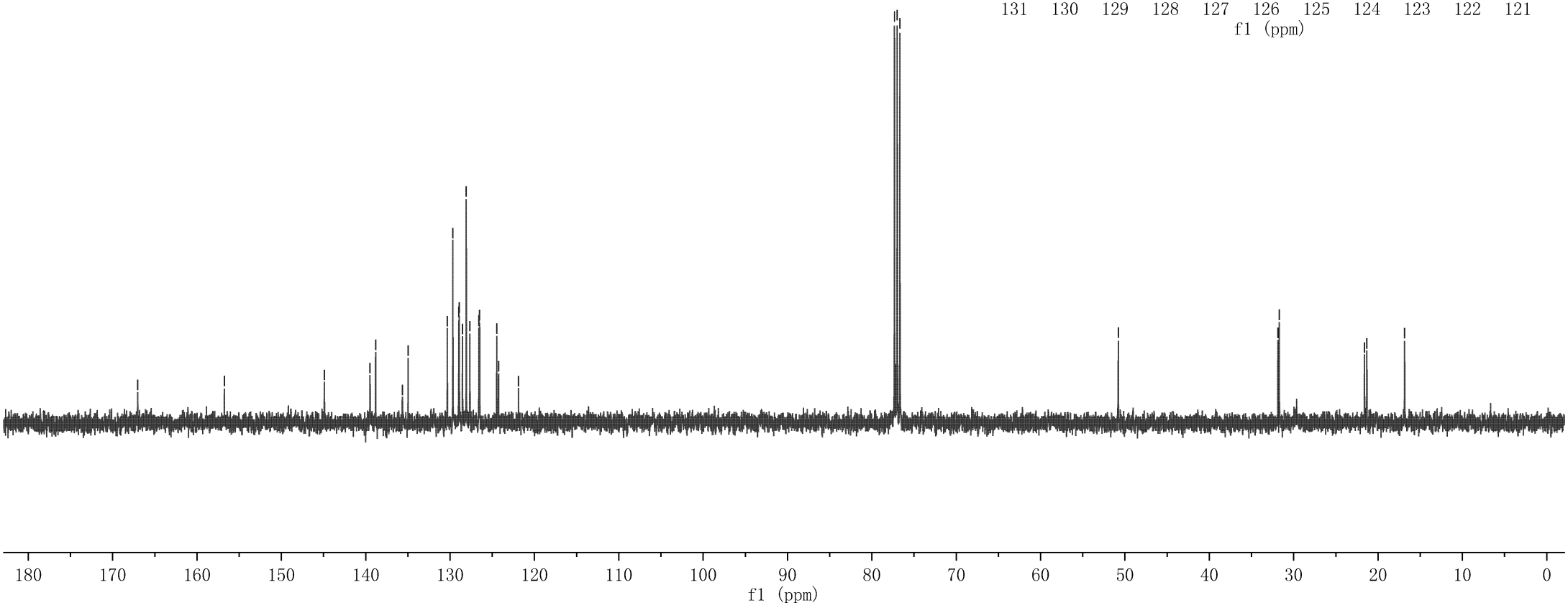
167.03
156.76
144.90
139.49
138.83
135.66
134.97
130.33
129.67
128.97
128.91
128.53
128.08
127.65
126.59
126.49
124.47
124.25
121.90
77.32
77.00
76.68
50.78
31.88
31.71
21.61
21.33
16.85

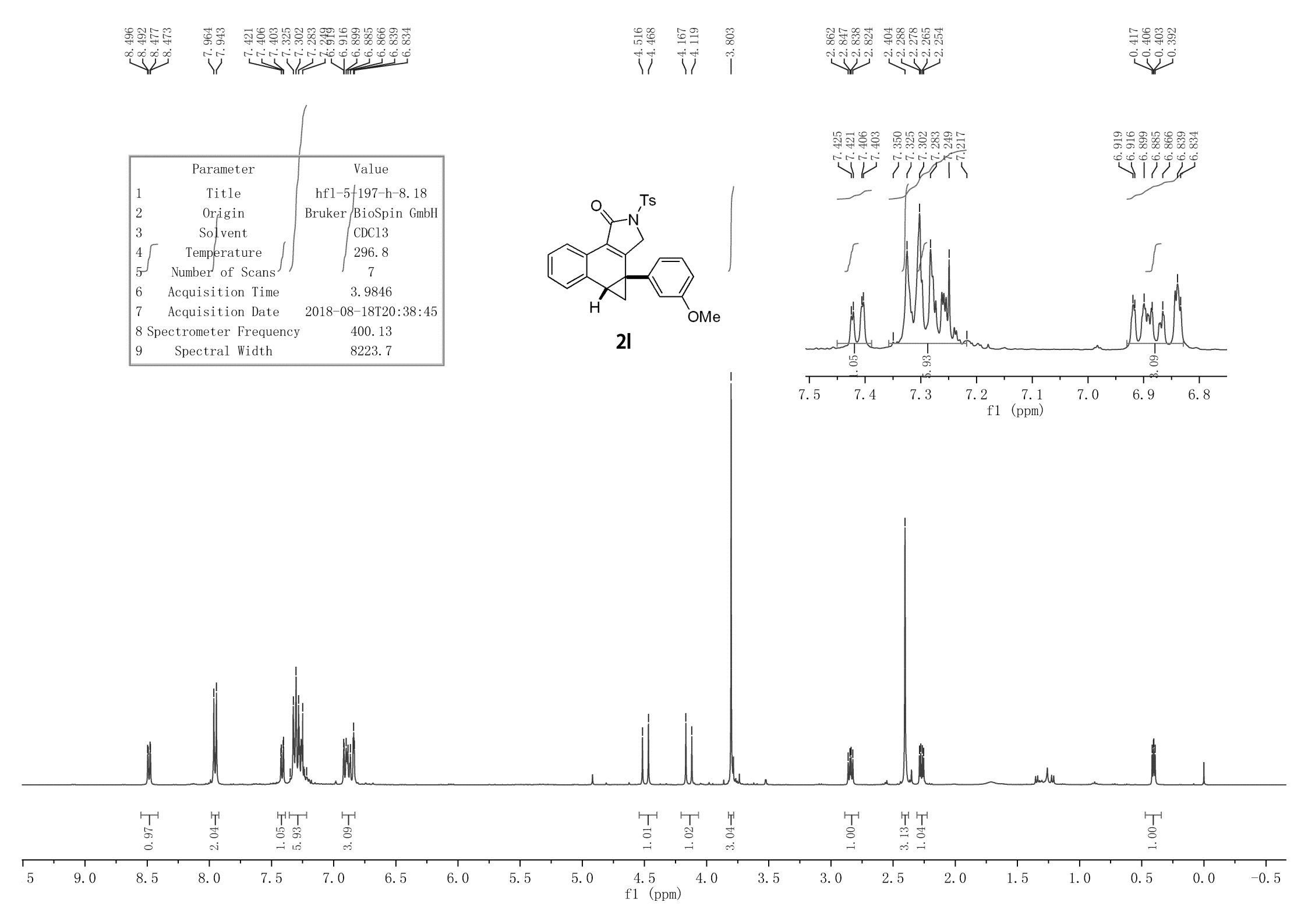
	Parameter	Value
1	Title	hfl-5-184-c-7.18
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.3
5	Number of Scans	51
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-18T11:32:46
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5

