Supporting Information

# One-pot synthesis of 2-hydroxymethylindoles via photoredox-catalyzed ketyl-ynamide coupling/1,3-allylic alcohol transposition

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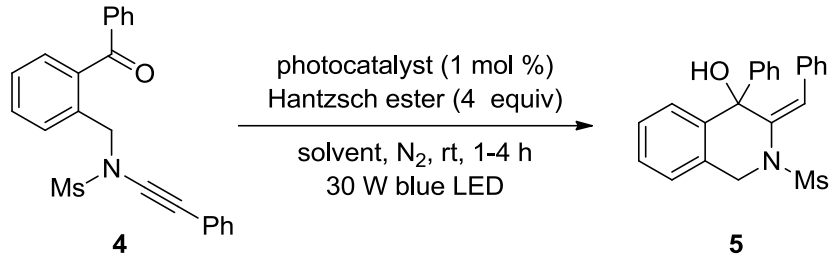
**General Information.** DMF, DMSO, DMA, MeCN, EtOAc, petroleum ether (PE), 1, 2-dichloroethane (DCE), dichloromethane (DCM), toluene, 1,4-dioxane and methanol (MeOH) which are all ACS grade were obtained commercially and used without further purification. Tetrahydrofuran (THF) was purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter ($cm^{-1}$). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

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

## More Reaction Condition

1. For the reaction condition studies on the photocatalysis of benzoyl ynamide **4**, please see as followed:[a]




**4** **5**

| Entry | Photocatalyst | Reaction Conditions | Yield[b] (%) |
|---|---|---|---|
| 1 | $[Ir(ppy)_2(dtbbpy)]PF_6$ | DMF, rt, 1 h | 25 |
| 2 | $[Ir(ppy)_2(dtbbpy)]PF_6$ | DMSO, rt, 1 h | 30 |
| **3** | **$[Ir(ppy)_2(dtbbpy)]PF_6$** | **DCE, rt, 1 h** | **53 (33)** |
| 4 | $[Ir(ppy)_2(dtbbpy)]PF_6$ | MeCN, rt, 1 h | 47 |
| 5 | $[Ir(dF(CF)_3ppy)_2(dtbbpy)]PF_6$ | DCE, rt, 1 h | 51 |
| 6 | *fac*-$Ir(ppy)_3$ | DCE, rt, 1 h | 27 |
| 7 | 4CzIPN | DCE, rt, 1 h | 44 |
| 8 | $Ru(bpy)_3(PF_6)_2$ | DCE, rt, 7 h | 20 |
| 9[c] | $[Ir(ppy)_2(dtbbpy)]PF_6$ | DCE, rt, 1 h | 45 |
| 10[d] | $[Ir(ppy)_2(dtbbpy)]PF_6$ | DCE, rt, 1 h | 27 |

[a]Reaction conditions: **3a** (0.03 mmol), Hantzsch ester (0.12 mmol), photocatalyst (0.3 umol), solvent (0.3 mL), $N_2$, rt, 2-4 h, $N_2$; 30 W blue LED is used and the distance between light soure and vail is about 3 cm. [b]Estimated by $^1H$ NMR using Hantzsch ester and Hantzsch pyridine as internal reference. [c]2 equiv of Hantzsch ester was used. [d]3 equiv of Hantzsch ester was used.

**Preliminary Cell Viability Assay.**

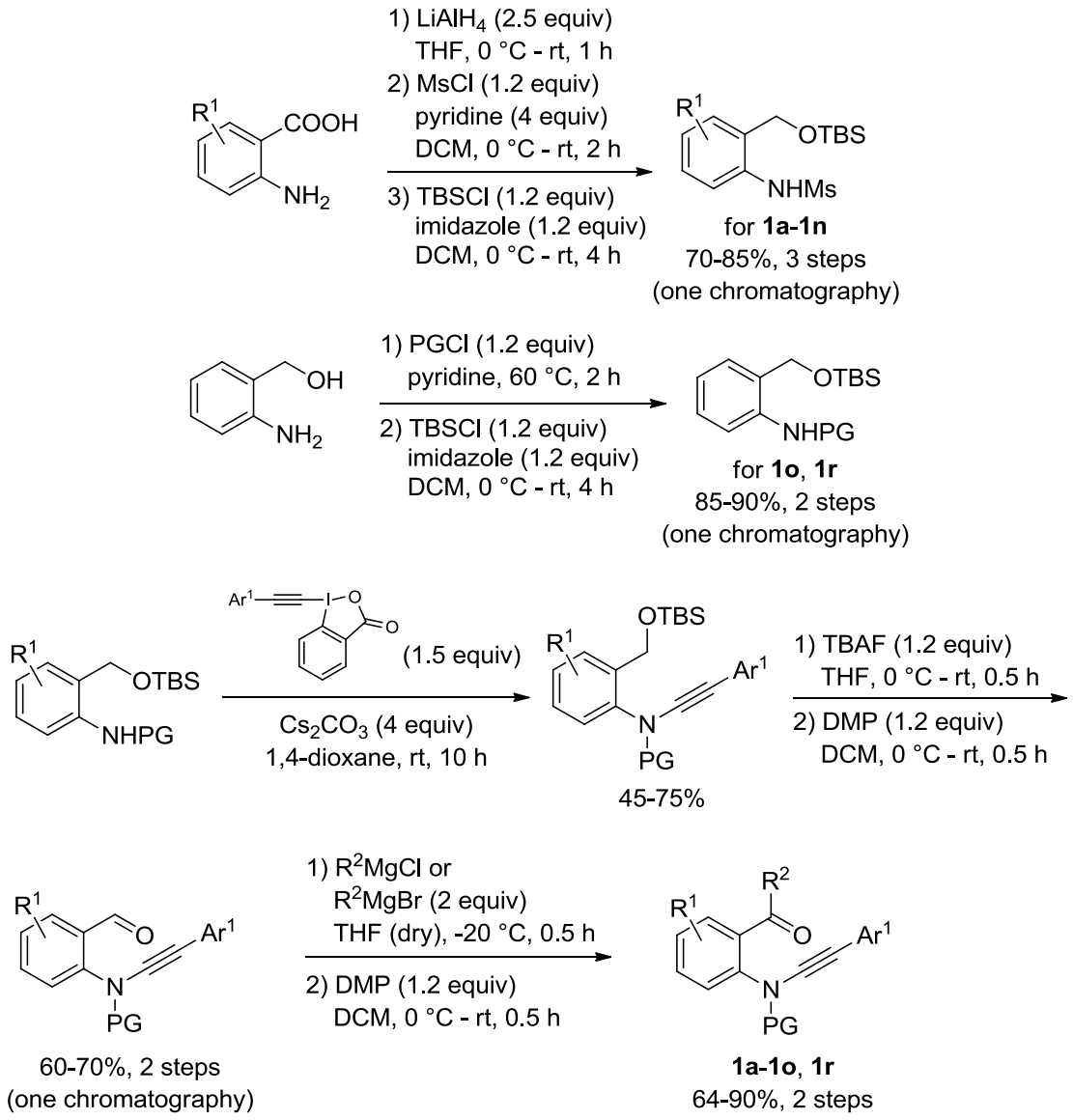
We also tested the newly synthesized 2-hydroxymethylindoles **3a**-**3h** and **3l**-**3n** for their bioactivity as antitumor agents. The cytotoxic effects of these compounds were evaluated against a panel of cancer cells, including breast cancer cells MDA-MB-231 and MCF-7, melanoma cells A375, and esophageal cancer cells SK-GT-4 and KYSE-450 based on cell viability assays, using a commercially available proliferation assay kit (Promega, US). Briefly, the cells were plated in 96-well culture plates at an appropriate density in culture medium and allowed to attach overnight. After treatment of vehicle (0.1% DMSO as control) or test compounds for indicated times and concentrations, 20 μL of MTS reaction solution (3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium, inner salt; MTS (a) and 100 μg/mL phenazine methosulfate; PES) was added to each well. The absorbance values were read at 490 nm wavelength with a spectrophotometer (Varioskan Flash, Thermo, US) after 1 to 4 hours incubation. The cell viability was calculated as: cell survival = (ODcompd. - ODblank)/(ODcontrol - ODblank)*100%.

**Table S1.** The cytotoxic effects of the newly synthesized 2-hydroxymethylindoles against cancer cells

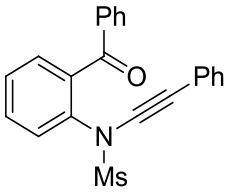
| Cmpd ID | Cell viability at 20 μM (%) | | | | |
|---|---|---|---|---|---|
| | MDA-MB-231 | A375 | MCF-7 | SK-GT-4 | KYSE-450 |
| **3a** | 89.92 | 0.79 | 56.73 | 23.02 | 111.06 |
| **3b** | 92.45 | 45.26 | 64.44 | 33.66 | 108.45 |
| **3c** | 92.45 | 7.97 | 35.66 | 25.24 | 112.66 |
| **3d** | 89.92 | 71.02 | 68.76 | 91.45 | 101.78 |
| **3e** | 91.43 | 75.33 | 57.00 | 75.22 | 117.71 |
| **3f** | 102.08 | 64.28 | 61.73 | 56.37 | 113.31 |
| **3g** | 102.67 | 72.33 | 71.76 | 60.89 | 114.27 |
| **3h** | 93.67 | 76.10 | 80.98 | 82.91 | 108.67 |
| **3l** | 93.96 | 74.62 | 59.95 | 54.06 | 92.99 |
| **3m** | 91.33 | 72.93 | 87.73 | 75.01 | 110.84 |
| **3n** | 92.68 | 86.64 | 96.80 | 93.25 | 94.38 |

Results are average of two experiments.

**Representative synthetic procedures for the preparation of benzoyl ynamides 1a-1o, 1r**[1,2]




***N*-(2-benzoylphenyl)-*N*-(phenylethynyl)methanesulfonamide (1a)**

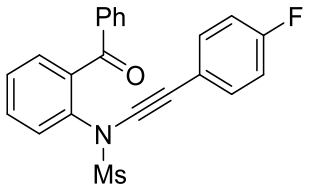


**1a**

Pale yellow solid (mp 101-102 $^{o}$C). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.82 (m, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.61 – 7.51 (m, 2H), 7.47 – 7.38 (m, 4H), 7.20 – 7.12 (m, 1H), 7.12 – 7.04 (m, 2H), 6.93 – 6.87 (m, 2H), 3.29 (s, 3H); $^{13}$C NMR (100 MHz,

$CDCl_3$) δ 195.1, 137.1, 136.6, 136.0, 133.4, 131.3, 131.2, 130.3, 129.6(1), 129.5(6), 128.4, 127.9(4), 127.8(5), 121.8, 82.3, 71.2, 38.3; IR (neat): 2955, 2925, 2852, 2241(s), 1667(s), 1366, 1167, 759, 700, 549; HRESIMS Calcd for $[C_{22}H_{17}NNaO_3S]^+$ ($M + Na^+$) 398.0821, found 398.0822.

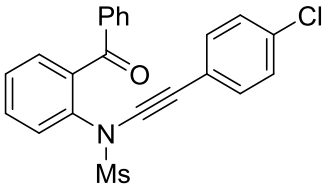
***N*-(2-benzoylphenyl)-*N*-((4-fluorophenyl)ethynyl)methanesulfonamide (1b)**




**1b**

White solid (mp 104-105 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.81 (m, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.50 (m, 2H), 7.46 – 7.35 (m, 4H), 6.92 – 6.82 (m, 2H), 6.81 – 6.73 (m, 2H), 3.29 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 194.9, 162.1 (d, *J* = 248.0 Hz), 137.0, 136.5, 135.9, 133.4 (d, *J* = 8.0 Hz), 131.1, 130.2, 129.4(4), 129.4(0), 128.4, 127.9, 117.7 (d, *J* = 3.0 Hz), 115.0 (d, *J* = 22.0 Hz), 82.0, 70.0, 38.2; IR (neat): 2954, 2926, 2852, 2244, 1667(s), 1598, 1509, 1366(s), 1169(s), 964, 837, 772; HRESIMS Calcd for $[C_{22}H_{16}FNNaO_3S]^+$ ($M + Na^+$) 416.0727, found 416.0725.

***N*-(2-benzoylphenyl)-*N*-((4-chlorophenyl)ethynyl)methanesulfonamide (1c)**

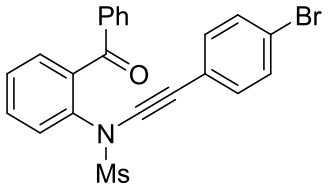



**1c**

White solid (mp 129-130 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.81 (m, 2H), 7.74 – 7.67 (m, 1H), 7.62 – 7.53 (m, 2H), 7.49 – 7.38 (m, 4H), 7.09 – 7.02 (m, 2H), 6.82 – 6.75 (m, 2H), 3.31 (s, 3H); $^{13}C$ NMR (100MHz, $CDCl_3$) δ 195.0, 137.0, 136.6, 135.9, 133.9, 133.5, 132.5, 131.3, 130.3, 129.6(4), 129.5(7), 128.5, 128.2, 128.0, 120.4, 83.2, 70.3, 38.5; IR (neat): 2955, 2927, 2853, 2241(s), 1665(s), 1597, 1448,

1366(s), 1168(s), 1091, 764, 701; HRESIMS Calcd for $[C_{22}H_{16}ClNNaO_3S]^+$ (M + $Na^+$) 432.0432, found 432.0428.

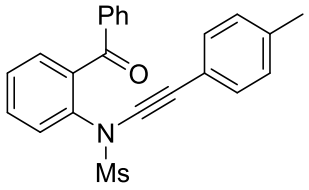
***N*-(2-benzoylphenyl)-*N*-((4-bromophenyl)ethynyl)methanesulfonamide (1d)**




**1d**

White solid (mp 133-134 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.81 (m, 2H), 7.74 – 7.68 (m, 1H), 7.61 – 7.53 (m, 2H), 7.47 – 7.38 (m, 4H), 7.24 – 7.17 (m, 2H), 6.75 – 6.67 (m, 2H), 3.31 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 195.0, 137.0, 136.6, 135.9, 133.5, 132.7, 131.2, 131.1, 130.3, 129.6(2), 129.5(6), 128.5, 128.0, 122.1, 120.8, 83.4, 70.4, 38.5; IR (neat): 2956, 2926, 2852, 2241(s), 1667, 1597, 1447, 1367(s), 1168(s), 1076, 763, 701; HRESIMS Calcd for $[C_{22}H_{16}BrNNaO_3S]^+$ (M + $Na^+$) 475.9926, found 475.9928.

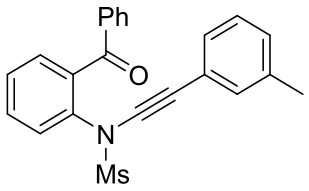
***N*-(2-benzoylphenyl)-*N*-(*p*-tolylethynyl)methanesulfonamide (1e)**




**1e**

White solid (mp 117-118 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ7.88 – 7.79 (m, 2H), 7.72 – 7.65 (m, 1H), 7.58 – 7.49 (m, 2H), 7.45 – 7.35 (m, 4H), 6.93 – 6.86 (m, 2H), 6.85 – 6.77 (m, 2H), 3.26 (s, 3H), 2.22 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 195.0, 138.1, 137.1, 136.6, 136.0, 133.3, 131.3, 131.2, 130.2, 129.5, 129.4, 128.6, 128.3, 127.8, 118.5, 81.6, 71.2, 38.0, 21.2; IR (neat): 2954, 2924, 2241, 1667, 1597, 1448, 1365, 1168, 963, 817, 768, 706; HRESIMS Calcd for $[C_{23}H_{19}NNaO_3S]^+$ (M + $Na^+$) 412.0978, found 412.0976.

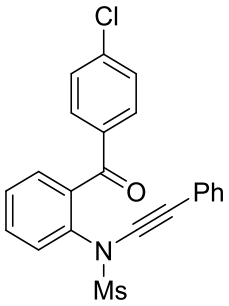
***N*-(2-benzoylphenyl)-*N*-(*m*-tolylethynyl)methanesulfonamide (1f)**




**1f**

Pale yellow solid (mp 67-68 $^{o}$C). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.79 (m, 2H), 7.74 – 7.65 (m, 1H), 7.60 – 7.49 (m, 2H), 7.46 – 7.34 (m, 4H), 7.01 – 6.90 (m, 2H), 6.78 – 6.71 (m, 1H), 6.61 (s, 1H), 3.27 (s, 3H), 2.12 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.9, 137.4, 137.1, 136.5, 135.9, 133.3, 131.7, 131.1, 130.2, 129.5, 129.4, 128.7, 128.3, 128.2, 127.8, 127.7, 121.5, 81.9, 71.3, 38.1, 20.8; IR (neat): 2955, 2925, 2240, 1667(s), 1597, 1448, 1366(s), 1168(s), 963, 768, 700; HRESIMS Calcd for $[C_{23}H_{19}NNaO_3S]^+$ (M + $Na^+$) 412.0978, found 412.0975.

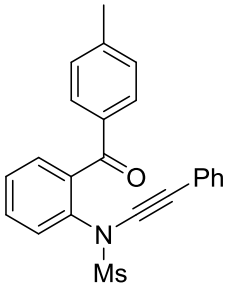
***N*-(2-(4-chlorobenzoyl)phenyl)-*N*-(phenylethynyl)methanesulfonamide (1g)**




**1g**

Pale yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.74 (m, 2H), 7.74 – 7.68 (m, 1H), 7.62 – 7.55 (m, 1H), 7.47 – 7.34 (m, 4H), 7.21 – 7.09 (m, 3H), 6.99 – 6.93 (m, 2H), 3.29 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.8, 140.0, 137.2, 135.7, 135.1, 131.6, 131.5, 131.4, 129.5, 129.4, 128.7, 128.2, 128.1, 128.0, 121.7, 82.4, 71.4, 38.3; IR (neat): 2955, 2926, 2241, 1668(s), 1587, 1367(s), 1168(s), 1091, 963, 746; HRESIMS Calcd for $[C_{22}H_{16}ClNNaO_3S]^+$ (M + $Na^+$) 432.0432, found 432.0430.

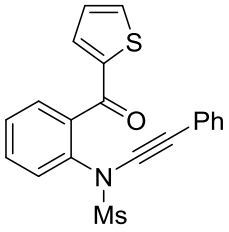
***N*-(2-(4-methylbenzoyl)phenyl)-*N*-(phenylethynyl)methanesulfonamide (1h)**




**1h**

Pale yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.73 (m, 2H), 7.72 – 7.68 (m, 1H), 7.59 – 7.54 (m, 1H), 7.47 – 7.38 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.13 (m, 1H), 7.12 – 7.06 (m, 2H), 6.93 – 6.86 (m, 2H), 3.30 (s, 3H), 2.39 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.8, 144.5, 137.1, 136.5, 134.3, 131.5, 131.0, 130.6, 129.7, 129.5, 129.2, 127.9, 127.8, 122.0, 82.4, 71.3, 38.4, 21.6; IR (neat): 2957, 2924, 2851, 2241, 1662, 1604, 1444, 1366, 1167, 963, 915, 759; HRESIMS Calcd for $[C_{23}H_{19}NNaO_3S]^+$ (M + $Na^+$) 412.0978, found 412.0978.

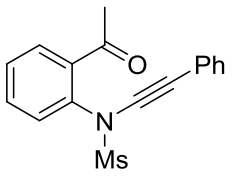
***N*-(phenylethynyl)-*N*-(2-(thiophene-2-carbonyl)phenyl)methanesulfonamide (1i)**




**1i**

Pale yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 2H), 7.61 – 7.54 (m, 2H), 7.51 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.21 – 7.15 (m, 1H), 7.14 – 7.05 (m, 3H), 6.98 – 6.92 (m, 2H), 3.36 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 187.0, 144.0, 136.9, 135.8, 135.3, 131.4, 131.3, 130.1, 129.4, 128.2, 128.0, 127.9(2), 127.8(9), 122.0, 82.3, 71.4, 38.5; IR (neat): 2956, 2925, 2852, 2242, 1643(s), 1411, 1365(s), 1167(s), 963, 759, 728; HRESIMS Calcd for $[C_{20}H_{15}NNaO_3S_2]^+$ (M + $Na^+$) 404.0386, found 404.0388.

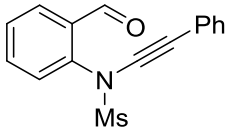
***N*-(2-acetylphenyl)-*N*-(phenylethynyl)methanesulfonamide (1j)**




**1j**

Pale yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.59 – 7.53 (m, 1H), 7.50 – 7.44 (m, 1H), 7.44 – 7.39 (m, 2H), 7.32 – 7.27 (m, 3H), 3.31 (s, 3H), 2.65 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 199.7, 137.3, 135.9, 132.2, 131.7, 129.2, 129.0, 128.3(0), 128.2(8), 122.0, 82.0, 70.9, 38.0, 29.6; IR (neat): 3020, 2928, 2850, 2240(s), 1698(s), 1597, 1484, 1444, 1363(s), 1167(s), 961, 757, 692; HRESIMS Calcd for $[C_{17}H_{15}NNaO_3S]^+$ (M + $Na^+$) 336.0665, found 336.0671.

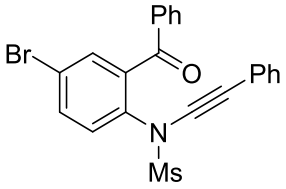
***N*-(2-formylphenyl)-*N*-(phenylethynyl)methanesulfonamide (1k)**




**1k**

Pale yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.04 – 7.97 (m, 1H), 7.74 – 7.64 (m, 2H), 7.59 – 7.51 (m, 1H), 7.49 – 7.41 (m, 2H), 7.34 – 7.24 (m, 3H), 3.27 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 188.5, 139.8, 134.9, 133.1, 131.6, 129.6, 129.4, 128.5, 128.3, 127.3, 121.5, 81.8, 71.0, 36.9; IR (neat): 2930, 2241, 1698(s), 1597, 1367, 1167, 961, 754, 550, 501; HRESIMS Calcd for $[C_{16}H_{13}NNaO_3S]^+$ (M + $Na^+$) 322.0508, found 322.0509.

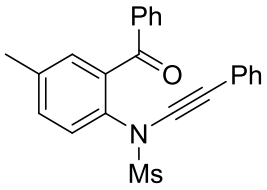
***N*-(2-benzoyl-4-bromophenyl)-*N*-(phenylethynyl)methanesulfonamide (1l)**




**1l**

White solid (mp 141-142 $^{o}$C). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.2 Hz, 2H), 7.68 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.61 – 7.50 (m, 3H), 7.47 – 7.39 (m, 2H), 7.20 – 7.12 (m, 1H), 7.12 – 7.03 (m, 2H), 6.92 – 6.84 (m, 2H), 3.28 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.5, 137.6, 136.2, 136.0, 134.1, 133.8, 132.1, 131.3, 131.0, 130.2, 128.6, 128.1, 127.9, 121.8, 121.5, 81.8, 71.7, 38.3; IR (neat): 2958, 2923, 2240, 1668, 1366, 1285, 1168, 1070, 963, 914, 756; HRESIMS Calcd for $[C_{22}H_{16}BrNNaO_3S]^+$ (M + $Na^+$) 475.9926, found 475.9922.

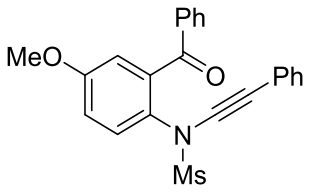
**_N_-(2-benzoyl-4-methylphenyl)-_N_-(phenylethynyl)methanesulfonamide (1m)**




**1m**

White solid (mp 95-96 $^{o}$C). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.2 Hz, 2H), 7.62 – 7.50 (m, 2H), 7.46 – 7.32 (m, 3H), 7.26 – 7.19 (m, 1H), 7.18 – 7.04 (m, 3H), 6.95 – 6.86 (m, 2H), 3.25 (s, 3H), 2.37 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.2, 138.4, 136.7, 135.9, 134.5, 133.3, 131.8, 131.3, 130.2, 129.9, 129.2, 128.4, 127.8, 121.9, 82.4, 70.9, 38.1, 20.9; IR (neat): 2955, 2926, 2852, 2240, 1668(s), 1365(s), 1167(s), 962, 758; HRESIMS Calcd for $[C_{23}H_{19}NNaO_3S]^+$ (M + $Na^+$) 412.0978, found 412.0976.

**_N_-(2-benzoyl-4-methoxyphenyl)-_N_-(phenylethynyl)methanesulfonamide (1n)**

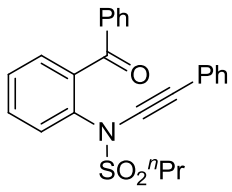



**1n**

Pale yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.83 (m, 2H), 7.61 (d, *J* = 8.8 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.46 – 7.39 (m, 2H), 7.20 – 7.13 (m, 1H), 7.13 – 7.04 (m, 3H), 6.96 – 6.89 (m, 3H), 3.81 (s, 3H), 3.24 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$)

δ 194.8, 158.9, 137.5, 136.6, 133.5, 131.4, 130.9, 130.3, 129.5, 128.5, 127.9, 122.0, 116.3, 114.9, 82.5, 70.9, 55.8, 38.1; IR (neat): 2955, 2927, 2851, 2240(s), 1668(s), 1492, 1365(s), 1167(s), 961, 758; HRESIMS Calcd for $[C_{23}H_{19}NNaO_4S]^+$ (M + $Na^+$) 428.0927, found 428.0925.

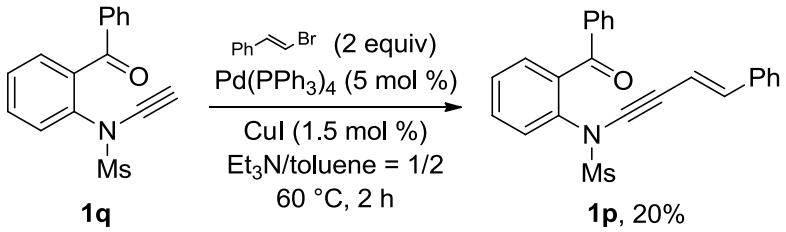
**_N_-(2-benzoylphenyl)-_N_-(phenylethynyl)propane-1-sulfonamide (1o)**




**1o**

Pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.81 (m, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.61 – 7.51 (m, 2H), 7.47 – 7.37 (m, 4H), 7.19 – 7.13 (m, 1H), 7.12 – 7.05 (m, 2H), 6.96 – 6.89 (m, 2H), 3.49 – 3.42 (m, 2H), 2.00 – 1.85 (m, 2H), 1.07 (t, *J* = 7.6 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.0, 137.2, 136.7, 136.2, 133.3, 131.3, 131.2, 130.3, 129.6, 129.3, 128.4, 127.9, 127.8, 122.0, 82.8, 70.7, 53.5, 16.9, 12.9; IR (neat): 3060, 2971, 2935, 2241(s), 1668(s), 1597, 1445, 1368(s), 1160(s), 761, 700; HRESIMS Calcd for $[C_{24}H_{21}NNaO_3S]^+$ (M + $Na^+$) 426.1134, found 426.1127.

**(*E*)-*N*-(2-benzoylphenyl)-*N*-(4-phenylbut-3-en-1-yn-1-yl)methanesulfonamide (1p)**[1]

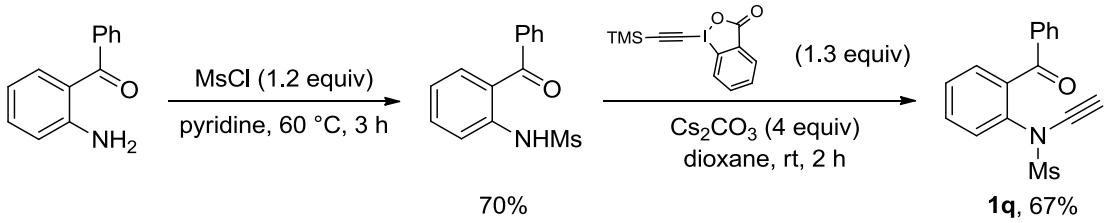



**1q** **1p**, 20%

To a solution of ynamide **1q** (2 mmol, 598 mg) in $Et_3N$/toluene (1:2) mixed solvent (30 mL) was added styrene (4 mmol, 0.51 mL). And then the reaction was stirred for a while followed by addition of $Pd(PPh_3)_4$ (0.1 mmol, 116 mg) and CuI (0.03 mmol, 5.9 mg). Then, the solution was stirred at 60 $^o$C until TLC analysis showed the complete consumption of substrate (about 2 h). The residue was filtered through a Celite pad

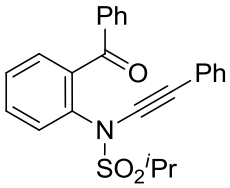
and the filtrate was concentrated. The resulting mixture was purified by chromatography on silica gel (eluent: PE/EtOAc) to afford the desired ynamide **1p** in 20% yield.[3] Pale red oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.85 (m, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.63 – 7.55 (m, 2H), 7.52 – 7.40 (m, 4H), 7.29 – 7.20 (m, 3H), 7.15 – 7.09 (m, 2H), 6.18 (d, *J* = 16.0 Hz, 1H), 5.82 (d, *J* = 16.0 Hz, 1H), 3.30 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.2, 140.0, 137.3, 136.7, 136.1, 136.0, 133.6, 131.2, 130.5, 129.7, 129.5, 128.6, 128.5, 128.4, 127.9, 126.0, 106.5, 84.5, 71.2, 38.4; IR (neat): 3030, 2923, 2225(s), 1667(s), 1597, 1448, 1366(s), 1167(s), 964, 701; HRESIMS Calcd for $[C_{24}H_{19}NNaO_3S]^+$ (M + $Na^+$) 424.0978, found 424.0976.

**_N_-(2-benzoylphenyl)-_N_-ethynylmethanesulfonamide (1q)**




Pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.79 (m, 2H), 7.68 – 7.63 (m, 1H), 7.63 – 7.55 (m, 2H), 7.50 – 7.42 (m, 4H), 3.22 (s, 3H), 2.72 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.0, 136.7, 136.3, 136.2, 133.4, 131.6, 130.2, 129.4, 128.4, 128.3, 75.7, 60.0, 38.2; IR (neat): 3294(s), 3061, 3029, 2932, 2133(s), 1667(s), 1597, 1449, 1366(s), 1170(s), 964, 768, 701; HRESIMS Calcd for $[C_{16}H_{13}NNaO_3S]^+$ (M + $Na^+$) 322.0508, found 336.0509.

**_N_-(2-benzoylphenyl)-_N_-(phenylethynyl)propane-2-sulfonamide (1r)**

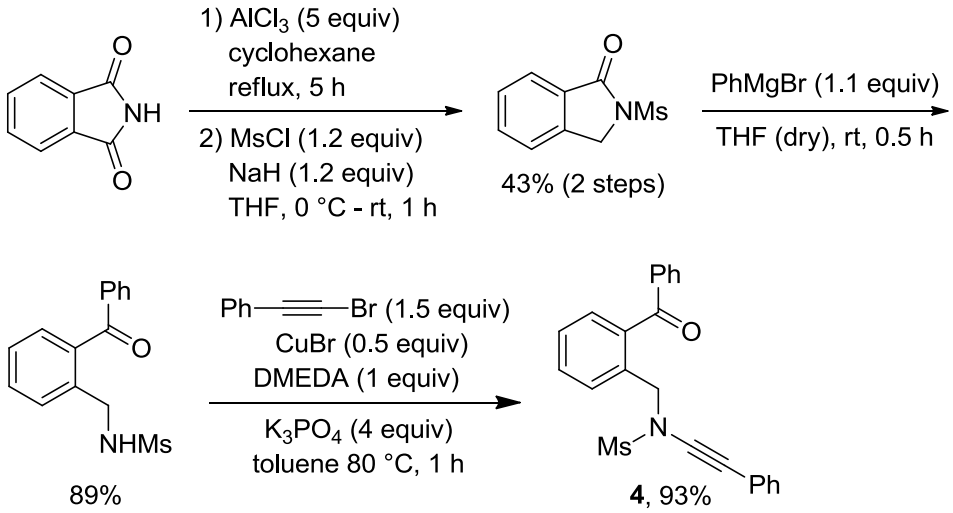



**1r**

Pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.81 (m, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.49 (m, 2H), 7.45 – 7.36 (m, 4H), 7.19 – 7.07 (m, 3H), 7.03 – 6.95

(m, 2H), 3.94 – 3.82 (m, 1H), 1.45 (d, *J* = 6.8 Hz, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.0, 137.4, 136.7, 136.5, 133.3, 131.2(1), 131.1(6), 130.2, 129.6, 128.9, 128.3, 127.9, 127.8, 127.7, 122.1, 83.8, 69.9, 55.5, 17.0; IR (neat): 3061, 2990, 2938, 2241(s), 1669(s), 1597, 1444, 1359(s), 1151, 758, 693; HRESIMS Calcd for $[C_{24}H_{21}NNaO_3S]$+ (M + Na+) 426.1134, found 426.1139.

**_N_-(2-benzoylbenzyl)-_N_-(phenylethynyl)methanesulfonamide (4)**[1]

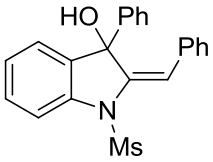



White solid (mp 96-97 $^{o}$C). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.77 (m, 2H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.61 – 7.49 (m, 2H), 7.44 – 7.32 (m, 4H), 7.23 – 7.15 (m, 3H), 7.15 – 7.10 (m, 2H), 4.95 (s, 2H), 3.04 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 197.4, 138.0, 137.4, 134.7, 133.2, 131.2, 131.1, 130.6, 130.4, 129.8, 128.3, 128.1, 127.8, 127.6, 122.3, 81.8, 71.7, 52.3, 38.3; IR (neat): 3057, 3023, 2928, 2238(s), 1660(s), 1597, 1448, 1359(s), 1165(s), 757, 703; HRESIMS Calcd for $[C_{23}H_{19}NNaO_3S]^+$ (M + $Na^+$) 412.0978, found 412.0977.

**General procedure for the synthesis of 2-hydroxymethylindoles 3:**


To a 10-mL oven-dried Schlenk tube containing a stirrer bar was mixed with substrate **1** (0.2 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (0.002 mmol, 1.8 mg), Hantzsch ester (0.8 mmol, 202.4 mg). After backfilled with $N_2$ (3 cycles), the mixture was dissolved with DMSO (2 mL) next charged with a $N_2$ balloon. The tube was then irradiated by a 30 W blue LED at room temperature. When the reaction was complete monitored by TLC (about 1 h), the reaction system was then charged with $O_2$ followed by being irradiated by a 30 W blue LED at room temperature. After TLC analysis showed the complete consumption of residual Hantzsch ester, the reaction system was then warmed up to 80 $^oC$. Until TLC analysis showed eneindolin-3-ols fully transferred into 2-hydroxymethylindoles **3**, the mixture was then extracted by EtOAc/$H_2O$. Organic phase was dried over $MgSO_4$ and concentrated. The resulting mixture was purified by chromatography on silica gel (eluent: PE/EtOAc) to afford the desired 2-hydroxymethylindoles **3**.

**(*E*)-2-benzylidene-1-(methylsulfonyl)-3-phenylindolin-3-ol ((*E*)-2a)**

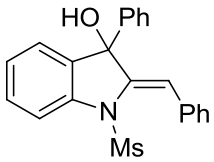



(*E*)-**2a**

Compound (*E*)-**2a** was prepared in 87% yield (56.3 mg) according to the general procedure without applying step 2. White solid (mp 179-181 $^oC$). $^1H$ NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.8 Hz, 1H), 7.41 (s, 1H), 7.36 – 7.30 (m, 1H), 7.26 – 7.22 (m, 2H), 7.15 – 7.00 (m, 9H), 6.94 (dd, *J* = 7.8, 0.6 Hz, 1H), 3.11 (s, 3H), 2.69 (s, 1H); $^{13}C$ NMR (150 MHz, $CDCl_3$) δ 145.4, 141.9, 140.2, 137.0, 133.9, 130.1, 129.5, 127.6,

127.5, 127.2, 127.1, 125.9, 125.7, 124.5, 121.6, 117.0, 80.8, 36.4; IR (neat): 3483(bs), 2959, 2926, 1600, 1463, 1165(s), 968, 753, 698; HRESIMS Calcd for $[C_{22}H_{19}NNaO_3S]^+$ (M + $Na^+$) 400.0978, found 400.0979.

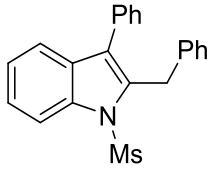
**(*Z*)-2-benzylidene-1-(methylsulfonyl)-3-phenylindolin-3-ol ((*Z*)-2a)**




(*Z*)-**2a**

Compound (*Z*)-**2a** was prepared in 9% yield (6.8 mg) according to the general procedure without applying step 2. Pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 6.8 Hz, 2H), 7.46 – 7.40 (m, 1H), 7.40 – 7.28 (m, 5H), 7.28 – 7.15 (m, 3H), 6.24 (s, 1H), 3.01 (s, 1H), 2.73 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 145.4, 142.2, 141.7, 138.1, 135.2, 130.3, 129.4, 128.3, 128.1, 127.9, 126.9, 126.7, 125.1, 123.8, 118.4, 82.7, 37.8; IR (neat): 3466(bs), 2958, 2926, 1730, 1602, 1461, 1357(s), 1163(s), 770, 700, 544; HRESIMS Calcd for $[C_{22}H_{19}NNaO_3S]^+$ (M + $Na^+$) 400.0978, found 400.0979.

**2-benzyl-1-(methylsulfonyl)-3-phenyl-1*H*-indole (2aa)**

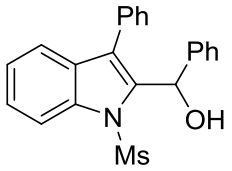



**2aa**

Compound **2aa** was prepared in 22% yield (15.9 mg) according to the general procedure except that the reaction was stirred at 80 $^o$C for 5 h after step 1. Pale yellow solid (mp 131-132 $^o$C). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.44 (m, 5H), 7.44 – 7.20 (m, 5H), 7.20 – 7.12 (m, 3H), 4.46 (s, 2H), 2.55 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 138.9, 136.0, 135.3, 132.9, 130.0, 129.6, 128.9, 128.7, 128.4, 127.7, 126.5, 124.7, 123.7, 123.5, 119.9, 113.9, 40.6, 31.5; IR (neat): 3061,

2990, 2938, 2241(s), 1669(s), 1597, 1444, 1359(s), 1151, 758, 693; HRESIMS Calcd for $[C_{22}H_{19}NNaO_2S]^+$ (M + $Na^+$) 384.1029, found 384.1030.

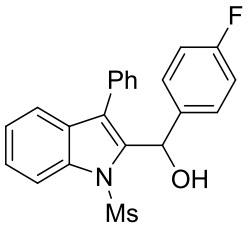
**(1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)(phenyl)methanol (3a)**




**3a**

Compound **3a** was prepared in 76% yield (57.7 mg) according to the general procedure. White solid (mp 149-150 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.53 (m, 3H), 7.53 – 7.45 (m, 2H), 7.45 – 7.37 (m, 2H), 7.37 – 7.24 (m, 5H), 7.24 – 7.18 (m, 1H), 6.24 (d, *J* = 12.0 Hz, 1H), 4.51 (d, *J* = 12.0 Hz, 1H), 2.60 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 142.2, 136.9, 136.3, 132.2, 130.1, 129.2, 128.9, 128.2, 127.2, 126.2, 125.9, 125.7, 123.9, 120.9, 113.9, 68.3, 40.6; IR (neat): 3533(bs), 2955, 2925, 2852, 1448, 1359(s), 1167(s), 1020, 771, 739, 702; HRESIMS Calcd for $[C_{22}H_{19}NNaO_3S]^+$ (M + $Na^+$) 400.0978, found 400.0976.

**(4-fluorophenyl)(1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)methanol (3b)**

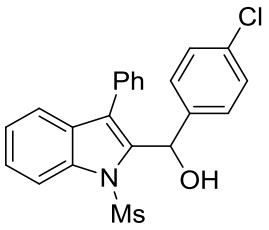



**3b**

Compound **3b** was prepared in 84% yield (66.4 mg) according to the general procedure. Pale yellow oil. $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.38 (m, 7H), 7.37 – 7.29 (m, 1H), 7.29 – 7.18 (m, 2H), 7.04 – 6.92 (m, 2H), 6.20 (d, *J* = 11.6 Hz, 1H), 4.47 (d, *J* = 11.6 Hz, 1H), 2.74 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 161.9 (d, *J* = 244.0 Hz), 138.0 (d, *J* = 3.0 Hz), 136.5, 136.3, 132.0, 130.1, 129.3, 128.9, 128.3, 127.3 (d, *J* = 8.0 Hz), 126.5, 126.1, 124.1, 120.9, 115.0 (d,

*J* = 21.0 Hz), 114.0, 67.9, 40.7; IR (neat): 3527(bs), 2957, 2926, 1726, 1506, 1361(s), 1226, 1168(s), 801, 768, 745; HRESIMS Calcd for $[C_{22}H_{18}FNNaO_3S]^+$ (M + $Na^+$) 418.0884, found 418.0881.

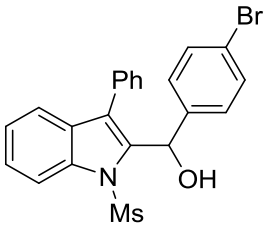
**(4-chlorophenyl)(1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)methanol (3c)**




**3c**

Compound **3c** was prepared in 83% yield (68.4 mg) according to the general procedure. Pale yellow solid (mp 131-132 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.38 (m, 6H), 7.37 – 7.31 (m, 1H), 7.30 – 7.18 (m, 4H), 6.18 (d, *J* = 12.0 Hz, 1H), 4.44 (d, *J* = 12.0 Hz, 1H), 2.76 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 140.9, 136.3, 136.1, 133.0, 131.9, 130.0, 129.3, 129.0, 128.3(2), 128.3(0), 127.1, 126.7, 126.1, 124.2, 121.0, 114.0, 67.9, 40.7; IR (neat): 3520(bs), 2955, 2925, 1727, 1489, 1361(s), 1167(s), 1021, 964, 747; HRESIMS Calcd for $[C_{22}H_{18}ClNNaO_3S]^+$ (M + $Na^+$) 434.0588, found 434.0587.