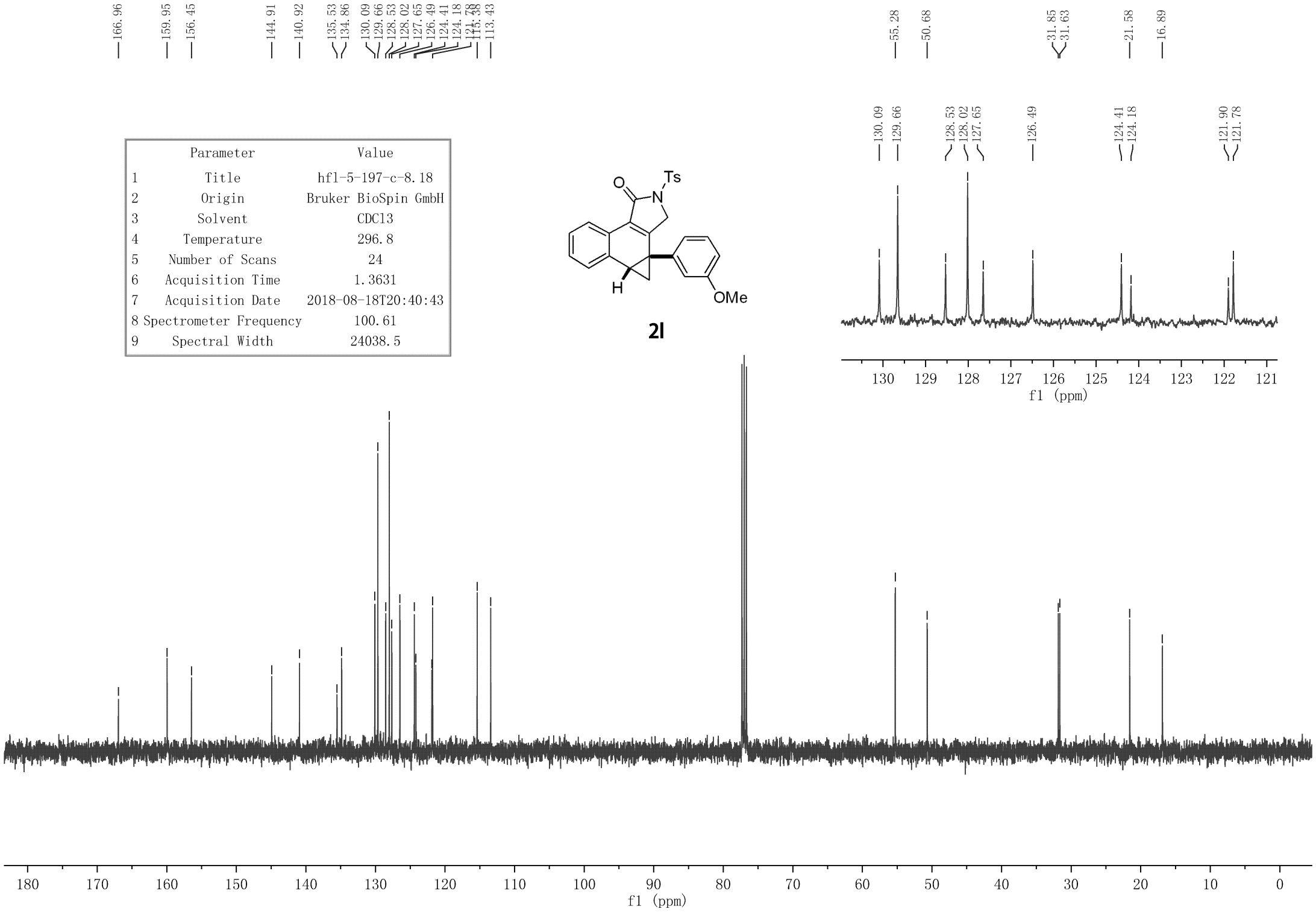


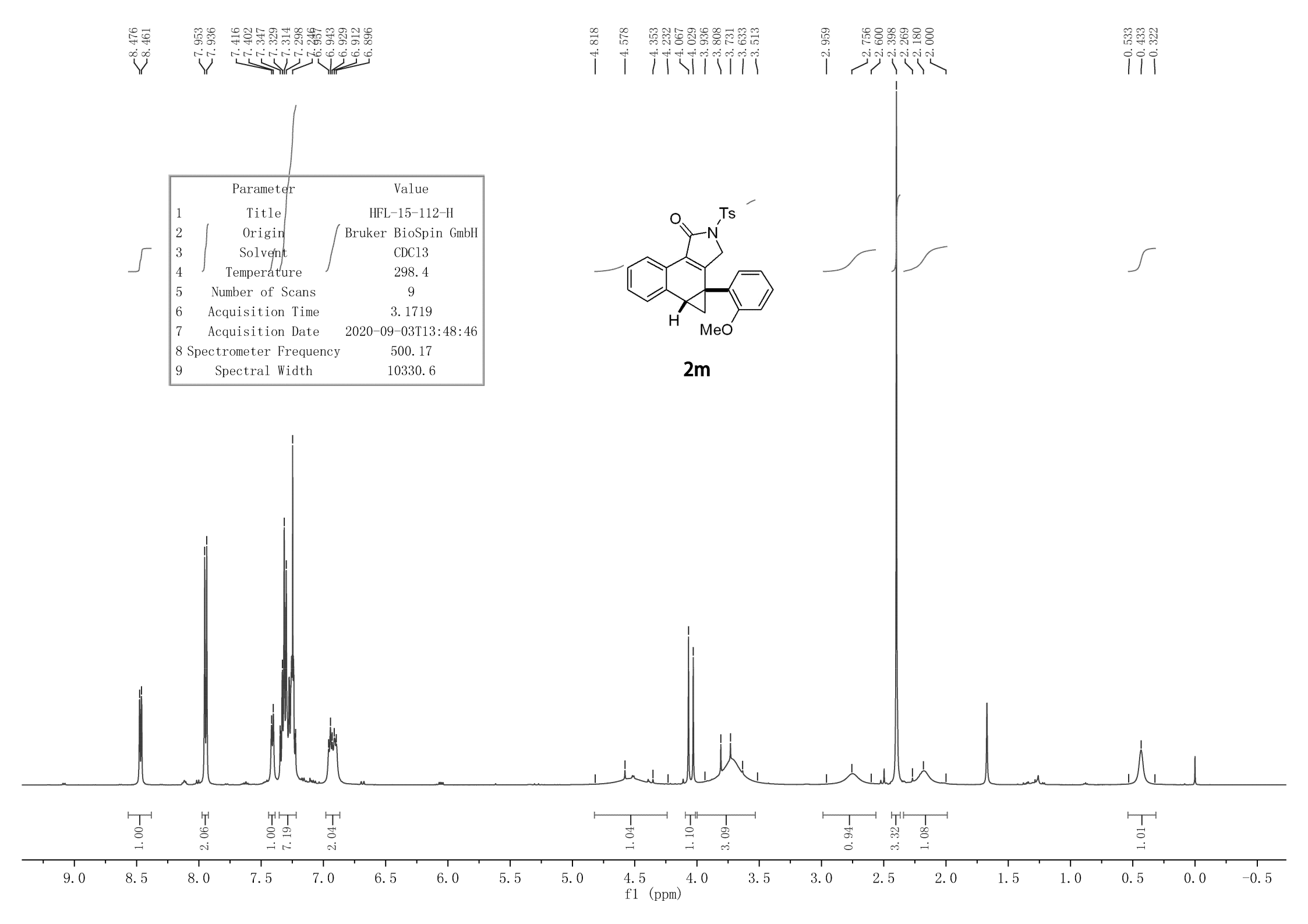
2k

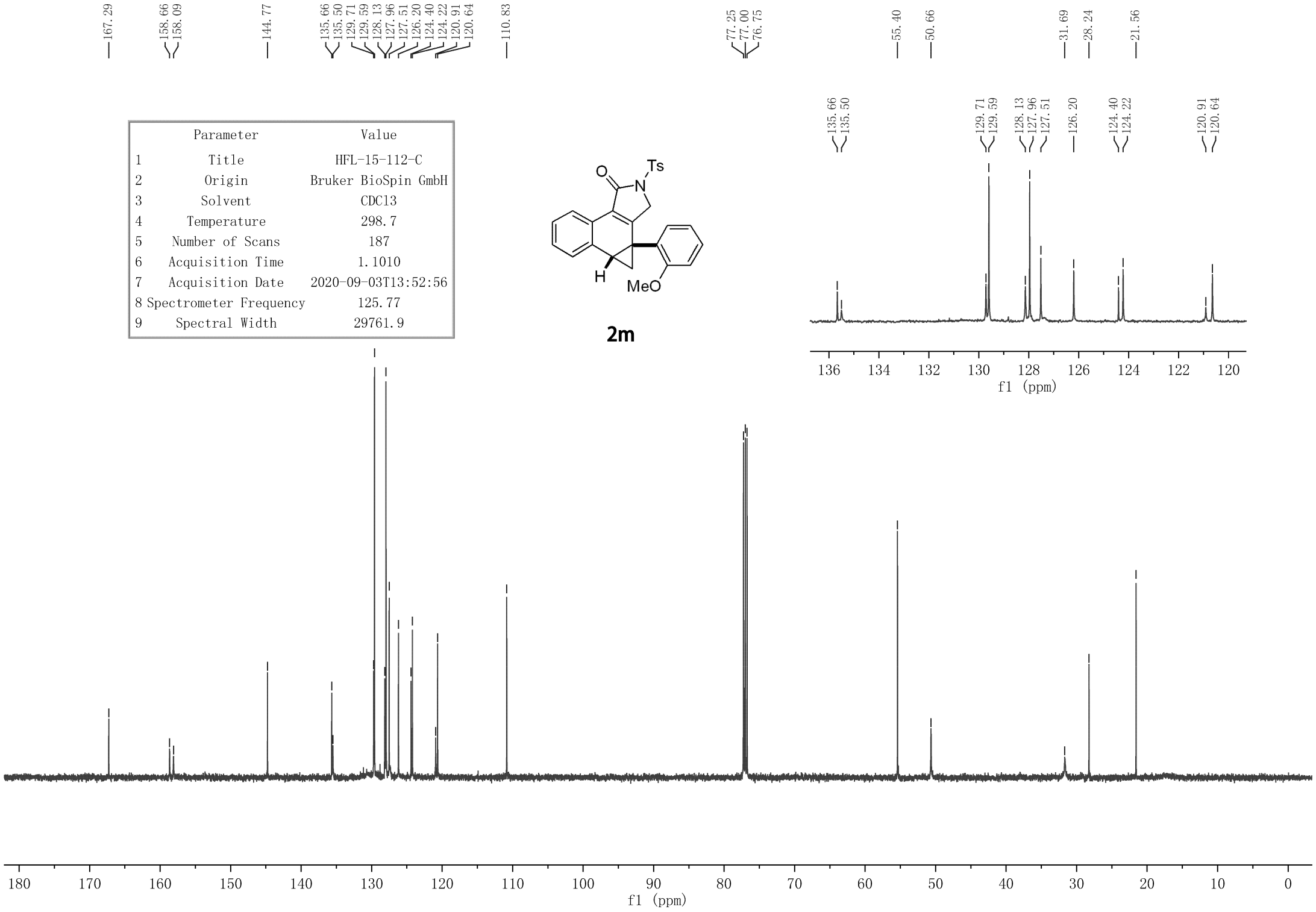




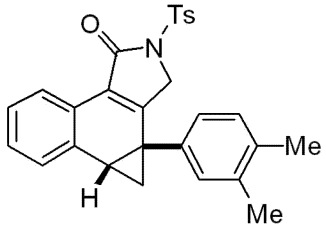

8.496
8.492
8.477
8.473
7.964
7.943
7.421
7.406
7.403
7.325
7.302
7.283
6.916
6.899
6.885
6.866
6.839
6.834
4.516
4.468
4.167
4.119
3.803
2.862
2.847
2.838
2.824
2.404
2.288
2.278
2.265
2.254
0.417
0.406
0.403
0.392
Parameter Value
1 Title hfl-5-197-h-8.18
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-08-18T20:38:45
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
H
OMe
2l
7.425
7.421
7.406
7.403
7.350
7.325
7.302
7.283
7.249
7.217
6.919
6.916
6.899
6.885
6.866
6.839
6.834
1.05
5.93
3.09
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)
0.97
2.04
1.05
5.93
3.09
1.01
1.02
3.04
1.00
3.13
1.04
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


166.96
159.95
156.45
144.91
140.92
135.53
134.86
130.09
129.66
128.53
128.02
127.65
126.49
124.41
124.18
121.78
113.43
55.28
50.68
31.85
31.63
21.58
16.89
Parameter Value
1 Title hfl-5-197-c-8.18
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 24
6 Acquisition Time 1.3631
7 Acquisition Date 2018-08-18T20:40:43
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
H
OMe
2l
f1 (ppm)
f1 (ppm)

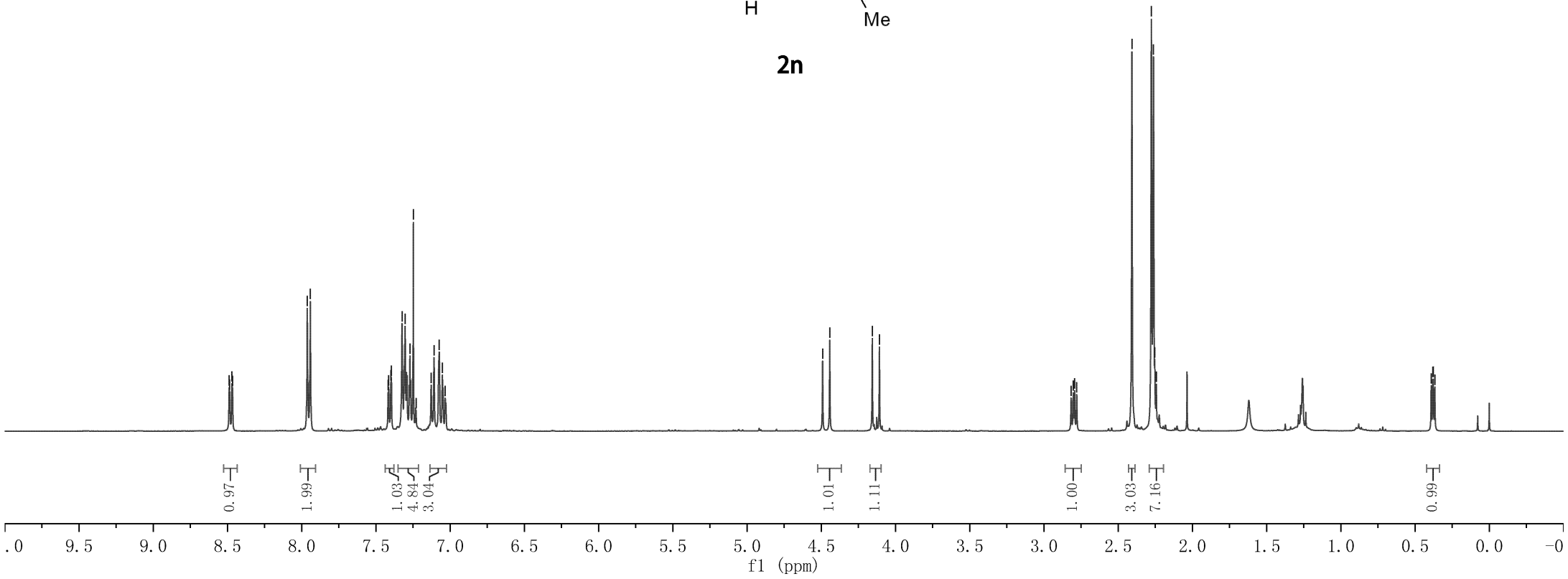

8.476
8.461
7.953
7.936
7.416
7.402
7.347
7.329
7.314
7.298
6.943
6.929
6.912
6.896
4.818
4.578
4.353
4.232
4.067
4.029
3.936
3.808
3.731
3.633
3.513
2.959
2.756
2.600
2.398
2.269
2.180
2.000
0.533
0.433
0.322
Parameter Value
1 Title HFL-15-112-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.4
5 Number of Scans 9
6 Acquisition Time 3.1719
7 Acquisition Date 2020-09-03T13:48:46
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
O
N
Ts
H
MeO
2m
1.00
2.06
1.00
7.19
2.04
1.04
1.10
3.09
0.94
3.32
1.08
1.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


167.29
158.66
158.09
144.77
135.66
135.50
129.71
129.59
128.13
127.96
127.51
126.20
124.40
124.22
120.91
120.64
110.83
77.25
77.00
76.75
55.40
50.66
31.69
28.24
21.56
Parameter Value
1 Title HFL-15-112-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.7
5 Number of Scans 187
6 Acquisition Time 1.1010
7 Acquisition Date 2020-09-03T13:52:56
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
O
N
Ts
H
MeO
2m
f1 (ppm)
f1 (ppm)

	Parameter	Value
1	Title	hfl-5-172-H
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	300.0
5	Number of Scans	9
6	Acquisition Time	3.9846
7	Acquisition Date	2018-07-14T16:50:22
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

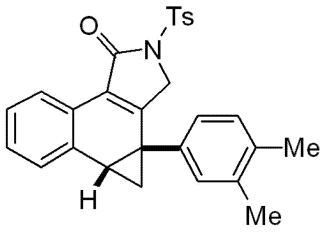


2n

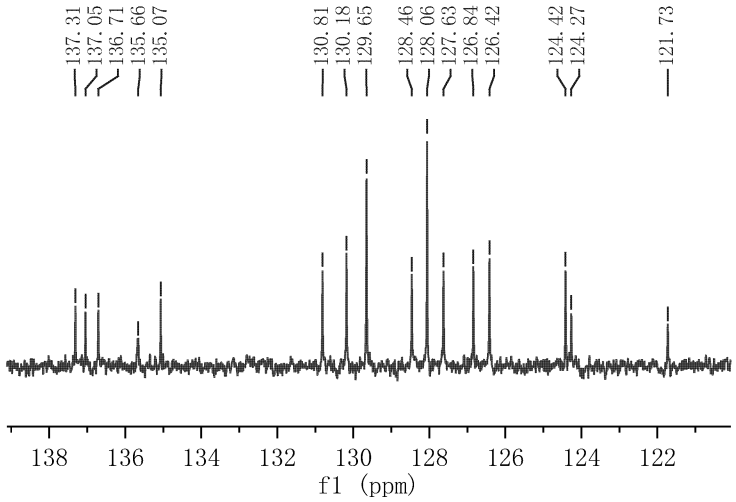


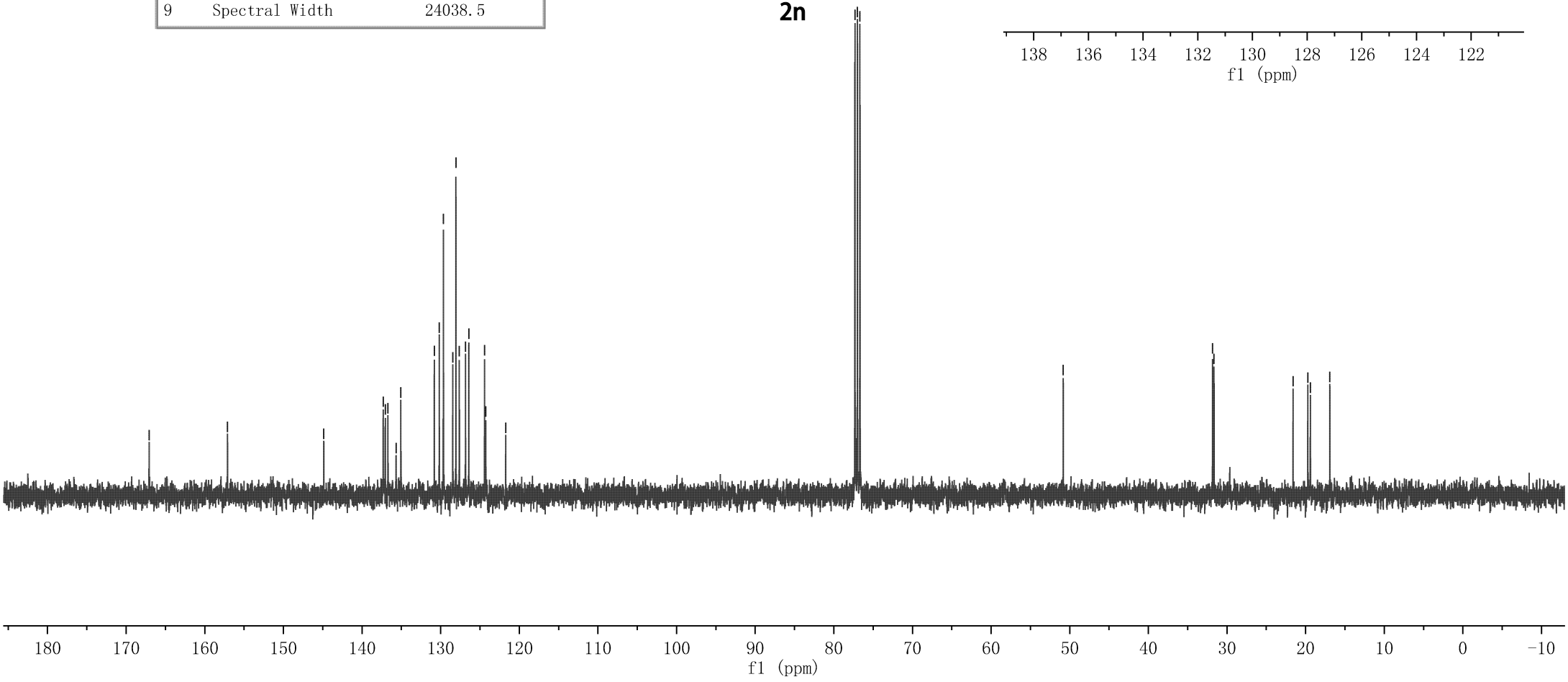
167.08
157.11
144.87
137.31
137.05
136.71
135.66
135.07
130.81
130.18
129.65
128.46
128.06
127.63
126.84
126.42
124.42
124.27
121.73
77.32
77.00
76.68
50.83
31.83
31.65
21.59
19.72
19.39
16.92

	Parameter	Value
1	Title	hfl-5-172-C
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	300.0
5	Number of Scans	36
6	Acquisition Time	1.3631
7	Acquisition Date	2018-07-14T16:52:33
8	Spectrometer Frequency	100.61
9	Spectral Width	24038.5



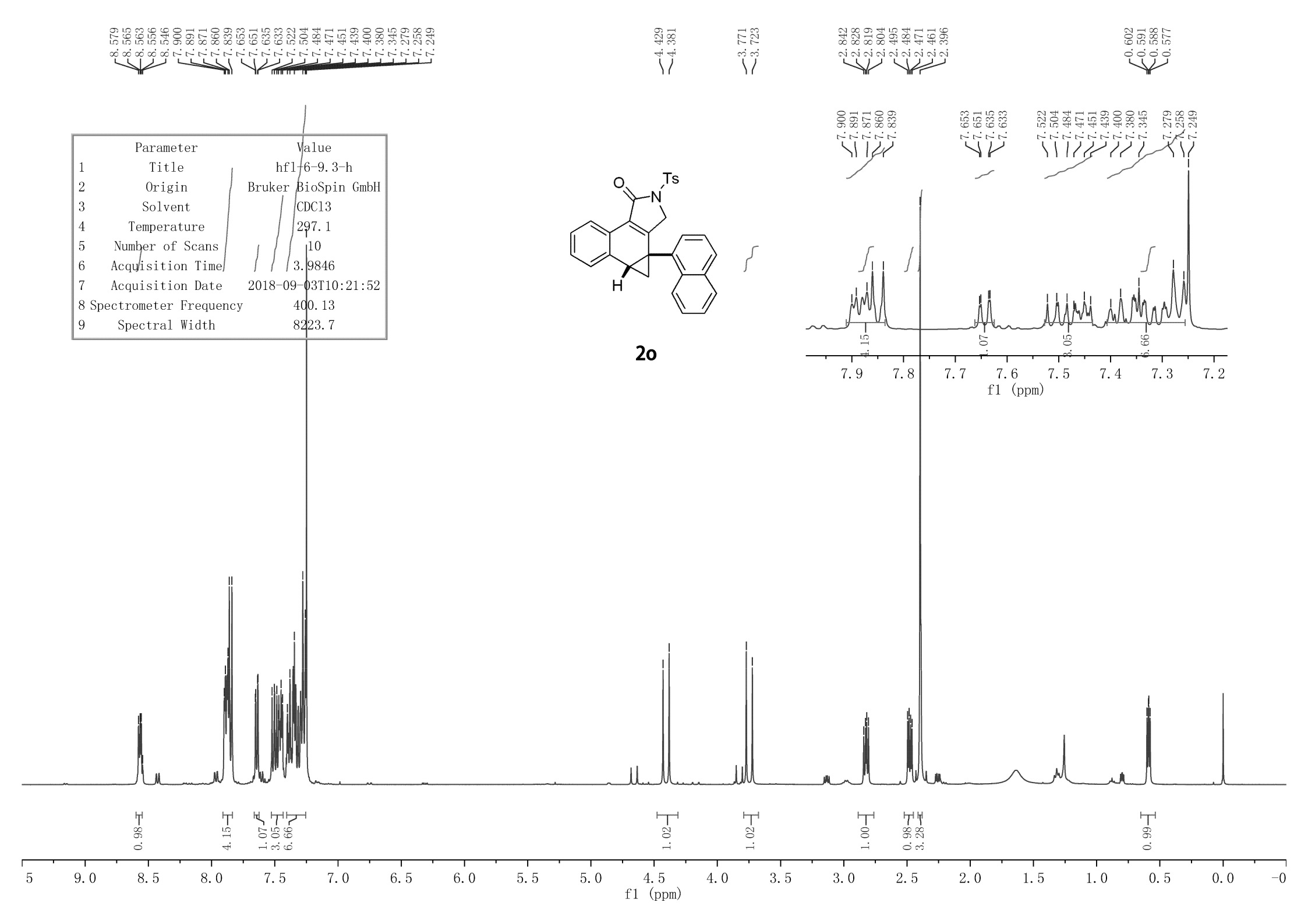
2n

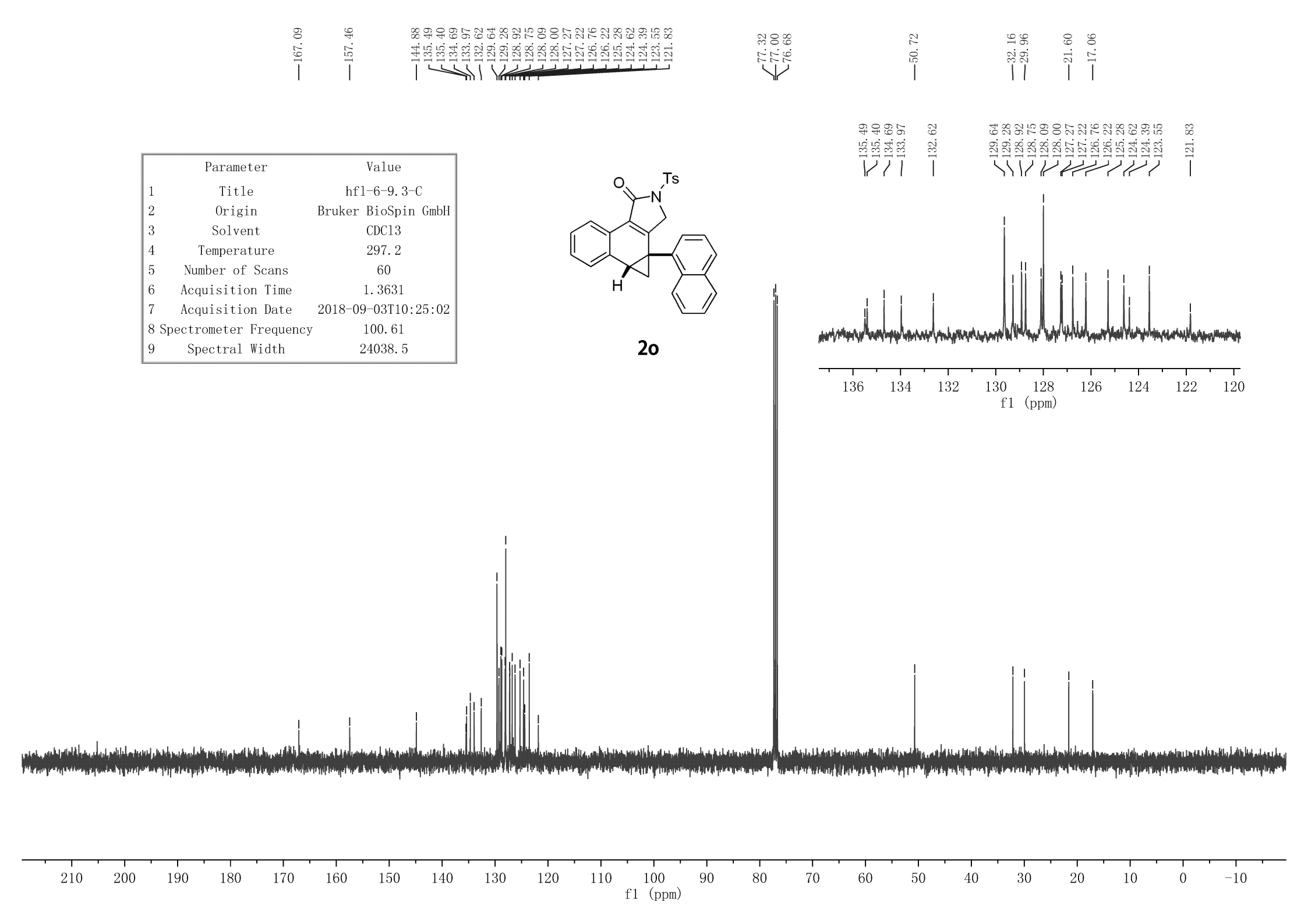


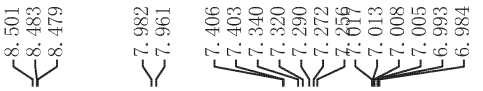


	Parameter	Value
1	Title	hfl-6-9.3-h
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	297.1
5	Number of Scans	10
6	Acquisition Time	3.9846
7	Acquisition Date	2018-09-03T10:21:52
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7

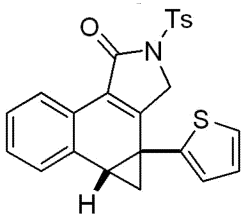
2o




167.09
157.46
144.88
135.49
135.40
134.69
133.97
132.62
129.64
129.28
128.92
128.75
128.09
128.00
127.27
127.22
126.76
126.22
125.28
124.62
124.39
123.55
121.83
77.32
77.00
76.68
50.72
32.16
29.96
21.60
17.06
Parameter Value
1 Title hf1-6-9.3-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.2
5 Number of Scans 60
6 Acquisition Time 1.3631
7 Acquisition Date 2018-09-03T10:25:02
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
H
2o
f1 (ppm)