**(4-bromophenyl)(1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)methanol (3d)**

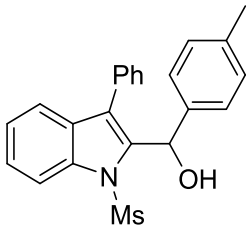



**3d**

Compound **3d** was prepared in 86% yield (78.4 mg) according to the general procedure. White solid (mp 160-161 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.37 (m, 8H), 7.37 – 7.29 (m, 1H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.16 (d, *J* = 12.0 Hz, 1H), 4.44 (d, *J* = 12.0 Hz, 1H), 2.77 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 141.4, 136.2, 135.9, 131.8, 131.2, 130.0, 129.2, 128.9,

128.3, 127.4, 126.6, 126.1, 124.1, 121.0, 120.9, 113.9, 67.9, 40.7; IR (neat): 3521(bs), 2955, 2925, 1485, 1453, 1360(s), 1167(s), 1021, 964, 746; HRESIMS Calcd for $[C_{22}H_{18}BrNNaO_3S]^+$ (M + $Na^+$) 478.0083, found 478.0087.

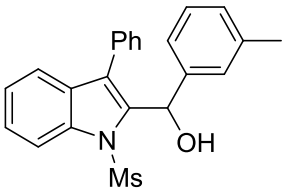
**(1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)(*p*-tolyl)methanol (3e)**




**3e**

Compound **3e** was prepared in 63% yield (49.3mg) according to the general procedure. White solid (mp 155-156 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.62 – 7.37 (m, 7H), 7.37 – 7.29 (m, 1H), 7.20 – 7.14 (m, 2H), 7.13 – 7.06 (m, 2H), 6.20 (d, *J* = 12.0 Hz, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 2.66 (s, 3H), 2.30 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 139.2, 137.1, 136.8, 136.3, 132.2, 130.1, 129.3, 128.9, 128.1, 126.1, 125.8, 125.6, 123.9, 120.9, 113.9, 68.2, 40.7, 21.0; IR (neat): 3515(bs), 2955, 2924, 1453, 1360, 1167(s), 1023, 964, 793, 744; HRESIMS Calcd for $[C_{23}H_{21}NNaO_3S]^+$ (M + $Na^+$) 414.1134, found 414.1131.

**(1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)(*m*-tolyl)methanol (3f)**

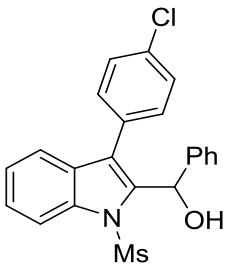



**3f**

Compound **3f** was prepared in 67% yield (52.4 mg) according to the general procedure. White solid (mp 145-146 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.64 – 7.37 (m, 7H), 7.37 – 7.29 (m, 1H), 7.21 – 7.10 (m, 2H), 7.08 – 6.97 (m, 2H), 6.21 (d, *J* = 12.0 Hz, 1H), 4.46 (d, *J* = 12.0 Hz, 1H), 2.64 (s, 3H), 2.30 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 142.1, 137.9, 137.0, 136.3, 132.2, 130.1,

129.3, 128.9, 128.2, 128.1, 127.9, 126.3, 126.1, 125.8, 123.9, 122.8, 120.9, 113.9, 68.2, 40.7, 21.5; IR (neat): 3533(bs), 2954, 2924, 1606, 1453, 1359(s), 1167(s), 1022, 965, 743; HRESIMS Calcd for $[C_{23}H_{21}NNaO_3S]^+$ (M + $Na^+$) 414.1134, found 414.1134.

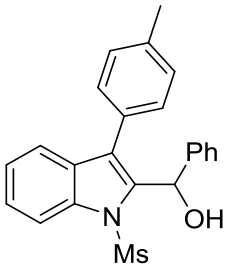
**(3-(4-chlorophenyl)-1-(methylsulfonyl)-1*H*-indol-2-yl)(phenyl)methanol (3g)**




**3g**

Compound **3g** was prepared in 78% yield (64.3 mg) according to the general procedure. White solid (mp 166-167 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.38 (m, 6H), 7.38 – 7.18 (m, 6H), 6.18 (d, *J* = 12.0 Hz, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 2.61 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 141.9, 137.1, 136.2, 134.3, 131.5, 130.7, 129.2, 128.9, 128.3, 127.3, 126.0, 125.6, 124.9, 124.1, 120.6, 114.0, 68.2, 40.7; IR (neat): 3533(bs), 2955, 2925, 1491, 1449, 1361(s), 1167(s), 1013, 770, 749; HRESIMS Calcd for $[C_{22}H_{18}ClNNaO_3S]^+$ (M + $Na^+$) 434.0588, found 434.0587.

**(1-(methylsulfonyl)-3-(*p*-tolyl)-1*H*-indol-2-yl)(phenyl)methanol (3h)**

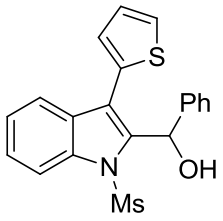



**3h**

Compound **3h** was prepared in 75% yield (58.7 mg) according to the general procedure. Pale yellow oil. $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 1H),

7.57 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.42 – 7.36 (m, 1H), 7.36 – 7.17 (m, 8H), 6.23 (d, *J* = 12.0 Hz, 1H), 4.51 (d, *J* = 12.0 Hz, 1H), 2.59 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 142.2, 138.0, 136.8, 136.3, 130.0, 129.6, 129.4, 129.1, 128.2, 127.1, 126.2, 125.8, 125.7, 123.9, 120.9, 113.9, 68.3, 40.6, 21.2; IR (neat): 3534(bs), 2981, 2928, 1724(s), 1597, 1446, 1369, 1285, 1232, 1105, 1045, 772; HRESIMS Calcd for $[C_{23}H_{21}NNaO_3S]^+$ (M + $Na^+$) 414.1134, found 414.1135.

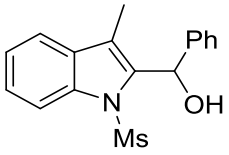
**(1-(methylsulfonyl)-3-(thiophen-2-yl)-1*H*-indol-2-yl)(phenyl)methanol (3i)**




**3i**

Compound **3i** was prepared in 71% yield (54.4 mg) according to the general procedure. White solid (mp 164-165 $^{o}$C). $^1$H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), δ 7.46 (d, *J* = 5.2 Hz, 1H), 7.44 – 7.28 (m, 6H), 7.28 – 7.21 (m, 2H), 7.16 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.43 (d, *J* = 12.0 Hz, 1H), 4.48 (d, *J* = 12.0 Hz, 1H), 2.60 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 141.9, 138.0, 136.1, 132.4, 129.2, 128.5, 128.2, 127.7, 127.2, 127.1, 126.1, 125.7, 124.1, 120.9, 119.1, 113.8, 68.3, 40.7; IR (neat): 3525(bs), 2954, 2924, 1449, 1361, 1361, 1170, 1008, 770, 701; HRESIMS Calcd for $[C_{20}H_{17}NNaO_3S_2]^+$ (M + $Na^+$) 406.0542, found 406.0543.

**(3-methyl-1-(methylsulfonyl)-1*H*-indol-2-yl)(phenyl)methanol (3j)**

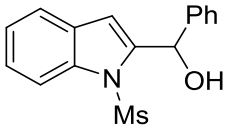



**3j**

Compound **3j** was prepared in 47% yield (29.4 mg) according to the general procedure except being operated on step 1 in 15 h without applying step 2. Pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 1H), 7.63 – 7.55 (m, 1H),

7.42 – 7.30 (m, 6H), 7.29 – 7.22 (m, 1H), 6.41 (d, *J* = 11.2 Hz, 1H), 4.34 (d, *J* = 11.2 Hz, 1H), 2.58 (s, 3H), 2.35 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 141.8, 136.5, 136.3, 130.5, 128.3, 127.3, 125.7(0), 125.6(7), 123.7, 119.7, 119.6, 114.1, 67.7, 40.1, 9.5; IR (neat): 3526(bs), 3028, 2926, 1452, 1359(s), 1167(s), 969, 747, 702; HRESIMS Calcd for $[C_{17}H_{17}NNaO_3S]^+$ (M + $Na^+$) 338.0821, found 338.0820.

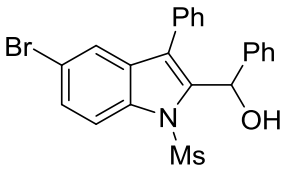
**(1-(methylsulfonyl)-1*H*-indol-2-yl)(phenyl)methanol (3k)**




**3k**

Compound **3k** was prepared in 23% yield (13.6 mg) according to the general procedure except step 1 being operated on step 1 in 2 h. Pale yellow solid (mp 126-127 $^o$C). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.96 (m, 1H), 7.51 – 7.45 (m, 3H), 7.44 – 7.30 (m, 4H), 7.29 – 7.22 (m, 1H), 6.38 (d, *J* = 5.2 Hz, 1H), 6.27 (s, 1H), 3.27 (d, *J* = 5.2 Hz, 1H), 3.04 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 143.0, 140.8, 137.2, 128.6, 128.4, 128.2, 127.1, 125.2, 123.8, 121.4, 113.9, 111.4, 69.3, 40.8; IR (neat): 3535(bs), 2927, 2850, 1452, 1364(s), 1169(s), 1143, 1057, 963, 767, 748; HRESIMS Calcd for $[C_{16}H_{15}NNaO_3S]^+$ (M + $Na^+$) 324.0665, found 324.0676.

**(5-bromo-1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)(phenyl)methanol (3l)**

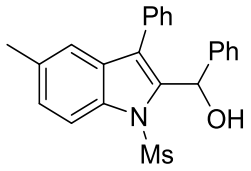



**3l**

Compound **3l** was prepared in 84% yield (76.6 mg) according to the general procedure. White solid (mp 126-127 $^o$C). $^1$H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 1.5 Hz, 1H), 7.57 – 7.46 (m, 5H), 7.47 – 7.40 (m, 1H), 7.34 – 7.20 (m, 5H), 6.22 (d, *J* = 12.0 Hz, 1H), 4.43 (d, *J* = 12.0 Hz, 1H), 2.59 (s, 3H); $^{13}$C NMR (150 MHz, $CDCl_3$) δ 141.7, 138.1, 134.9, 131.4, 131.0, 130.0, 129.1, 128.7,

128.5, 128.3, 127.3, 125.6, 125.3, 123.5, 117.5, 115.4, 68.2, 40.8; IR (neat): 3527(bs), 3026, 2925, 1725, 1446, 1356, 1167(s), 965, 699; HRESIMS Calcd for $[C_{22}H_{18}BrNNaO_3S]^+$ (M + $Na^+$) 478.0083, found 478.0087.

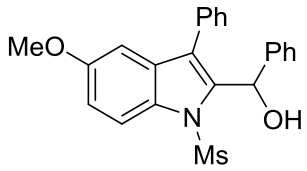
**(5-methyl-1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)(phenyl)methanol (3m)**




**3m**

Compound **3m** was prepared in 71% yield (55.5 mg) according to the general procedure. Pale yellow solid (mp 67-68 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.53 (m, 2H), 7.53 – 7.45 (m, 2H), 7.45 – 7.39 (m, 1H), 7.37 – 7.18 (m, 7H), 6.21 (d, *J* = 12.0 Hz, 1H), 4.51 (d, *J* = 12.0 Hz, 1H), 2.59 (s, 3H), 2.43 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 142.2, 137.0, 134.5, 133.8, 132.3, 130.1, 129.5, 128.9, 128.2, 128.1, 127.2, 127.1, 126.1, 125.7, 120.6, 113.6, 68.3, 40.5, 21.2; IR (neat): 3425(bs), 2977, 2928, 1718(s), 1591, 1444, 1302, 1223, 1045, 772; HRESIMS Calcd for $[C_{23}H_{21}NNaO_3S]^+$ (M + $Na^+$) 414.1134, found 414.1133.

**(5-methoxy-1-(methylsulfonyl)-3-phenyl-1*H*-indol-2-yl)(phenyl)methanol (3n)**

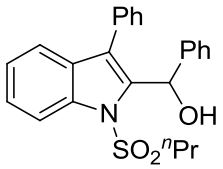



**3n**

Compound **3n** was prepared in 70% yield (57.0 mg) according to the general procedure. White solid (mp 182-183 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 9.2 Hz, 1H), 7.59 – 7.52 (m, 2H), 7.52 – 7.45 (m, 2H), 7.45 – 7.38 (m, 1H), 7.34 – 7.17 (m, 5H), 7.06 – 6.94 (m, 2H), 6.20 (d, *J* = 12.0 Hz, 1H), 4.50 (d, *J* = 12.0 Hz, 1H), 3.80 (s, 3H), 2.59 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 156.9, 142.1, 137.5, 132.2, 130.7, 130.2, 130.0, 129.0, 128.2, 127.1, 126.2, 125.6, 114.8, 103.0, 68.2, 55.8,

40.5; IR (neat): 3526(bs), 2955, 2925, 1610, 1474, 1360, 1217, 1154(s), 1037, 732; HRESIMS Calcd for $[C_{23}H_{21}NNaO_4S]^+$ (M + $Na^+$) 430.1083, found 430.1084.

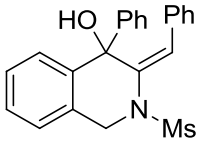
**phenyl(3-phenyl-1-(propylsulfonyl)-1*H*-indol-2-yl)methanol (3o)**




**3o**

Compound **3o** was prepared in 33% yield (26.8 mg) according to the general procedure. Pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.61 – 7.53 (m, 3H), 7.53 – 7.46 (m, 2H), 7.45 – 7.35 (m, 2H), 7.34 – 7.26 (m, 4H), 7.26 – 7.19 (m, 2H), 6.24 (d, *J* = 12.0 Hz, 1H), 4.62 (d, *J* = 12.0 Hz, 1H), 2.72 – 2.18 (m, 2H), 1.75 – 1.49 (m, 2H), 0.77 (t, *J* = 7.6 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 142.3, 137.1, 136.7, 132.3, 130.2, 129.0, 128.9, 128.1, 127.1, 126.1, 125.7(3), 125.6(9), 123.7, 120.8, 114.2, 68.2, 55.8, 16.5, 12.6; IR (neat): 3523(bs), 3060, 2969, 2932, 1493, 1448, 1360(s), 1152(s), 1020, 741, 702; HRESIMS Calcd for $[C_{24}H_{23}NNaO_3S]^+$ (M + $Na^+$) 428.1291, found 428.1297.

**(*E*)-3-benzylidene-2-(methylsulfonyl)-4-phenyl-1,2,3,4-tetrahydroisoquinolin-4-ol (5)**

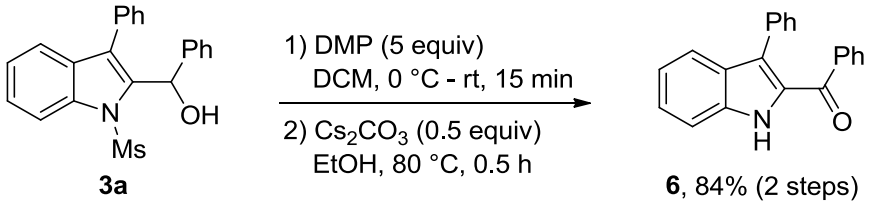



**5**

Compound **5** was prepared in 33% yield (25.7 mg) according to the general procedure without applying step 2. White solid (mp 148-149 $^o$C). $^1$H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.38 (m, 1H), 7.29 – 7.22 (m, 5H), 7.22 – 7.02 (m, 9H), 4.99 (d, *J* = 16.4 Hz, 1H), 4.71 (d, *J* = 16.4 Hz, 1H), 3.31 (s, 1H), 2.67 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 145.0, 141.5, 140.5, 134.7, 131.2, 130.8, 128.9, 128.3, 127.9, 127.8, 127.5, 127.3, 127.1, 126.3, 125.2, 75.4, 49.0, 39.3; IR (neat): 3494(bs), 2923, 2851, 1491,

1447, 1339, 1151(s), 957, 697; HRESIMS Calcd for $[C_{23}H_{21}NNaO_3S]^+$ (M + $Na^+$) 414.1134, found 414.1135.

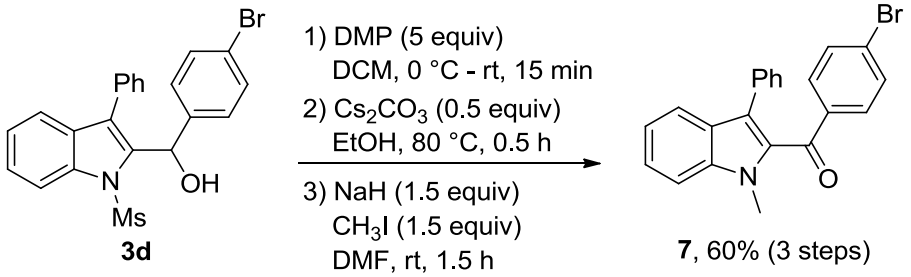
**phenyl(3-phenyl-1*H*-indol-2-yl)methanone (6)**




**3a** **6**, 84% (2 steps)

Compound **6** was prepared in 84% yield (59.0 mg, 2 steps) according to the following procedures. 2-Hydroxymethylindole **3a** (0.24 mmol, 89 mg) dissolved in DCM (5 mL) was cooled to 0 $^oC$. Then, DMP (1.2 mmol, 509 mg) was added slowed to the mixture. The reaction was stirred at room temperature for 15 min. Aqueous saturated $NaHCO_3$ was added to quench extra DMP. Next, the resulting mixture was extracted by DCM/$H_2O$. Organic phase was dried over $MgSO_4$ and concentrated. The resulting mixture was purified by chromatography on silica gel (eluent: PE/DCM) to afford the crude product. To a flask containing the above crude product and EtOH (2 mL) was added $Cs_2CO_3$ (0.12 mmol, 39 mg) followed by being stirred at 80 $^oC$ until TLC analysis showed the complete consumption of substrate (about 30 min). The residue was filtered through a Celite pad and the filtrate was concentrated. The resulting mixture was purified by chromatography on silica gel (eluent: PE/EtOAc) to afford the desired 2-acylindole **6** (84%, 2 steps). White solid (mp 204-205 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 9.47 (s, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.47 (m, 3H), 7.47 – 7.35 (m, 1H), 7.31 – 7.00 (m, 9H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 189.6, 137.6, 136.4, 133.7, 131.6, 130.9, 129.5, 127.9, 127.7, 127.5, 126.8, 126.6, 125.3, 122.1, 121.1, 112.0; IR (neat): 3319(bs), 2955, 2924, 1616(s), 1335, 1266, 1018, 737, 696; HRESIMS Calcd for $[C_{21}H_{15}NNaO]^+$ (M + $Na^+$) 320.1046, found 320.1046.

**(4-bromophenyl)(1-methyl-3-phenyl-1*H*-indol-2-yl)methanone (7)**




Compound **7** was prepared in 60% yield (79.5 mg, 3 steps) according to the following procedures. Step 1 and step 2 were referred to above procedures. A round-bottom flask was charged with corresponding 2-acylindole (0.2 mmol, 74 mg) and DMF (2 mL). Then, 60% NaH (0.3 mmol, 12 mg) was added in one portion to the solution. After being stirred in 10 min, $CH_3I$ (0.3 mmol, 18.7 uL) was added to the mixture. The reaction was then stirred at room temperature for 1.5 h until TLC analysis showed the complete consumption of substrate. Appropriate $H_2O$ was poured into carefully to quench extra NaH. Then, the mixture was extracted by EtOAc/$H_2O$. Organic phase was dried over $MgSO_4$ and concentrated. The resulting mixture was purified by chromatography on silica gel (eluent: PE/EtOAc) to afford the desired product **7** (60%, 3 steps). Pale yellow solid (mp 60-61 $^oC$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.75 (d, $J$ = 8.4 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.47 – 7.37 (m, 2H), 7.27 – 7.17 (m, 5H), 7.17 – 7.06 (m, 3H), 3.94 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 189.3, 138.7, 137.0, 133.7, 132.4, 131.5, 131.0, 130.4, 128.1, 127.5, 126.7, 125.8, 125.5, 123.9, 121.5, 121.0, 110.2, 31.6; IR (neat): 2954, 2923, 1633, 1585, 1257, 1067, 1011, 958, 743, 701; HRESIMS Calcd for $[C_{22}H_{16}BrNNaO]^+$ (M + $Na^+$) 412.0307, found 412.0314.

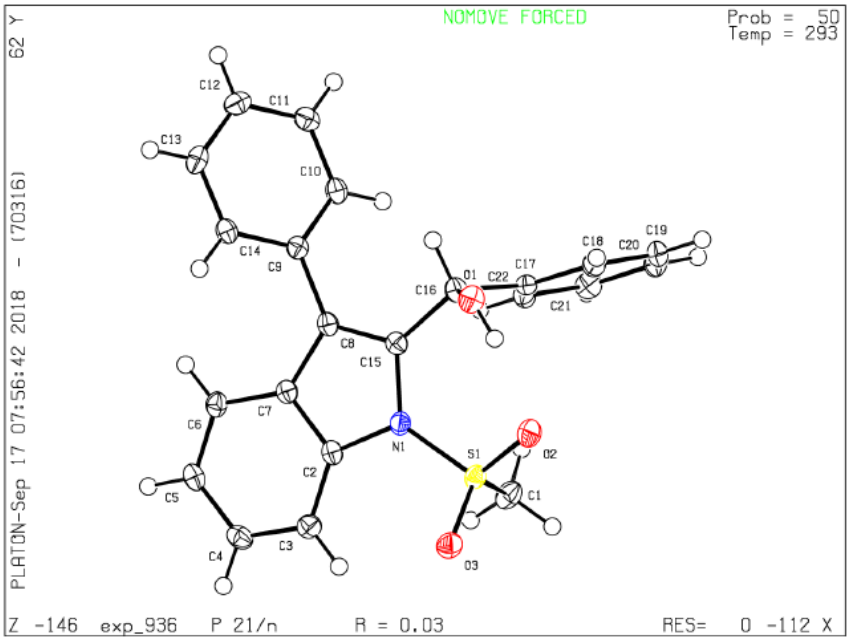
**Reference:**

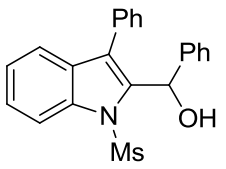

1 Z.-S. Wang, Y.-B. Chen, H.-W. Zhang, Z. Sun, C. Zhu and L.-W. Ye, *J. Am. Chem. Soc.*, 2020, **142**, 3636.

2 B. Zhou, L. Li, X.-Q. Zhu, J.-Z. Yan, Y.-L. Guo and L.-W. Ye, *Angew. Chem. Int. Ed.*, 2017, **56**, 4015.

3 M. R. Tracey, Y. Zhang, M. O. Frederick, J. A. Mulder and R. P. Hsung, *Org. Lett.*, 2004, **6**, 2209.

**Crystal data and structure refinement for 3a. CCDC Number = 1998433**

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Temperature:     293 K

                 Calculated                Reported
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Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C22 H19 N O3 S            ?
Sum formula      C22 H19 N O3 S            C22 H19 N O3 S
Mr               377.44                    377.44
Dx,g cm-3        1.408                     1.408
Z                4                         4
Mu (mm-1)        1.807                     1.807
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F000'            795.54
h,k,lmax         10,16,16                  10,16,16
Nref             3174                      3171
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Tmin'            0.835

Correction method= # Reported T Limits: Tmin=0.851 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 67.052

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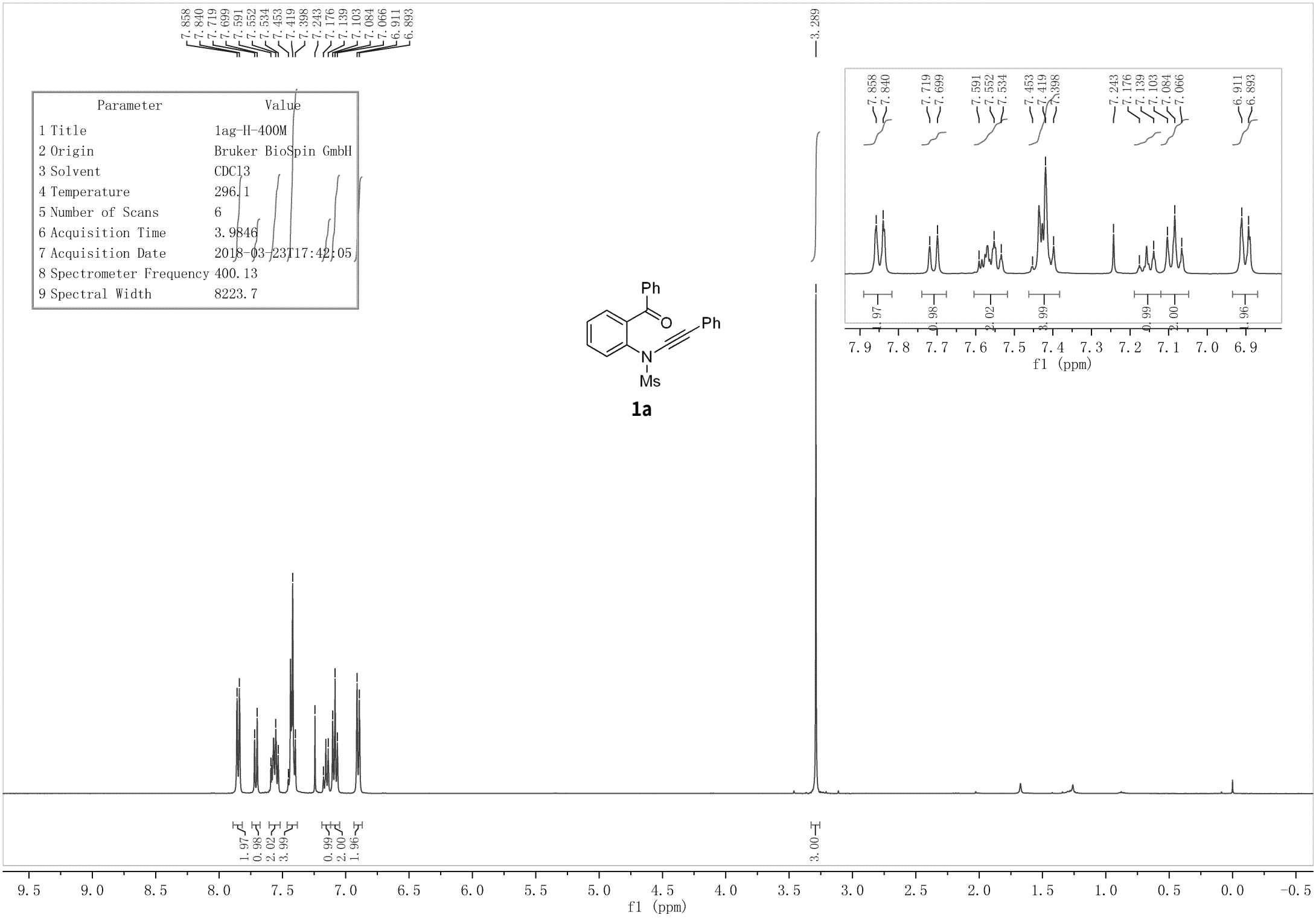
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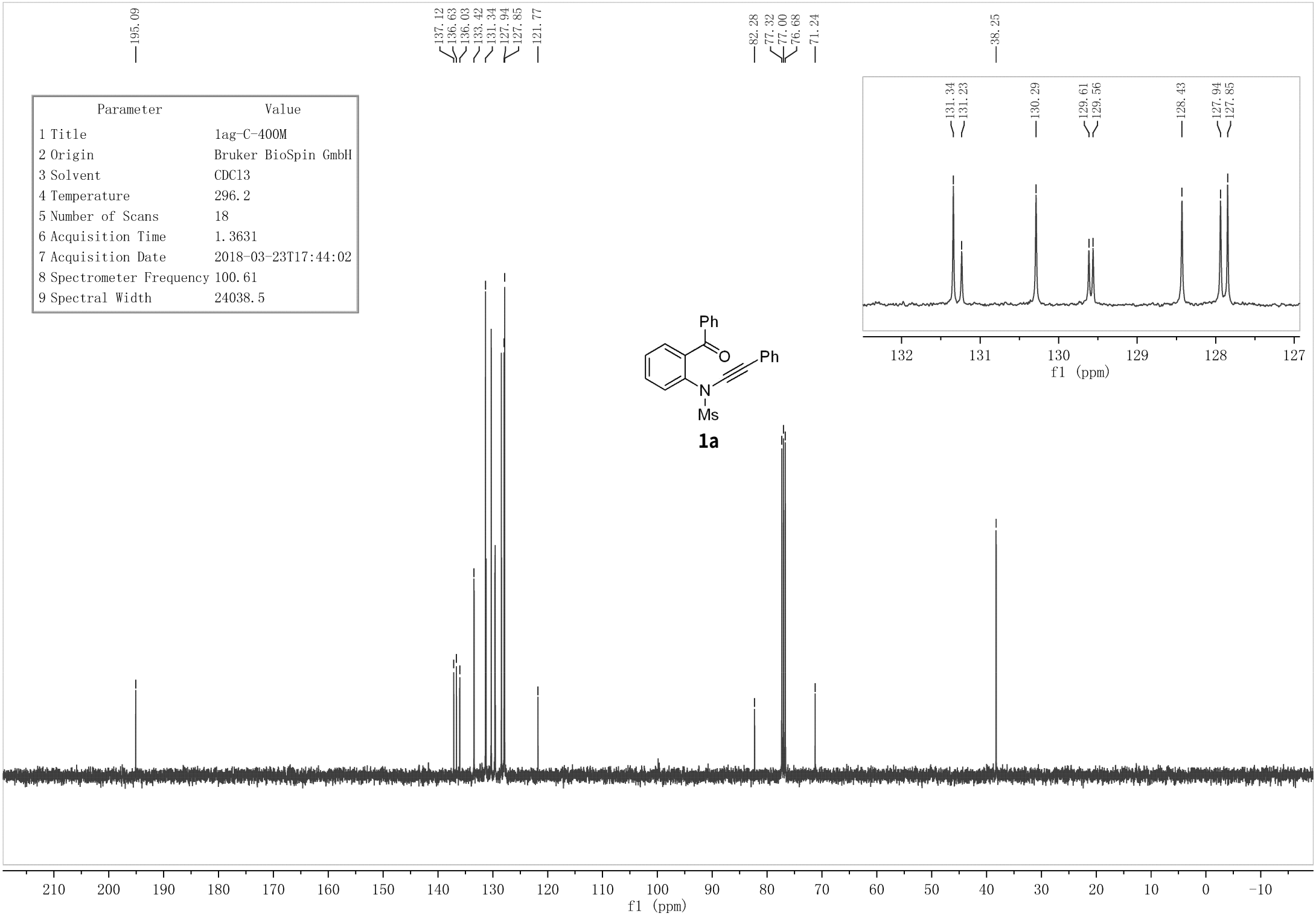
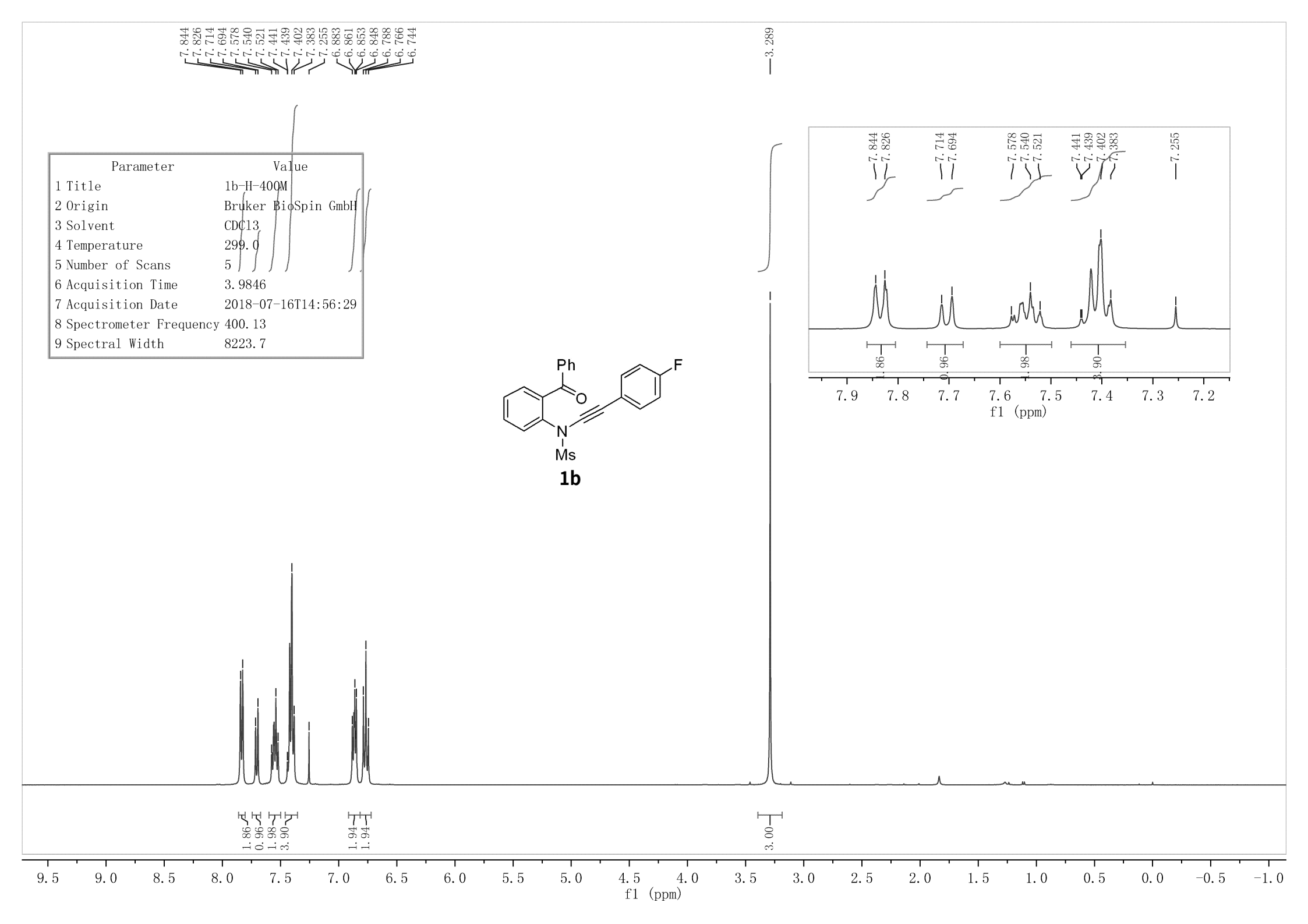
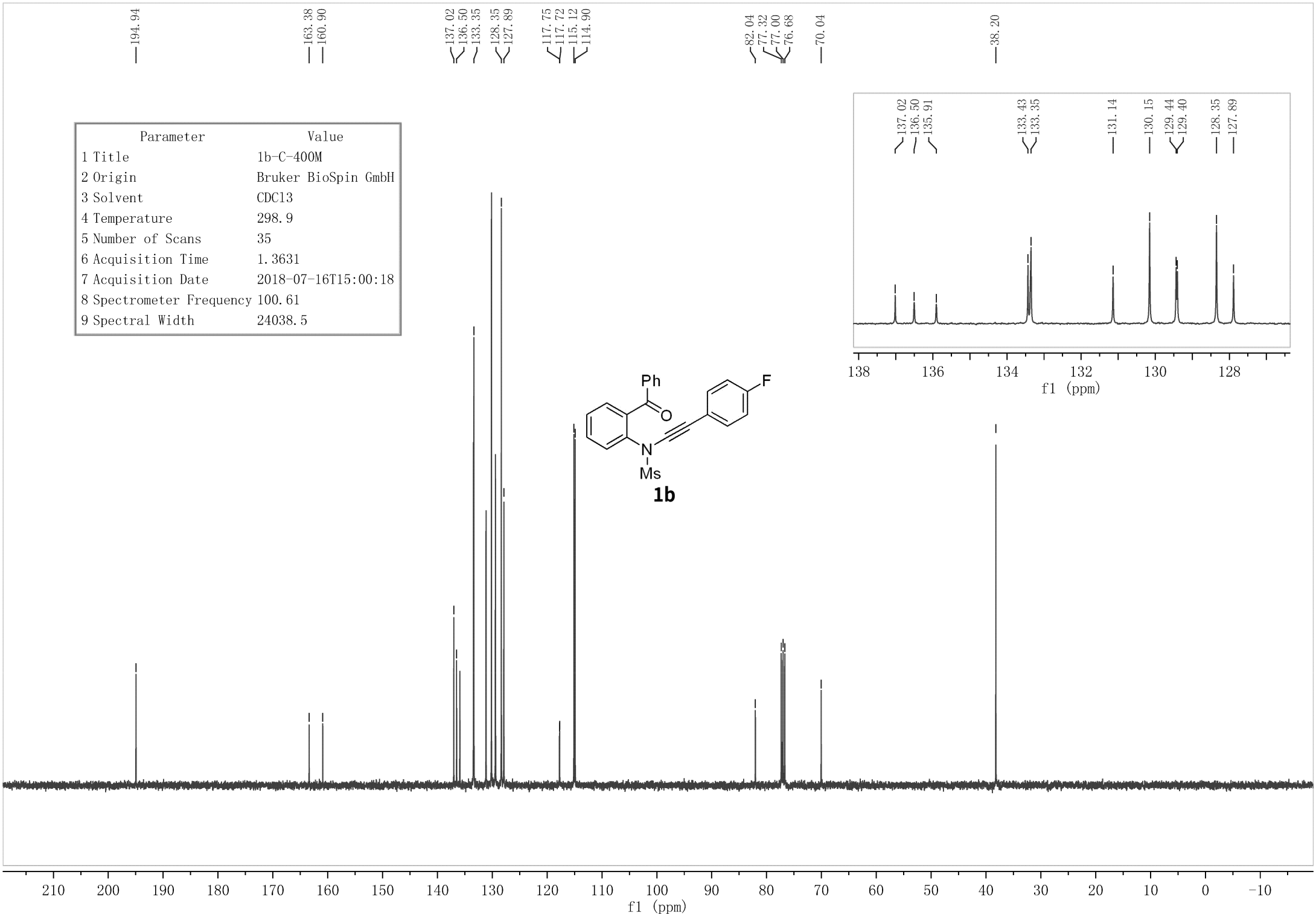
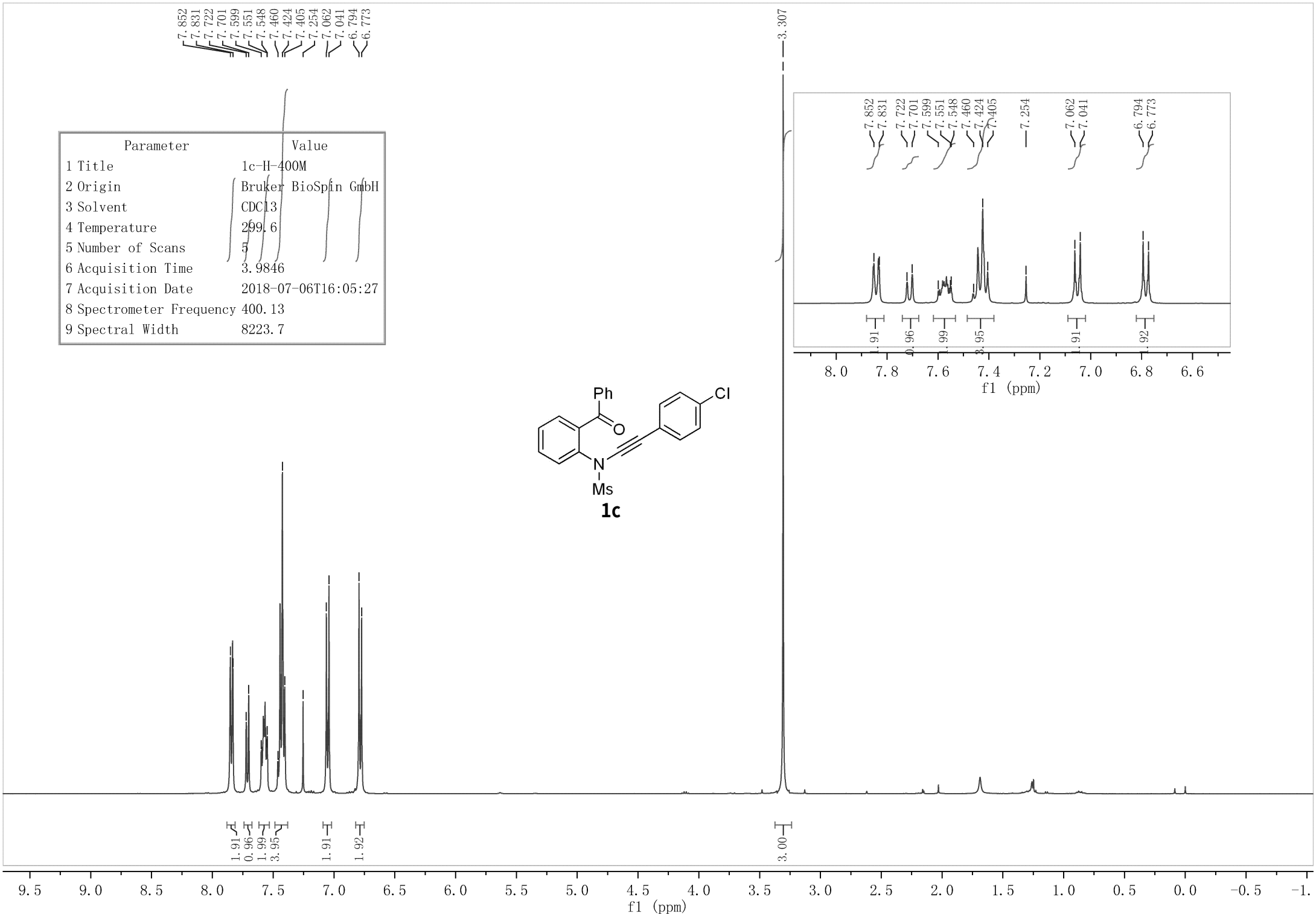
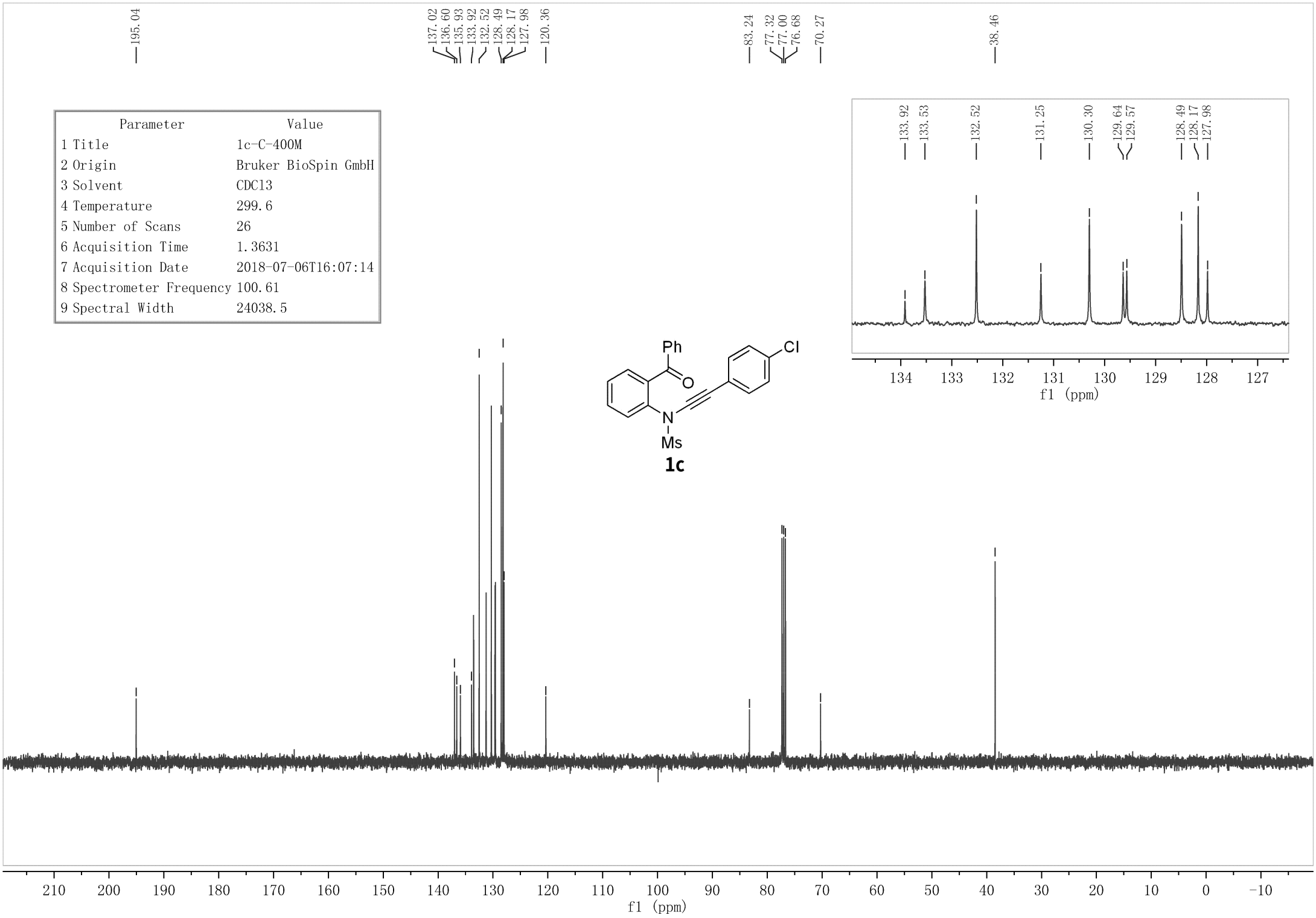
Parameter Value
1 Title 1ag-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.1
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-03-23T17:42:05
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
Ph
N
Ms
1a
1.97
0.98
2.02
3.99
0.99
2.00
1.96
3.00
9.5 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 -0.5
f1 (ppm)
0.97
0.98
2.02
3.99
0.99
2.00
0.96
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)