	Parameter	Value
1	Title	HFL-5-142-7.10-H
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	299.1
5	Number of Scans	8
6	Acquisition Time	3.9846
7	Acquisition Date	2018-07-10T21:55:24
8	Spectrometer Frequency	400.13
9	Spectral Width	8223.7



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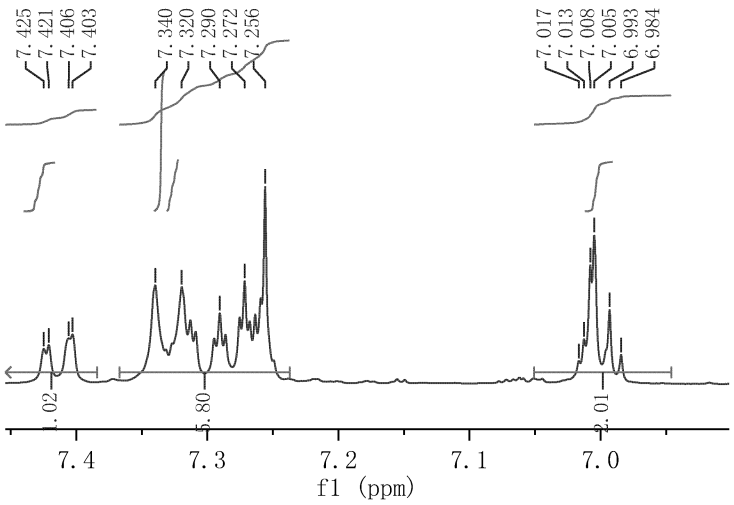
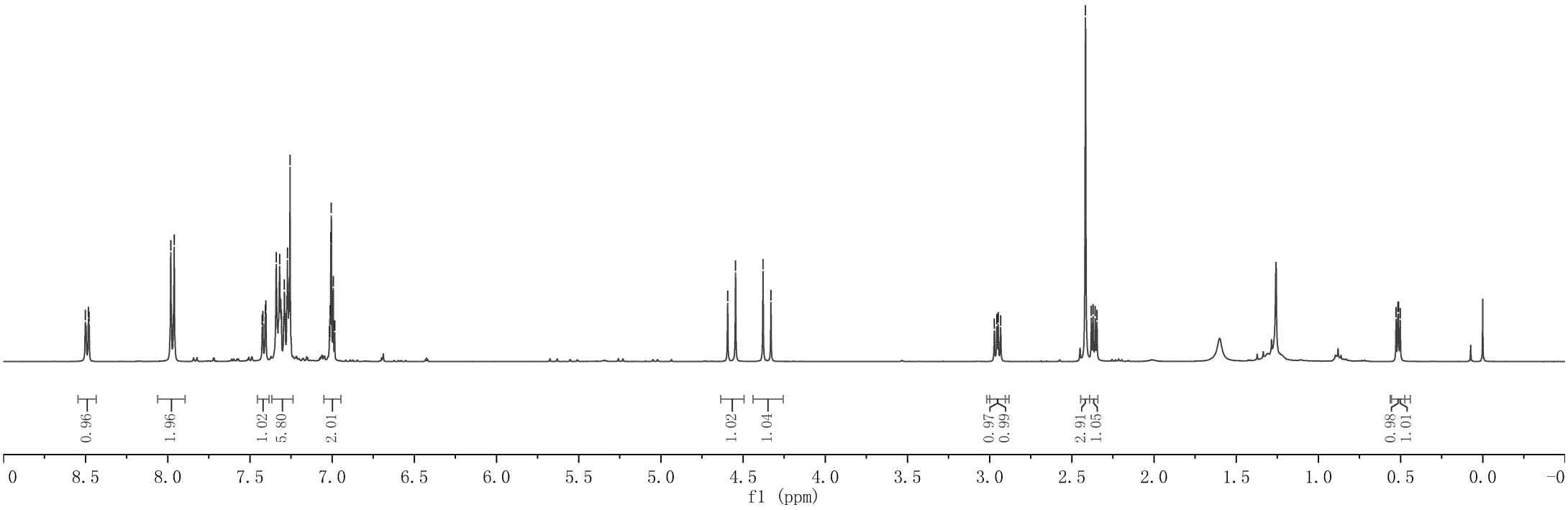
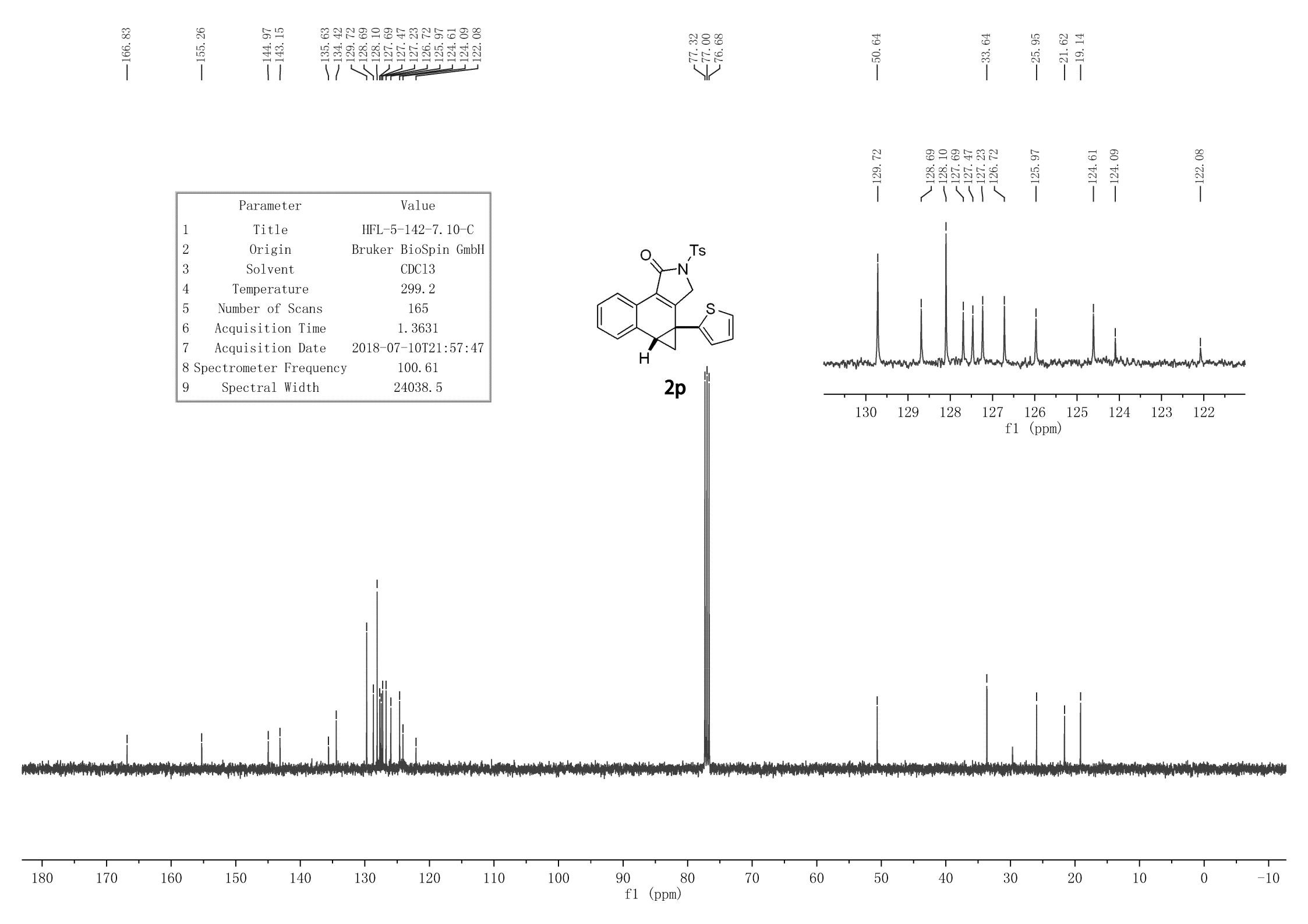
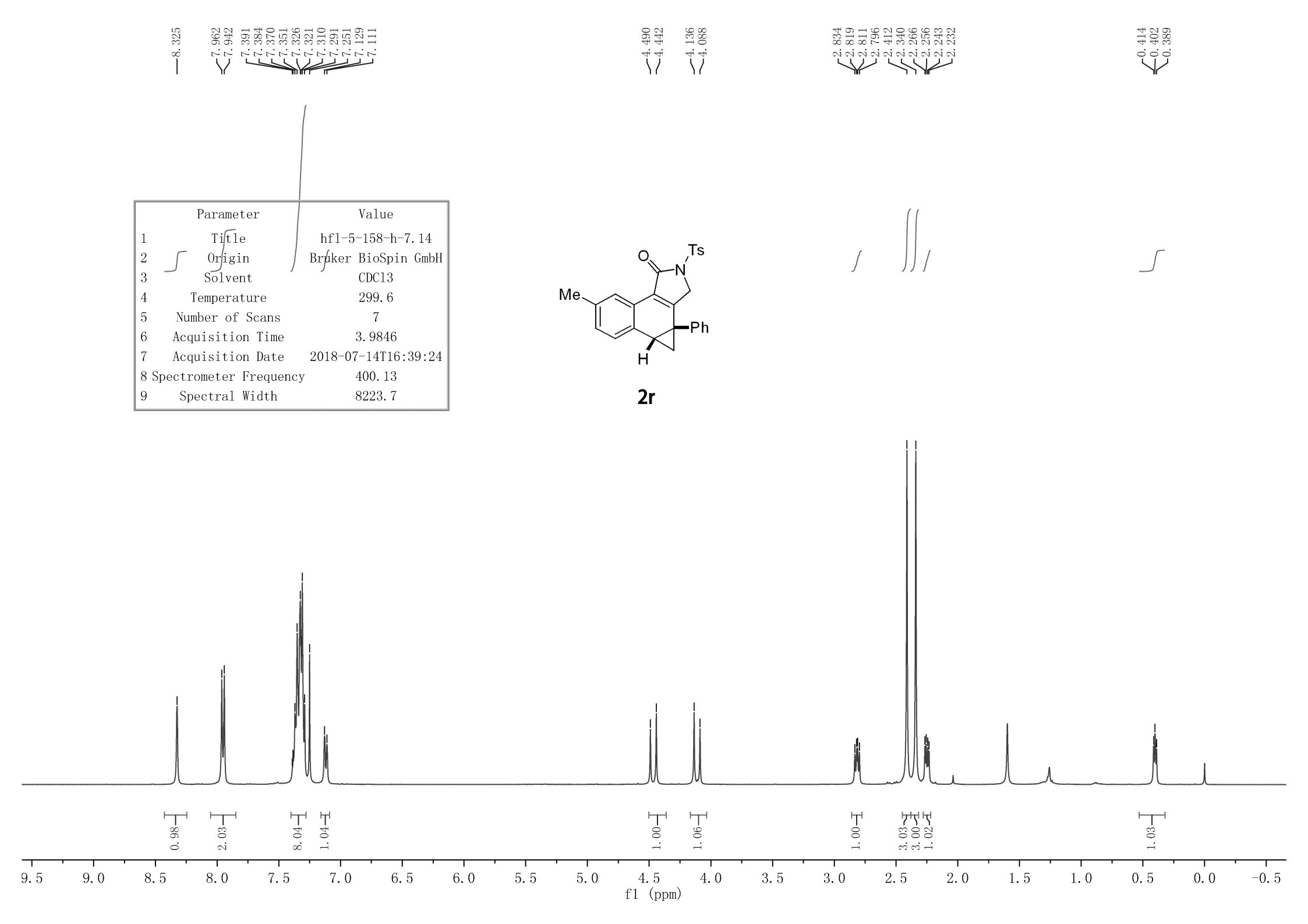
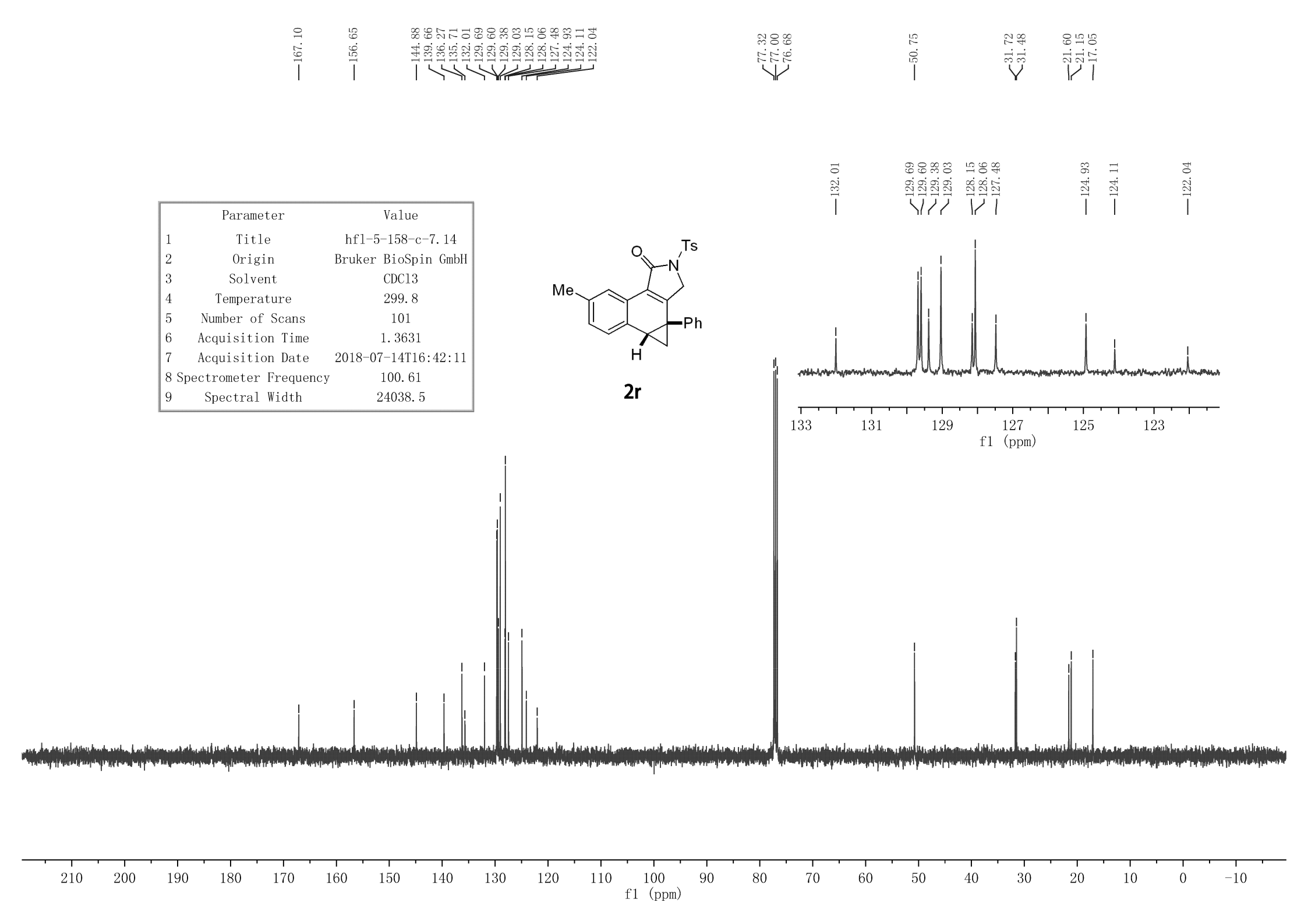


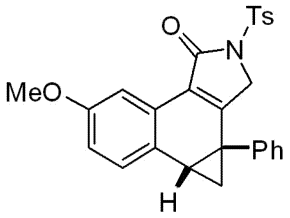



166.83
155.26
144.97
143.15
135.63
134.42
129.72
128.69
128.10
127.69
127.47
127.23
126.72
125.97
124.61
124.09
122.08
77.32
77.00
76.68
50.64
33.64
25.95
21.62
19.14
Parameter Value
1 Title HFL-5-142-7.10-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.2
5 Number of Scans 165
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-10T21:57:47
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
S
H
2p
f1 (ppm)


8.325
7.962
7.942
7.391
7.384
7.370
7.351
7.326
7.321
7.310
7.291
7.251
7.129
7.111
4.490
4.442
4.136
4.088
2.834
2.819
2.811
2.796
2.412
2.340
2.266
2.256
2.243
2.232
0.414
0.402
0.389
Parameter Value
1 Title hf1-5-158-h-7.14
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-14T16:39:24
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
Me
Ph
H
2r
0.98
2.03
8.04
1.04
1.00
1.06
1.00
3.03
3.00
1.02
1.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

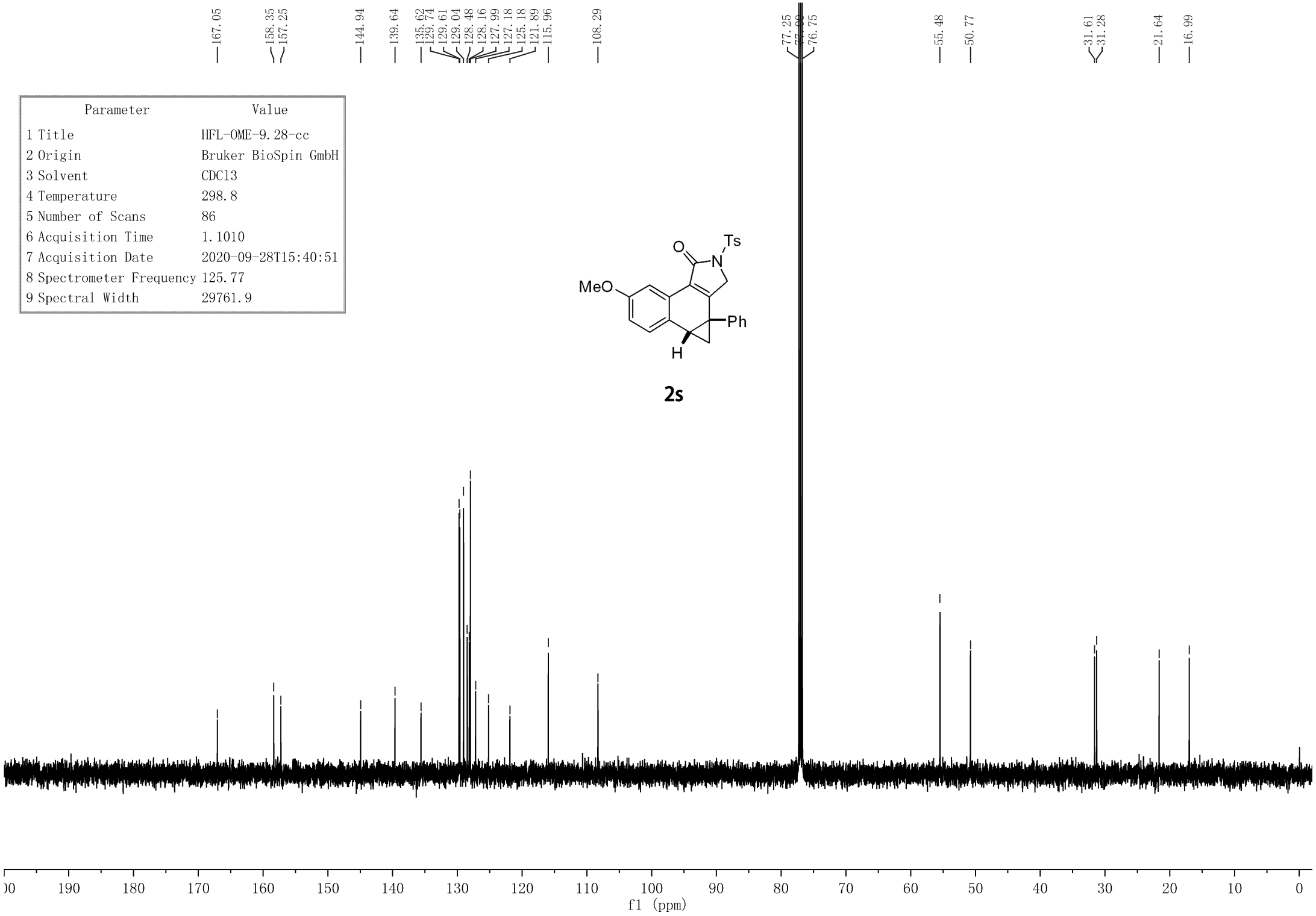

167.10
156.65
144.88
139.66
136.27
135.71
132.01
129.69
129.60
129.38
129.03
128.15
128.06
127.48
124.93
124.11
122.04
77.32
77.00
76.68
50.75
31.72
31.48
21.60
21.15
17.05
Parameter Value
1 Title hfl-5-158-c-7.14
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.8
5 Number of Scans 101
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-14T16:42:11
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
Me
Ph
H
2r
f1 (ppm)

Parameter	Value
1 Title	HFL-OME-9.28-HH
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	5
6 Acquisition Time	3.1719
7 Acquisition Date	2020-09-28T15:36:01
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6