195.09
137.12
136.63
136.03
133.42
131.34
127.94
127.85
121.77
82.28
77.32
77.00
76.68
71.24
38.25
Parameter Value
1 Title 1ag-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.2
5 Number of Scans 18
6 Acquisition Time 1.3631
7 Acquisition Date 2018-03-23T17:44:02
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.34
131.23
130.29
129.61
129.56
128.43
127.94
127.85
132 131 130 129 128 127
f1 (ppm)
Ph
O
Ph
N
Ms
1a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

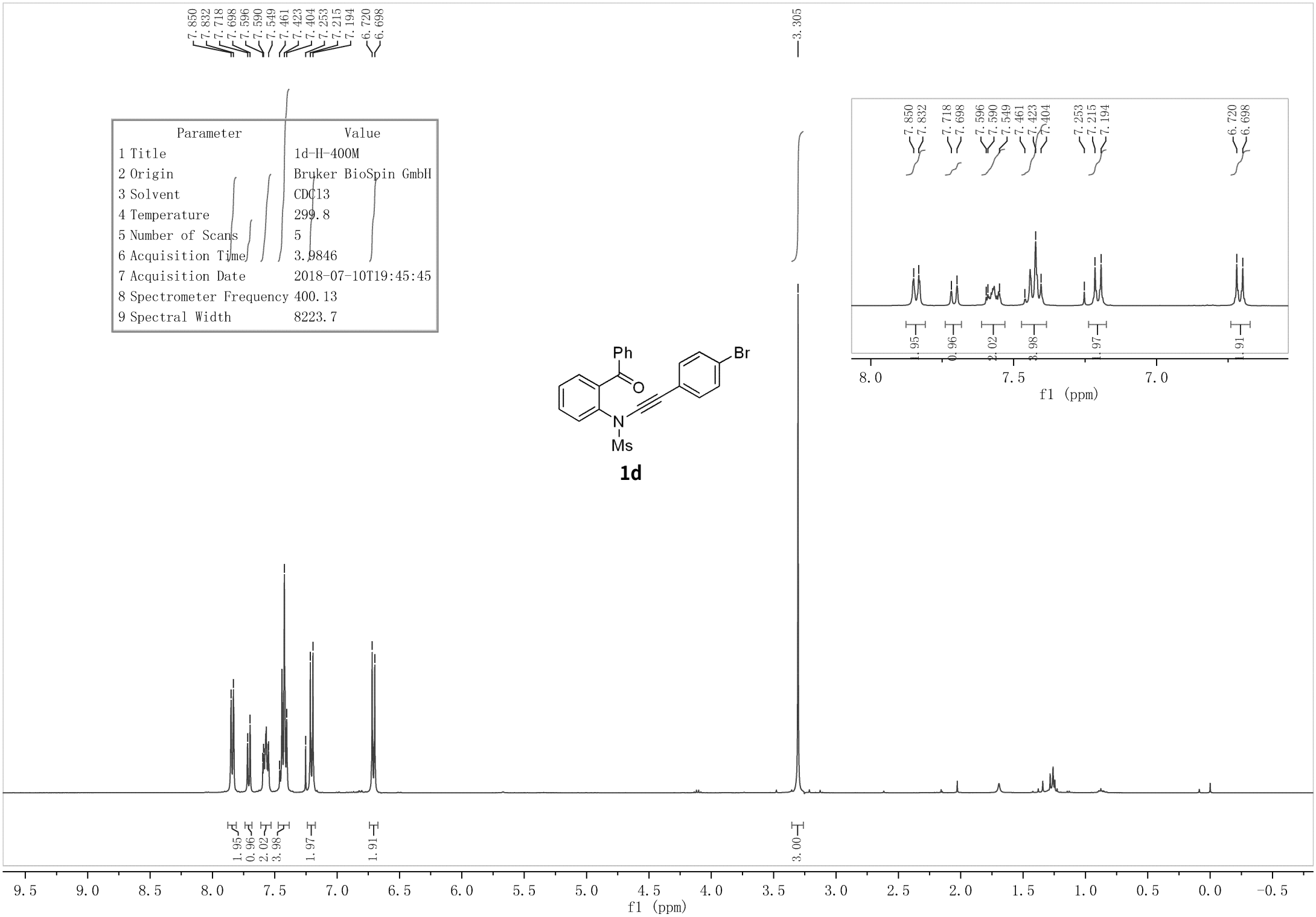

7.844
7.826
7.714
7.694
7.578
7.540
7.521
7.441
7.439
7.402
7.383
7.255
6.883
6.861
6.853
6.848
6.788
6.766
6.744
3.289
Parameter Value
1 Title 1b-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.0
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-16T14:56:29
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
N
Ms
F
1b
1.86
0.96
1.98
3.90
1.94
1.94
3.00
f1 (ppm)

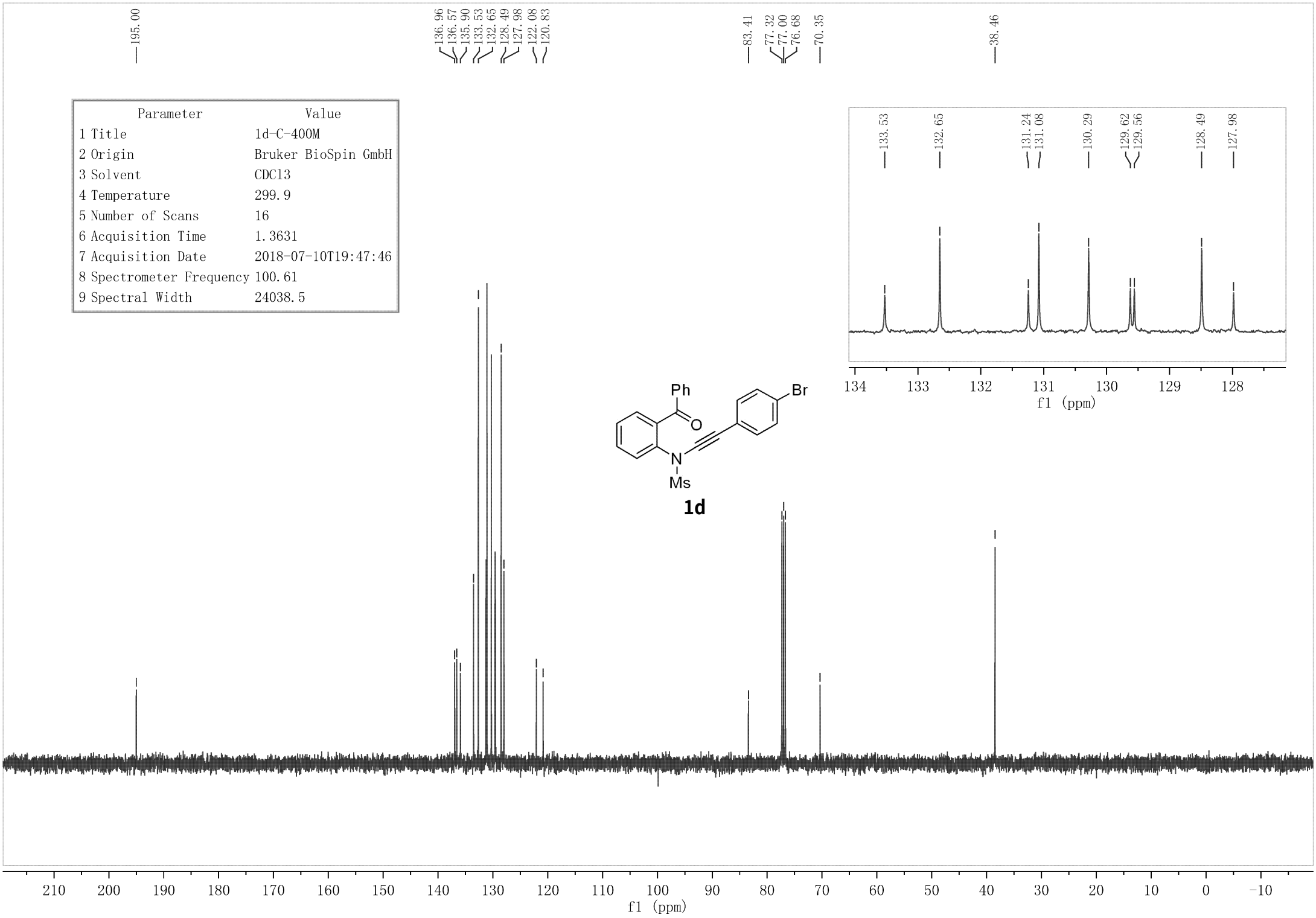

194.94
163.38
160.90
137.02
136.50
133.35
128.35
127.89
117.75
117.72
115.12
114.90
82.04
77.32
77.00
76.68
70.04
38.20
Parameter Value
1 Title 1b-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 35
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-16T15:00:18
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
137.02
136.50
135.91
133.43
133.35
131.14
130.15
129.44
129.40
128.35
127.89
138
136
134
132
130
128
f1 (ppm)
Ph
O
F
N
Ms
1b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

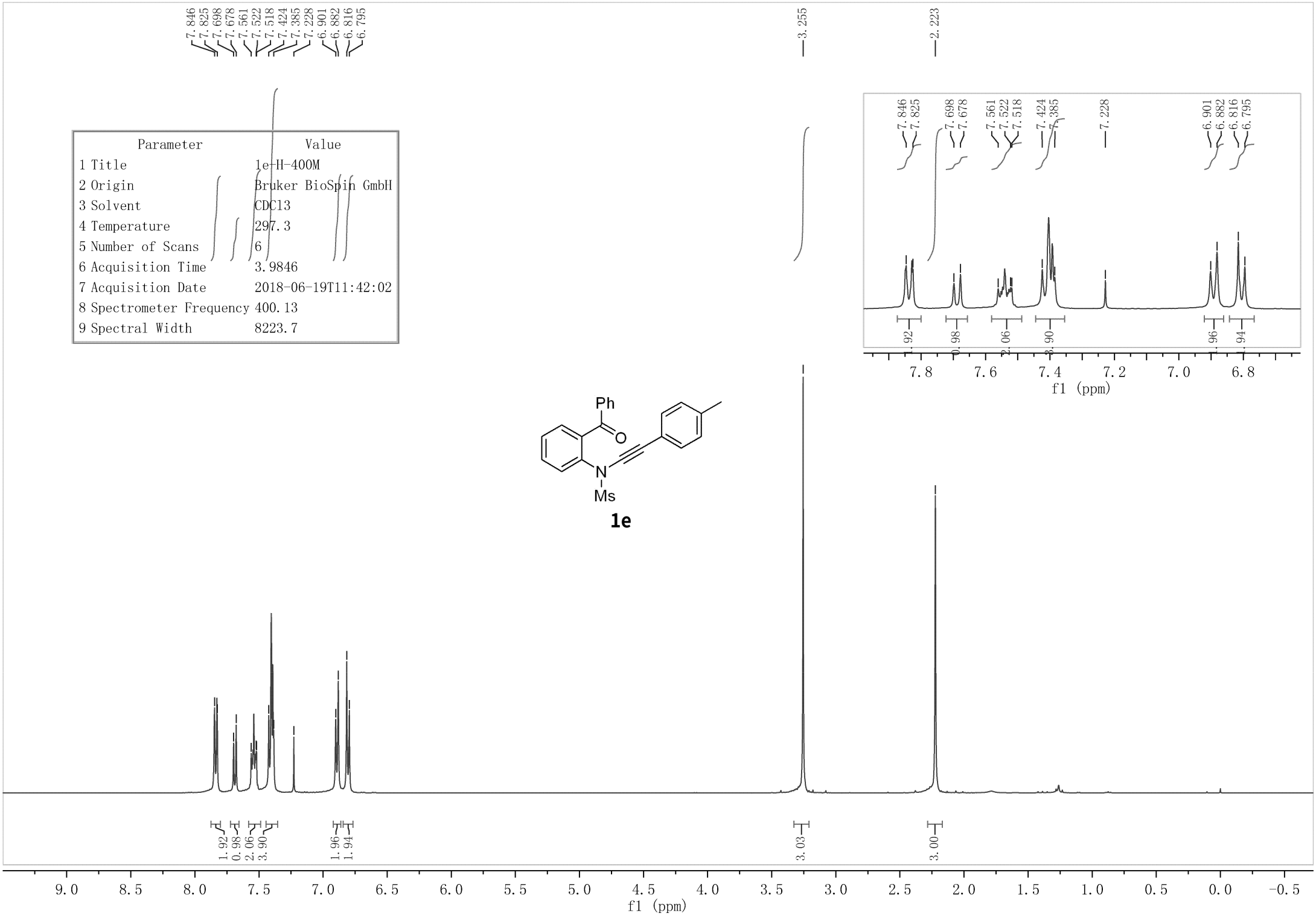

7.852
7.831
7.722
7.701
7.599
7.551
7.548
7.460
7.424
7.405
7.254
7.062
7.041
6.794
6.773
3.307
Parameter Value
1 Title 1c-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-06T16:05:27
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
N
Ms
Cl
1c
1.91
0.96
1.99
3.95
1.91
1.92
3.00
f1 (ppm)

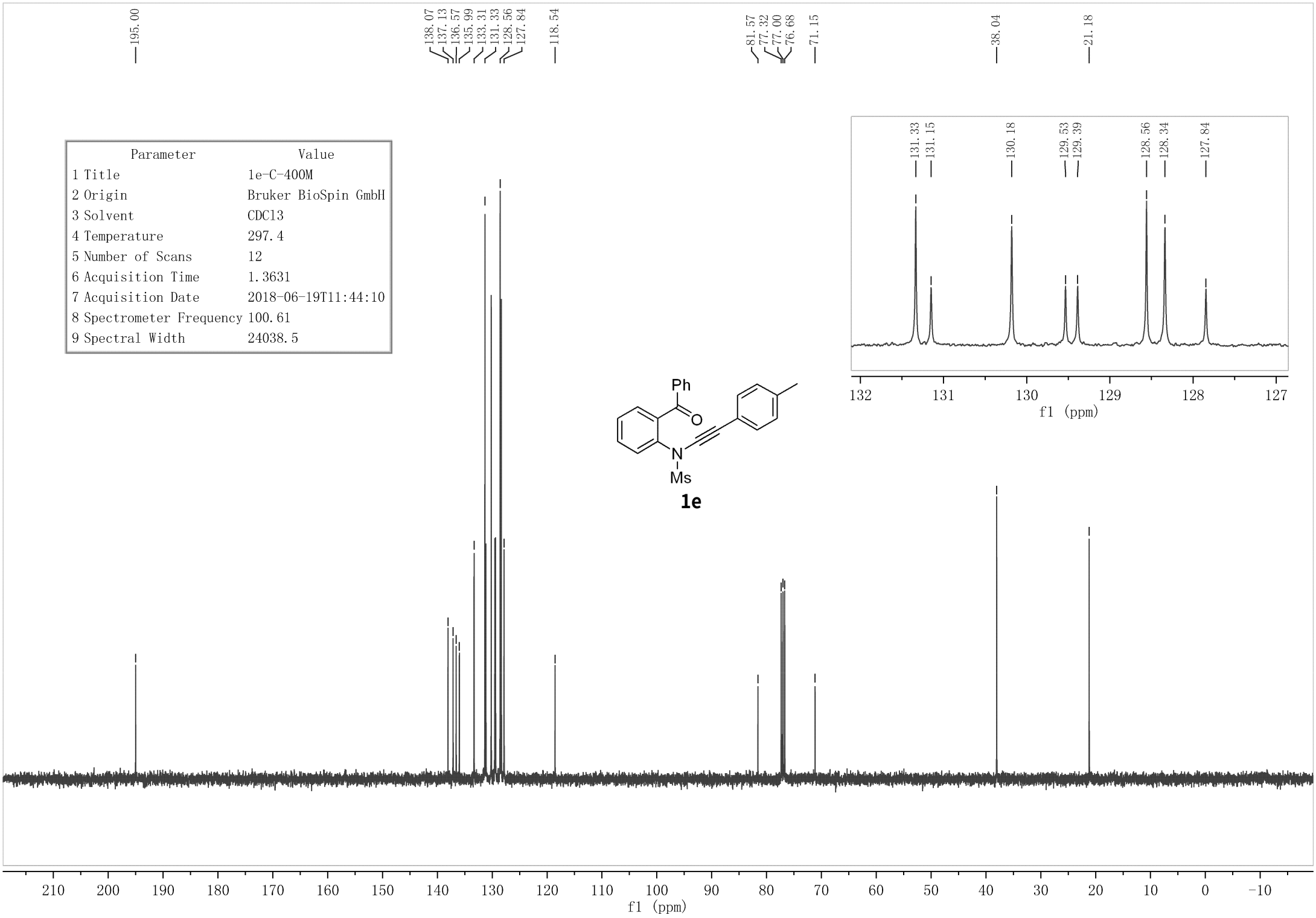


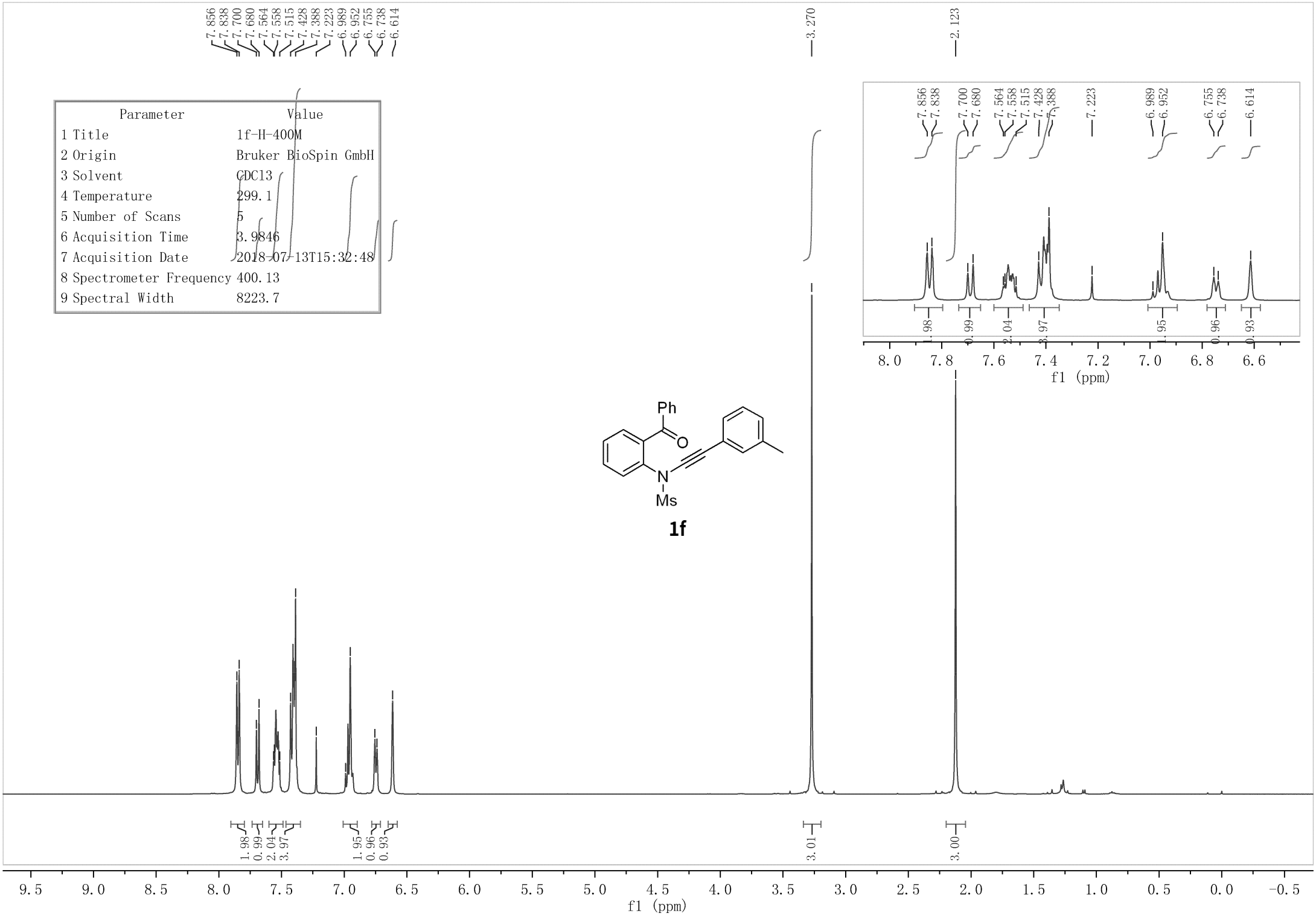

| Parameter | Value |
|---|---|
| 1 Title | 1c-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.6 |
| 5 Number of Scans | 26 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-07-06T16:07:14 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |


7.850
7.832
7.718
7.698
7.596
7.590
7.549
7.461
7.423
7.404
7.253
7.215
7.194
6.720
6.698
3.305
Parameter Value
1 Title 1d-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.8
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-10T19:45:45
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
N
Ms
Br
1d
1.95
0.96
2.02
3.98
1.97
1.91
3.00
f1 (ppm)


195.00
136.96
136.57
135.90
133.53
132.65
128.49
127.98
122.08
120.83
83.41
77.32
77.00
76.68
70.35
38.46
Parameter Value
1 Title 1d-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.9
5 Number of Scans 16
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-10T19:47:46
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
133.53
132.65
131.24
131.08
130.29
129.62
129.56
128.49
127.98
134 133 132 131 130 129 128
f1 (ppm)
Ph
O
N
Ms
Br
1d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

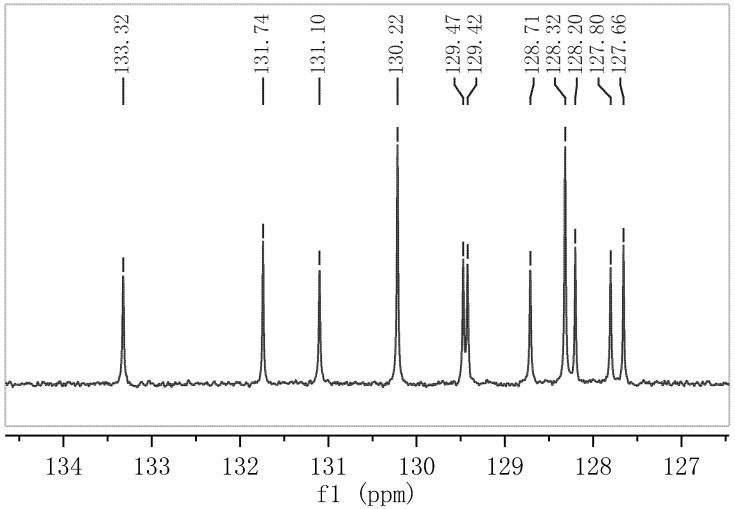

7.846
7.825
7.698
7.678
7.561
7.522
7.518
7.424
7.385
7.228
6.901
6.882
6.816
6.795
3.255
2.223
Parameter Value
1 Title 1e-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.3
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-19T11:42:02
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
N
Ms
1e
1.92
0.98
2.06
3.90
1.96
1.94
3.03
3.00
f1 (ppm)

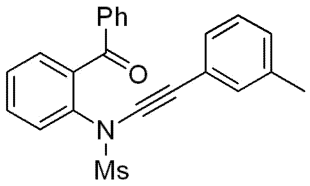

195.00
138.07
137.13
136.57
135.99
133.31
131.33
128.56
127.84
118.54
81.57
77.32
77.00
76.68
71.15
38.04
21.18
Parameter Value
1 Title 1e-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.4
5 Number of Scans 12
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-19T11:44:10
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.33
131.15
130.18
129.53
129.39
128.56
128.34
127.84
132
131
130
129
128
127
f1 (ppm)
Ph
O
N
Ms
1e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.856
7.838
7.700
7.680
7.564
7.558
7.515
7.428
7.388
7.223
6.989
6.952
6.755
6.738
6.614
3.270
2.123
Parameter Value
1 Title 1f-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.1
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-13T15:32:48
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
N
Ms
1f
1.98
0.99
2.04
3.97
1.95
0.96
0.93
3.01
3.00
f1 (ppm)

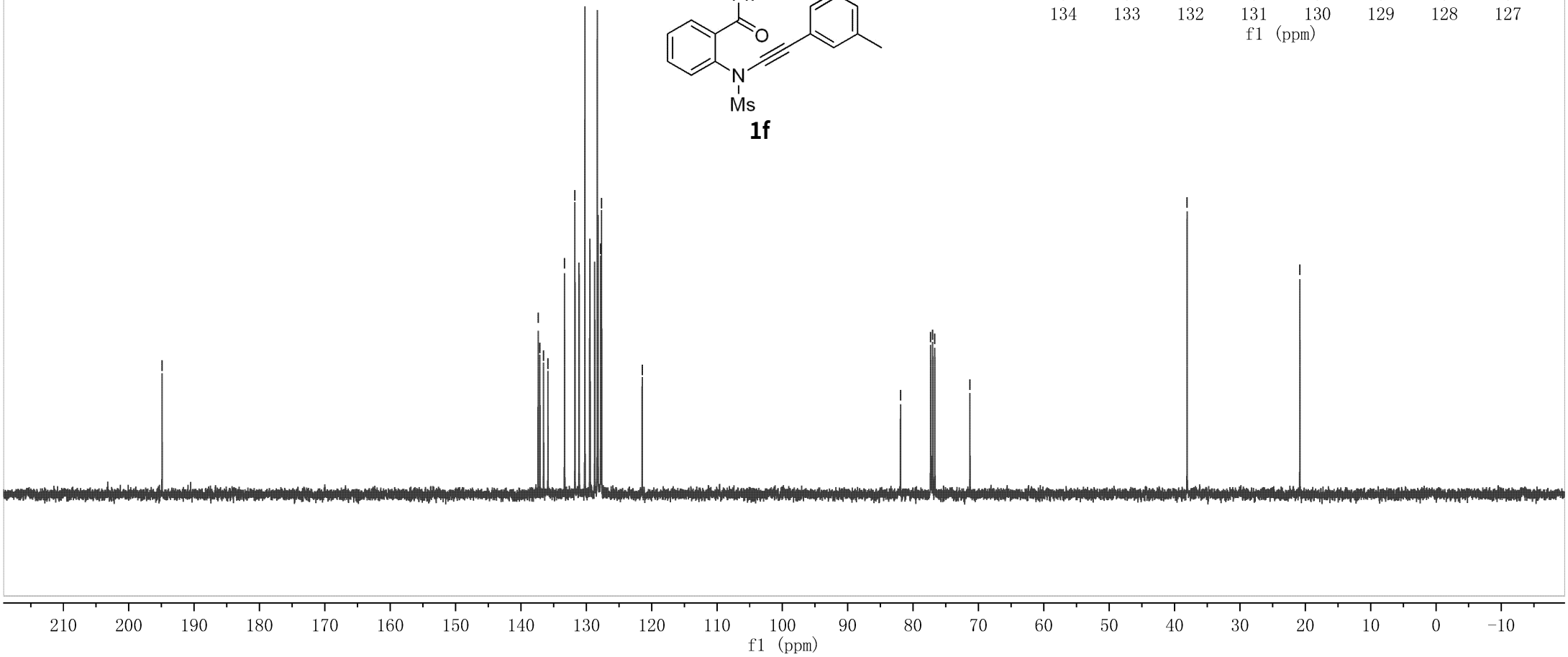
194.90
137.36
137.10
136.54
135.87
133.32
131.74
127.80
127.66
121.45
81.93
77.32
77.00
76.68
71.30
38.08
20.82

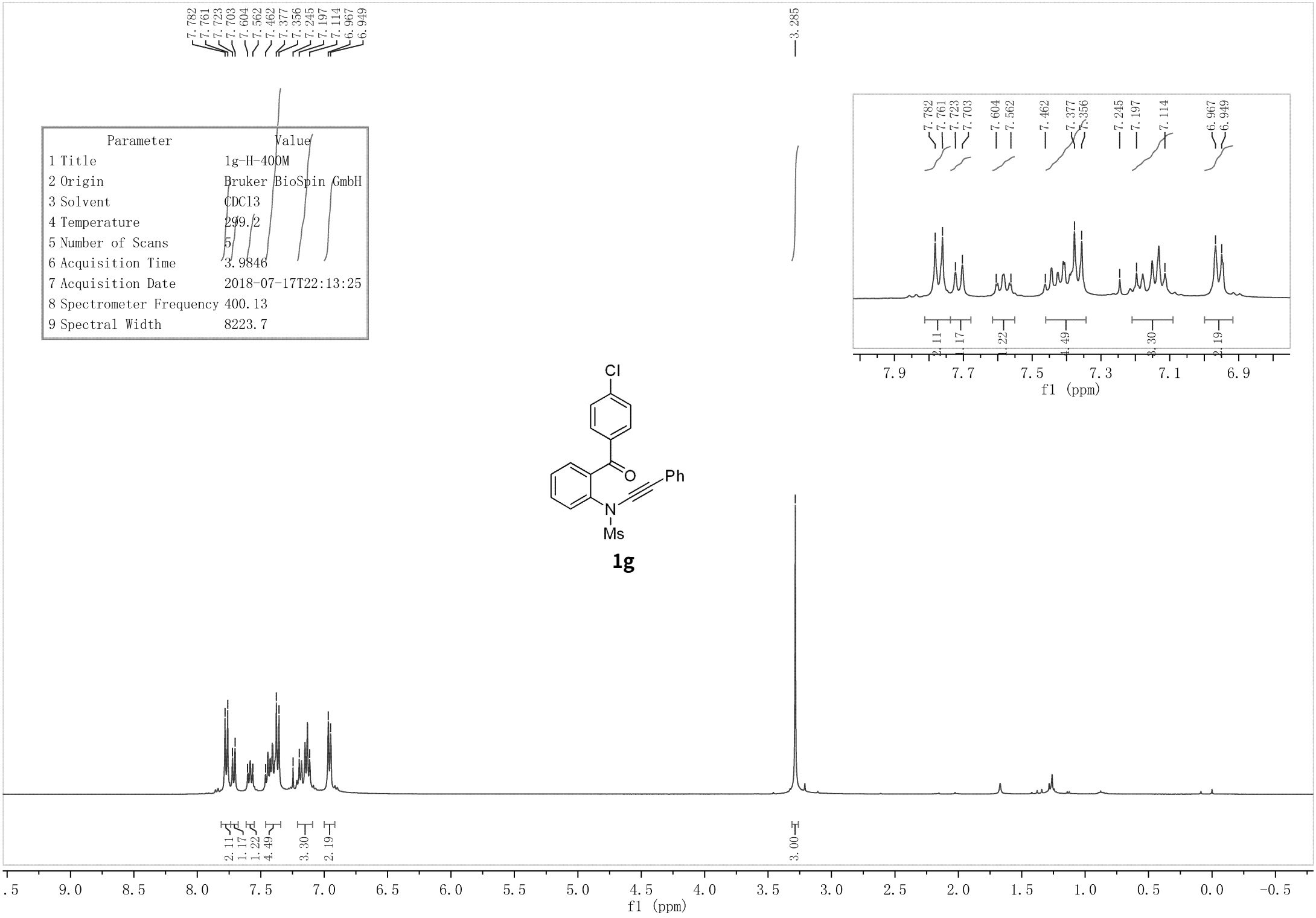
| Parameter | Value |
|---|---|
| 1 Title | 1f-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.2 |
| 5 Number of Scans | 12 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-07-13T15:35:11 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