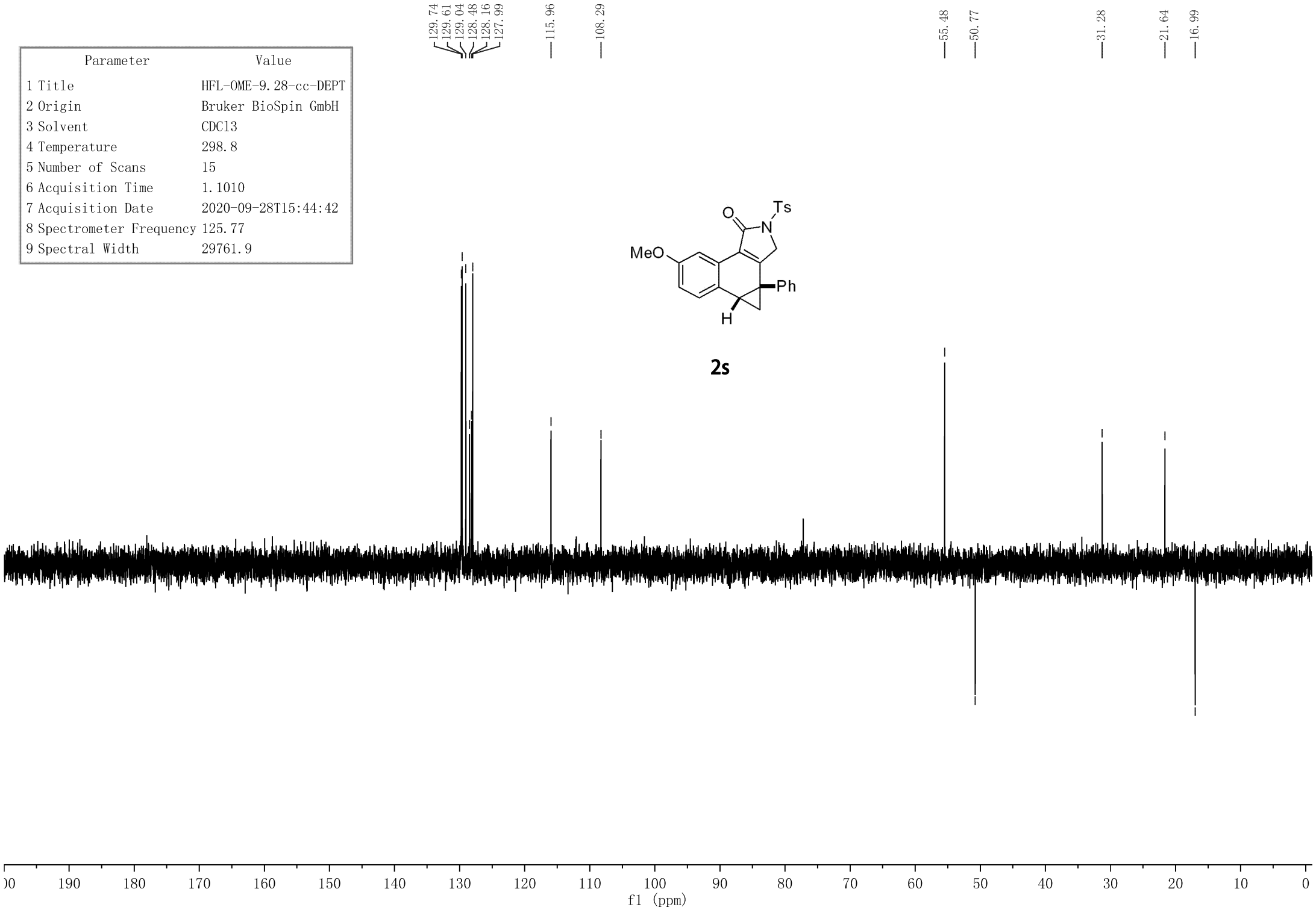
2s

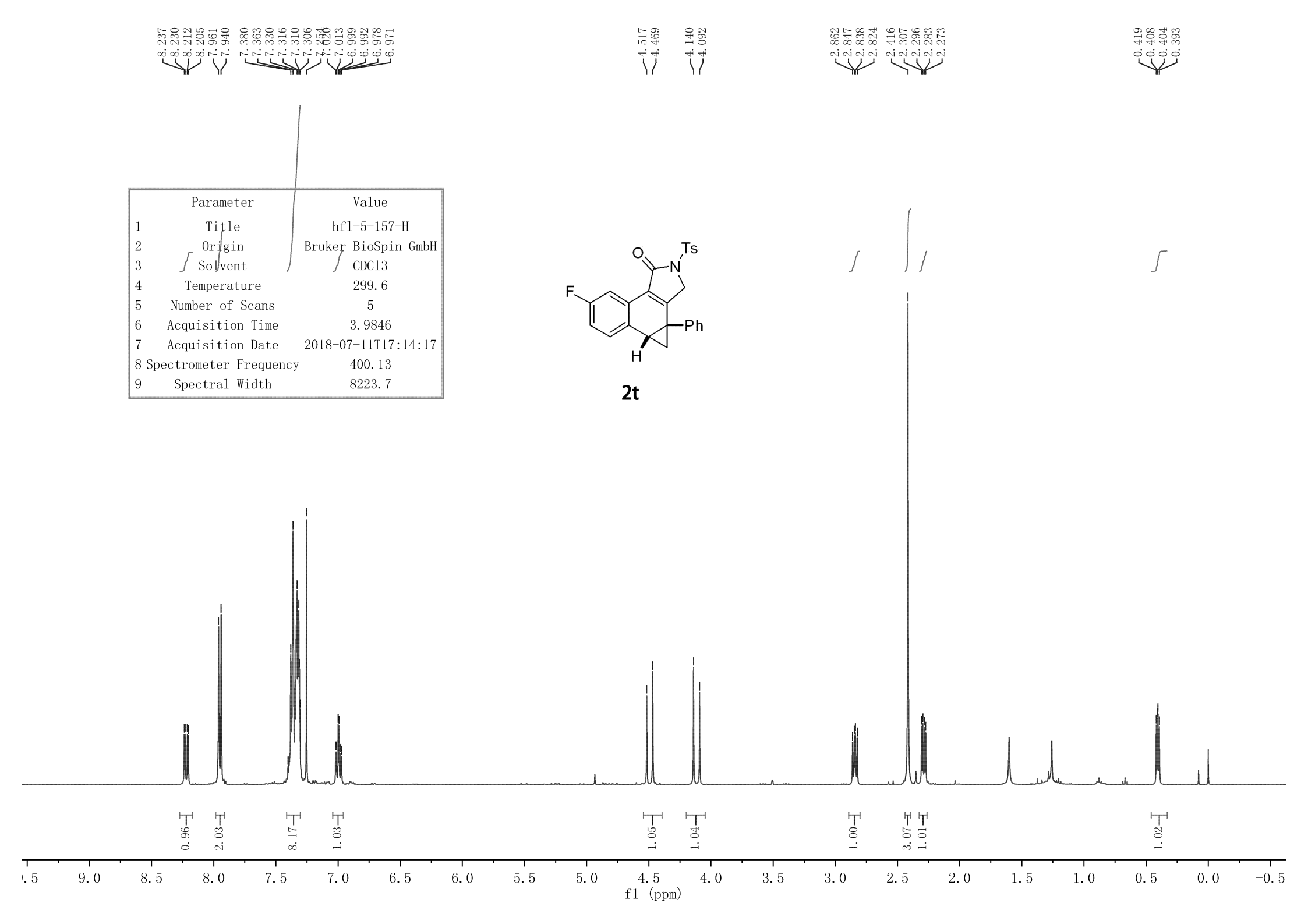
f1 (ppm)

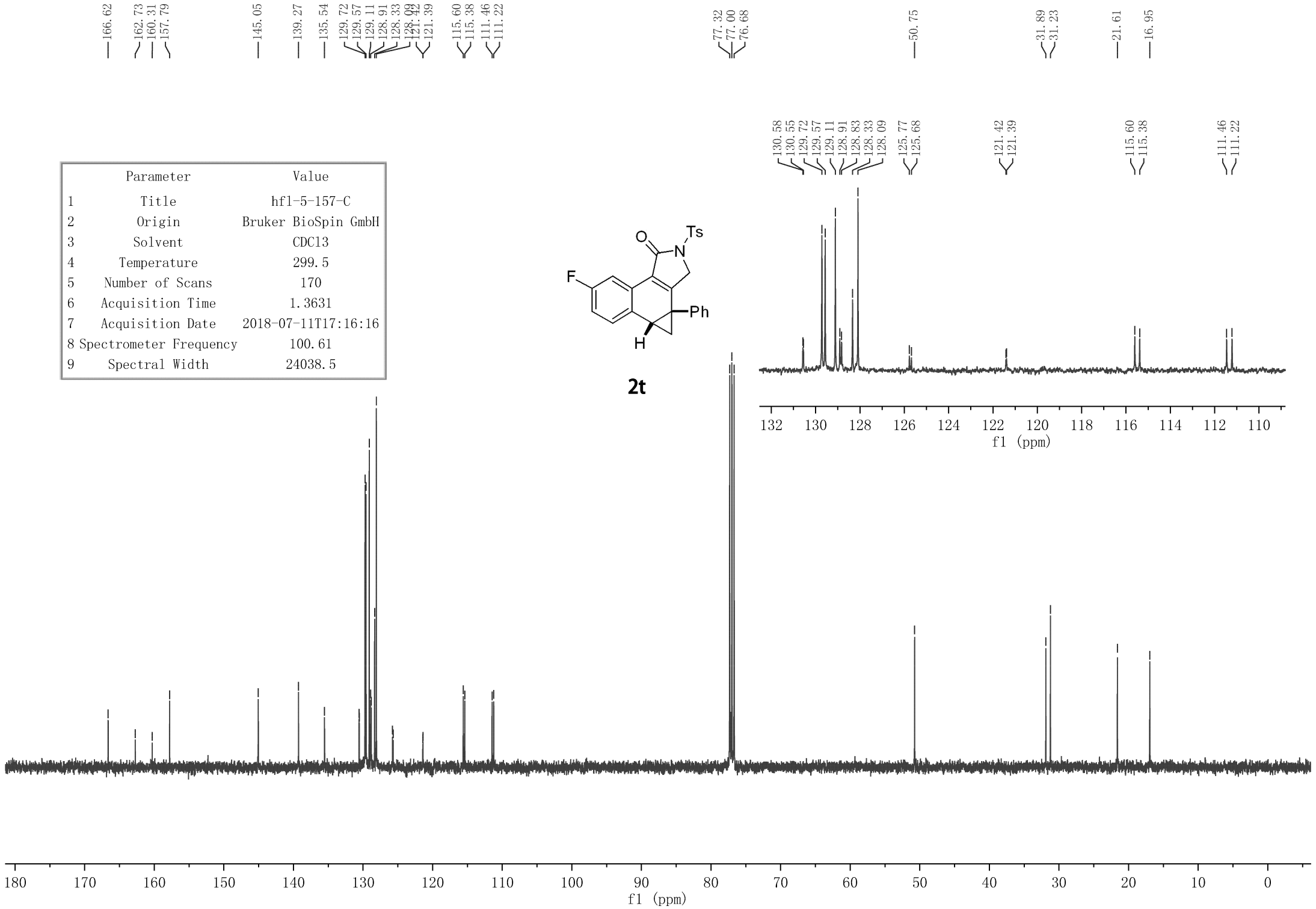

167.05
158.35
157.25
144.94
139.64
135.62
129.74
129.61
129.04
128.48
128.16
127.99
127.18
125.18
121.89
115.96
108.29
77.25
77.00
76.75
55.48
50.77
31.61
31.28
21.64
16.99
Parameter Value
1 Title HFL-OME-9.28-cc
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.8
5 Number of Scans 86
6 Acquisition Time 1.1010
7 Acquisition Date 2020-09-28T15:40:51
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
O
N
Ts
MeO
Ph
H
2s
f1 (ppm)

Parameter	Value
1 Title	HFL-OME-9.28-cc-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	15
6 Acquisition Time	1.1010
7 Acquisition Date	2020-09-28T15:44:42
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

2s

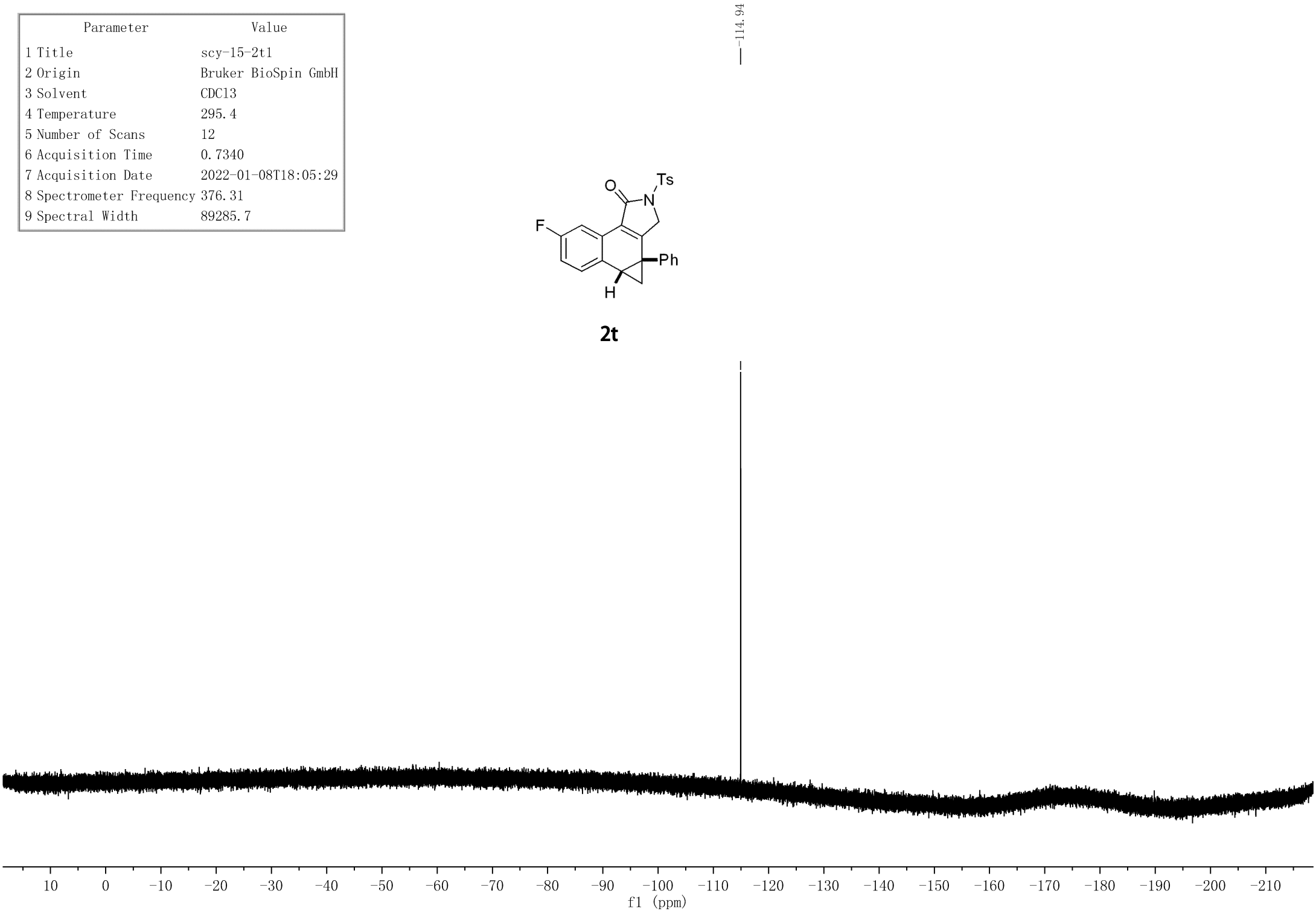



8.237
8.230
8.212
8.205
7.961
7.940
7.380
7.363
7.330
7.316
7.310
7.306
7.254
7.020
7.013
6.999
6.992
6.978
6.971
4.517
4.469
4.140
4.092
2.862
2.847
2.838
2.824
2.416
2.307
2.296
2.283
2.273
0.419
0.408
0.404
0.393
Parameter Value
1 Title hfl-5-157-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-11T17:14:17
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
N
Ts
F
Ph
H
2t
0.96
2.03
8.17
1.03
1.05
1.04
1.00
3.07
1.01
1.02
f1 (ppm)