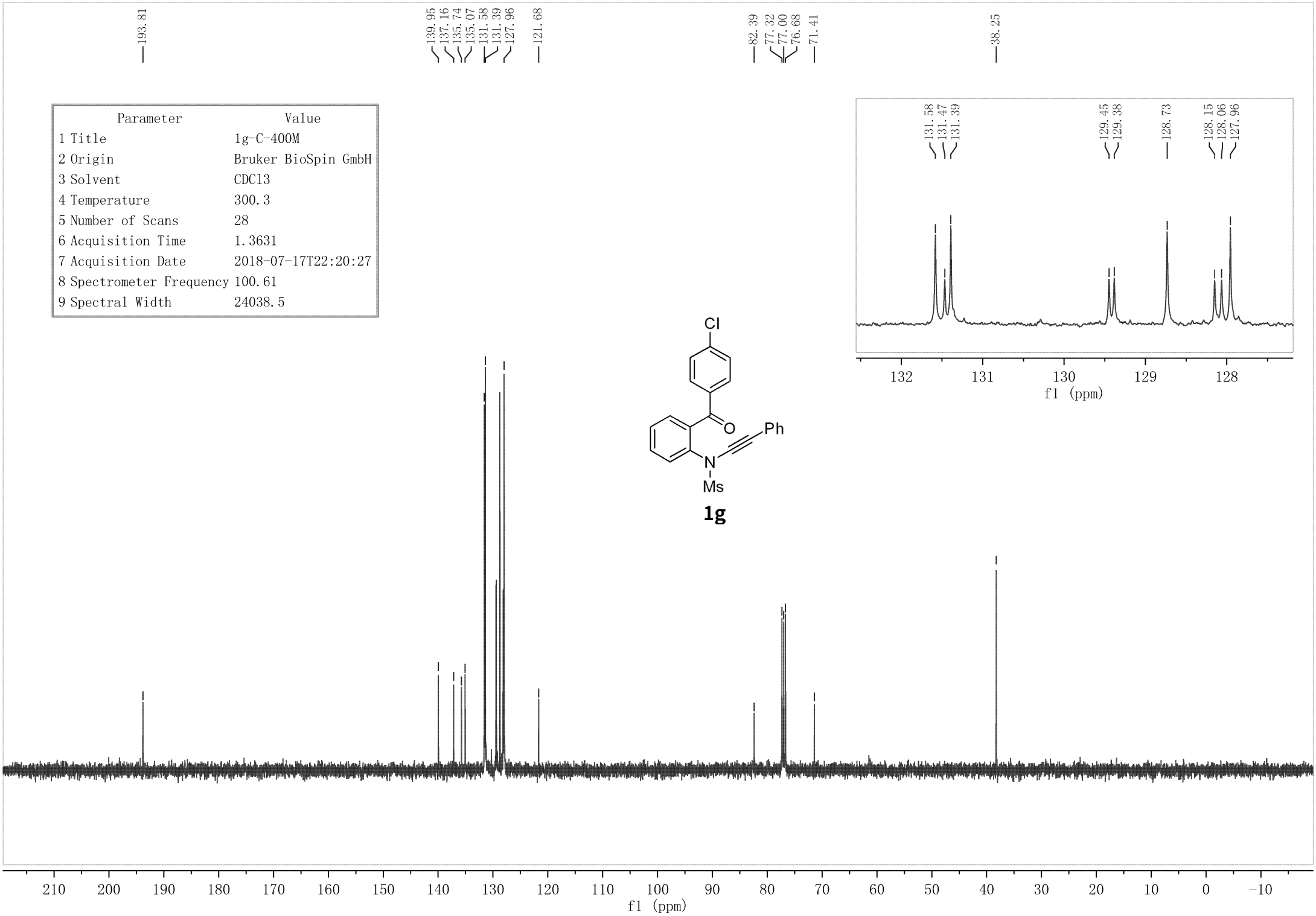


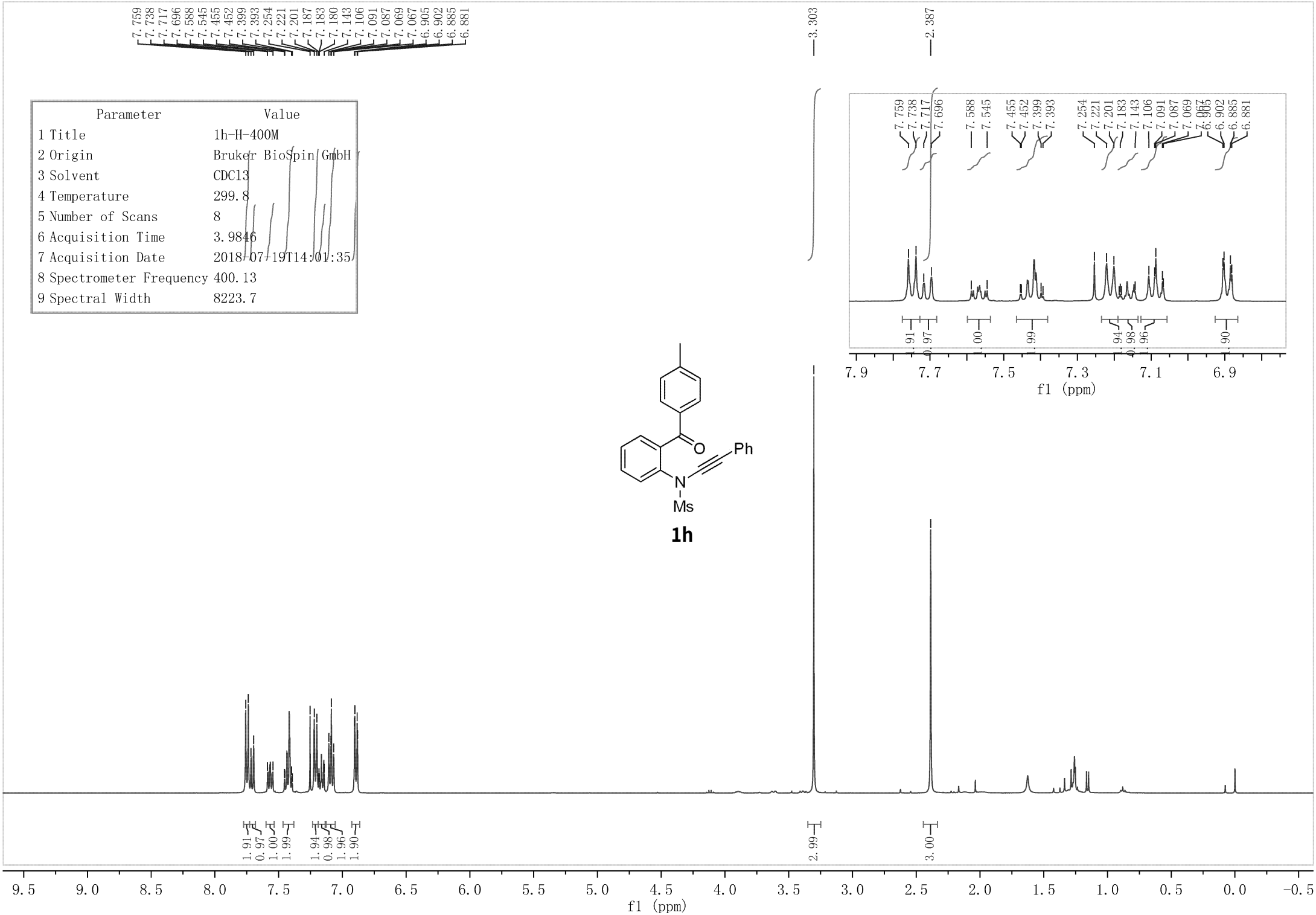



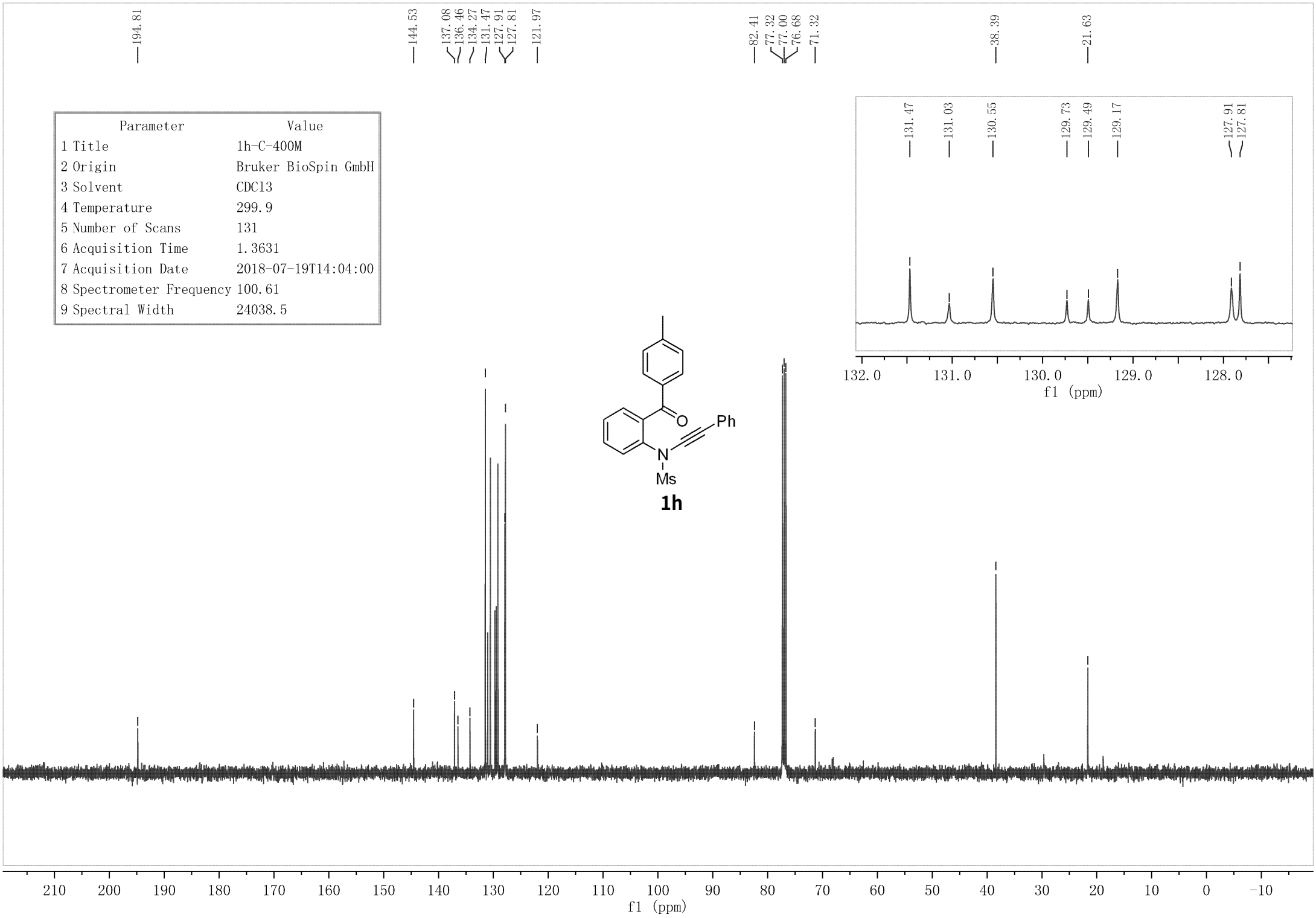

**1f**

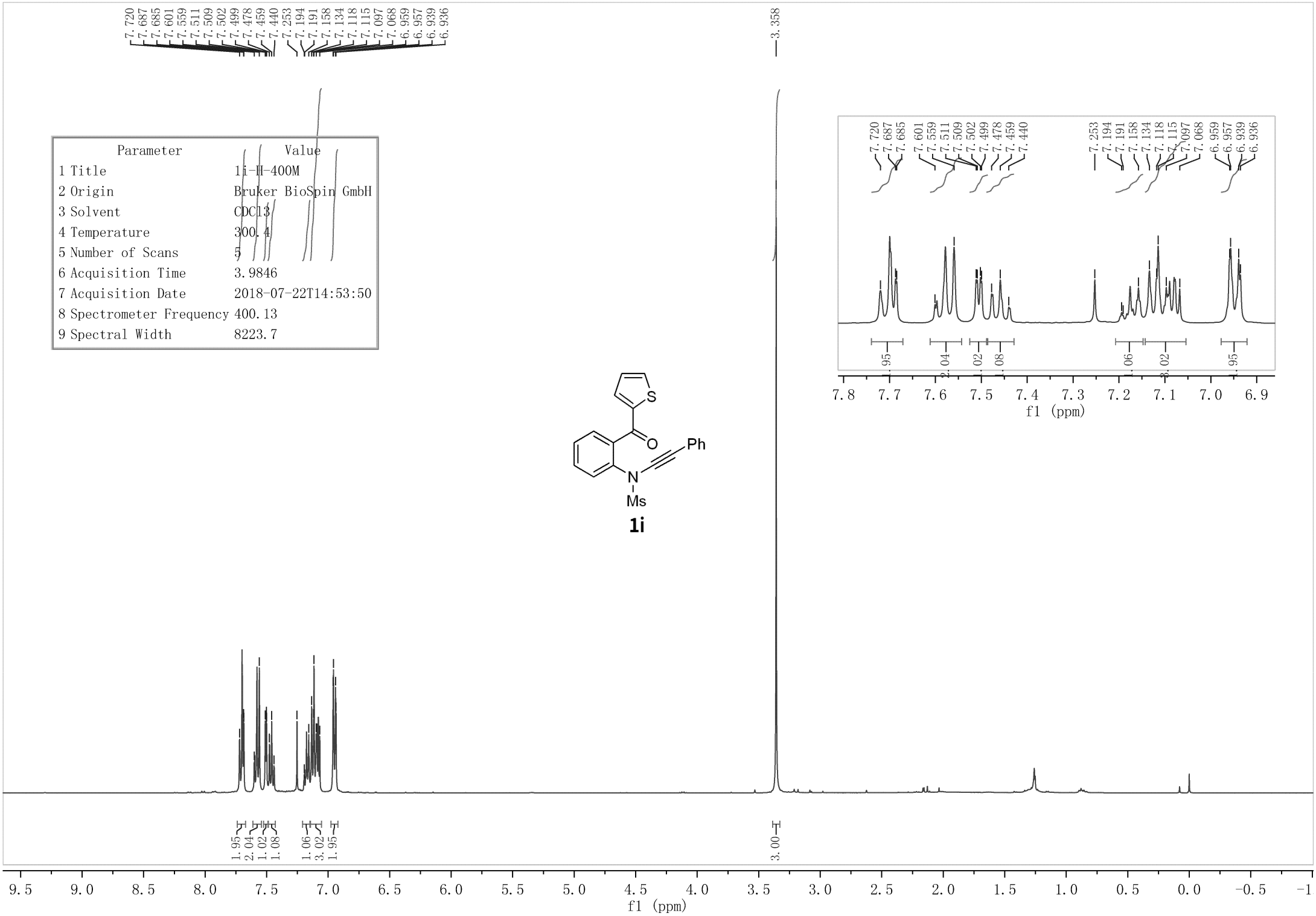


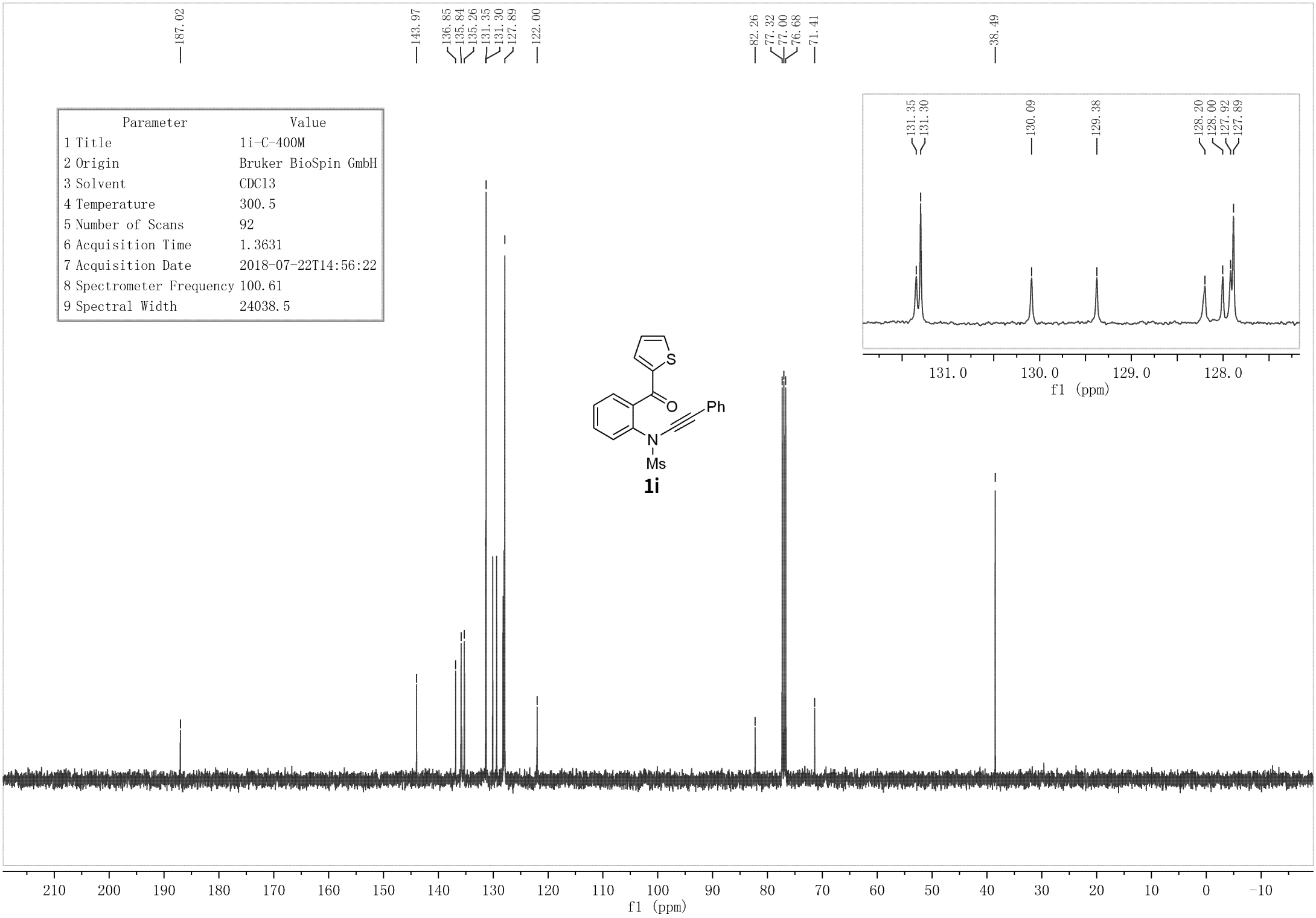

7.782
7.761
7.723
7.703
7.604
7.562
7.462
7.377
7.356
7.245
7.197
7.114
6.967
6.949
3.285
Parameter Value
1 Title 1g-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.2
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-17T22:13:25
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
2.11
1.17
1.22
4.49
3.30
2.19
3.00
f1 (ppm)
Cl
O
Ph
N
Ms
1g

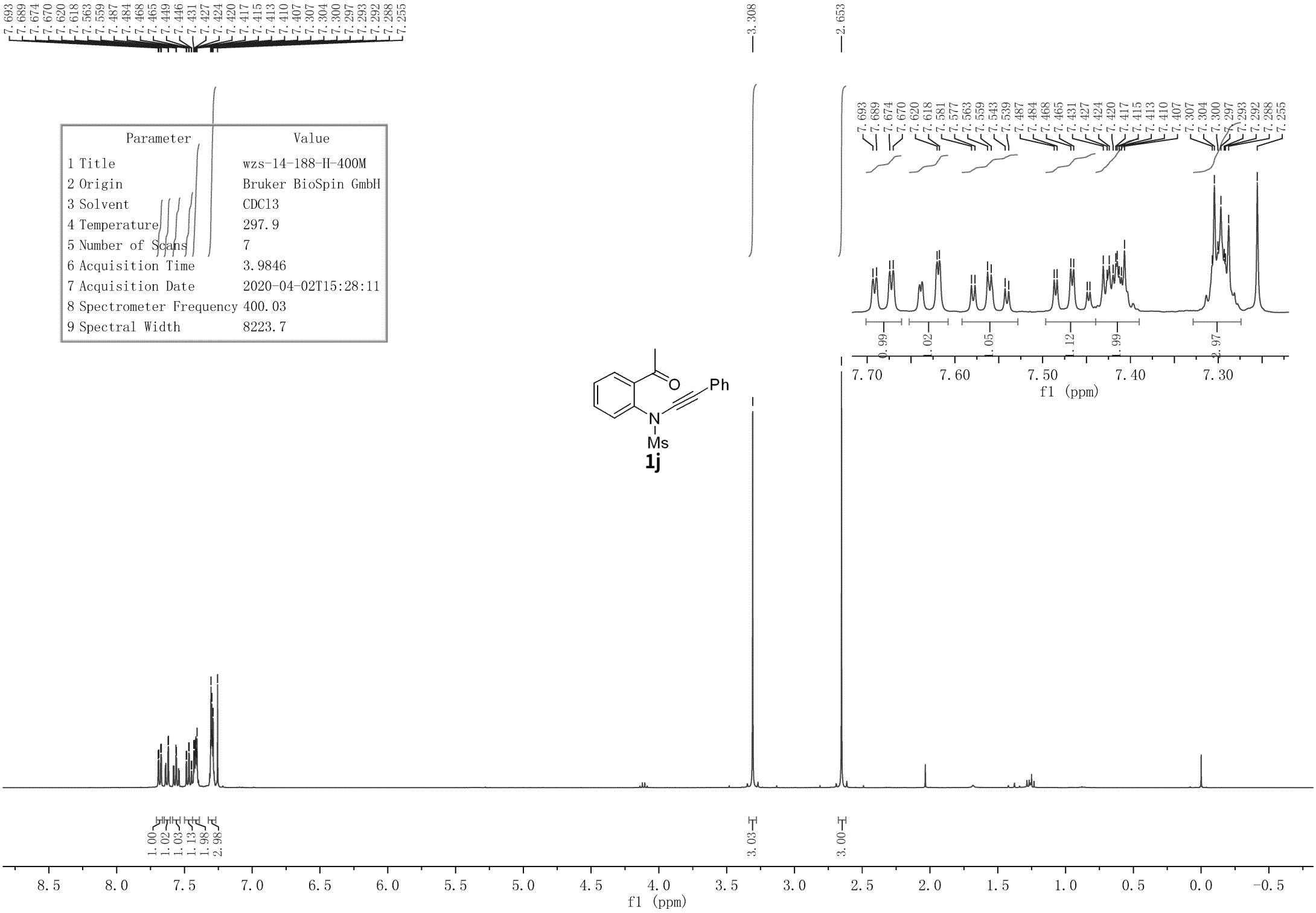

193.81
139.95
137.16
135.74
135.07
131.58
131.39
127.96
121.68
82.39
77.32
77.00
76.68
71.41
38.25
Parameter Value
1 Title 1g-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.3
5 Number of Scans 28
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-17T22:20:27
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.58
131.47
131.39
129.45
129.38
128.73
128.15
128.06
127.96
132
131
130
129
128
f1 (ppm)
Cl
O
Ph
N
Ms
1g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.759
7.738
7.717
7.696
7.588
7.545
7.455
7.452
7.399
7.393
7.254
7.221
7.201
7.187
7.183
7.180
7.143
7.106
7.091
7.087
7.069
7.067
6.905
6.902
6.885
6.881
3.303
2.387
Parameter Value
1 Title 1h-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.8
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-19T14:01:35
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
O
Ph
N
Ms
1h
1.91
0.97
1.00
1.99
1.94
0.98
1.96
1.90
2.99
3.00
f1 (ppm)


194.81
144.53
137.08
136.46
134.27
131.47
127.91
127.81
121.97
82.41
77.32
77.00
76.68
71.32
38.39
21.63
Parameter Value
1 Title 1h-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.9
5 Number of Scans 131
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-19T14:04:00
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.47
131.03
130.55
129.73
129.49
129.17
127.91
127.81
132.0
131.0
130.0
129.0
128.0
f1 (ppm)
O
Ph
N
Ms
1h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

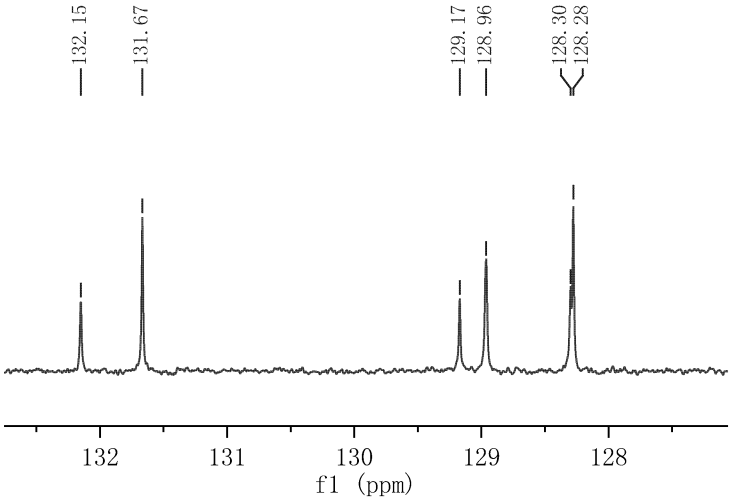

7.720
7.687
7.685
7.601
7.559
7.511
7.509
7.502
7.499
7.478
7.459
7.440
7.253
7.194
7.191
7.158
7.134
7.118
7.115
7.097
7.068
6.959
6.957
6.939
6.936
3.358
Parameter Value
1 Title 1i-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.4
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-22T14:53:50
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
S
O
Ph
N
Ms
1i
1.95
2.04
1.02
1.08
1.06
3.02
1.95
3.00
f1 (ppm)

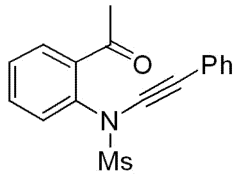

187.02
143.97
136.85
135.84
135.26
131.35
131.30
127.89
122.00
82.26
77.32
77.00
76.68
71.41
38.49
Parameter Value
1 Title 1i-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.5
5 Number of Scans 92
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-22T14:56:22
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.35
131.30
130.09
129.38
128.20
128.00
127.92
127.89
131.0
130.0
129.0
128.0
f1 (ppm)
S
O
Ph
N
Ms
1i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.693 7.689 7.674 7.670 7.620 7.618 7.563 7.559 7.487 7.484 7.468 7.465 7.449 7.446 7.431 7.427 7.424 7.420 7.417 7.415 7.413 7.410 7.407 7.307 7.304 7.300 7.297 7.293 7.292 7.288 7.255
3.308
2.653
Parameter Value
1 Title wzs-14-188-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.9
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2020-04-02T15:28:11
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
O
Ph
N
Ms
1j
0.99 1.02 1.05 1.12 1.99 2.97
7.70 7.60 7.50 7.40 7.30
f1 (ppm)
1.00 1.02 1.03 1.13 1.98 2.98
3.03
3.00
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)

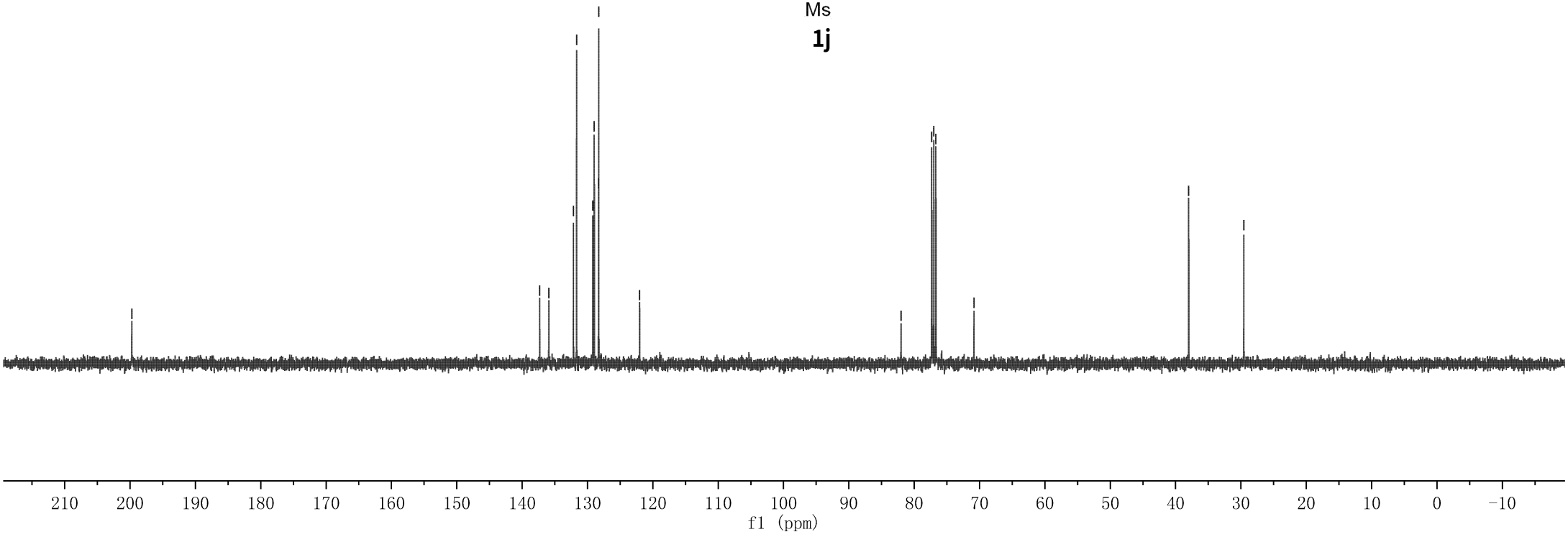
199.73
137.32
135.92
132.15
131.67
129.17
128.96
128.30
128.28
122.02
82.01
77.32
77.00
76.68
70.86
37.99
29.56

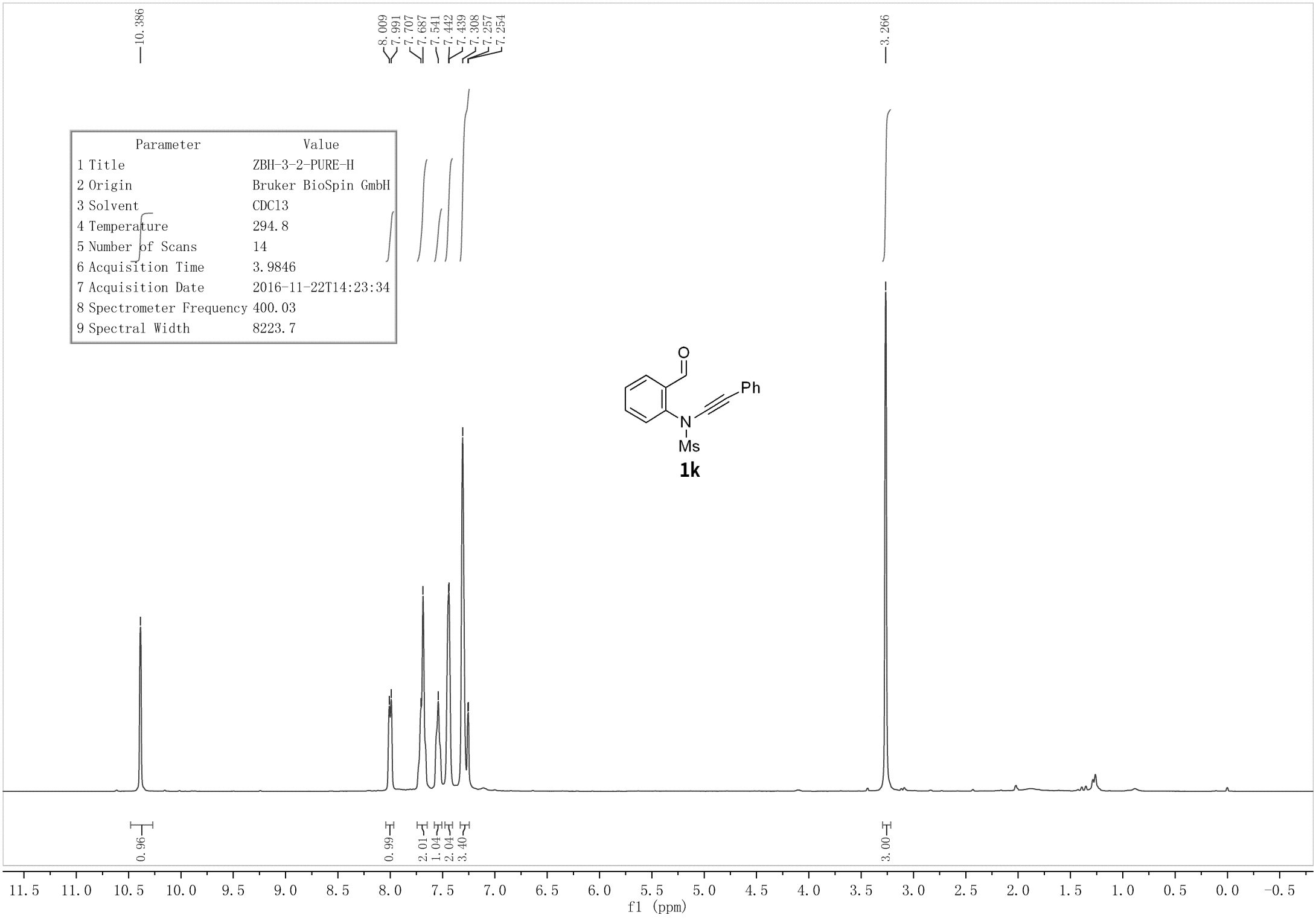
| Parameter | Value |
|---|---|
| 1 Title | wzs-14-188-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.3 |
| 5 Number of Scans | 22 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-04-02T15:30:35 |
| 8 Spectrometer Frequency | 100.59 |
| 9 Spectral Width | 24038.5 |

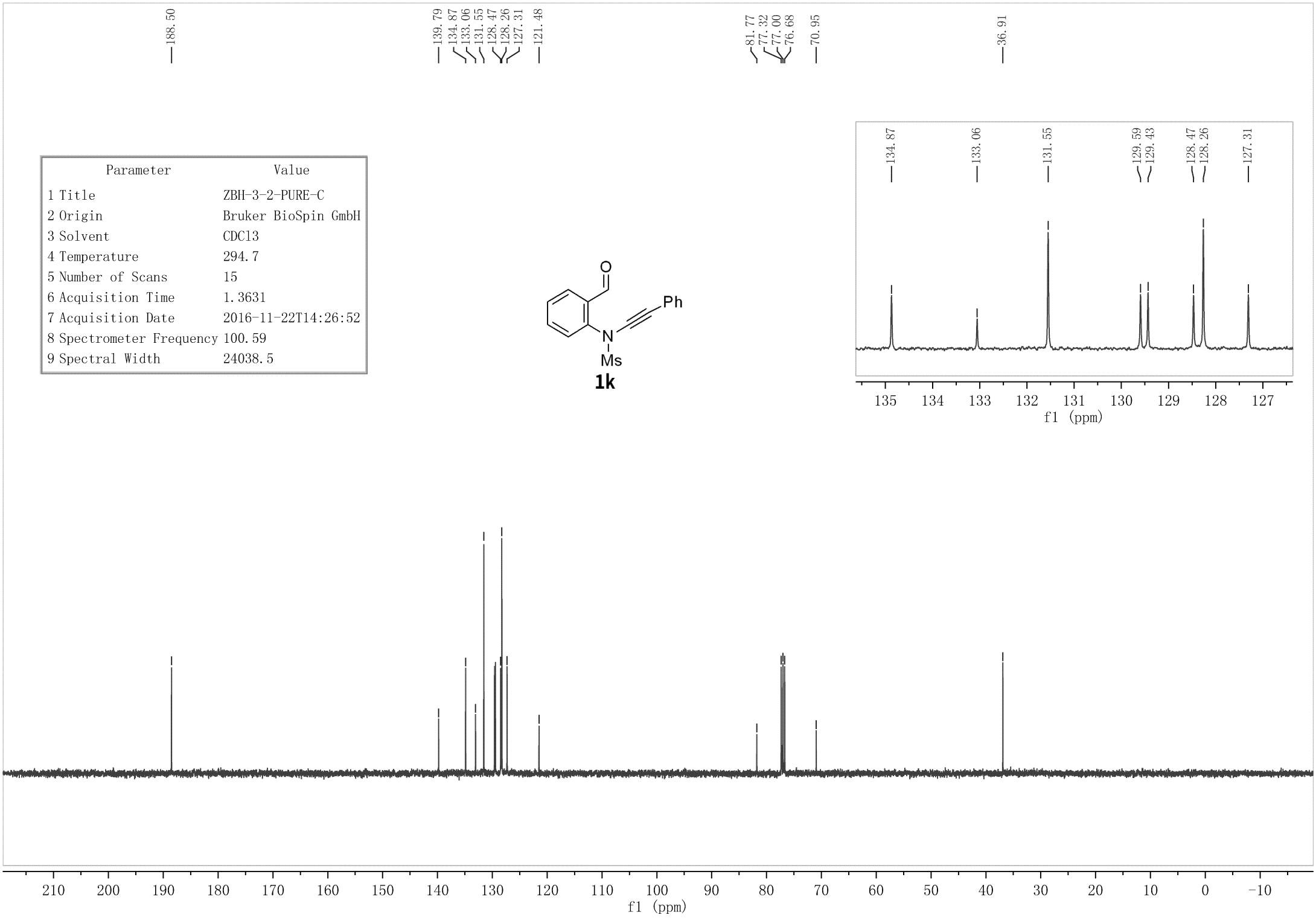


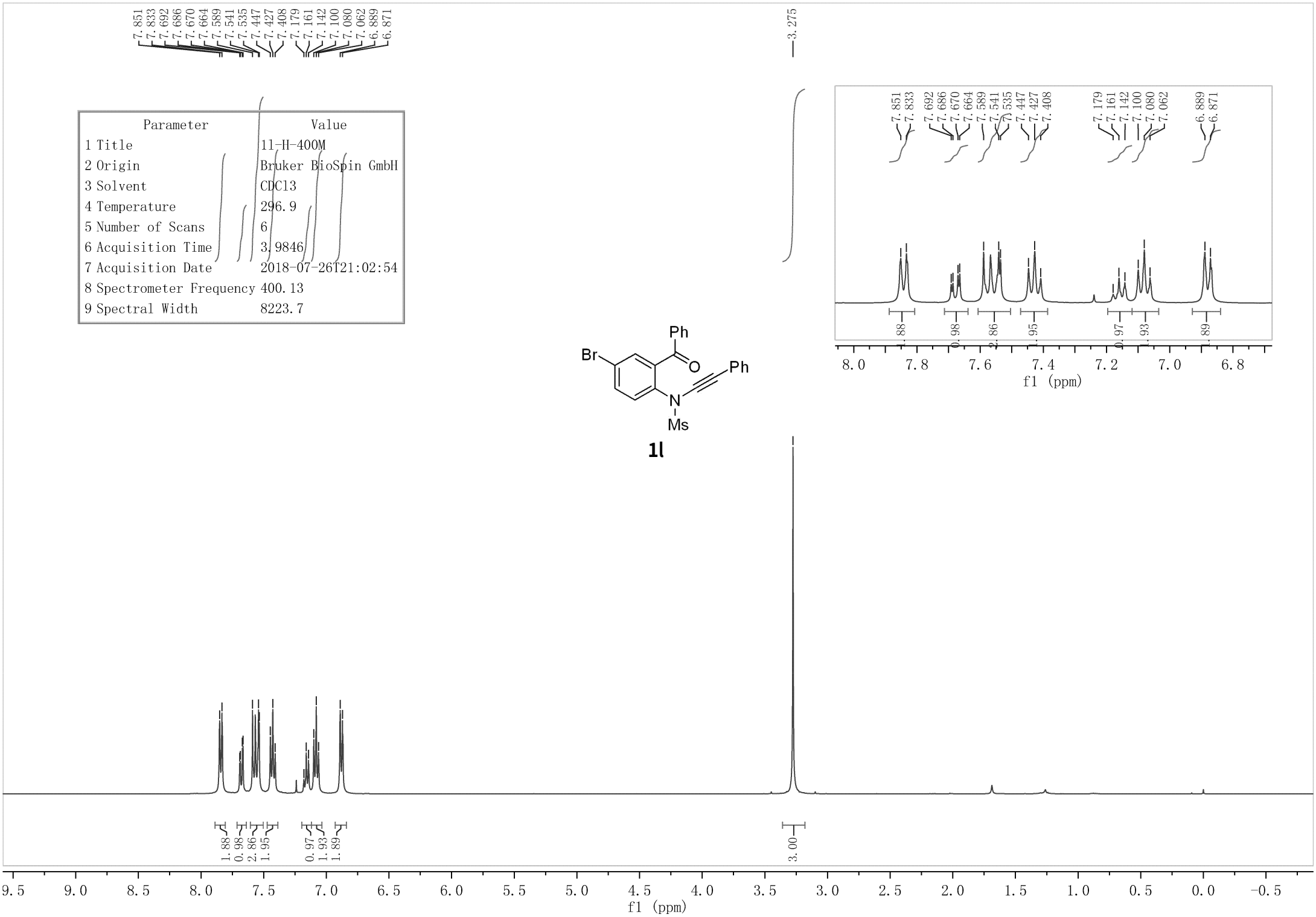



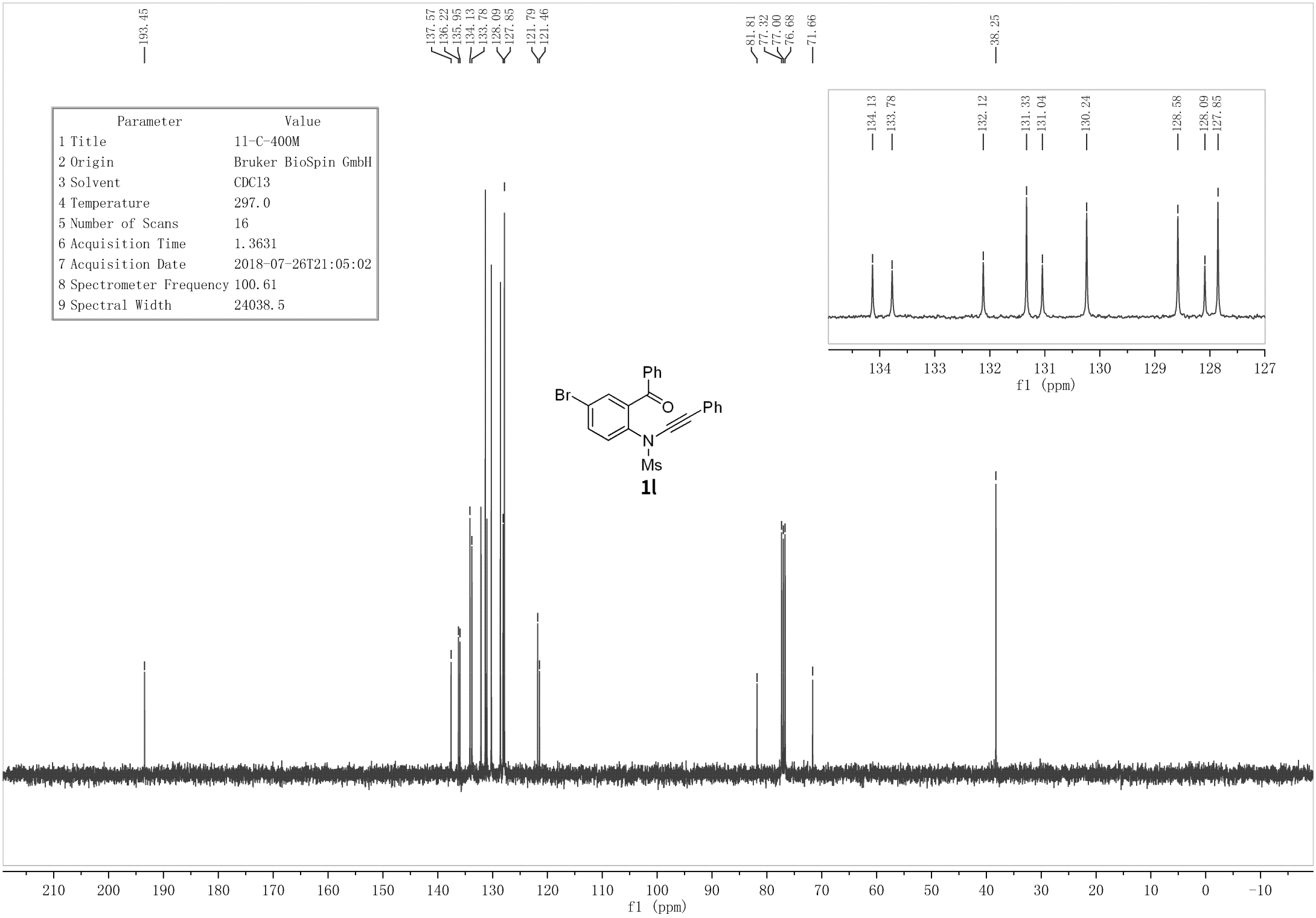

**1j**

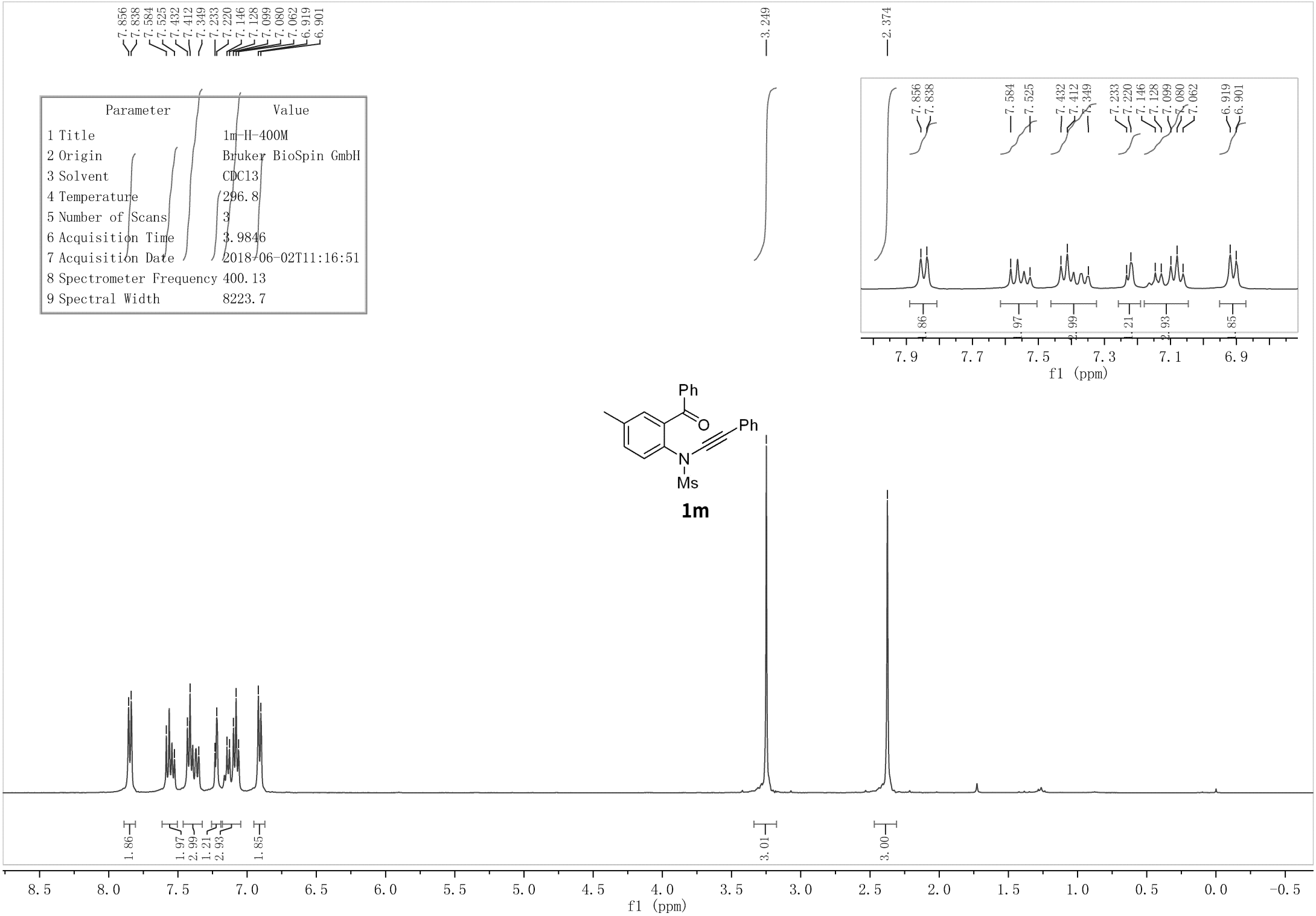


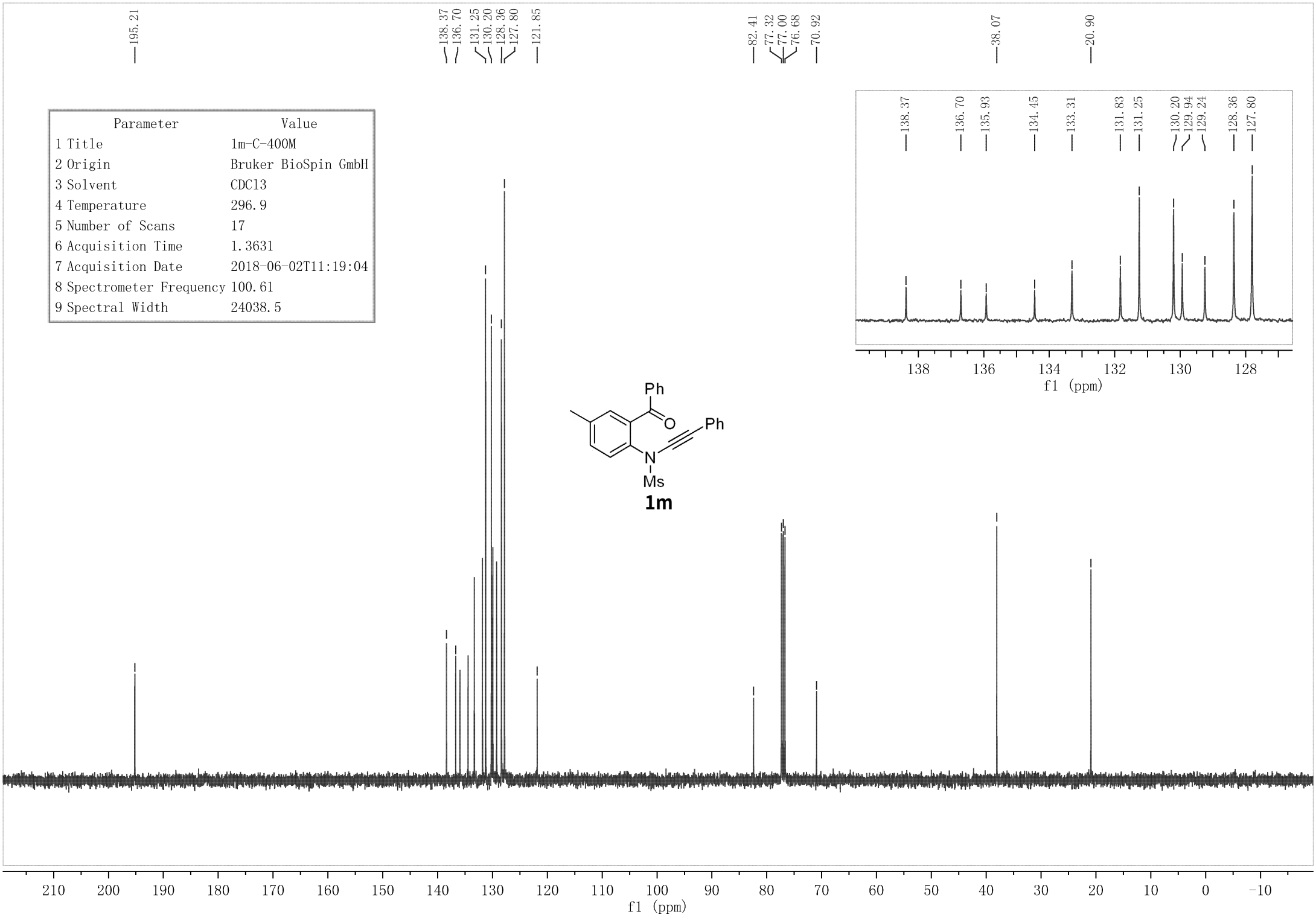

10.386
8.009
7.991
7.707
7.687
7.541
7.442
7.439
7.308
7.257
7.254
3.266
Parameter Value
1 Title ZBH-3-2-PURE-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.8
5 Number of Scans 14
6 Acquisition Time 3.9846
7 Acquisition Date 2016-11-22T14:23:34
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
O
Ph
N
Ms
1k
0.96
0.99
2.01
1.04
2.04
3.40
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