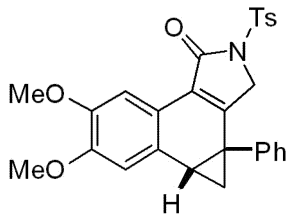

166.62
162.73
160.31
157.79
145.05
139.27
135.54
129.72
129.57
129.11
128.91
128.33
121.39
115.60
115.38
111.46
111.22
77.32
77.00
76.68
50.75
31.89
31.23
21.61
16.95
130.58
130.55
129.72
129.57
129.11
128.91
128.83
128.33
128.09
125.77
125.68
121.42
121.39
115.60
115.38
111.46
111.22
Parameter Value
1 Title hfl-5-157-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.5
5 Number of Scans 170
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-11T17:16:16
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
O
N
Ts
F
Ph
H
2t
132 130 128 126 124 122 120 118 116 114 112 110
f1 (ppm)
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	scy-15-2t1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	12
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-08T18:05:29
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

2t



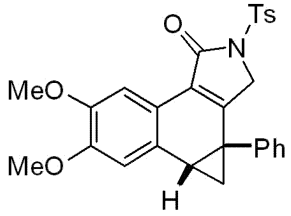
Parameter	Value
1 Title	HFL-DIOME-H-10.1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.4
5 Number of Scans	7
6 Acquisition Time	3.1719
7 Acquisition Date	2020-10-01T14:40:26
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6



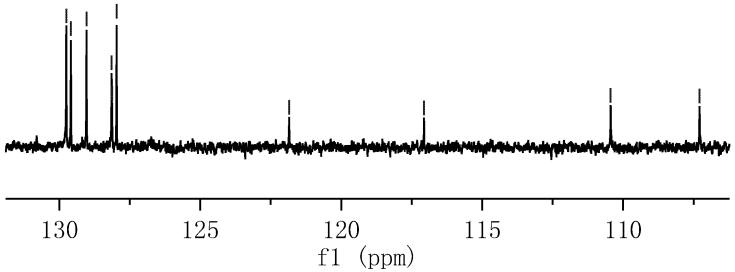
2u

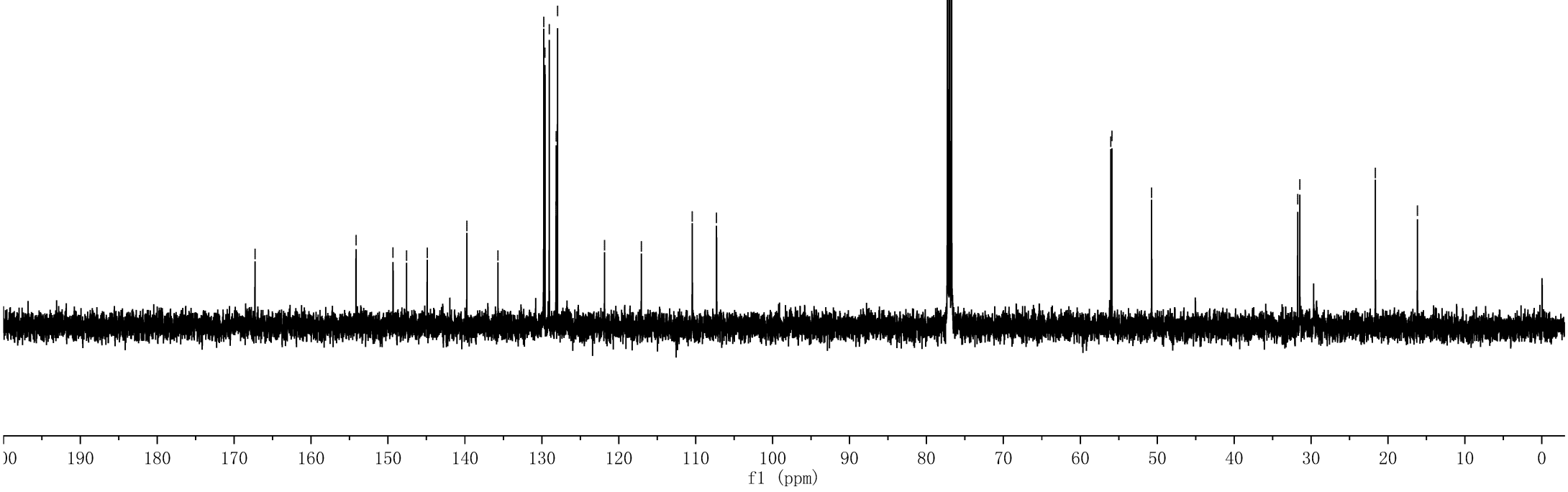
f1 (ppm)

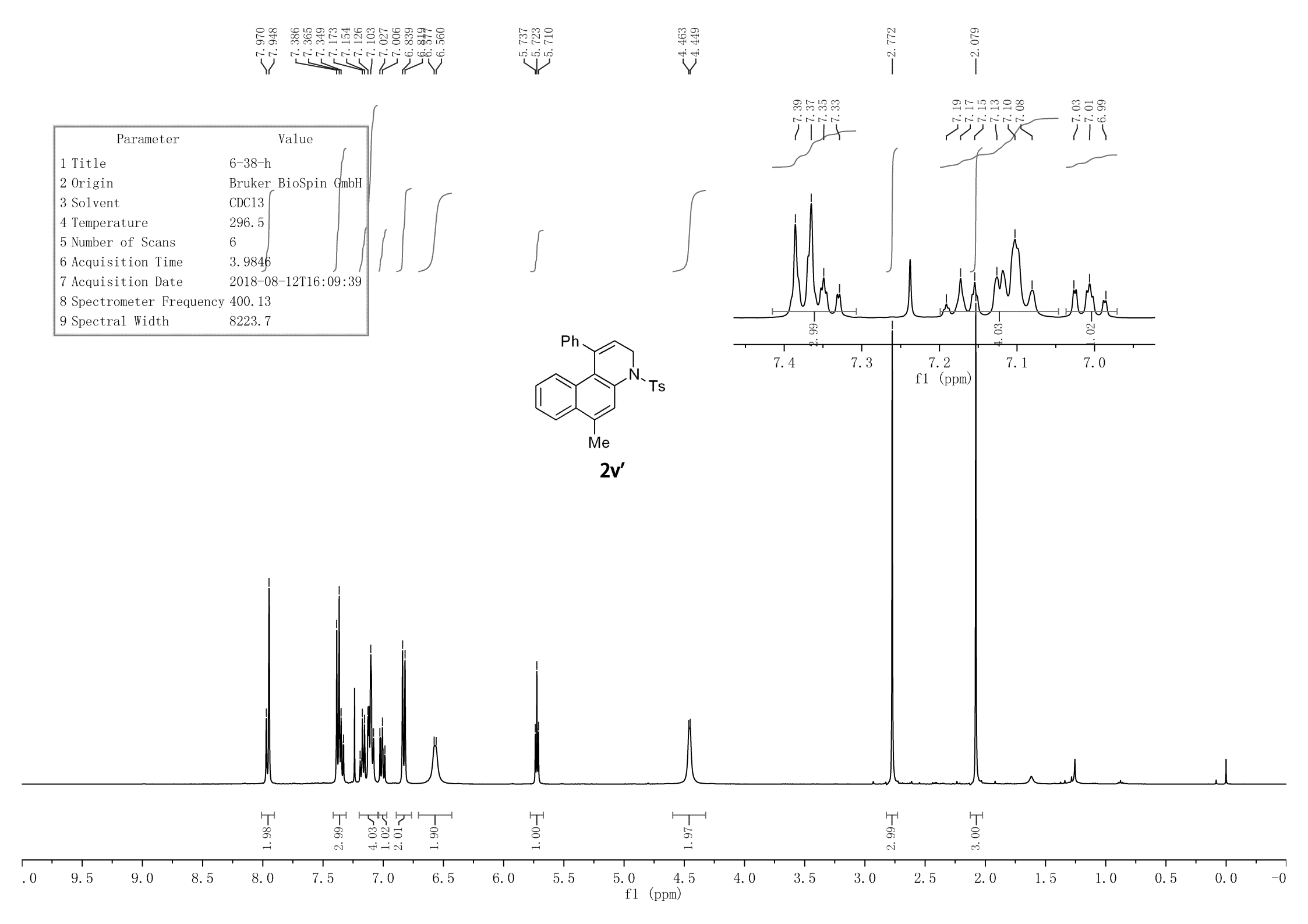
Parameter	Value
1 Title	HFL-DIOME-C-10.1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.4
5 Number of Scans	157
6 Acquisition Time	1.1010
7 Acquisition Date	2020-10-01T14:47:45
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9



2u

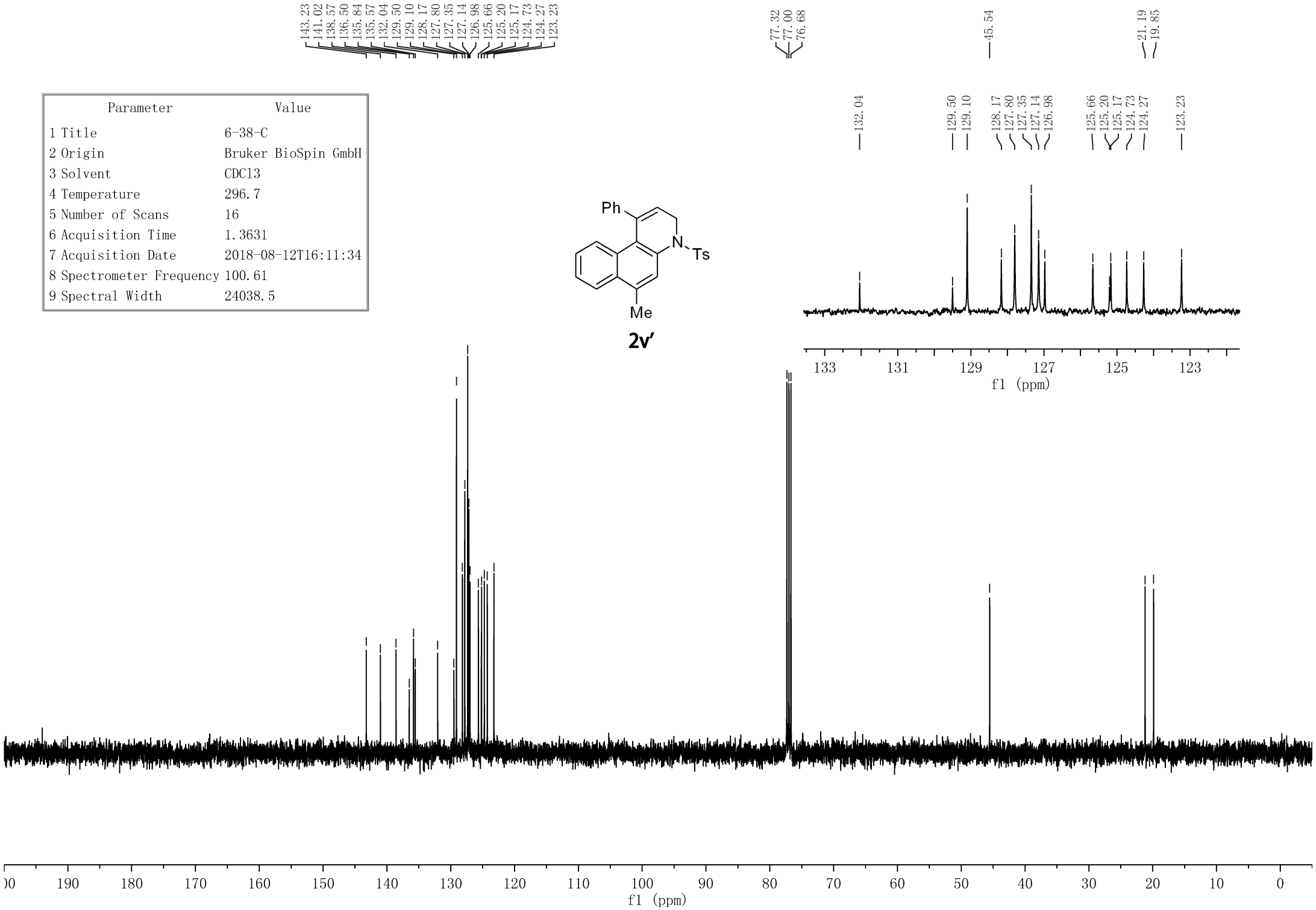


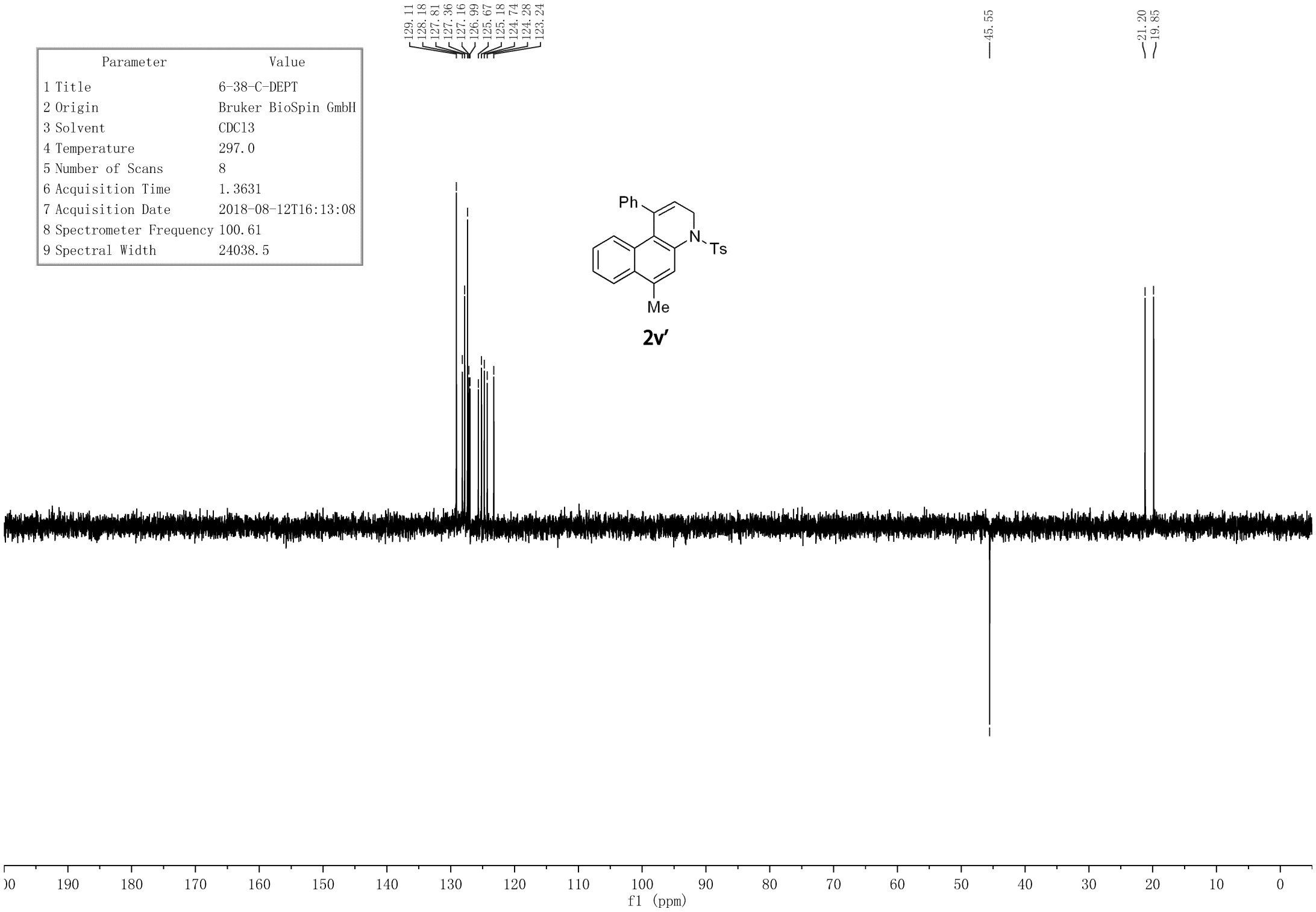



7.970
7.948
7.386
7.365
7.349
7.173
7.154
7.126
7.103
7.027
7.006
6.839
6.560
5.737
5.723
5.710
4.463
4.449
2.772
2.079
7.39
7.37
7.35
7.33
7.19
7.17
7.15
7.13
7.10
7.08
7.03
7.01
6.99
Parameter Value
1 Title 6-38-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.5
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-08-12T16:09:39
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
N
Ts
Me
2v′
2.99
4.03
1.02
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
1.98
2.99
4.03
1.02
2.01
1.90
1.00
1.97
2.99
3.00
f1 (ppm)

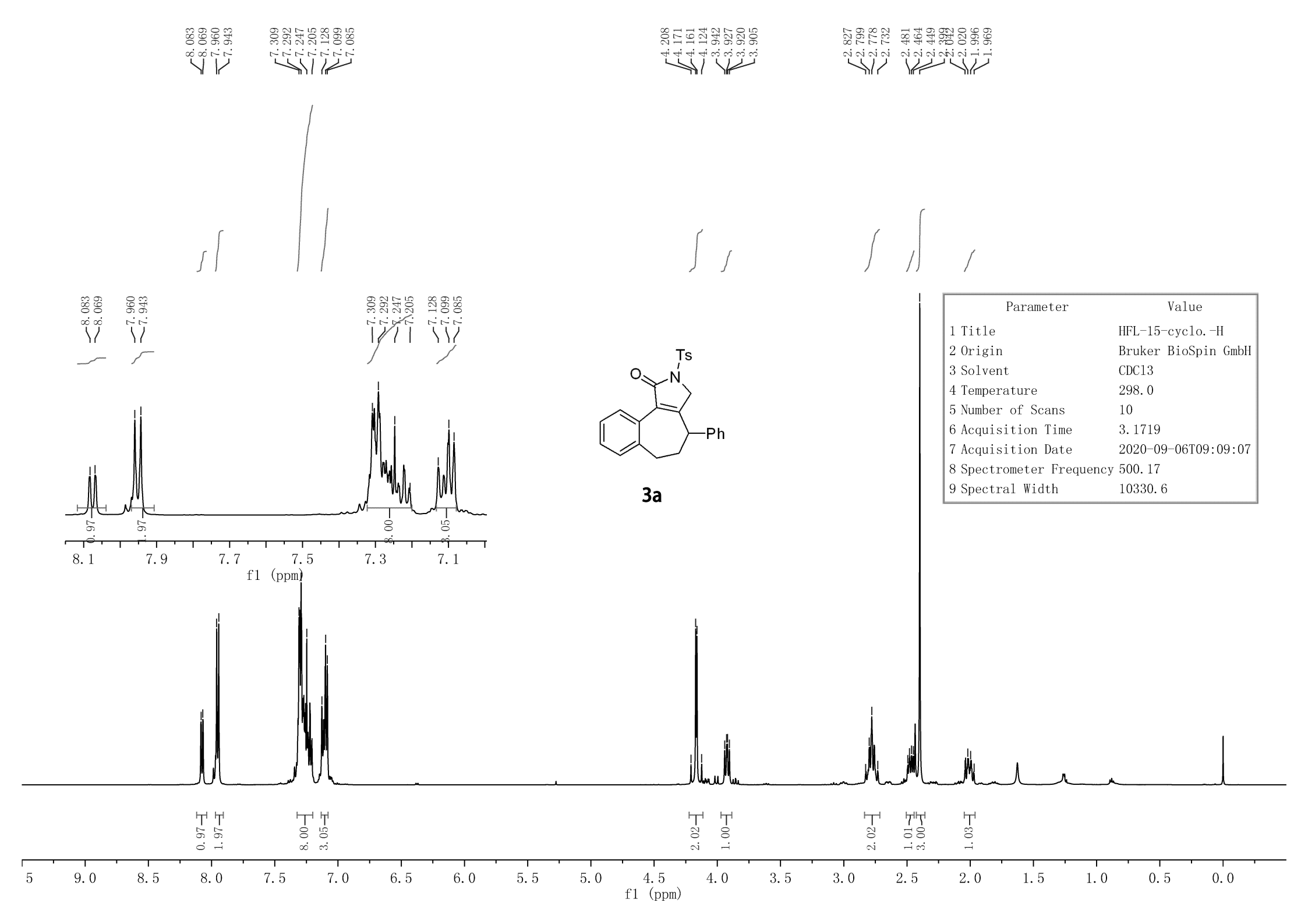
Parameter	Value
1 Title	6-38-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.7
5 Number of Scans	16
6 Acquisition Time	1.3631
7 Acquisition Date	2018-08-12T16:11:34
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

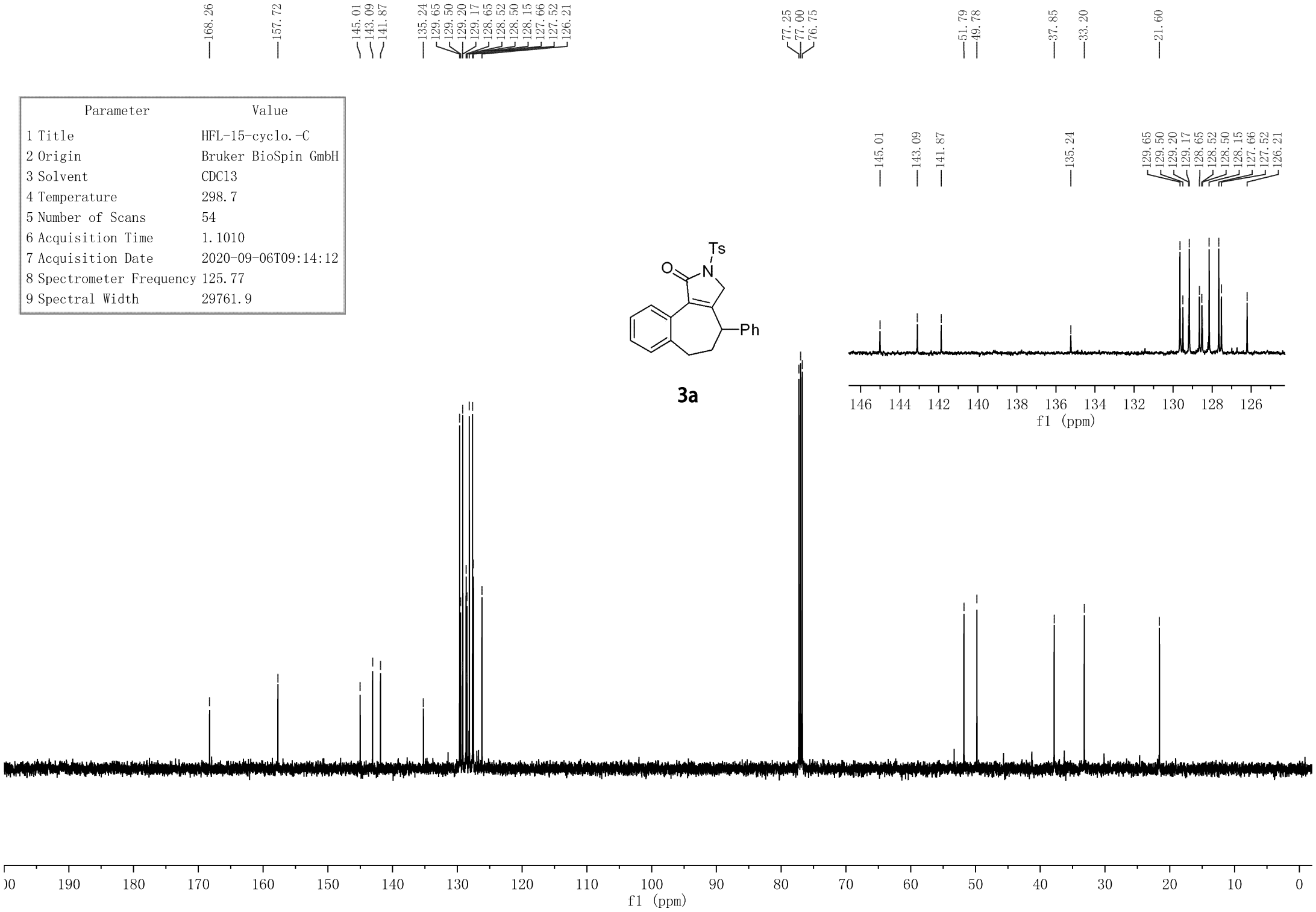
2v′





Parameter	Value
1 Title	6-38-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	8
6 Acquisition Time	1.3631
7 Acquisition Date	2018-08-12T16:13:08
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5


8.083
8.069
7.960
7.943
7.309
7.292
7.247
7.205
7.128
7.099
7.085
4.208
4.171
4.161
4.124
3.942
3.927
3.920
3.905
2.827
2.799
2.778
2.732
2.481
2.464
2.449
2.020
1.996
1.969
Ts
N
O
Ph
3a
Parameter Value
1 Title HFL-15-cyclo.-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDC13
4 Temperature 298.0
5 Number of Scans 10
6 Acquisition Time 3.1719
7 Acquisition Date 2020-09-06T09:09:07
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
0.97
1.97
8.00
3.05
2.02
1.00
2.02
1.01
3.00
1.03
f1 (ppm)


168.26
157.72
145.01
143.09
141.87
135.24
129.65
129.50
129.20
129.17
128.65
128.52
128.50
128.15
127.66
127.52
126.21
77.25
77.00
76.75
51.79
49.78
37.85
33.20
21.60
Parameter Value
1 Title HFL-15-cyclo.-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.7
5 Number of Scans 54
6 Acquisition Time 1.1010
7 Acquisition Date 2020-09-06T09:14:12
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
Ts
O
N
Ph
3a
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	HFL-15-cyclo.-C-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.6
5 Number of Scans	13
6 Acquisition Time	1.1010
7 Acquisition Date	2020-09-06T09:16:21
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9