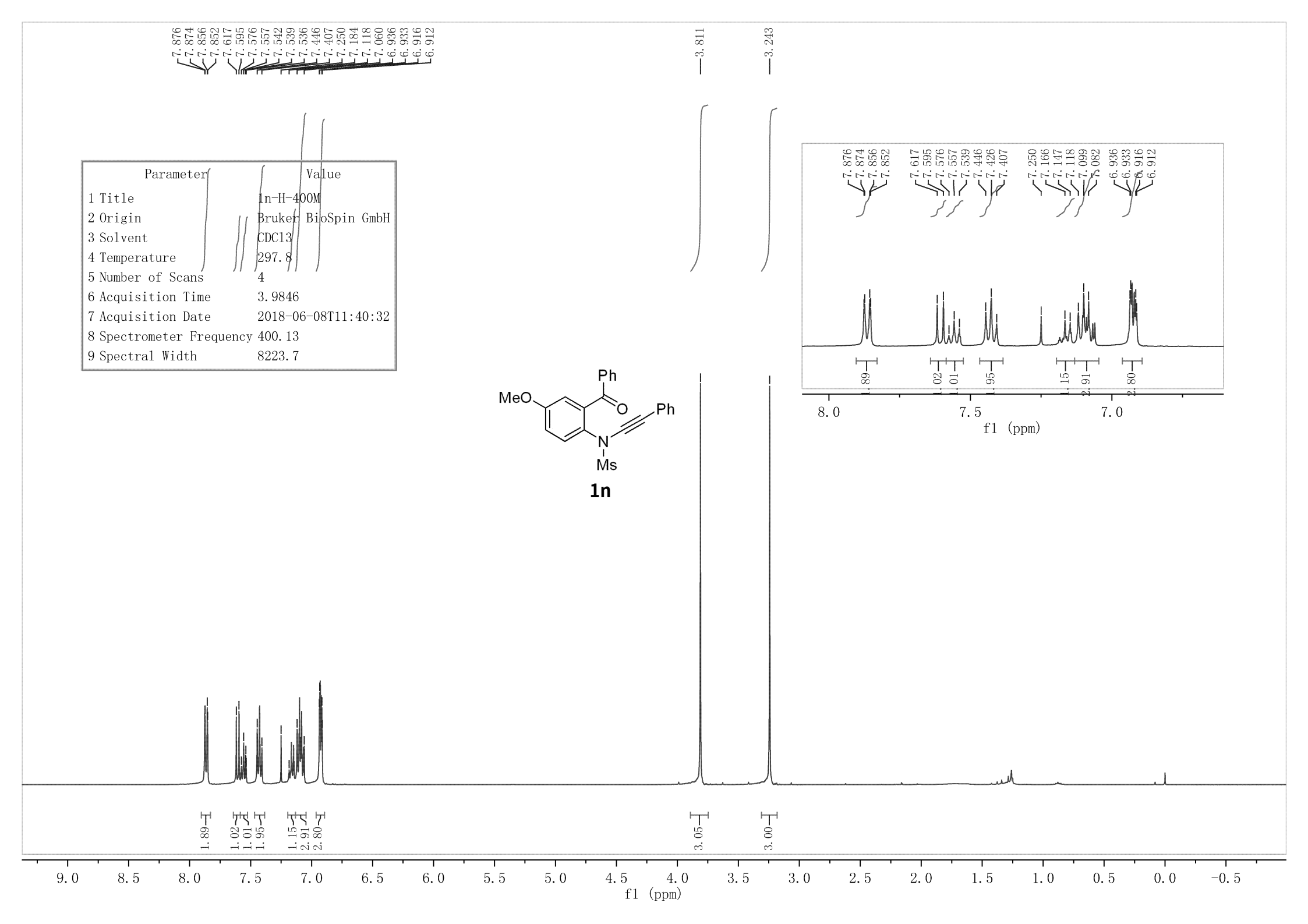

188.50
139.79
134.87
133.06
131.55
128.47
128.26
127.31
121.48
81.77
77.32
77.00
76.68
70.95
36.91
Parameter Value
1 Title ZBH-3-2-PURE-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.7
5 Number of Scans 15
6 Acquisition Time 1.3631
7 Acquisition Date 2016-11-22T14:26:52
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
O
Ph
N
Ms
1k
134.87
133.06
131.55
129.59
129.43
128.47
128.26
127.31
135 134 133 132 131 130 129 128 127
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.851
7.833
7.692
7.686
7.670
7.664
7.589
7.541
7.535
7.447
7.427
7.408
7.179
7.161
7.142
7.100
7.080
7.062
6.889
6.871
3.275
Parameter Value
1 Title 11-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.9
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-26T21:02:54
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Br
Ph
O
Ph
N
Ms
1l
1.88
0.98
2.86
1.95
0.97
1.93
1.89
3.00
f1 (ppm)


193.45
137.57
136.22
135.95
134.13
133.78
128.09
127.85
121.79
121.46
81.81
77.32
77.00
76.68
71.66
38.25
Parameter Value
1 Title 11-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.0
5 Number of Scans 16
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-26T21:05:02
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
134.13
133.78
132.12
131.33
131.04
130.24
128.58
128.09
127.85
f1 (ppm)
Ph
Br
O
Ph
N
Ms
1l
f1 (ppm)

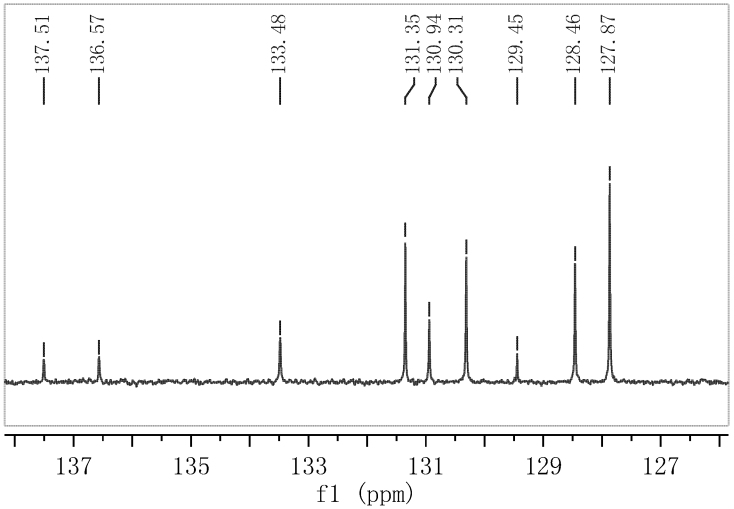

7.856
7.838
7.584
7.525
7.432
7.412
7.349
7.233
7.220
7.146
7.128
7.099
7.080
7.062
6.919
6.901
3.249
2.374
Parameter Value
1 Title 1m-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 3
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-02T11:16:51
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
1.86
1.97
2.99
1.21
2.93
1.85
3.01
3.00
f1 (ppm)
Ph
O
Ph
N
Ms
1m


195.21
138.37
136.70
131.25
130.20
128.36
127.80
121.85
82.41
77.32
77.00
76.68
70.92
38.07
20.90
Parameter Value
1 Title 1m-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.9
5 Number of Scans 17
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-02T11:19:04
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
138.37
136.70
135.93
134.45
133.31
131.83
131.25
130.20
129.94
129.24
128.36
127.80
138
136
134
132
130
128
f1 (ppm)
Ph
O
Ph
N
Ms
1m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.876
7.874
7.856
7.852
7.617
7.595
7.576
7.557
7.542
7.539
7.536
7.446
7.407
7.250
7.184
7.118
7.060
6.936
6.933
6.916
6.912
3.811
3.243
Parameter Value
1 Title 1n-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.8
5 Number of Scans 4
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-08T11:40:32
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
MeO
Ph
O
Ph
N
Ms
1n
1.89
1.02
1.01
1.95
1.15
2.91
2.80
3.05
3.00
f1 (ppm)

194.83
158.92
137.51
136.57
133.48
131.35
130.94
130.31
129.45
128.46
127.87
121.98
116.30
114.89
82.53
77.32
77.00
76.68
70.86
55.75
38.08

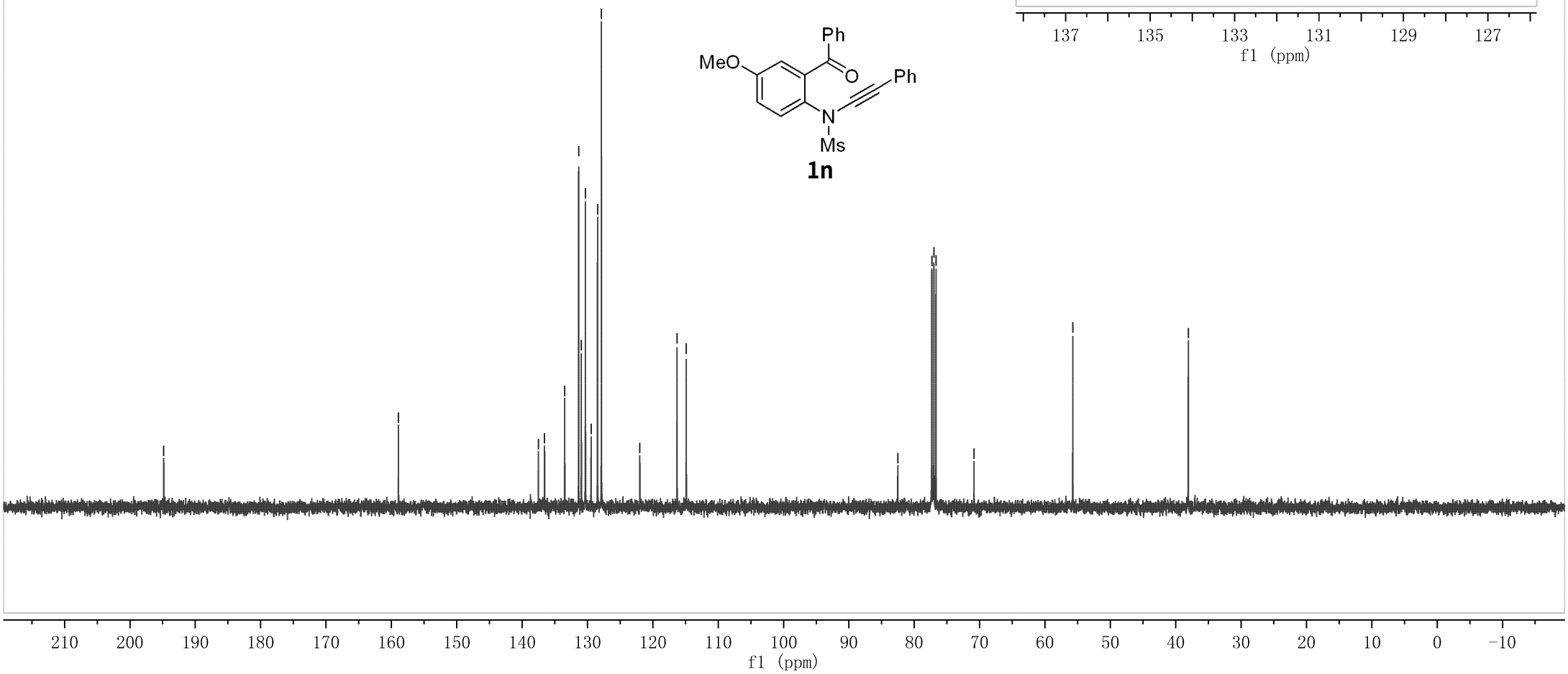
| Parameter | Value |
|---|---|
| 1 Title | 1n-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 297.9 |
| 5 Number of Scans | 33 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-06-08T11:42:46 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |



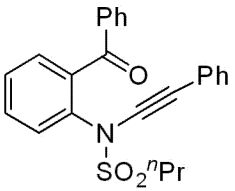




**1n**

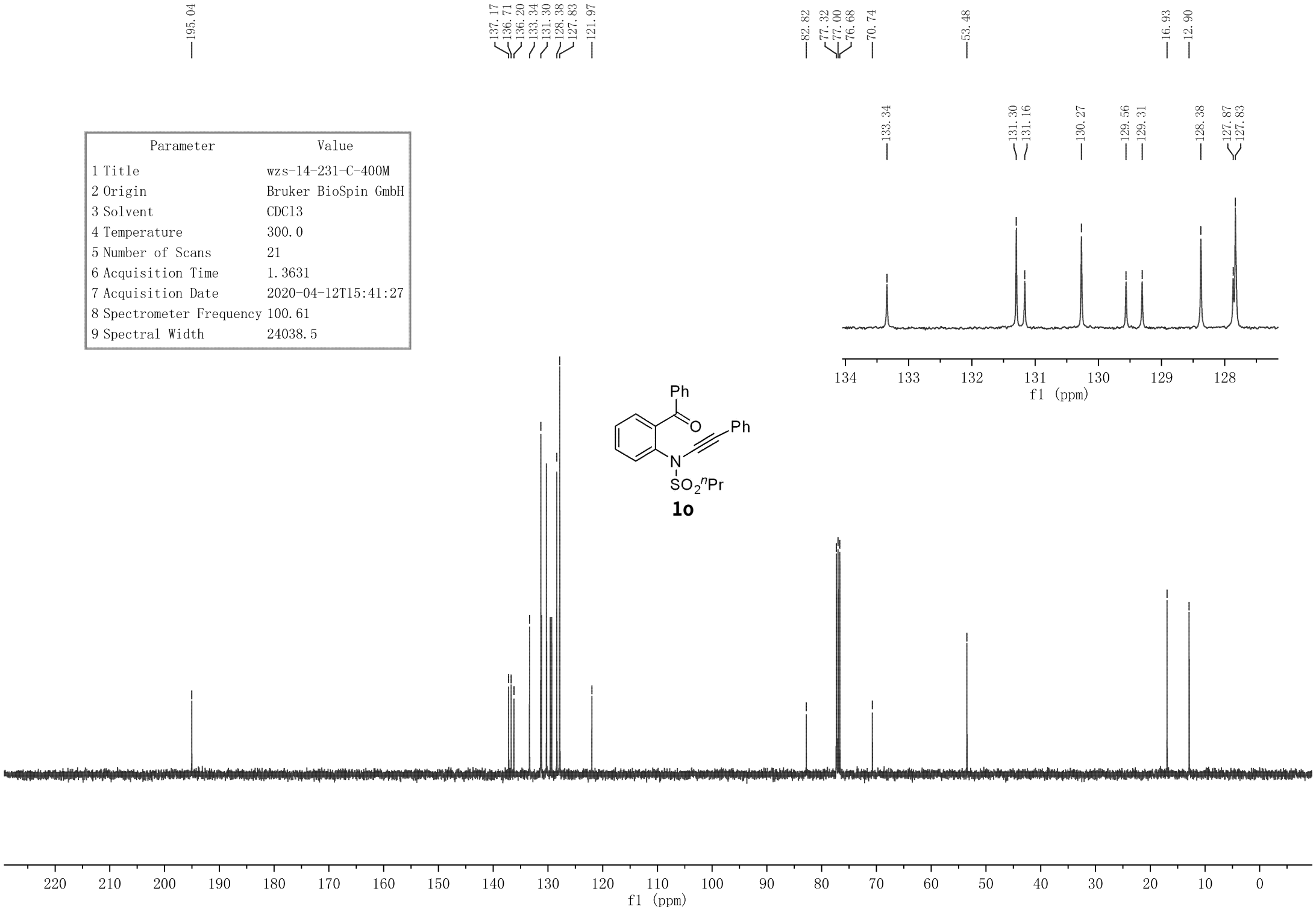


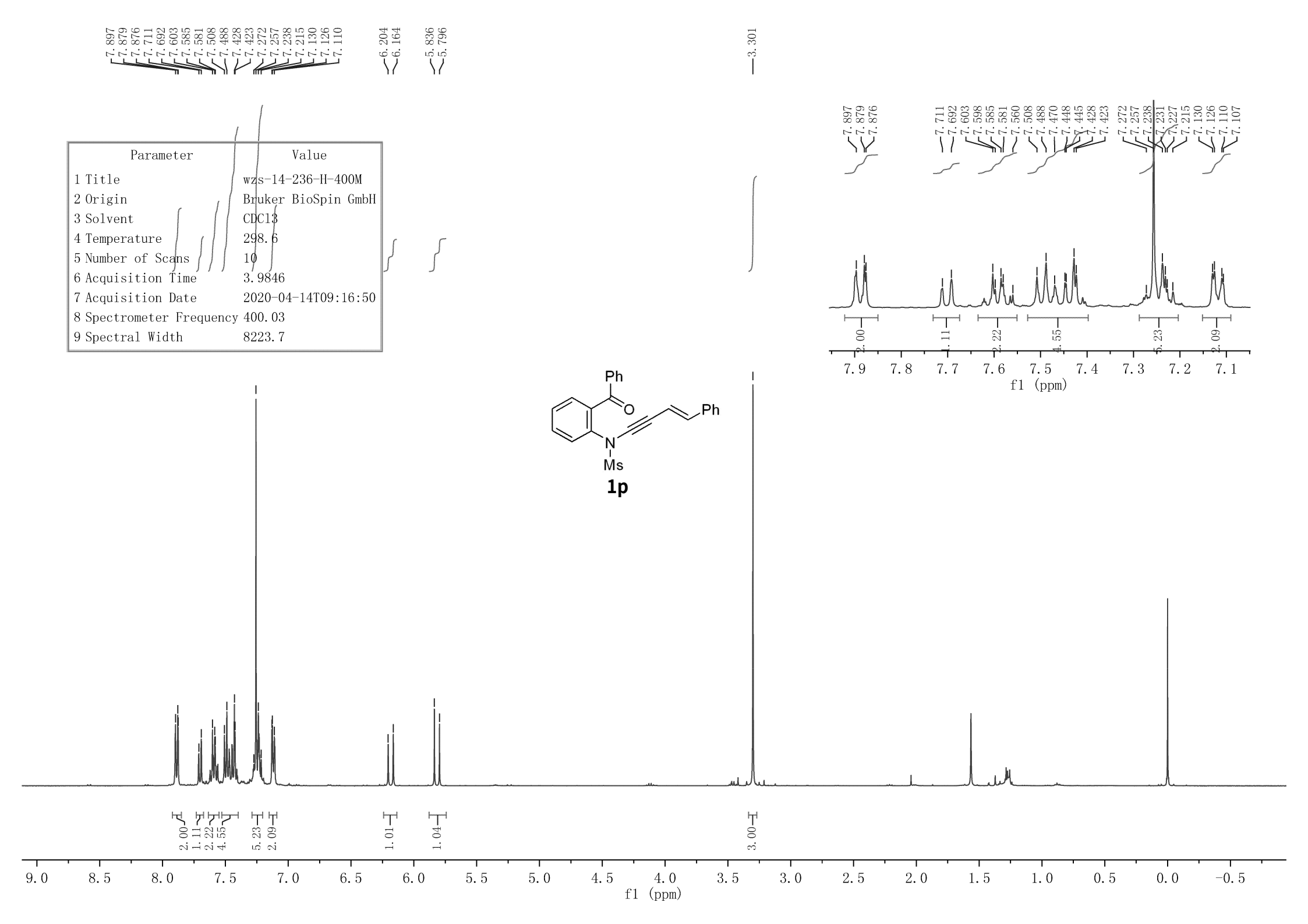
| Parameter | Value |
|---|---|
| 1 Title | wzs-14-231-H-400M-1 |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.0 |
| 5 Number of Scans | 7 |
| 6 Acquisition Time | 4.0894 |
| 7 Acquisition Date | 2020-04-12T16:50:33 |
| 8 Spectrometer Frequency | 400.13 |
| 9 Spectral Width | 8012.8 |

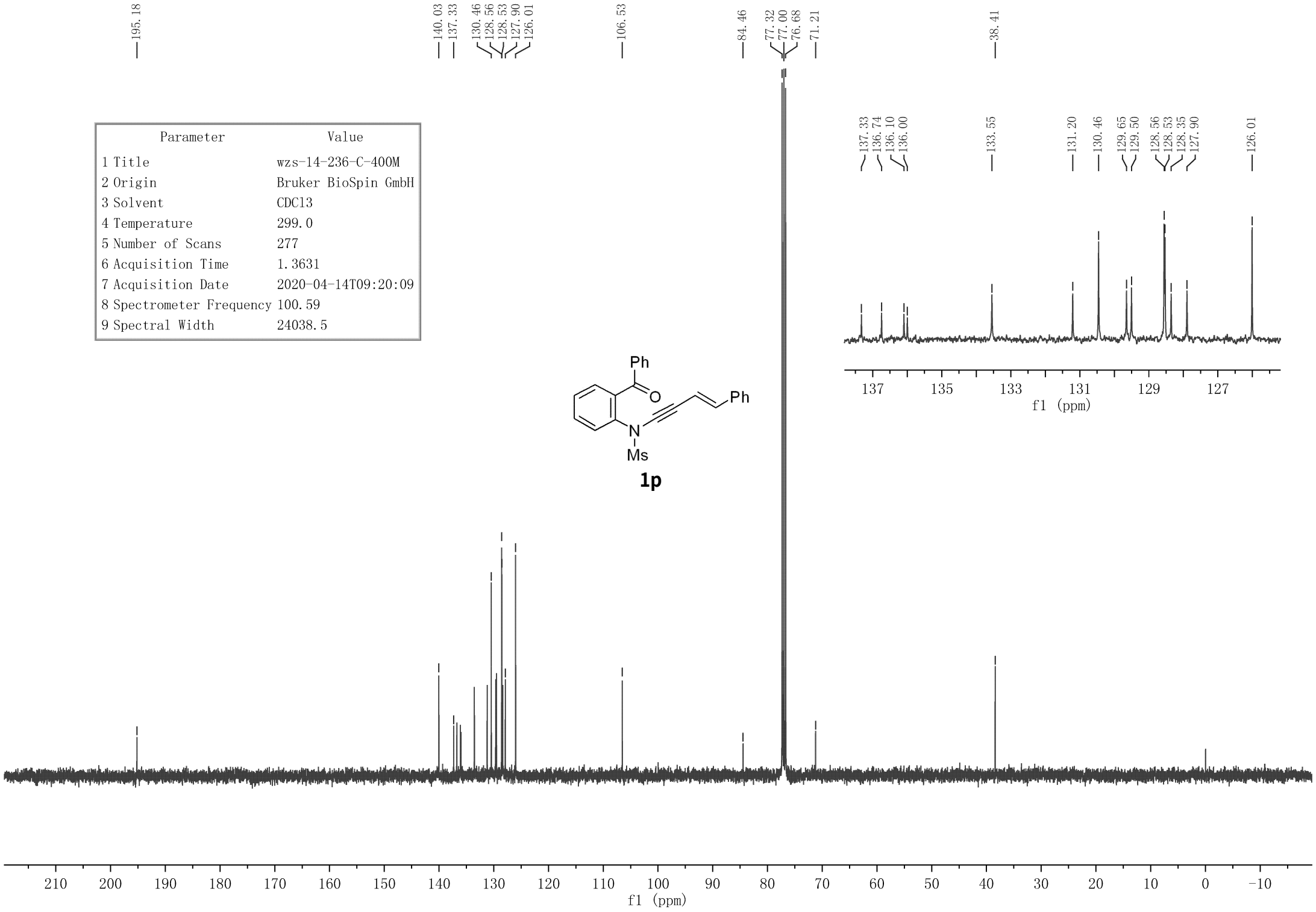


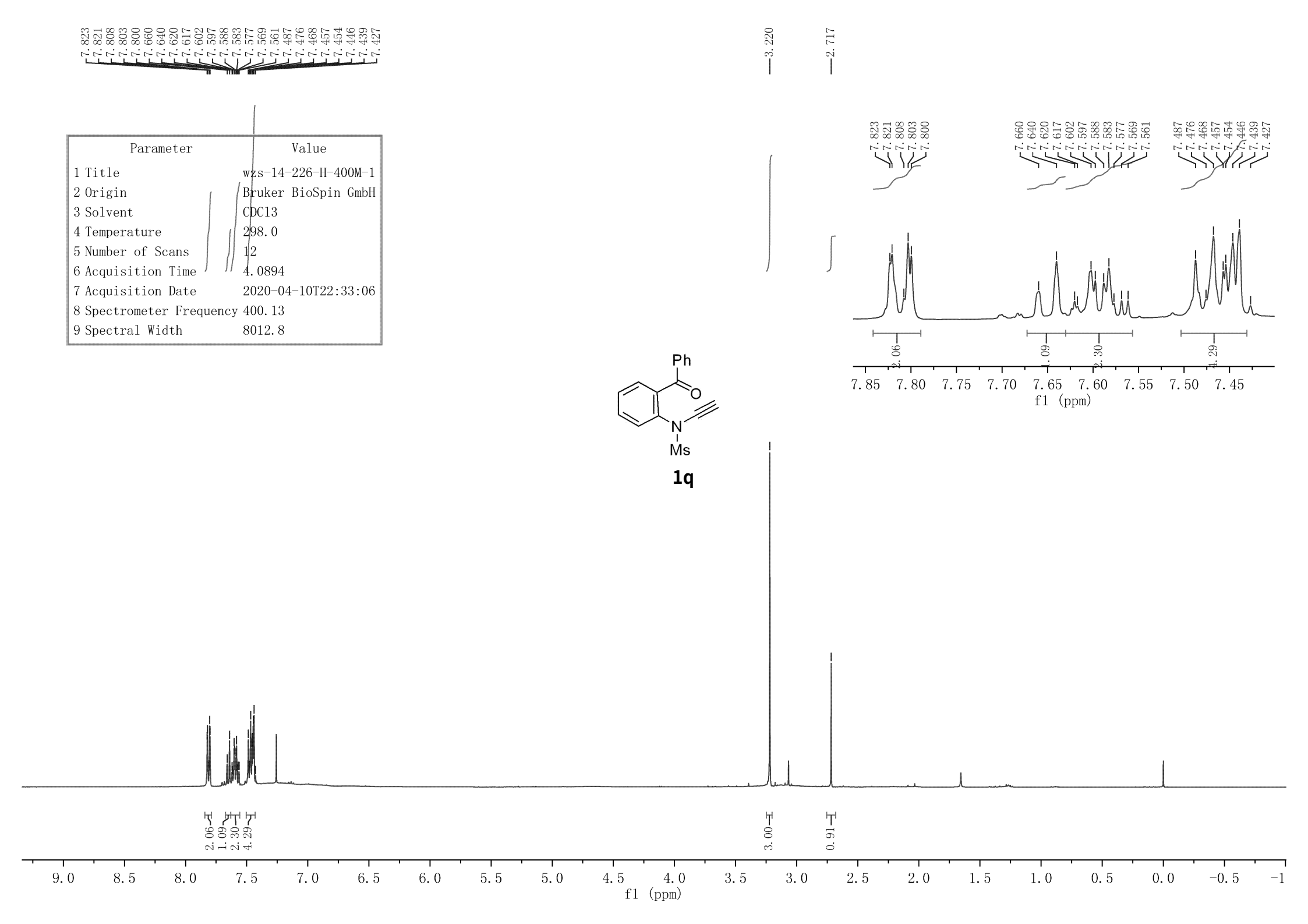

**1o**

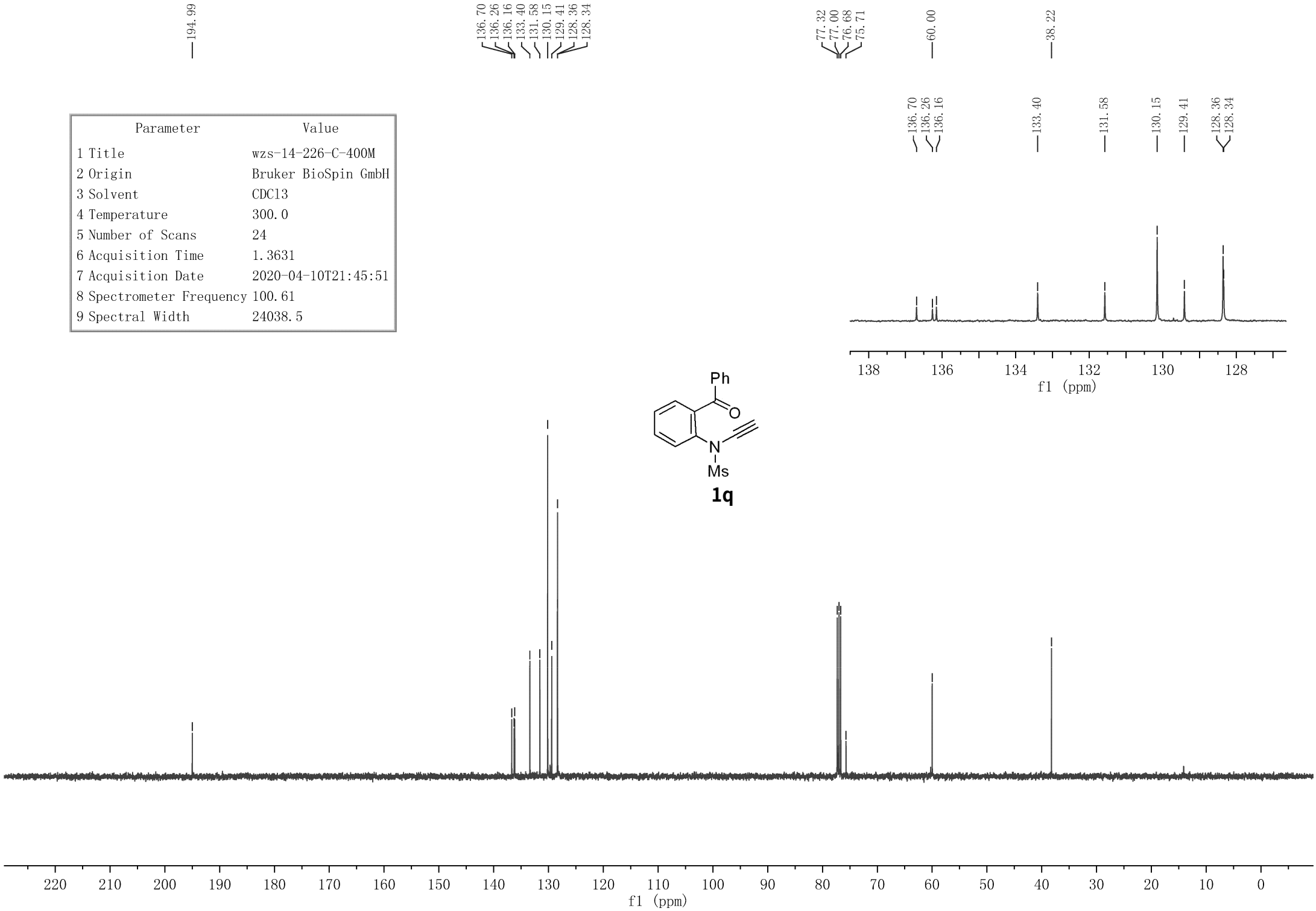
f1 (ppm)

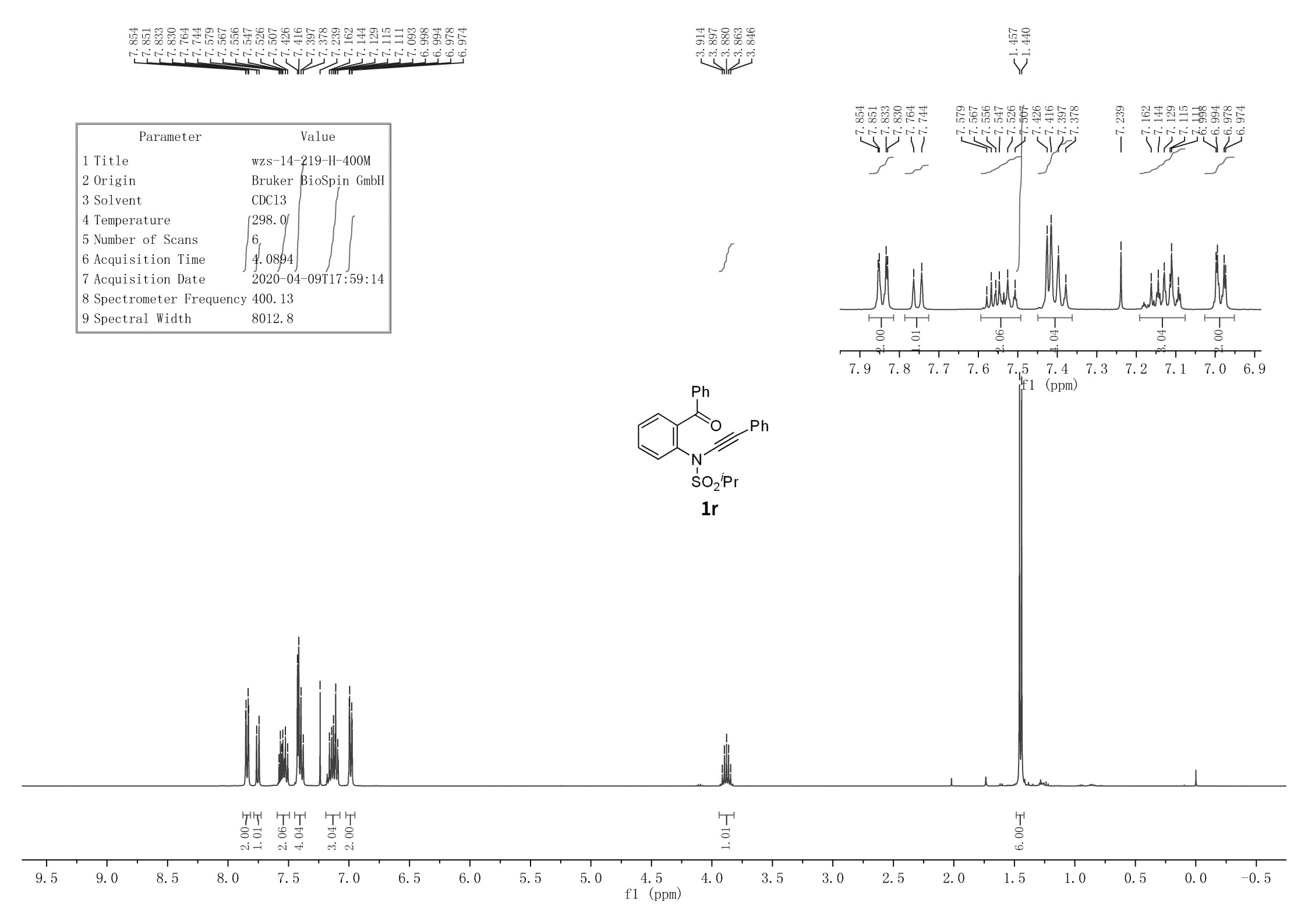

195.04
137.17
136.71
136.20
133.34
131.30
128.38
127.83
121.97
82.82
77.32
77.00
76.68
70.74
53.48
16.93
12.90
133.34
131.30
131.16
130.27
129.56
129.31
128.38
127.87
127.83
Parameter Value
1 Title wzs-14-231-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 21
6 Acquisition Time 1.3631
7 Acquisition Date 2020-04-12T15:41:27
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ph
O
Ph
N
SO2nPr
1o
f1 (ppm)
f1 (ppm)

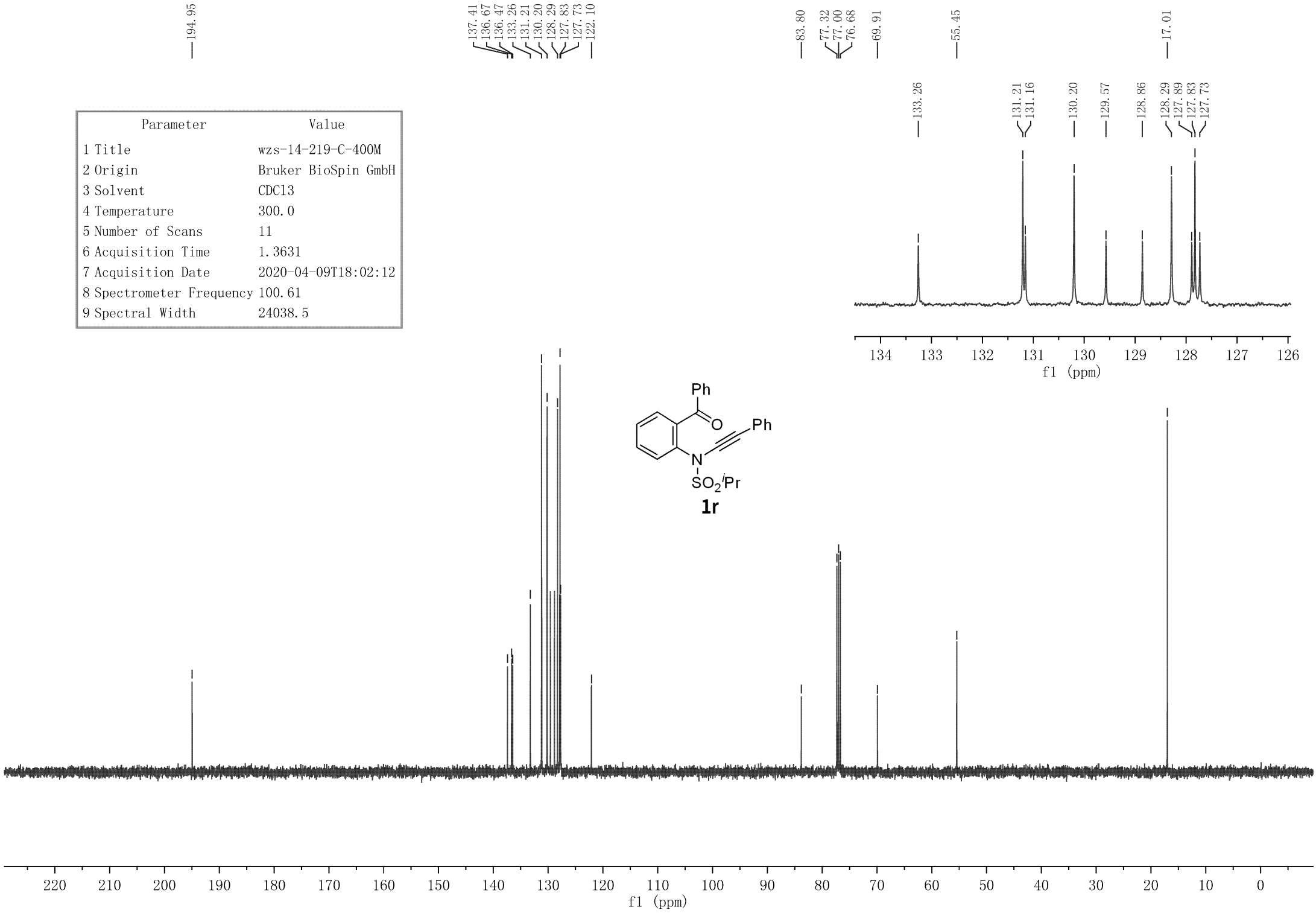

7.897
7.879
7.876
7.711
7.692
7.603
7.585
7.581
7.508
7.488
7.428
7.423
7.272
7.257
7.238
7.215
7.130
7.126
7.110
6.204
6.164
5.836
5.796
3.301
Parameter Value
1 Title wzs-14-236-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.6
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2020-04-14T09:16:50
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ph
O
Ph
N
Ms
1p
2.00
1.11
2.22
4.55
5.23
2.09
1.01
1.04
3.00
f1 (ppm)


195.18
140.03
137.33
130.46
128.56
128.53
127.90
126.01
106.53
84.46
77.32
77.00
76.68
71.21
38.41
Parameter Value
1 Title wzs-14-236-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.0
5 Number of Scans 277
6 Acquisition Time 1.3631
7 Acquisition Date 2020-04-14T09:20:09
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
Ph
O
Ph
N
Ms
1p
137.33
136.74
136.10
136.00
133.55
131.20
130.46
129.65
129.50
128.56
128.53
128.35
127.90
126.01
137
135
133
131
129
127
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

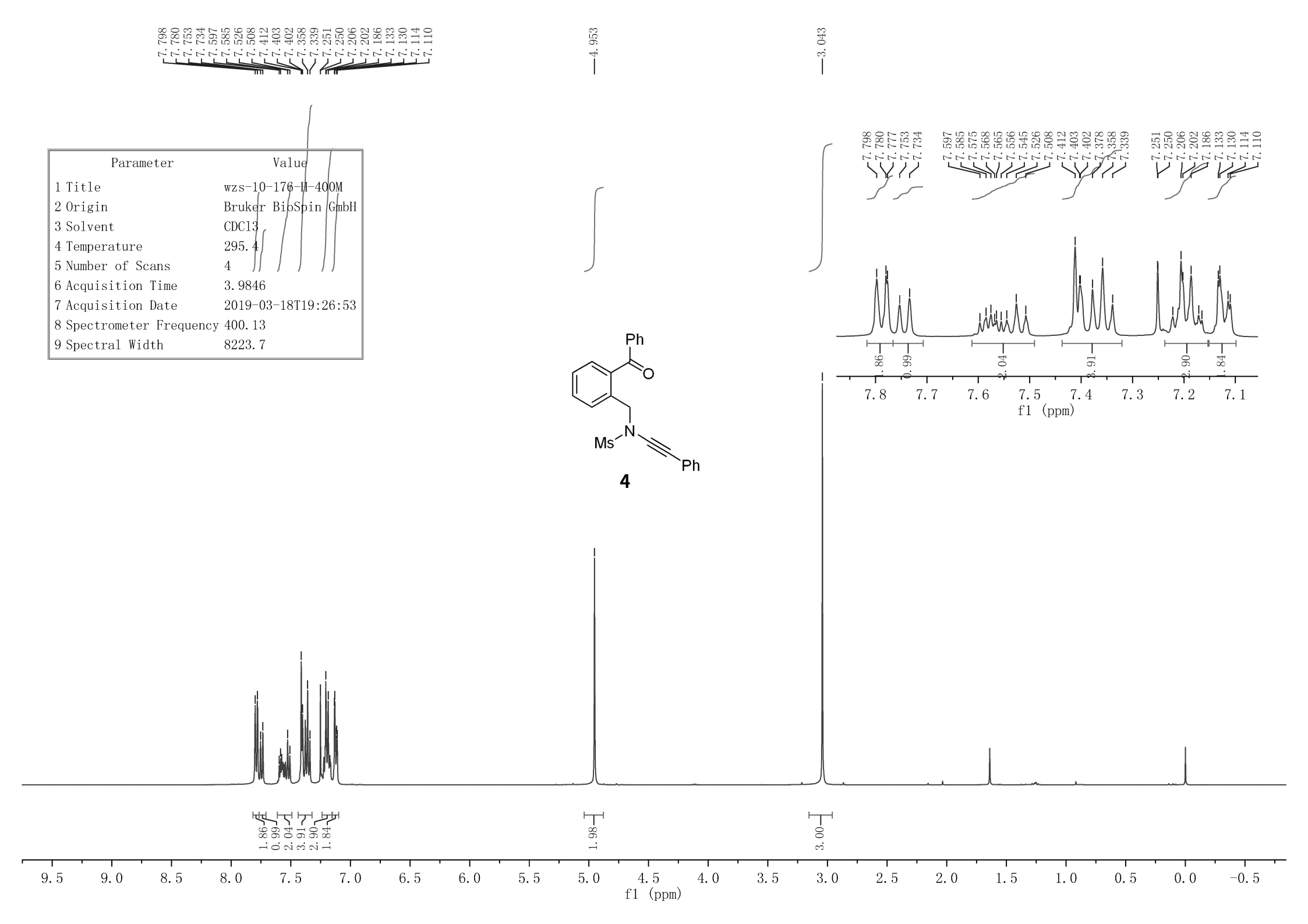

7.823
7.821
7.808
7.803
7.800
7.660
7.640
7.620
7.617
7.602
7.597
7.588
7.583
7.577
7.569
7.561
7.487
7.476
7.468
7.457
7.454
7.446
7.439
7.427
3.220
2.717
Parameter Value
1 Title wzs-14-226-H-400M-1
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 12
6 Acquisition Time 4.0894
7 Acquisition Date 2020-04-10T22:33:06
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ph
O
N
Ms
1q
2.06
1.09
2.30
4.29
3.00
0.91
f1 (ppm)

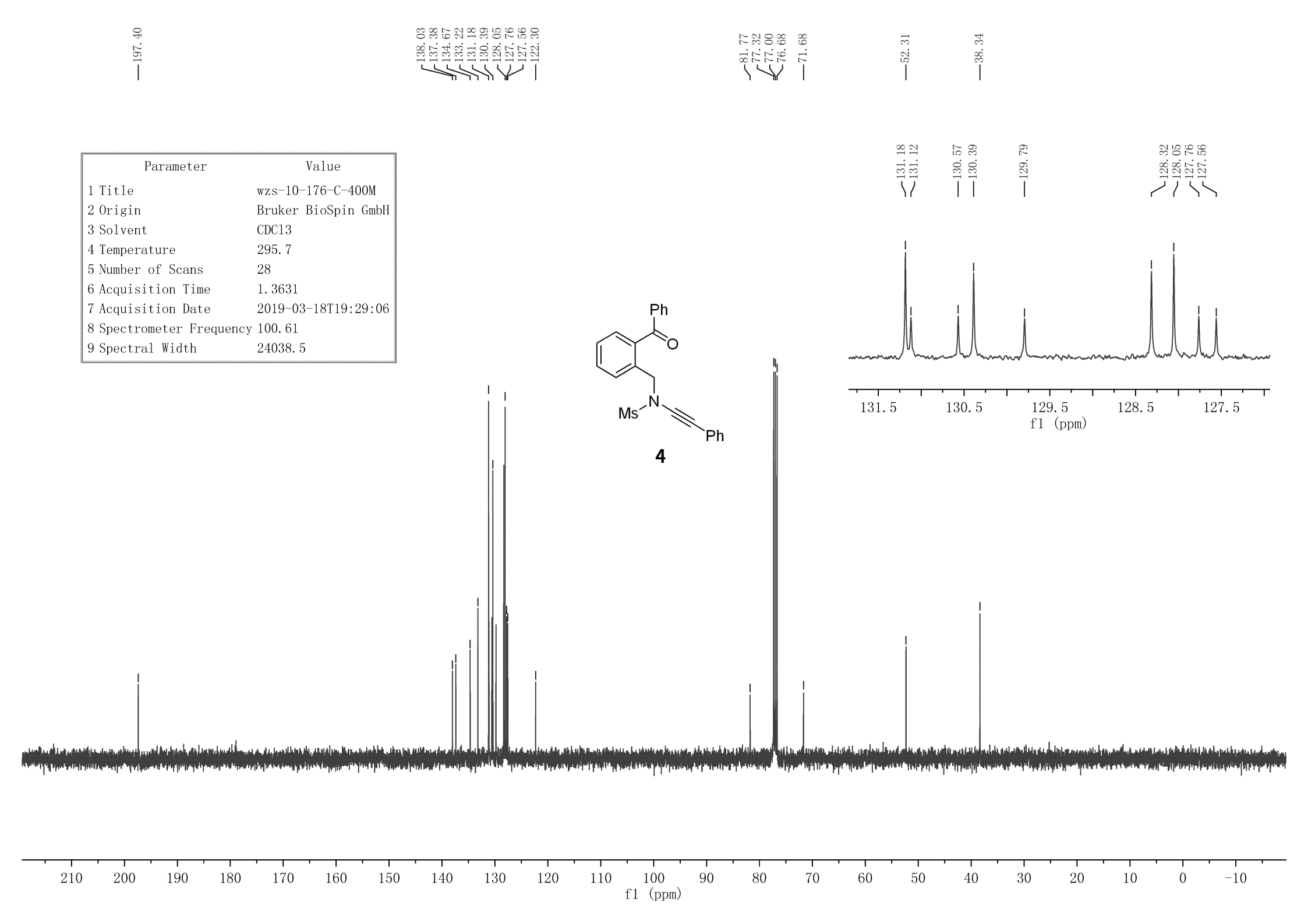

194.99
136.70
136.26
136.16
133.40
131.58
130.15
129.41
128.36
128.34
77.32
77.00
76.68
75.71
60.00
38.22
Parameter Value
1 Title wzs-14-226-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 24
6 Acquisition Time 1.3631
7 Acquisition Date 2020-04-10T21:45:51
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ph
O
N
Ms
1q
f1 (ppm)


7.854
7.851
7.833
7.830
7.764
7.744
7.579
7.567
7.556
7.547
7.526
7.507
7.426
7.416
7.397
7.378
7.239
7.162
7.144
7.129
7.115
7.111
7.093
6.998
6.994
6.978
6.974
3.914
3.897
3.880
3.863
3.846
1.457
1.440
Parameter Value
1 Title wzs-14-219-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2020-04-09T17:59:14
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ph
O
Ph
N
SO2iPr
1r
2.00
1.01
2.06
4.04
3.04
2.00
1.01
6.00
f1 (ppm)

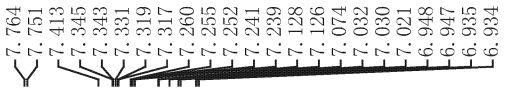



| Parameter | Value |
|---|---|
| 1 Title | wzs-14-219-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Number of Scans | 11 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-04-09T18:02:12 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |


7.798
7.780
7.753
7.734
7.597
7.585
7.526
7.508
7.412
7.403
7.402
7.358
7.339
7.251
7.250
7.206
7.202
7.186
7.133
7.130
7.114
7.110
4.953
3.043
Parameter Value
1 Title wzs-10-176-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.4
5 Number of Scans 4
6 Acquisition Time 3.9846
7 Acquisition Date 2019-03-18T19:26:53
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
O
N
Ms
Ph
4
1.86
0.99
2.04
3.91
2.90
1.84
1.98
3.00
f1 (ppm)

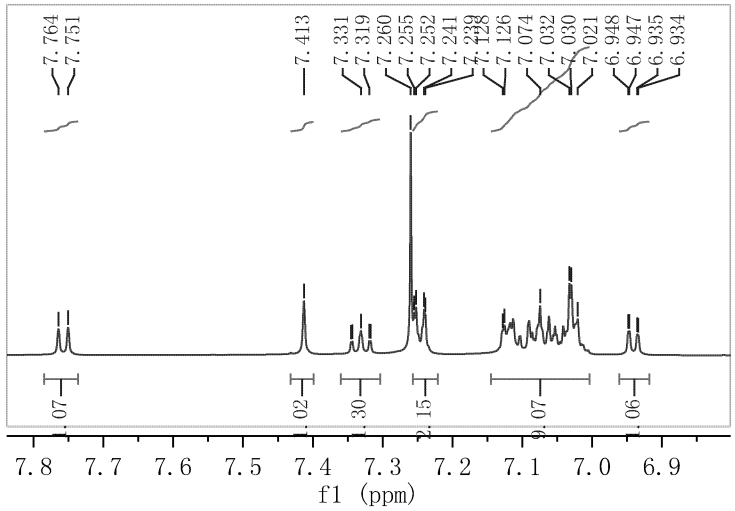


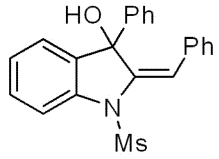

| Parameter | Value |
|---|---|
| 1 Title | wzs-10-176-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 295.7 |
| 5 Number of Scans | 28 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2019-03-18T19:29:06 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |



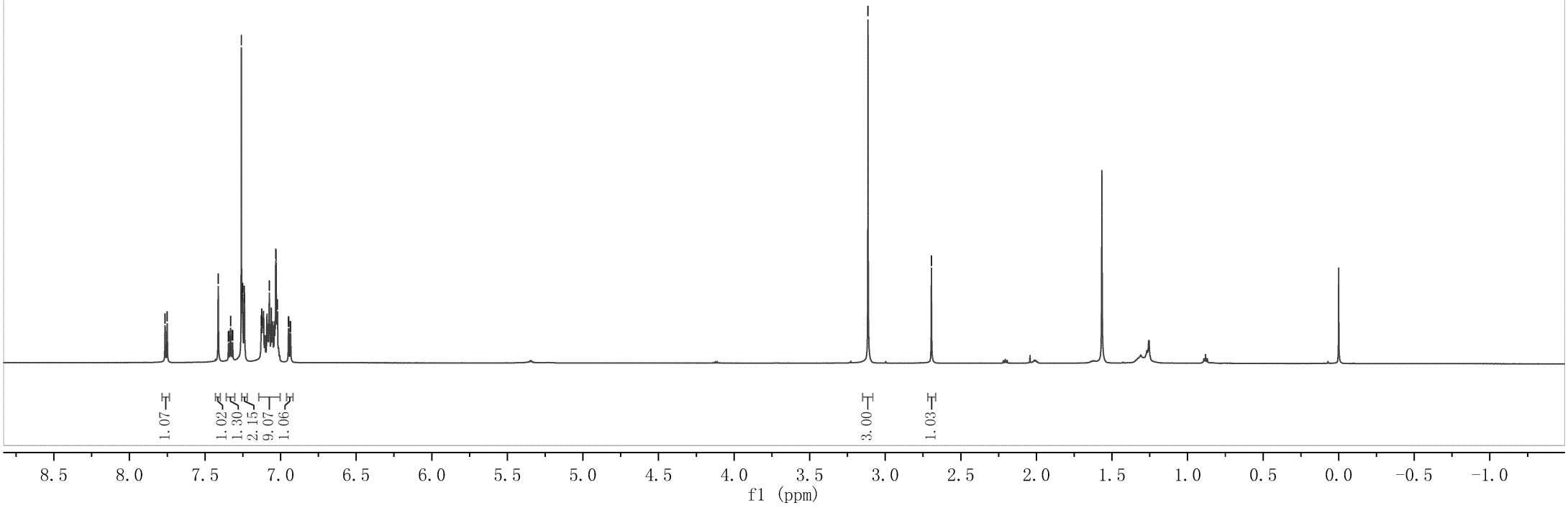


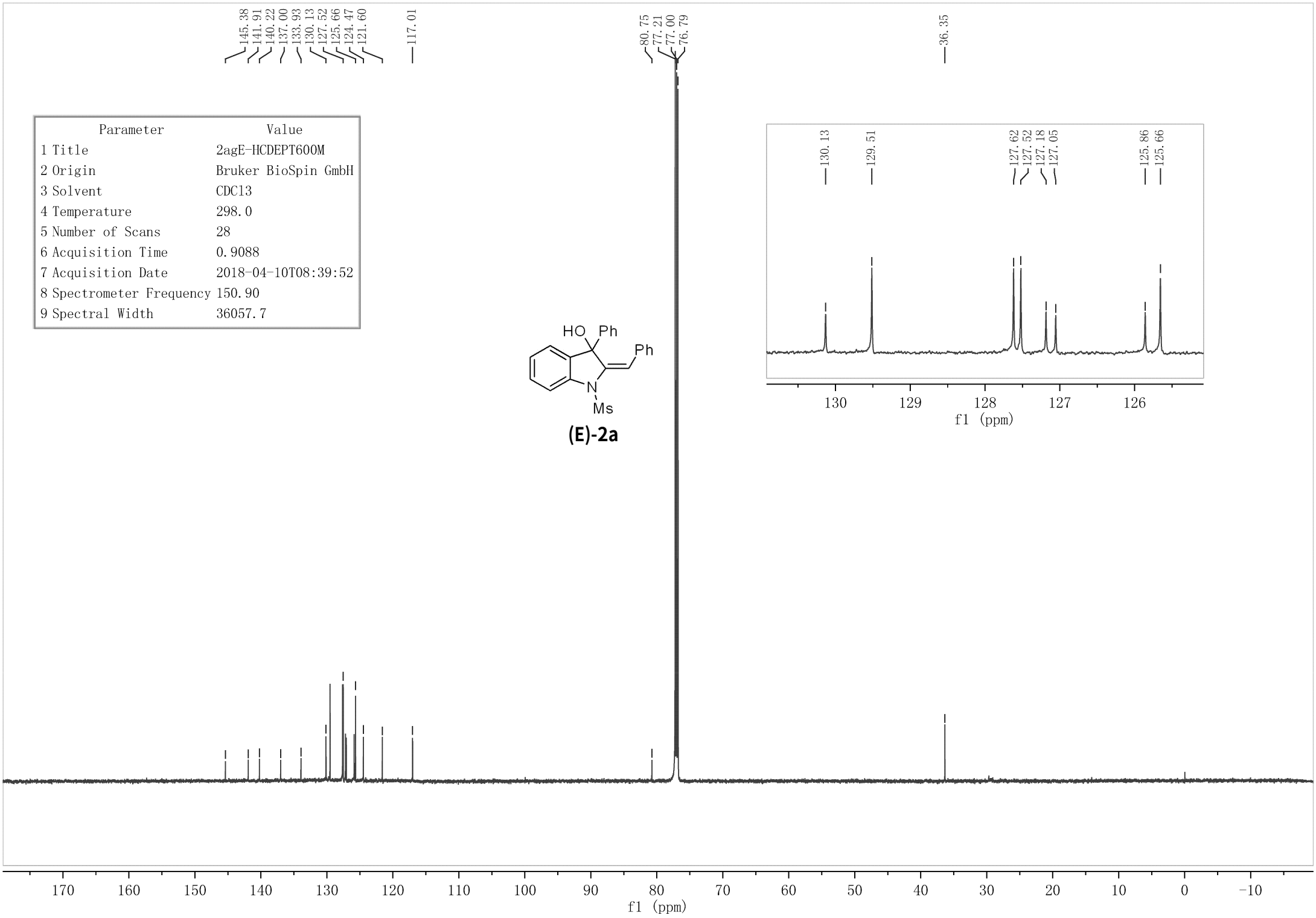
| Parameter | Value |
|---|---|
| 1 Title | 2gE-HCDEPT600M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.0 |
| 5 Number of Scans | 16 |
| 6 Acquisition Time | 2.7263 |
| 7 Acquisition Date | 2018-04-10T08:31:22 |
| 8 Spectrometer Frequency | 600.13 |
| 9 Spectral Width | 12019.2 |




**(E)-2a**



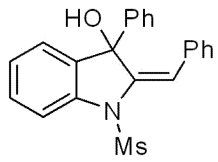

145.38
141.91
140.22
137.00
133.93
130.13
127.52
125.66
124.47
121.60
117.01
80.75
77.21
77.00
76.79
36.35
Parameter Value
1 Title 2agE-HCDEPT600M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 28
6 Acquisition Time 0.9088
7 Acquisition Date 2018-04-10T08:39:52
8 Spectrometer Frequency 150.90
9 Spectral Width 36057.7
HO
Ph
Ph
N
Ms
(E)-2a
130.13
129.51
127.62
127.52
127.18
127.05
125.86
125.66
130
129
128
127
126
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

130.13
129.51
127.61
127.52
127.18
127.05
125.85
125.65
124.46
121.59
117.01

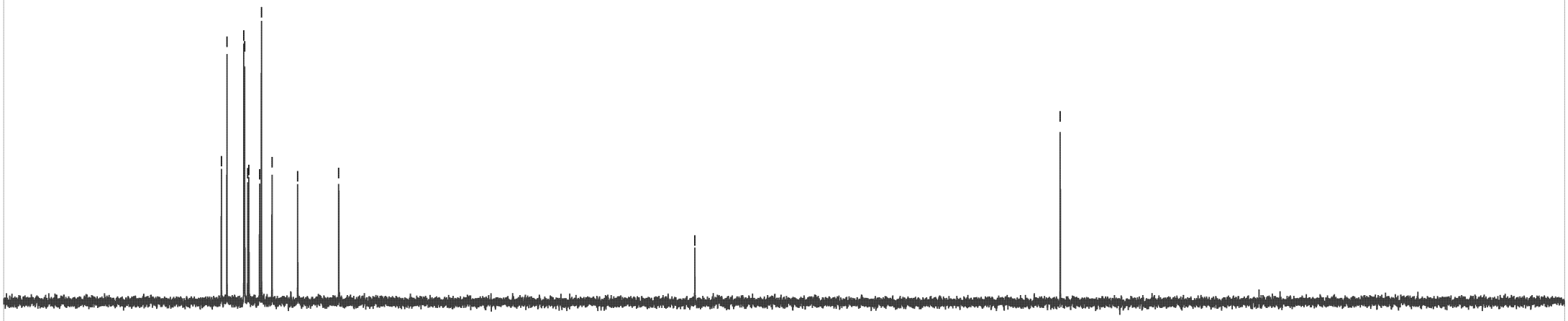
77.20

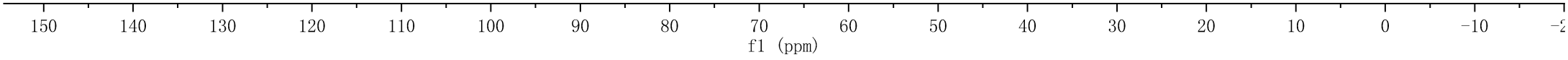
36.34

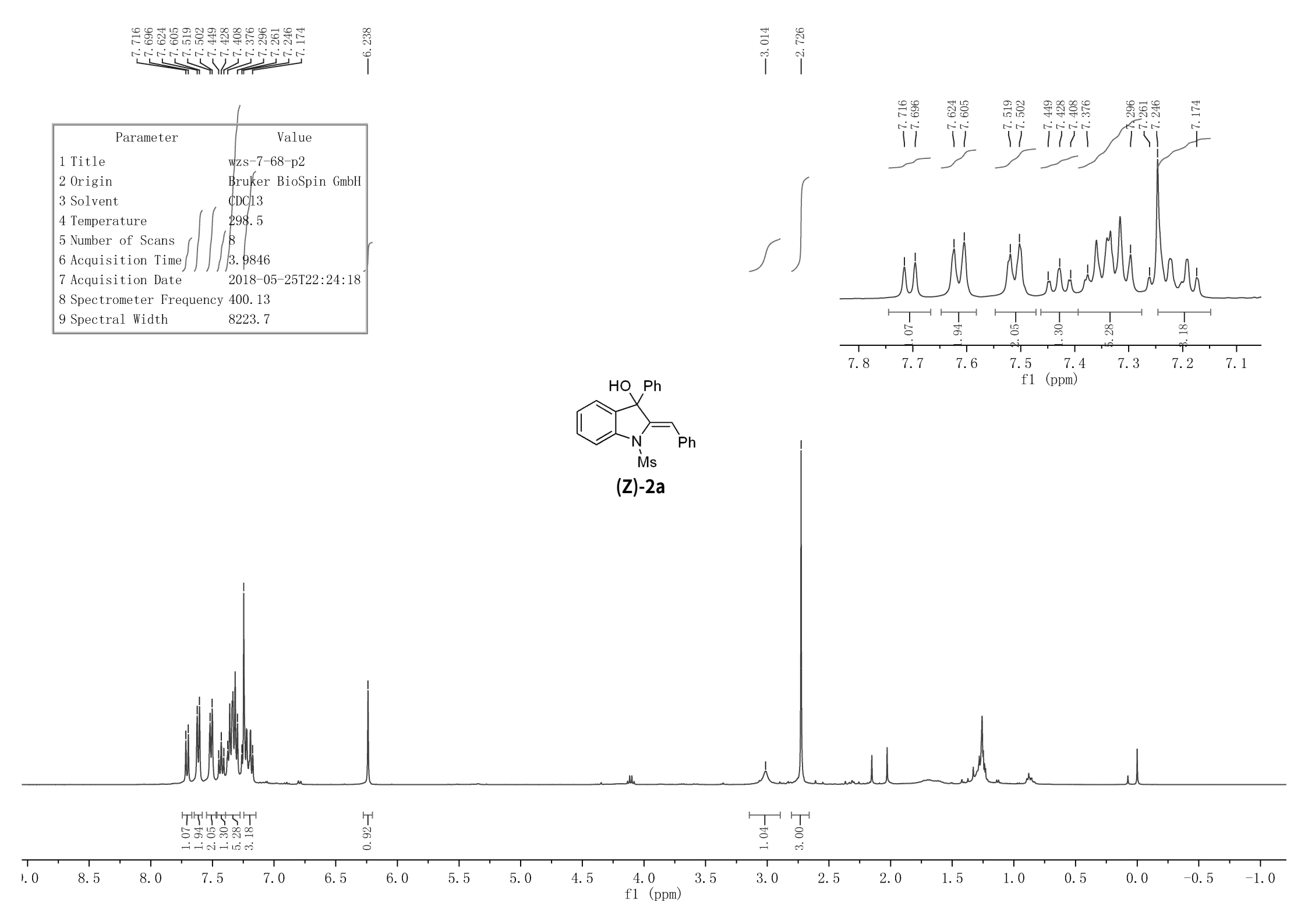
| Parameter | Value |
|---|---|
| 1 Title | 2agE-HCDEPT600M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.0 |
| 5 Number of Scans | 8 |
| 6 Acquisition Time | 0.9044 |
| 7 Acquisition Date | 2018-04-10T08:47:13 |
| 8 Spectrometer Frequency | 150.90 |
| 9 Spectral Width | 36231.9 |



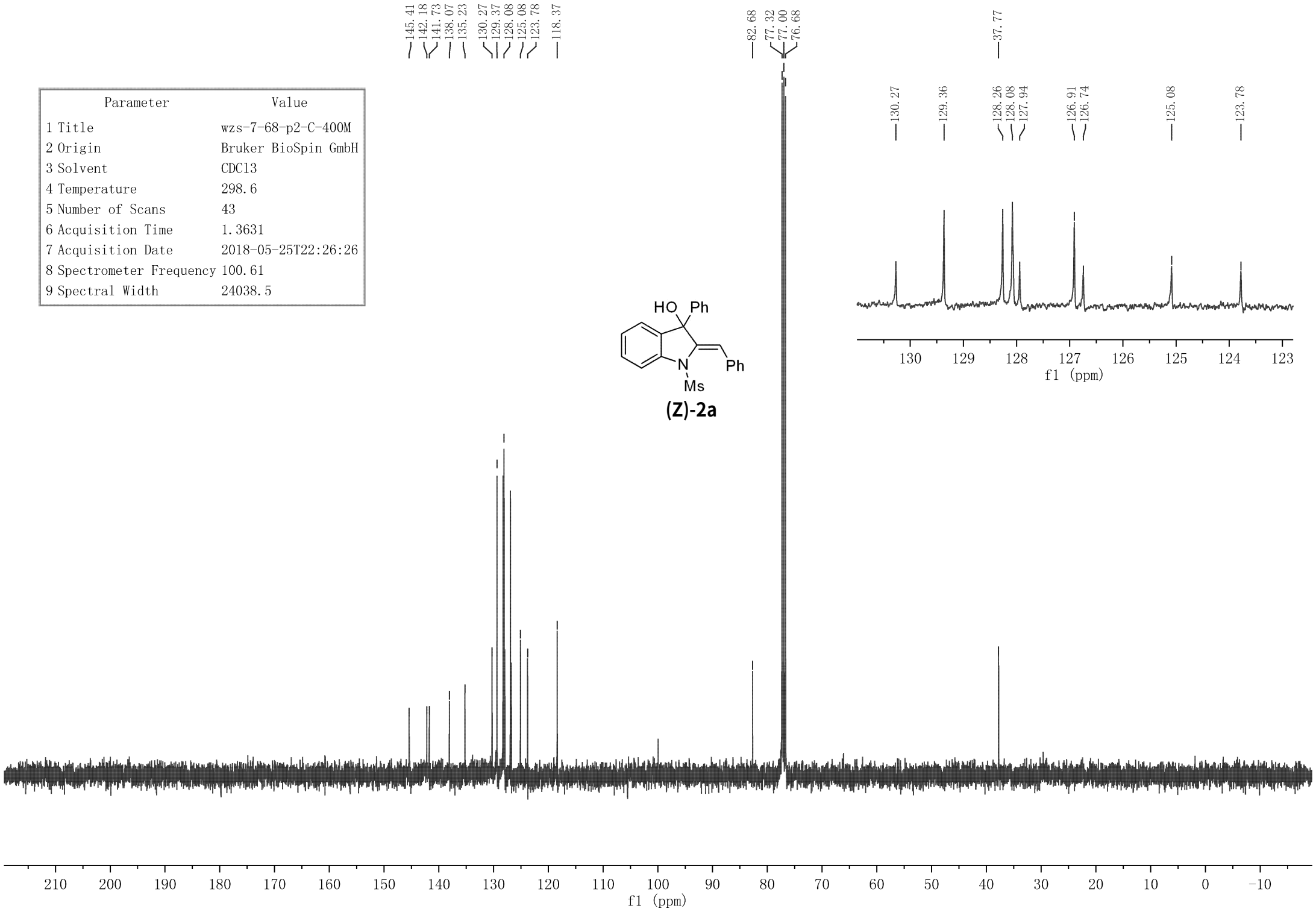

**(E)-2a**






7.716
7.696
7.624
7.605
7.519
7.502
7.449
7.428
7.408
7.376
7.296
7.261
7.246
7.174
6.238
3.014
2.726
Parameter Value
1 Title wzs-7-68-p2
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.5
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2018-05-25T22:24:18
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
1.07
1.94
2.05
1.30
5.28
3.18
0.92
1.04
3.00
f1 (ppm)
HO
Ph
N
Ms
Ph
(Z)-2a

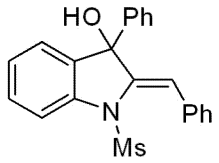
| Parameter | Value |
|---|---|
| 1 Title | wzs-7-68-p2-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.6 |
| 5 Number of Scans | 43 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-05-25T22:26:26 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |



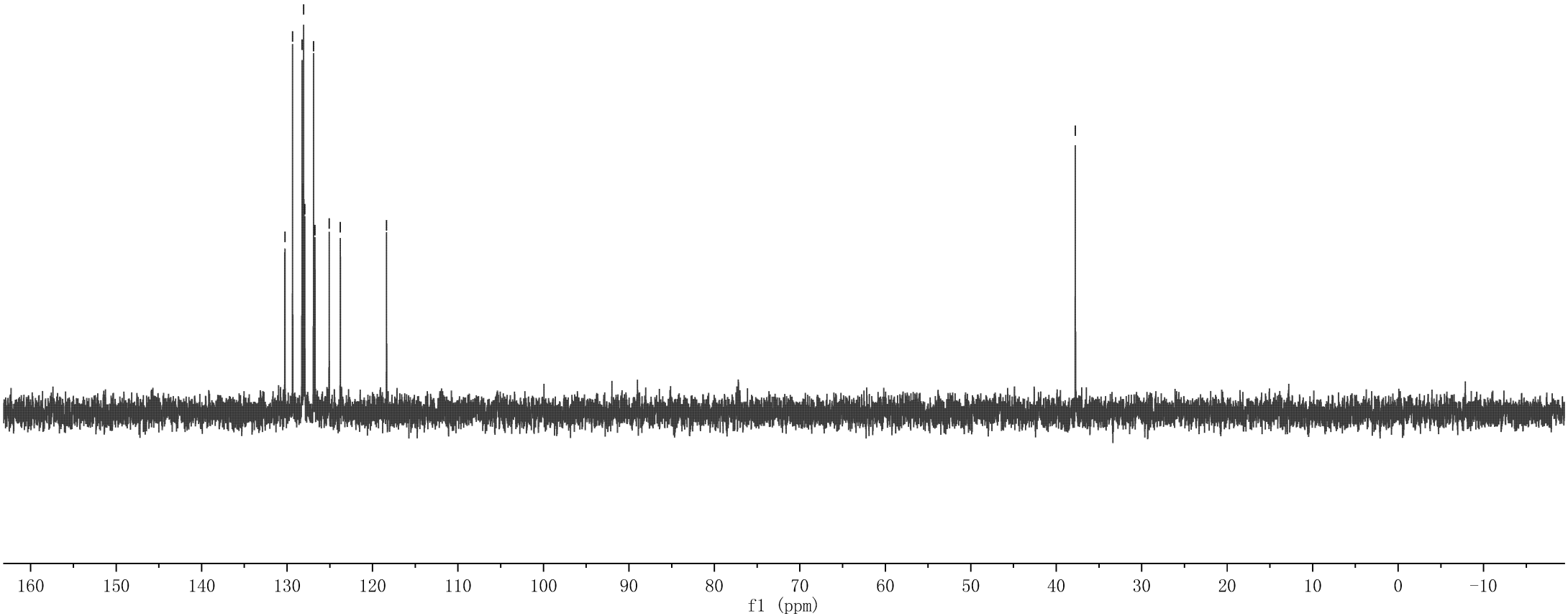
130.25
129.36
128.25
128.07
127.93
126.90
126.73
125.07
123.77
118.36

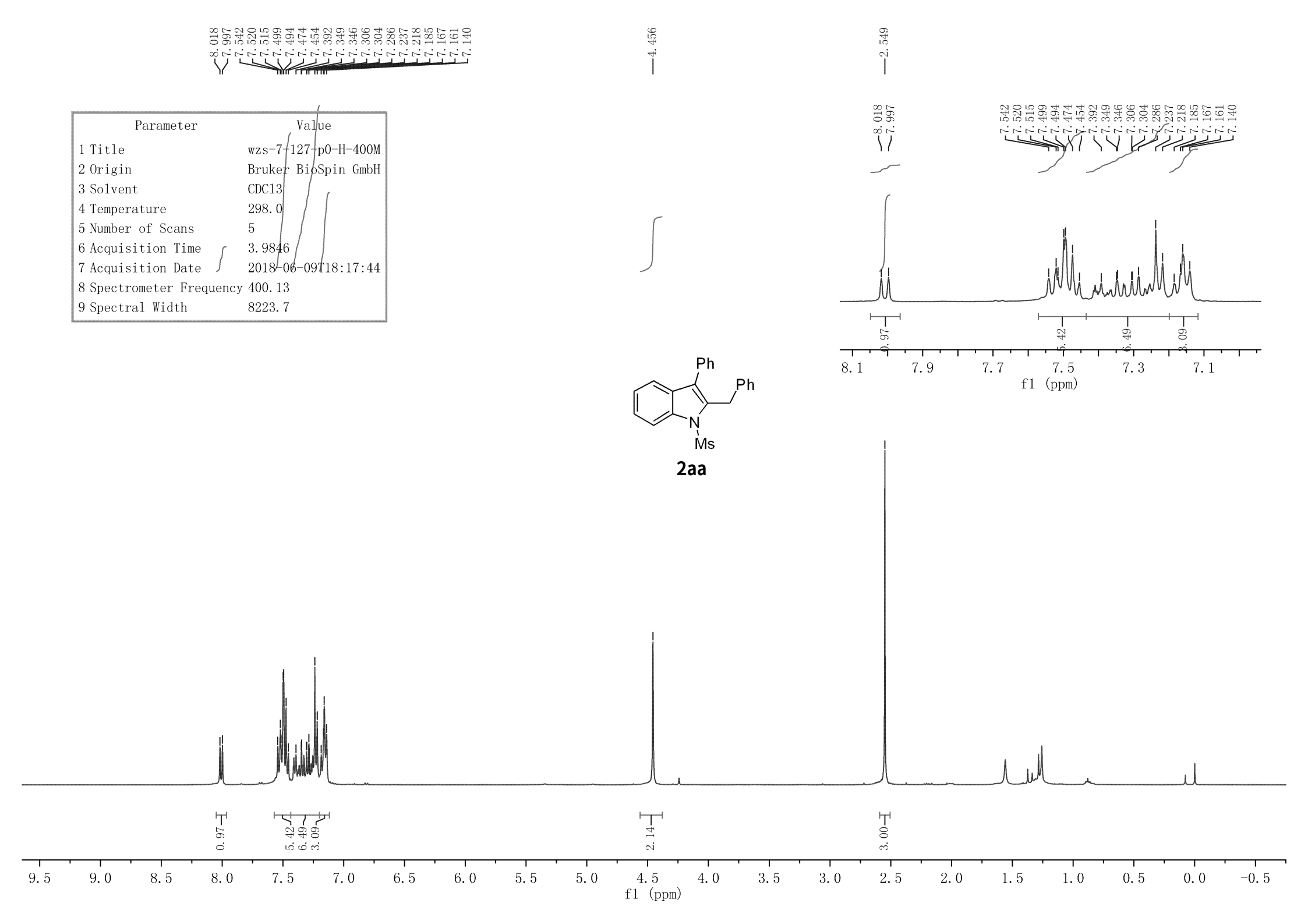
37.77

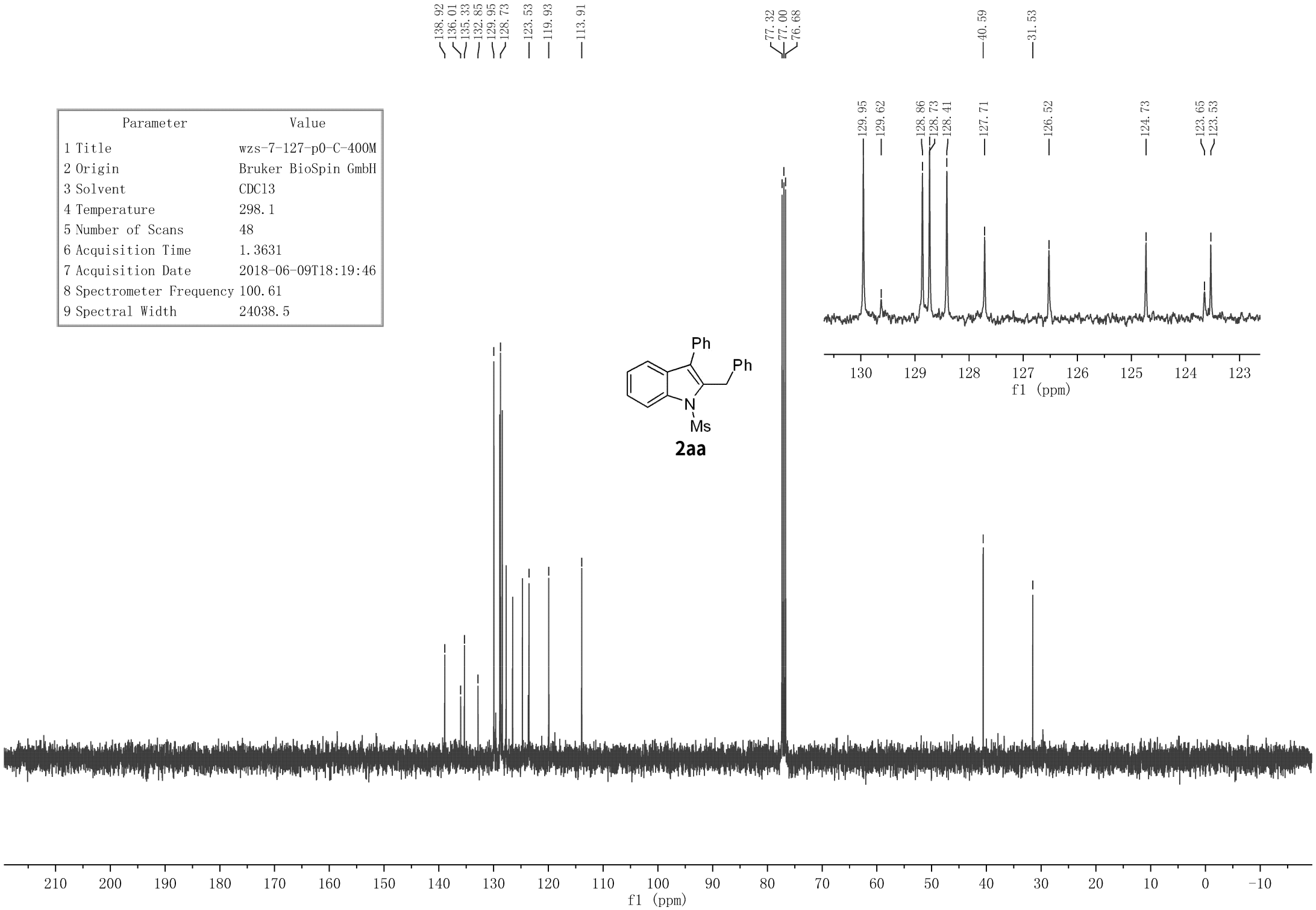
| Parameter | Value |
|---|---|
| 1 Title | wzs-7-68-p2-C-dept-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.1 |
| 5 Number of Scans | 13 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-05-25T22:29:24 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

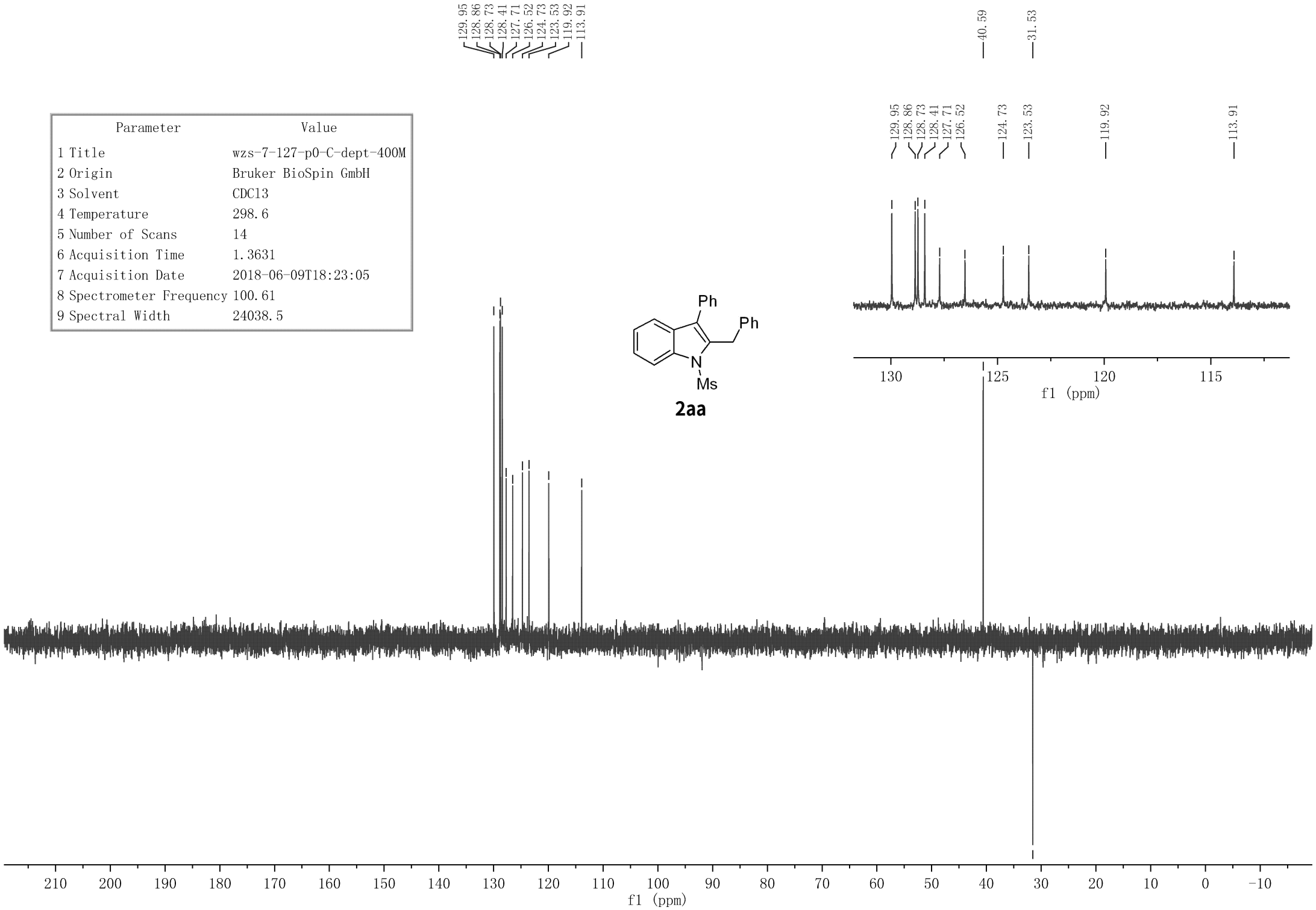


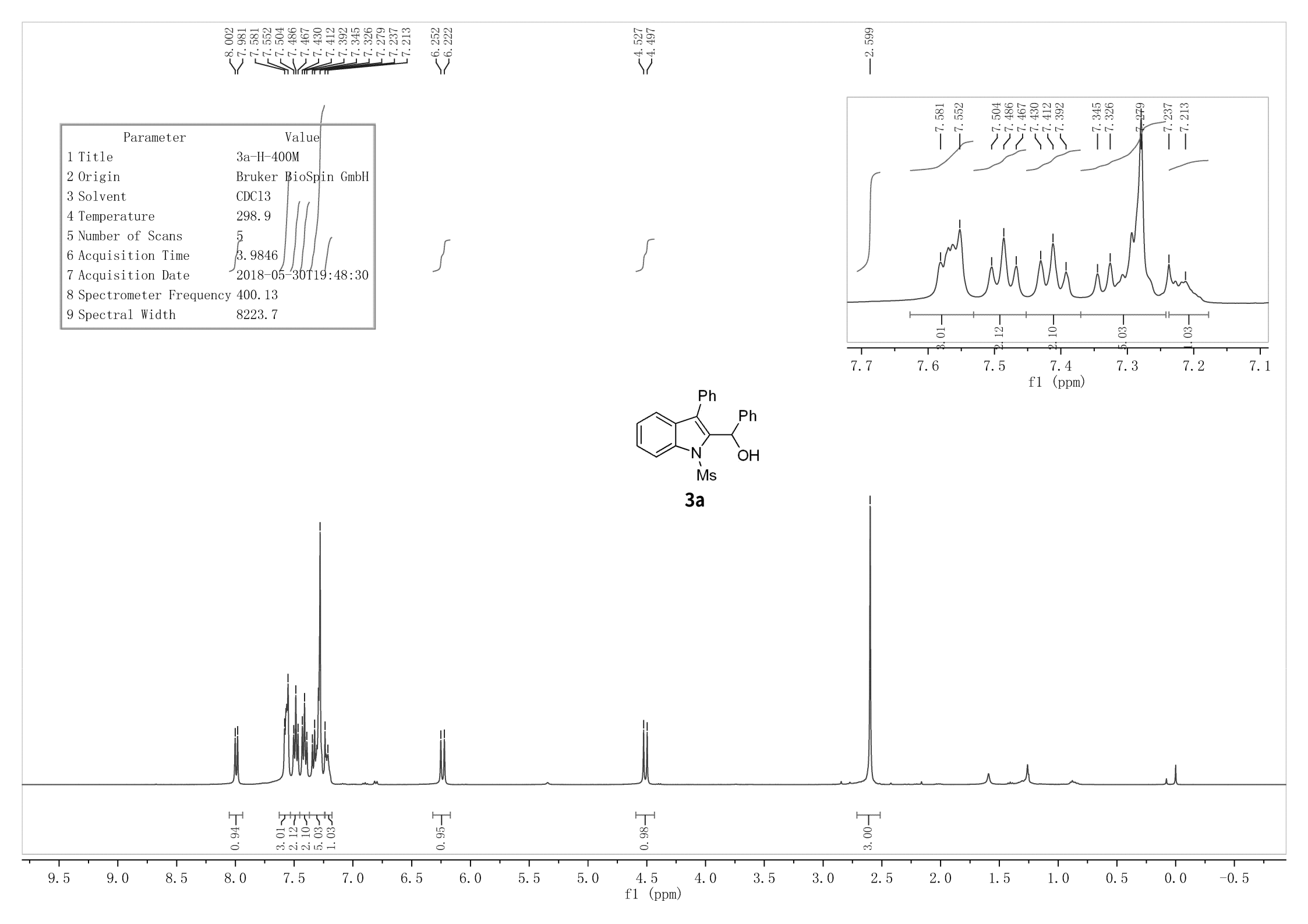

**(Z)-2a**

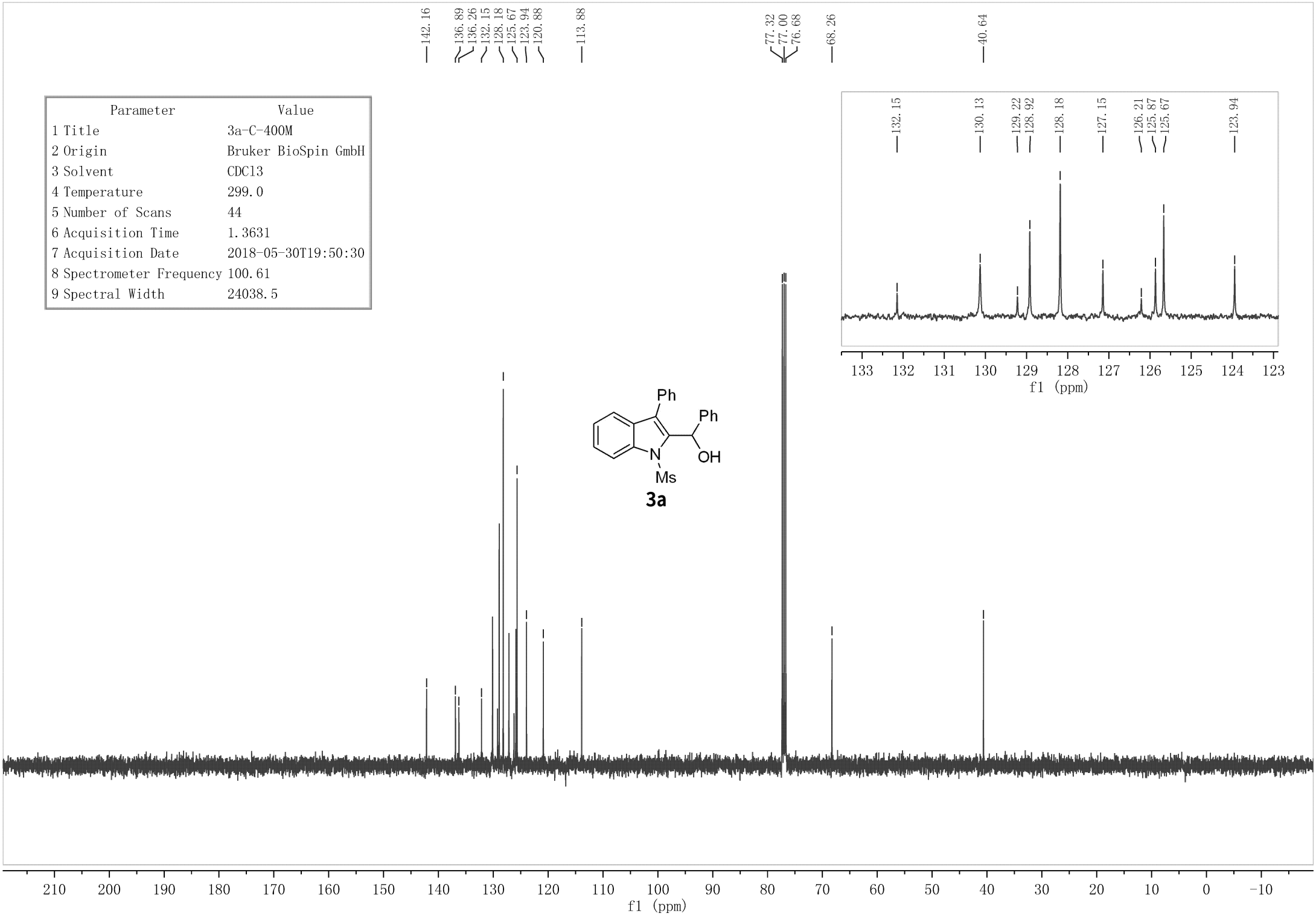


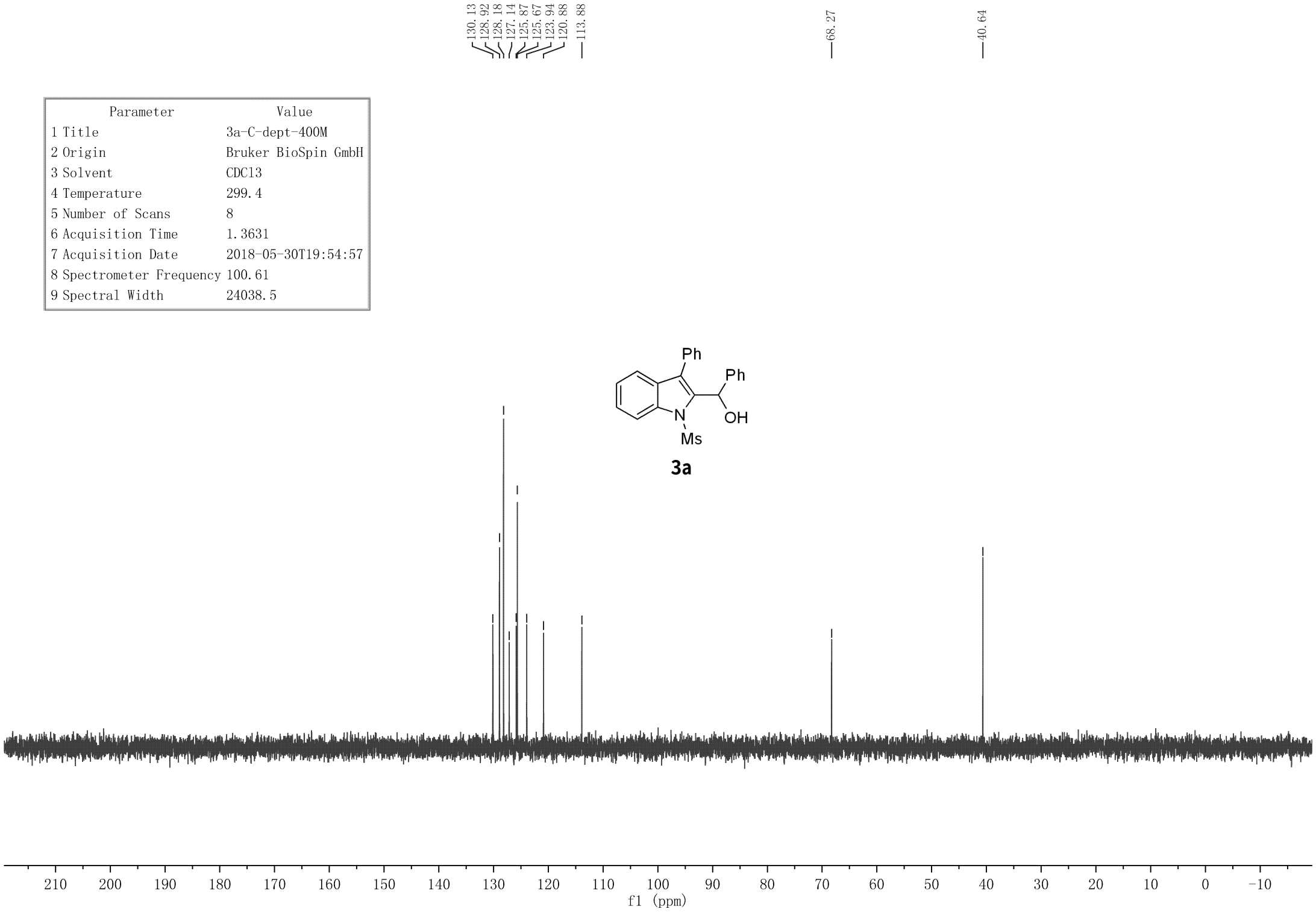

8.018
7.997
7.542
7.520
7.515
7.499
7.494
7.474
7.454
7.392
7.349
7.346
7.306
7.304
7.286
7.237
7.218
7.185
7.167
7.161
7.140
4.456
2.549
Parameter Value
1 Title wzs-7-127-p0-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-09T18:17:44
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
Ph
N
Ms
2aa
0.97
5.42
6.49
3.09
2.14
3.00
f1 (ppm)


138.92
136.01
135.33
132.85
129.95
128.73
123.53
119.93
113.91
77.32
77.00
76.68
40.59
31.53
Parameter Value
1 Title wzs-7-127-p0-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.1
5 Number of Scans 48
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-09T18:19:46
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ph
Ph
N
Ms
2aa
129.95
129.62
128.86
128.73
128.41
127.71
126.52
124.73
123.65
123.53
130 129 128 127 126 125 124 123
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


129.95
128.86
128.73
128.41
127.71
126.52
124.73
123.53
119.92
113.91
40.59
31.53
Parameter Value
1 Title wzs-7-127-p0-C-dept-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.6
5 Number of Scans 14
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-09T18:23:05
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ph
Ph
N
Ms
2aa
130
125
120
115
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

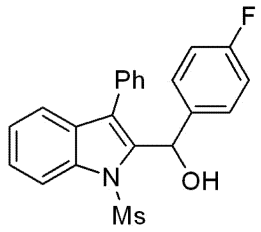

8.002
7.981
7.581
7.552
7.504
7.486
7.467
7.430
7.412
7.392
7.345
7.326
7.279
7.237
7.213
6.252
6.222
4.527
4.497
2.599
Parameter Value
1 Title 3a-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-05-30T19:48:30
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
3.01
2.12
2.10
5.03
1.03
f1 (ppm)
Ph
Ph
OH
N
Ms
3a
0.94
3.01
2.12
2.10
5.03
1.03
0.95
0.98
3.00
f1 (ppm)


142.16
136.89
136.26
132.15
128.18
125.67
123.94
120.88
113.88
77.32
77.00
76.68
68.26
40.64
Parameter Value
1 Title 3a-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.0
5 Number of Scans 44
6 Acquisition Time 1.3631
7 Acquisition Date 2018-05-30T19:50:30
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
132.15
130.13
129.22
128.92
128.18
127.15
126.21
125.87
125.67
123.94
133 132 131 130 129 128 127 126 125 124 123
f1 (ppm)
Ph
Ph
OH
N
Ms
3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



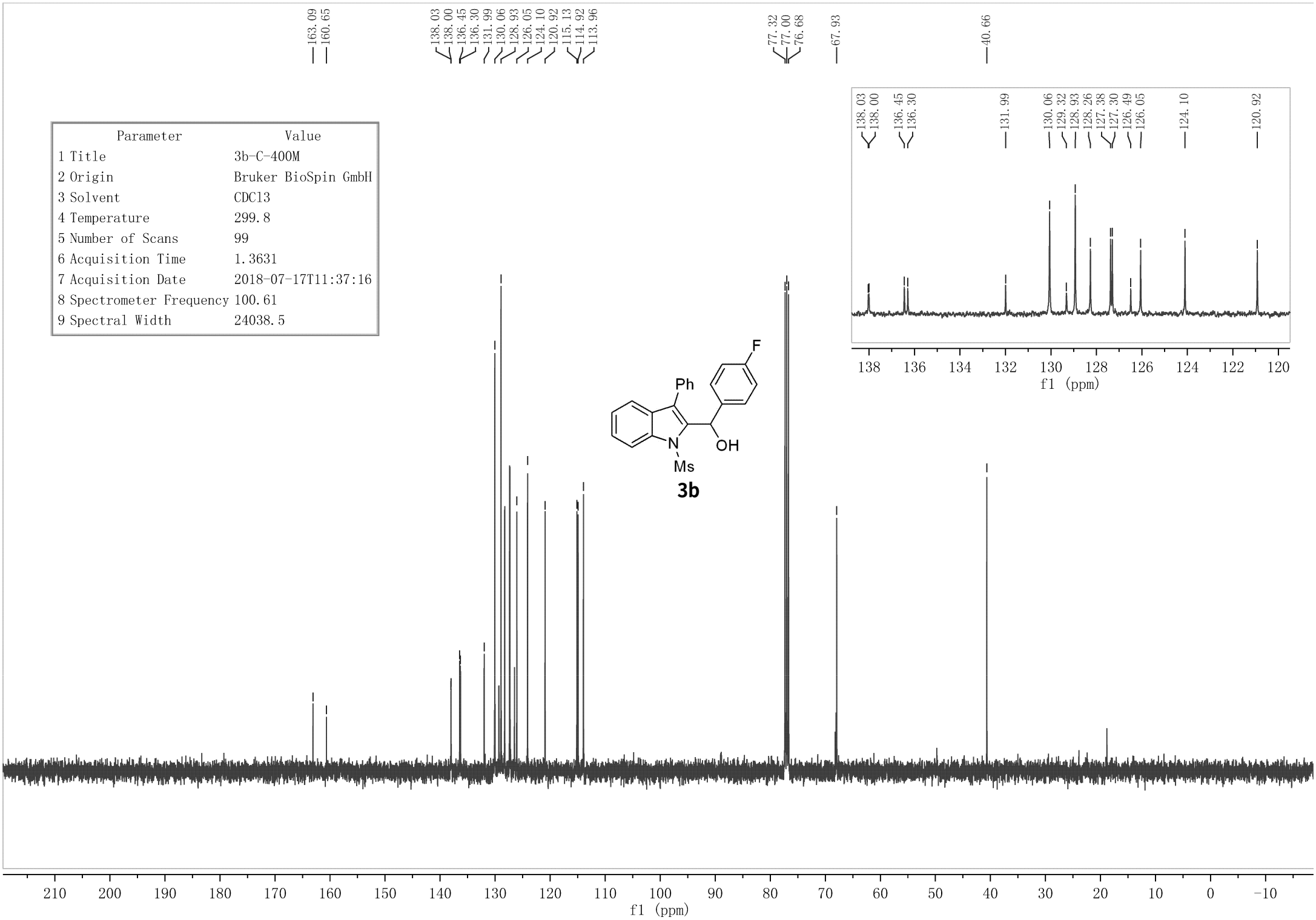

| Parameter | Value |
|---|---|
| 1 Title | 3a-C-dept-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.4 |
| 5 Number of Scans | 8 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-05-30T19:54:57 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

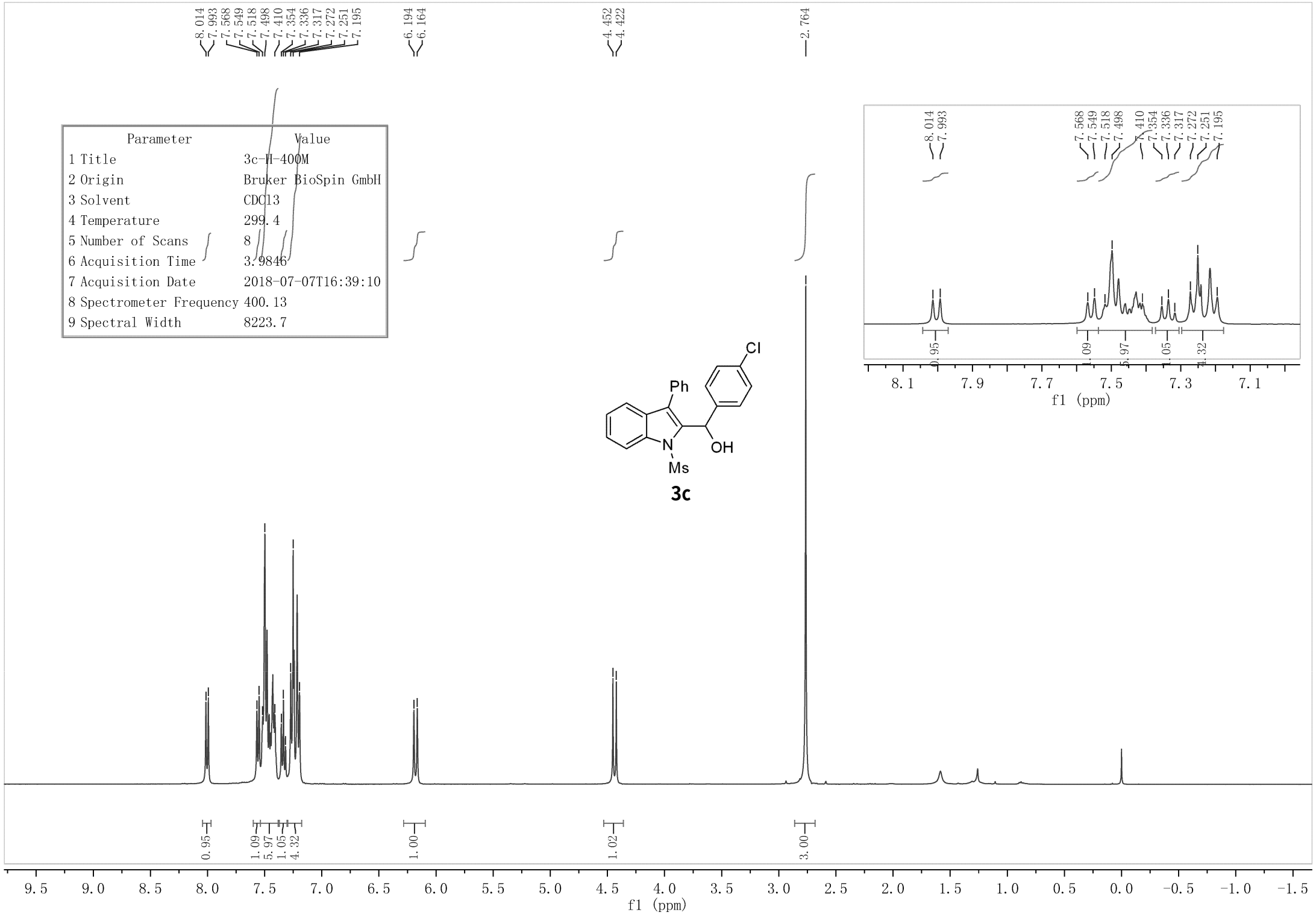
| Parameter | Value |
|---|---|
| 1 Title | 3b-H-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.8 |
| 5 Number of Scans | 12 |
| 6 Acquisition Time | 3.9846 |
| 7 Acquisition Date | 2018-07-17T11:34:29 |
| 8 Spectrometer Frequency | 400.13 |
| 9 Spectral Width | 8223.7 |

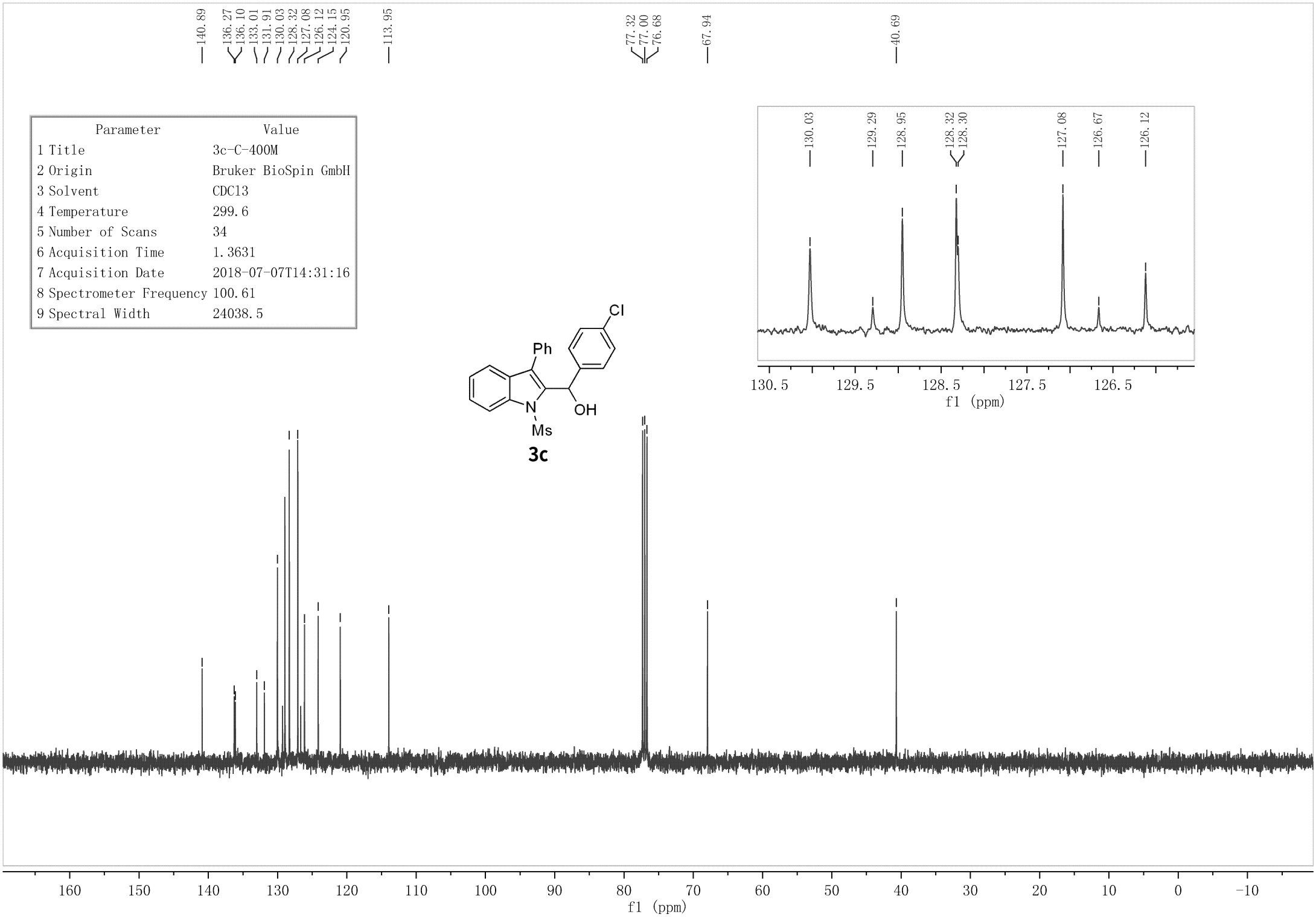


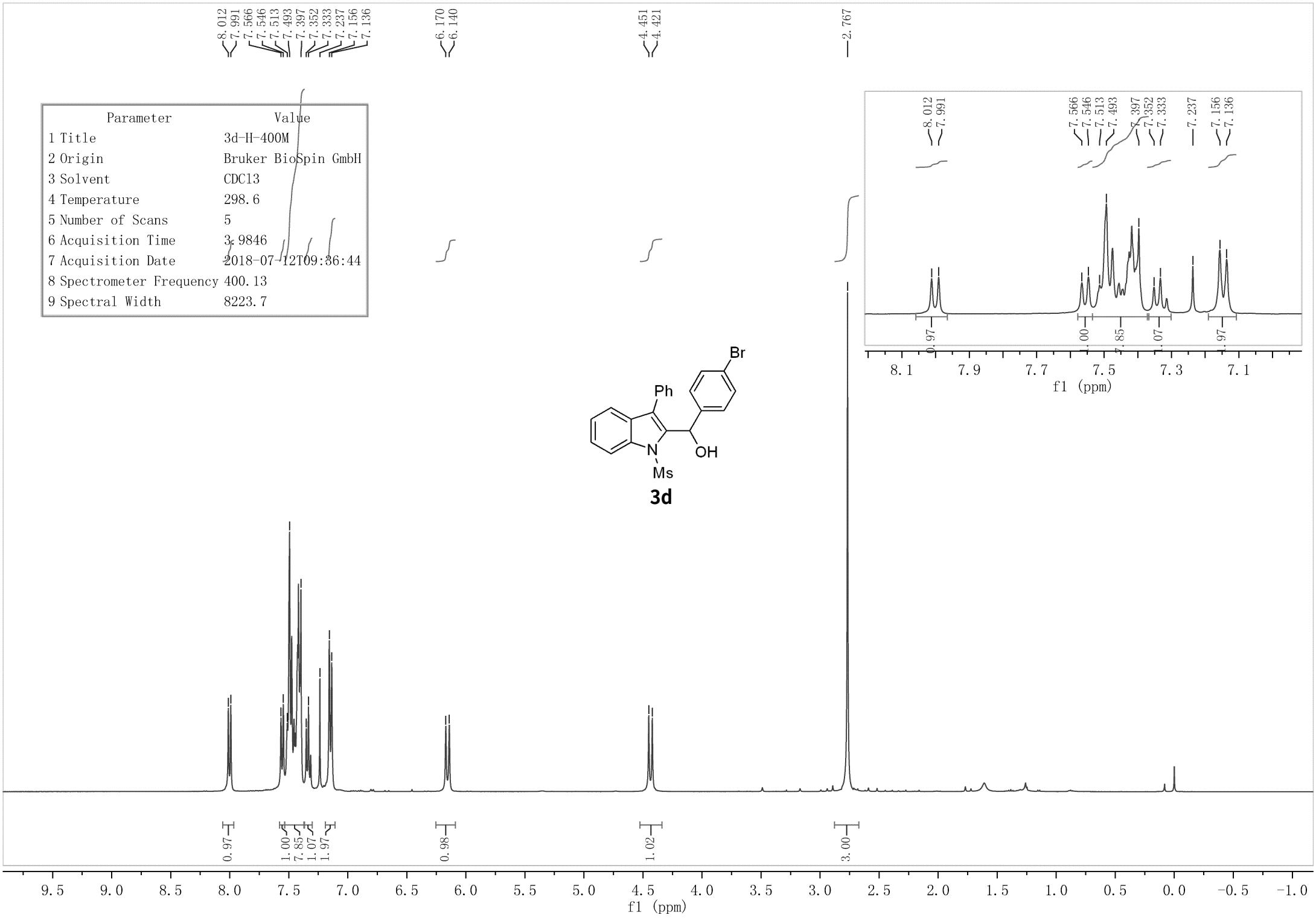

**3b**

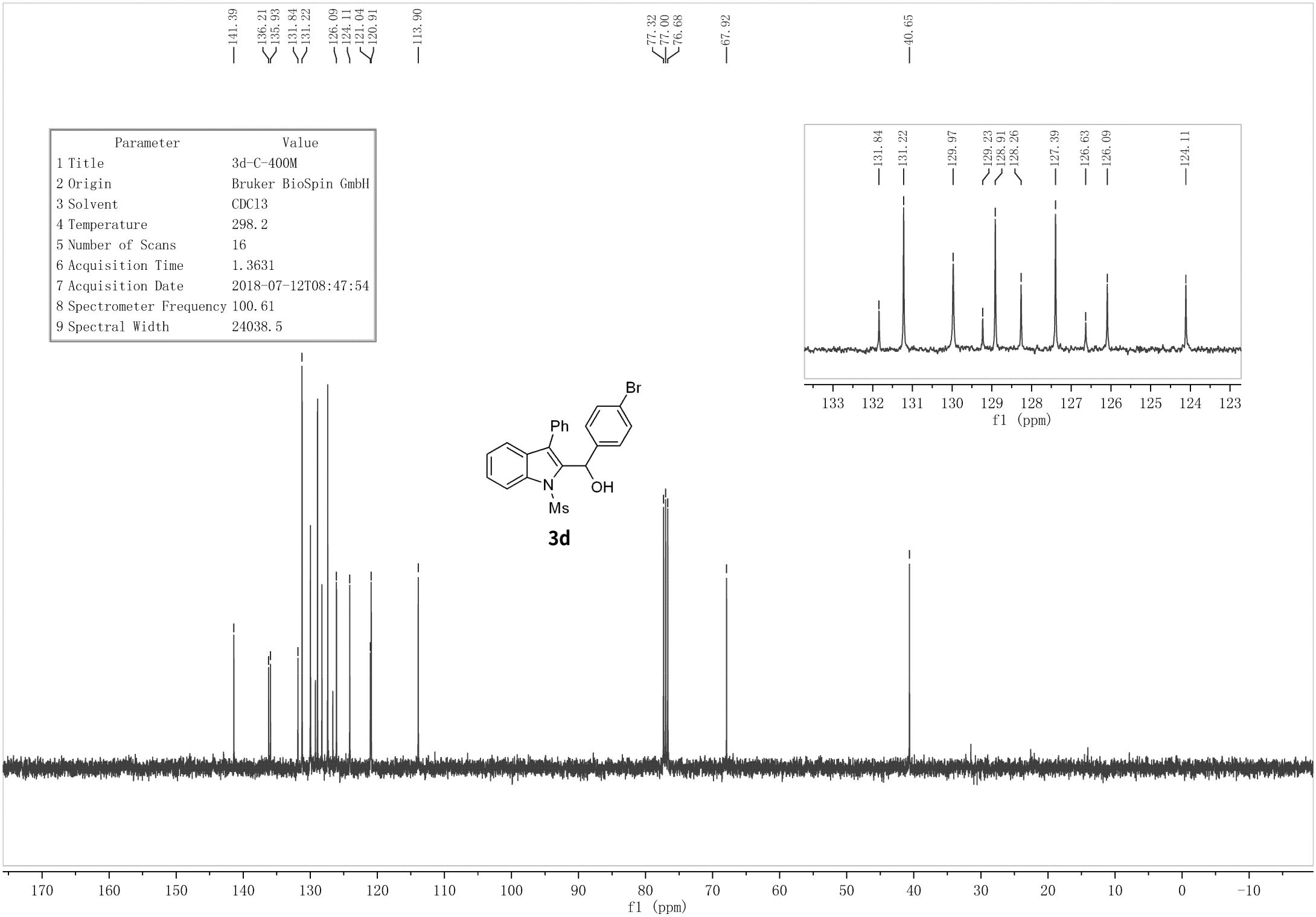
f1 (ppm)

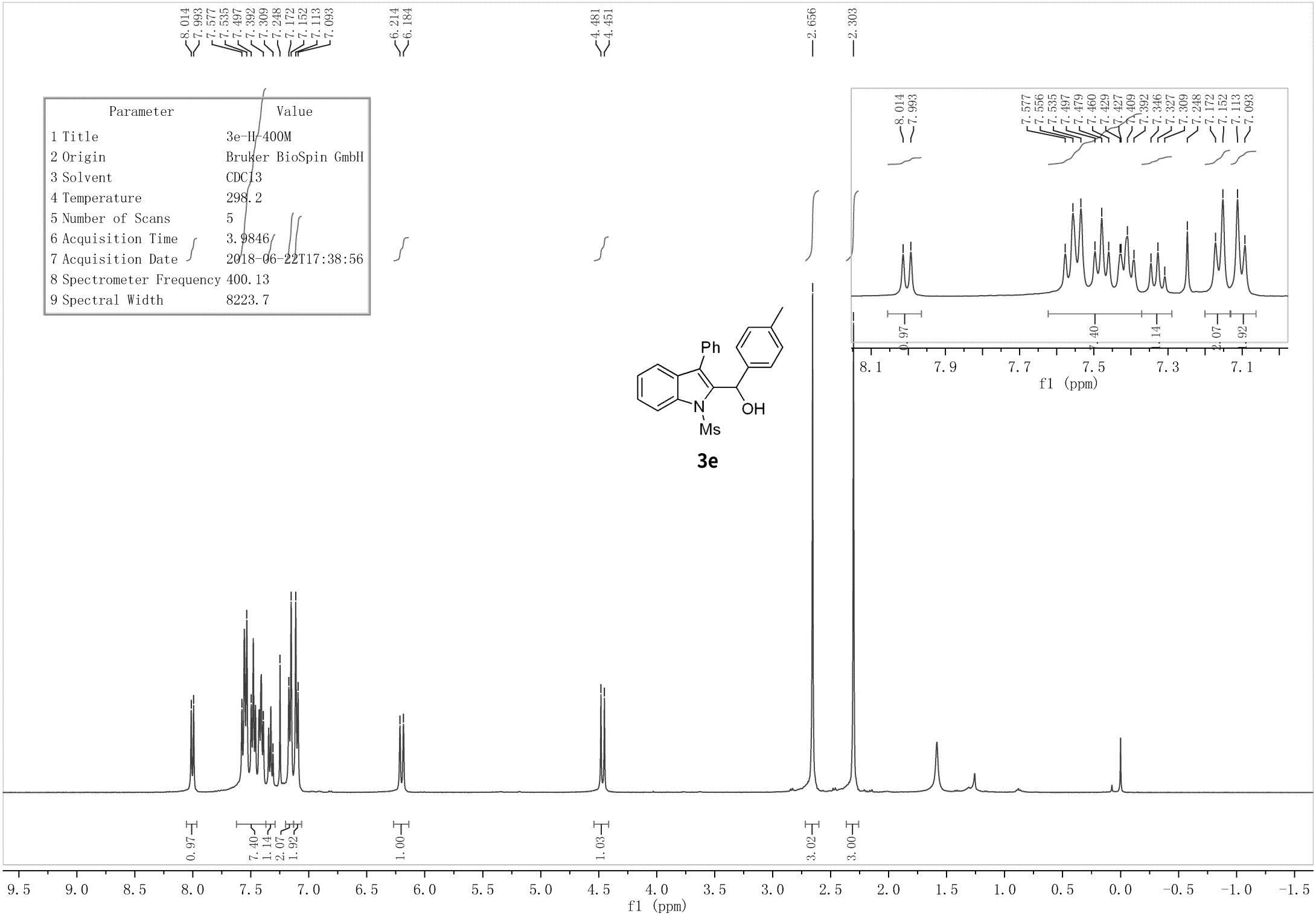

163.09
160.65
138.03
138.00
136.45
136.30
131.99
130.06
128.93
126.05
124.10
120.92
115.13
114.92
113.96
77.32
77.00
76.68
67.93
40.66
Parameter Value
1 Title 3b-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.8
5 Number of Scans 99
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-17T11:37:16
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
F
Ph
OH
N
Ms
3b
f1 (ppm)

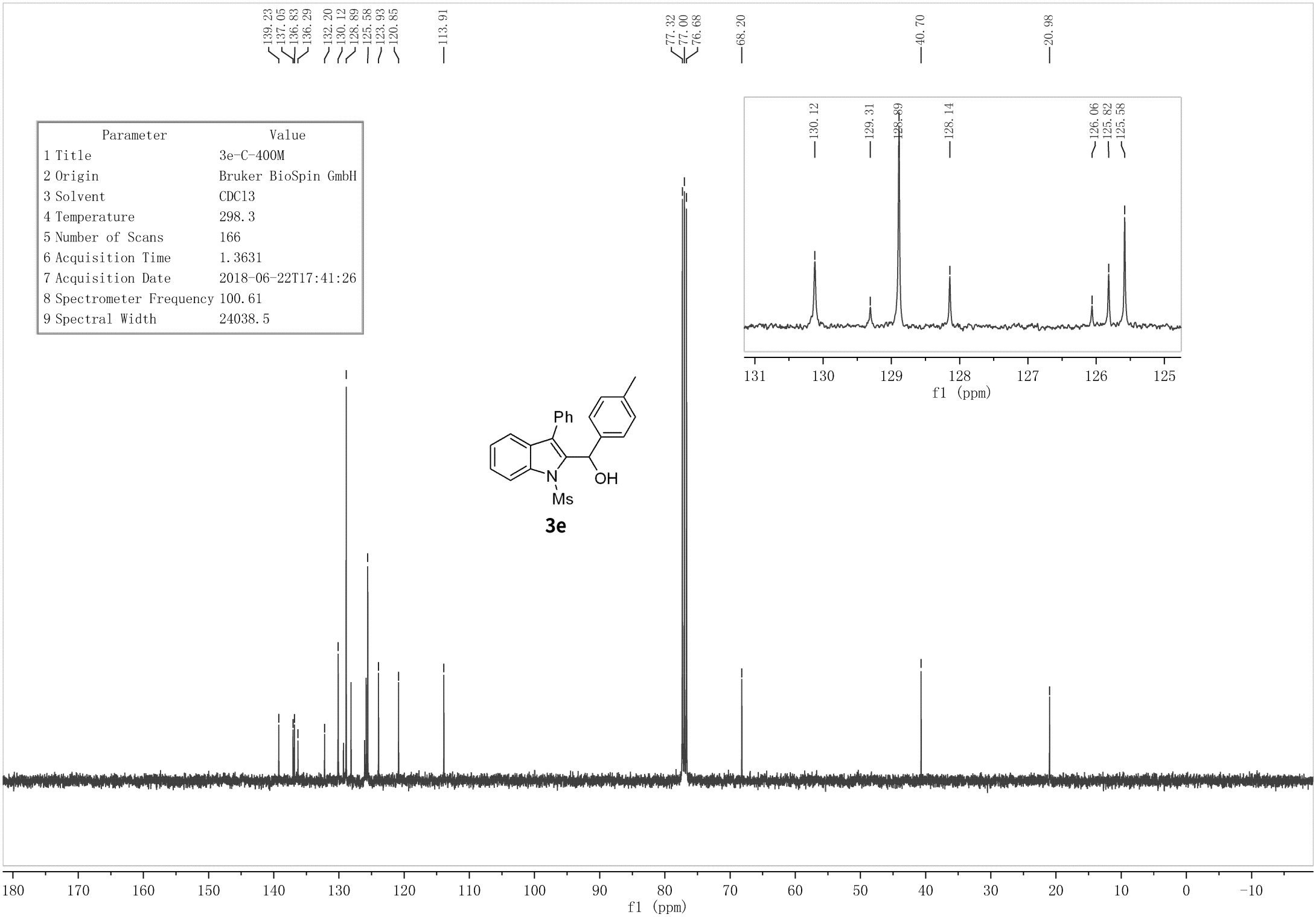

8.014
7.993
7.568
7.549
7.518
7.498
7.410
7.354
7.336
7.317
7.272
7.251
7.195
6.194
6.164
4.452
4.422
2.764
Parameter Value
1 Title 3c-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.4
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-07T16:39:10
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Cl
Ph
OH
N
Ms
3c
0.95
1.09
5.97
1.05
4.32
1.00
1.02
3.00
f1 (ppm)


140.89
136.27
136.10
133.01
131.91
130.03
128.32
127.08
126.12
124.15
120.95
113.95
77.32
77.00
76.68
67.94
40.69
Parameter Value
1 Title 3c-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 34
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-07T14:31:16
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Cl
Ph
OH
N
Ms
3c
130.03
129.29
128.95
128.32
128.30
127.08
126.67
126.12
130.5
129.5
128.5
127.5
126.5
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

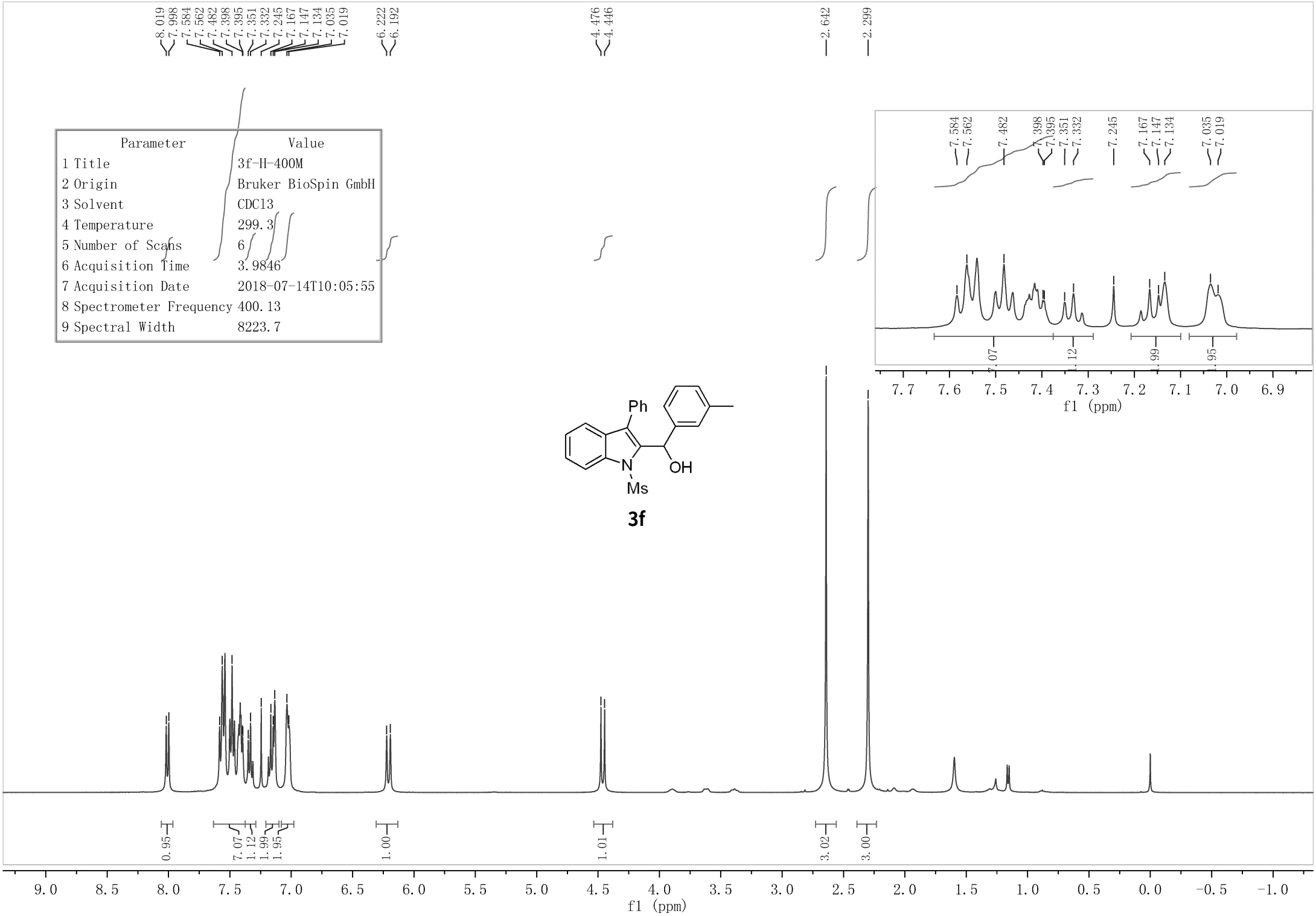

8.012
7.991
7.566
7.546
7.513
7.493
7.397
7.352
7.333
7.237
7.156
7.136
6.170
6.140
4.451
4.421
2.767
Parameter Value
1 Title 3d-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.6
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-12T09:36:44
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Br
Ph
N
OH
Ms
3d
0.97
1.00
7.85
1.07
1.97
0.98
1.02
3.00
f1 (ppm)

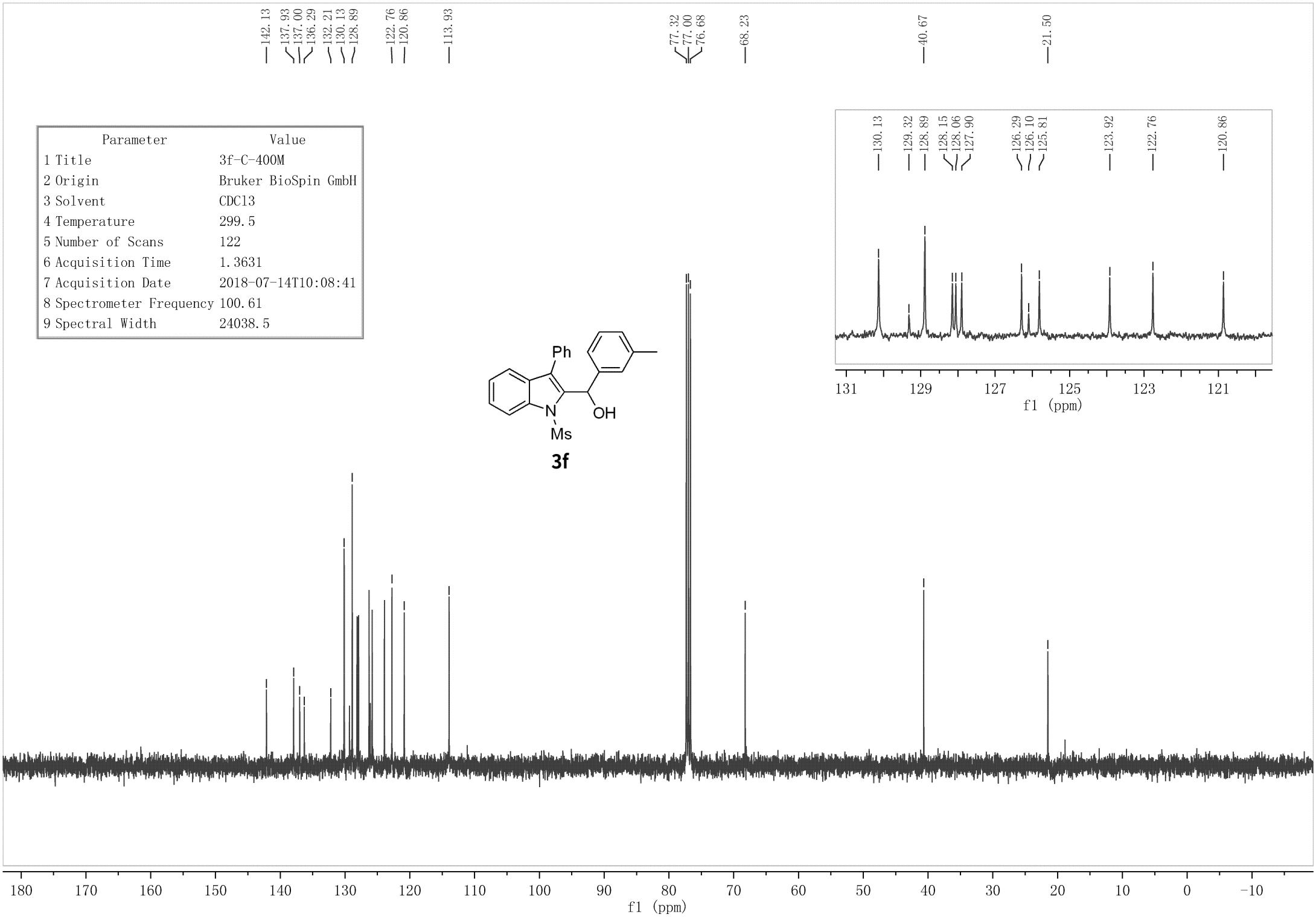

141.39
136.21
135.93
131.84
131.22
126.09
124.11
121.04
120.91
113.90
77.32
77.00
76.68
67.92
40.65
Parameter Value
1 Title 3d-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 16
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-12T08:47:54
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.84
131.22
129.97
129.23
128.91
128.26
127.39
126.63
126.09
124.11
133 132 131 130 129 128 127 126 125 124 123
f1 (ppm)
Br
Ph
N
OH
Ms
3d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.014
7.993
7.577
7.535
7.497
7.392
7.309
7.248
7.172
7.152
7.113
7.093
6.214
6.184
4.481
4.451
2.656
2.303
Parameter Value
1 Title 3e-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 5
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-22T17:38:56
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
OH
N
Ms
3e
0.97
7.40
1.14
2.07
1.92
1.00
1.03
3.02
3.00
f1 (ppm)




| Parameter | Value |
|---|---|
| 1 Title | 3e-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.3 |
| 5 Number of Scans | 166 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-06-22T17:41:26 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |


8.019
7.998
7.584
7.562
7.482
7.398
7.395
7.351
7.332
7.245
7.167
7.147
7.134
7.035
7.019
6.222
6.192
4.476
4.446
2.642
2.299
Parameter Value
1 Title 3f-H-400M
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 2018-07-14T10:05:55
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
OH
N
Ms
3f
0.95
7.07
1.12
1.99
1.95
1.00
1.01
3.02
3.00
f1 (ppm)

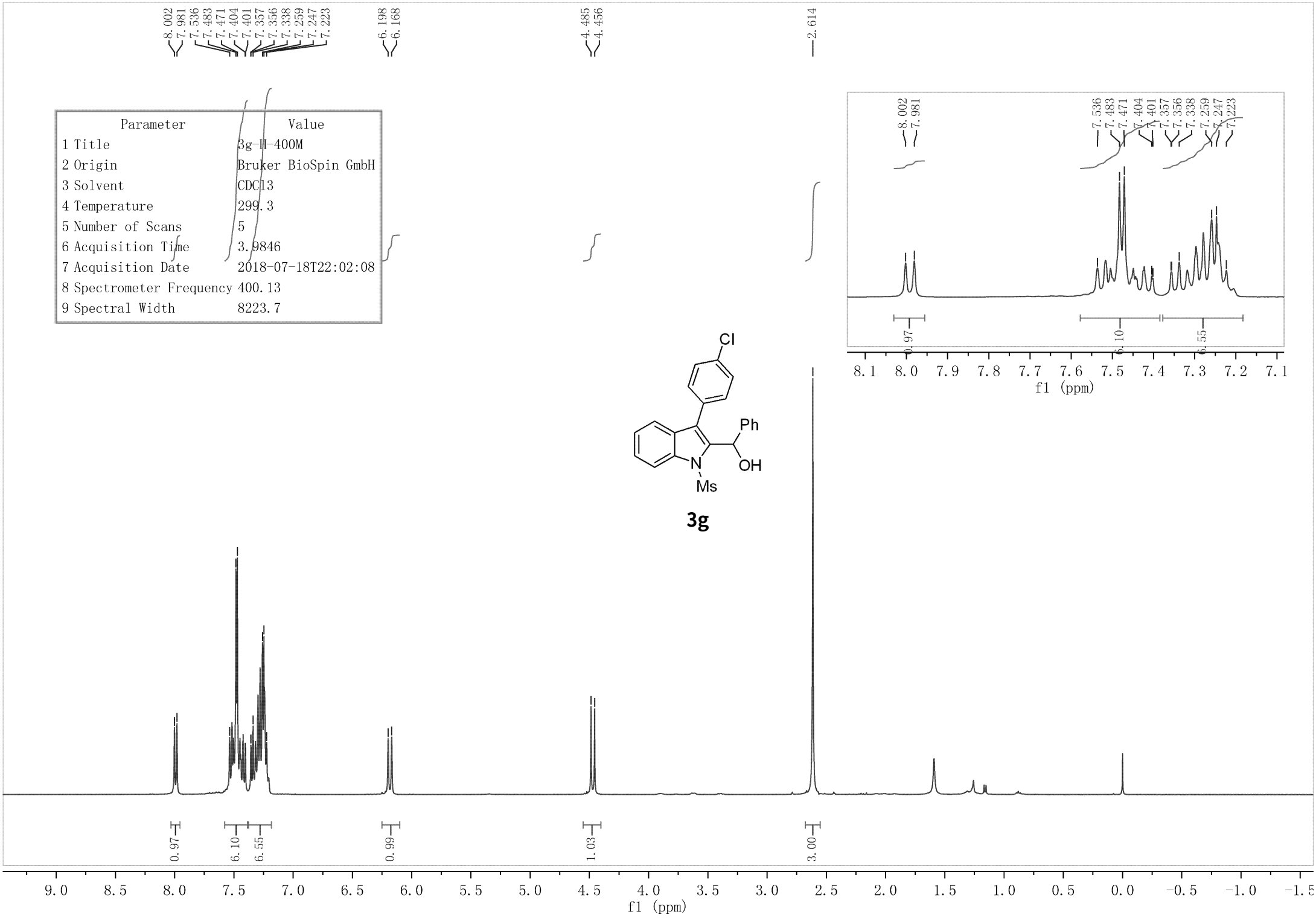


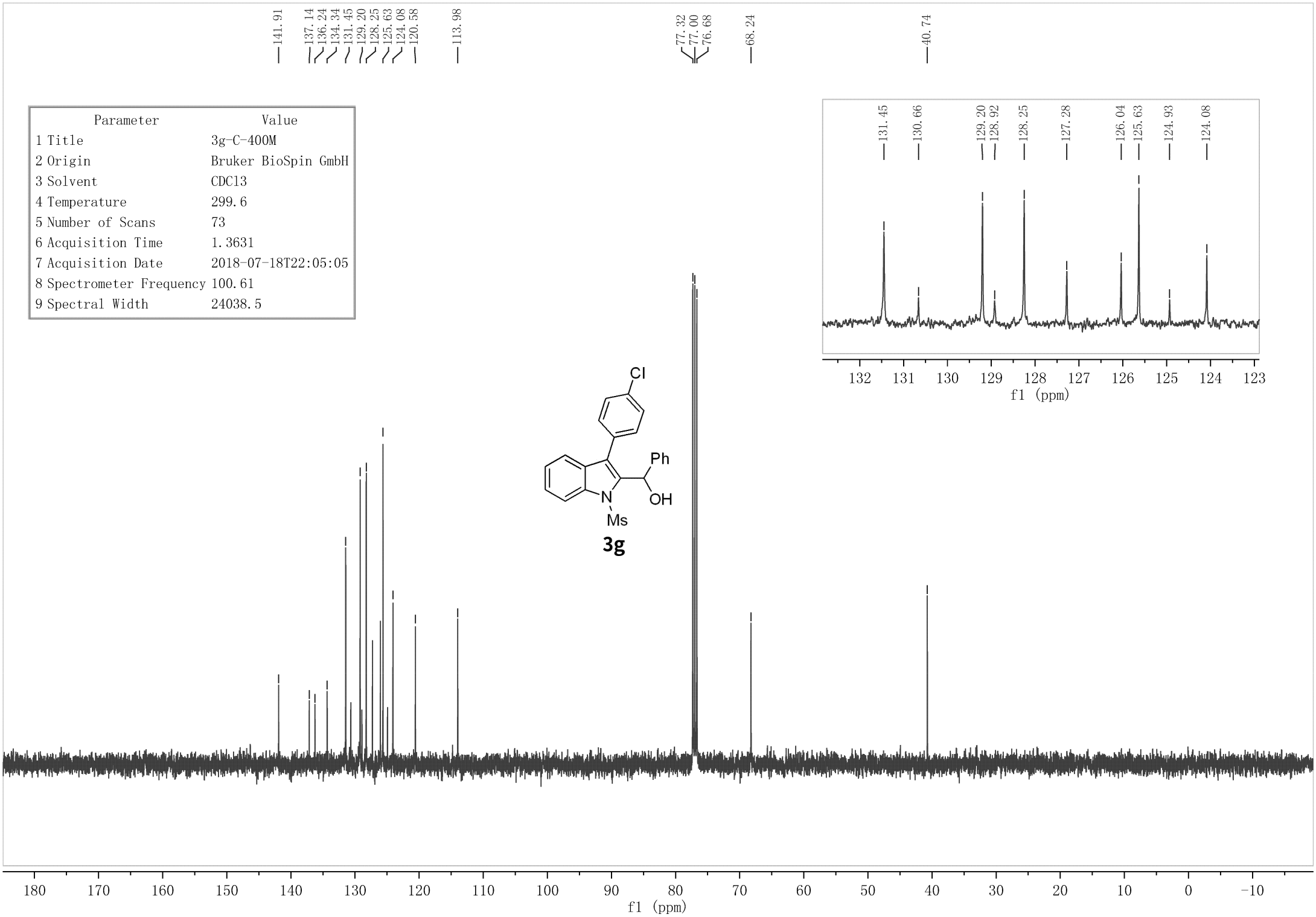

| Parameter | Value |
|---|---|
| 1 Title | 3f-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.5 |
| 5 Number of Scans | 122 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-07-14T10:08:41 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

| Parameter | Value |
|---|---|
| 1 Title | 3g-H-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.3 |
| 5 Number of Scans | 5 |
| 6 Acquisition Time | 3.9846 |
| 7 Acquisition Date | 2018-07-18T22:02:08 |
| 8 Spectrometer Frequency | 400.13 |
| 9 Spectral Width | 8223.7 |

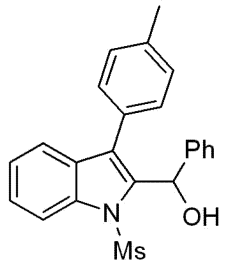



**3g**



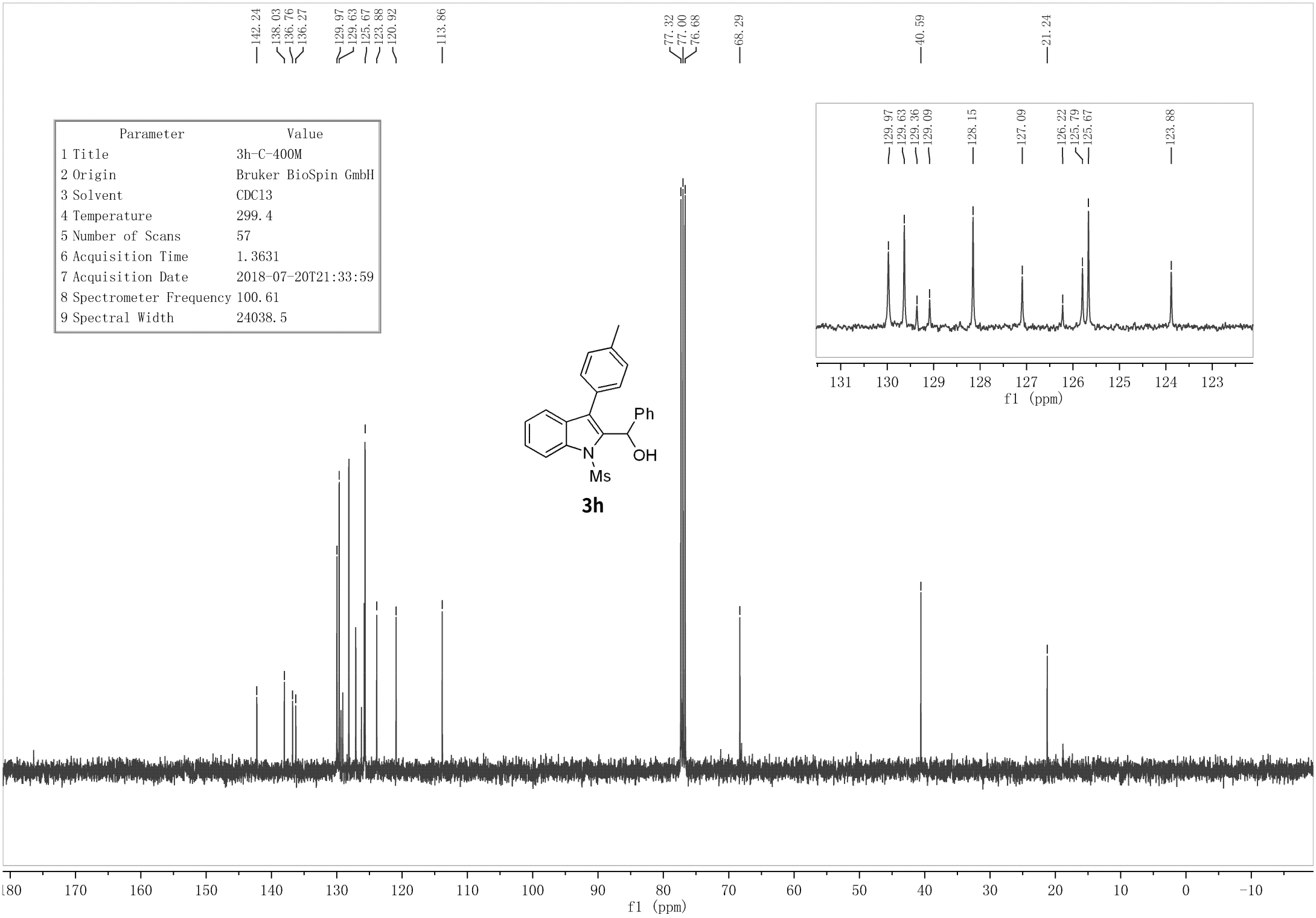

141.91
137.14
136.24
134.34
131.45
129.20
128.25
125.63
124.08
120.58
113.98
77.32
77.00
76.68
68.24
40.74
Parameter Value
1 Title 3g-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 73
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-18T22:05:05
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.45
130.66
129.20
128.92
128.25
127.28
126.04
125.63
124.93
124.08
132 131 130 129 128 127 126 125 124 123
f1 (ppm)
Cl
Ph
OH
N
Ms
3g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

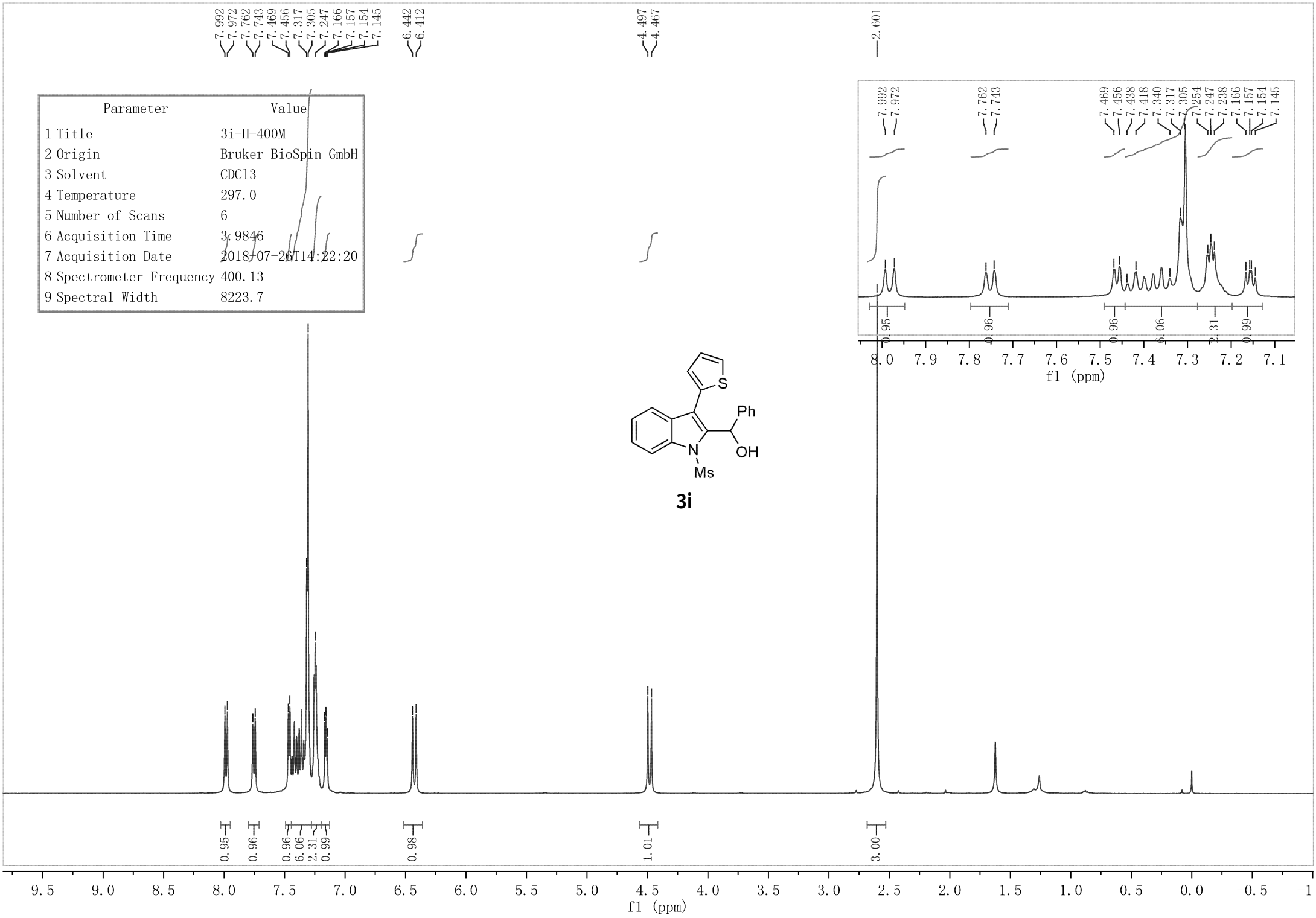
| Parameter | Value |
|---|---|
| 1 Title | 3h-H-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.3 |
| 5 Number of Scans | 6 |
| 6 Acquisition Time | 3.9846 |
| 7 Acquisition Date | 2018-07-20T21:31:21 |
| 8 Spectrometer Frequency | 400.13 |
| 9 Spectral Width | 8223.7 |

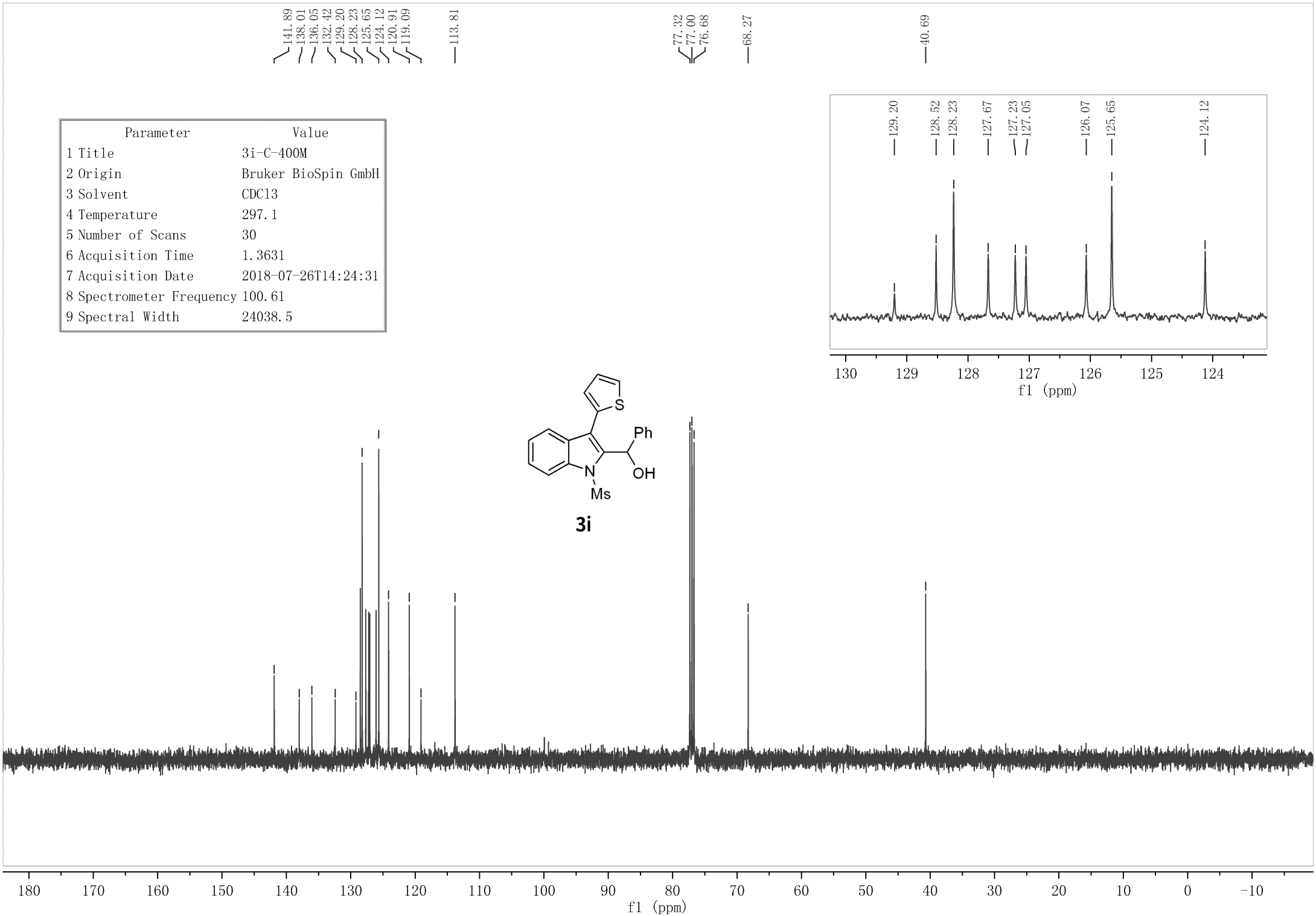


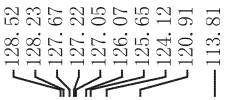

**3h**

f1 (ppm)


142.24
138.03
136.76
136.27
129.97
129.63
125.67
123.88
120.92
113.86
77.32
77.00
76.68
68.29
40.59
21.24
Parameter Value
1 Title 3h-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.4
5 Number of Scans 57
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-20T21:33:59
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
129.97
129.63
129.36
129.09
128.15
127.09
126.22
125.79
125.67
123.88
131 130 129 128 127 126 125 124 123
f1 (ppm)
Ph
OH
N
Ms
3h
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

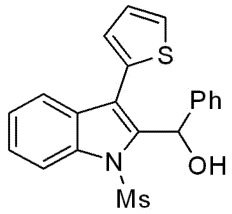

7.992
7.972
7.762
7.743
7.469
7.456
7.317
7.305
7.247
7.166
7.157
7.154
7.145
6.442
6.412
4.497
4.467
2.601
Parameter Value
1 Title 3i-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.0
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-26T14:22:20
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
S
Ph
OH
N
Ms
3i
0.95
0.96
0.96
6.06
2.31
0.99
0.98
1.01
3.00
f1 (ppm)


141.89
138.01
136.05
132.42
129.20
128.23
125.65
124.12
120.91
119.09
113.81
77.32
77.00
76.68
68.27
40.69
Parameter Value
1 Title 3i-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.1
5 Number of Scans 30
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-26T14:24:31
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
129.20
128.52
128.23
127.67
127.23
127.05
126.07
125.65
124.12
130 129 128 127 126 125 124
f1 (ppm)
S
Ph
OH
N
Ms
3i
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

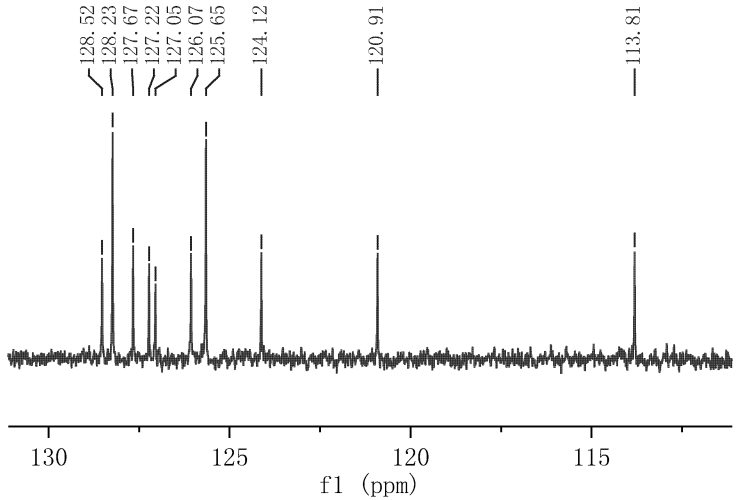


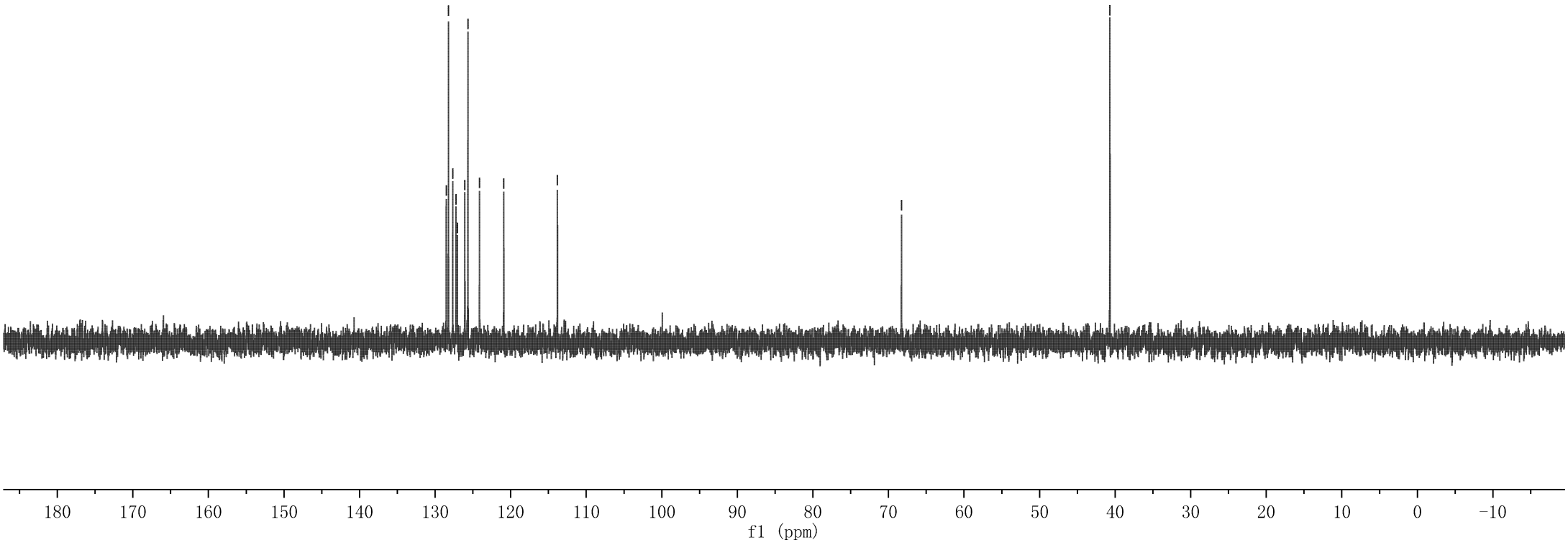


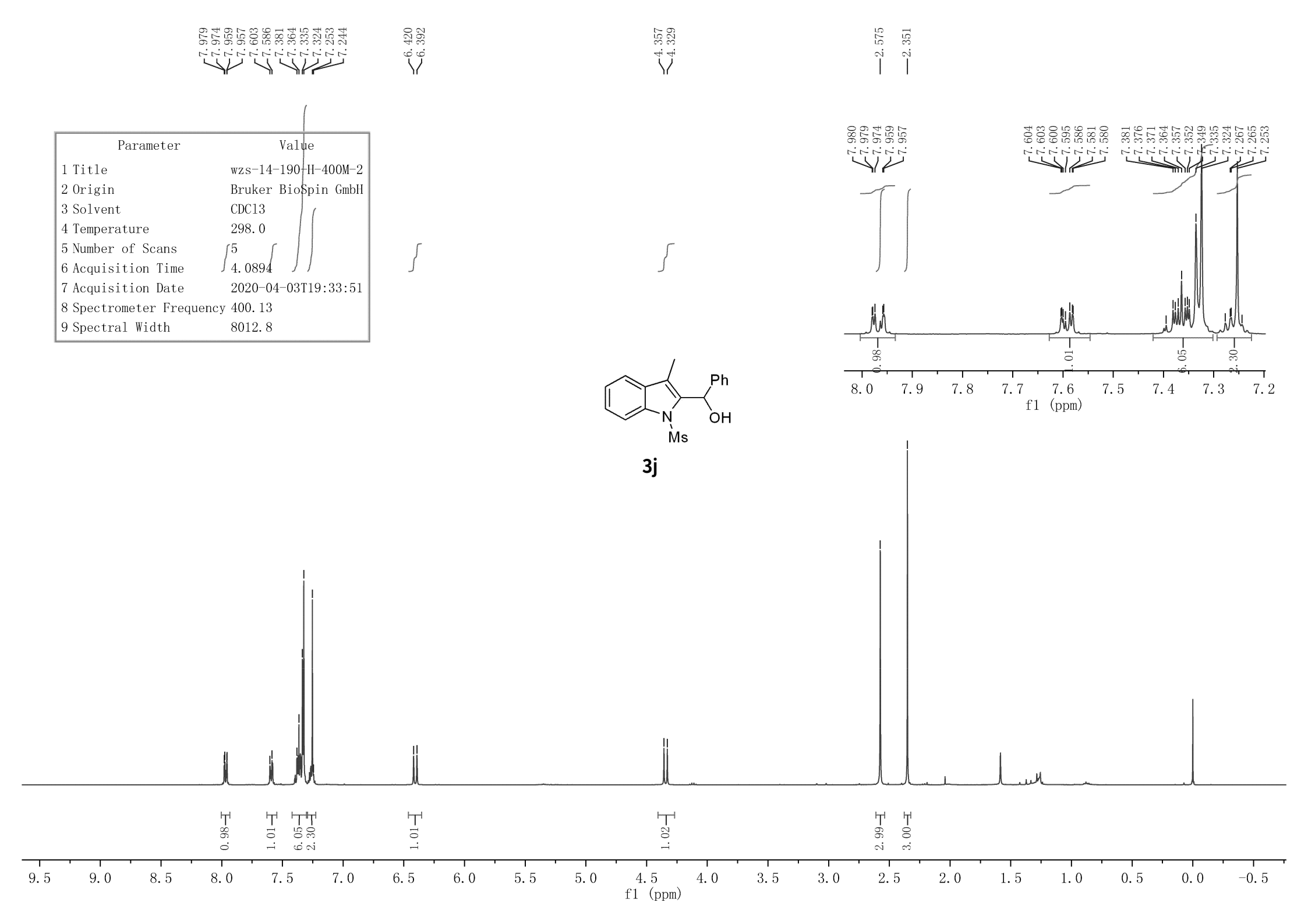
| Parameter | Value |
|---|---|
| 1 Title | 3i-C-dept-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 297.6 |
| 5 Number of Scans | 10 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-07-26T14:26:38 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

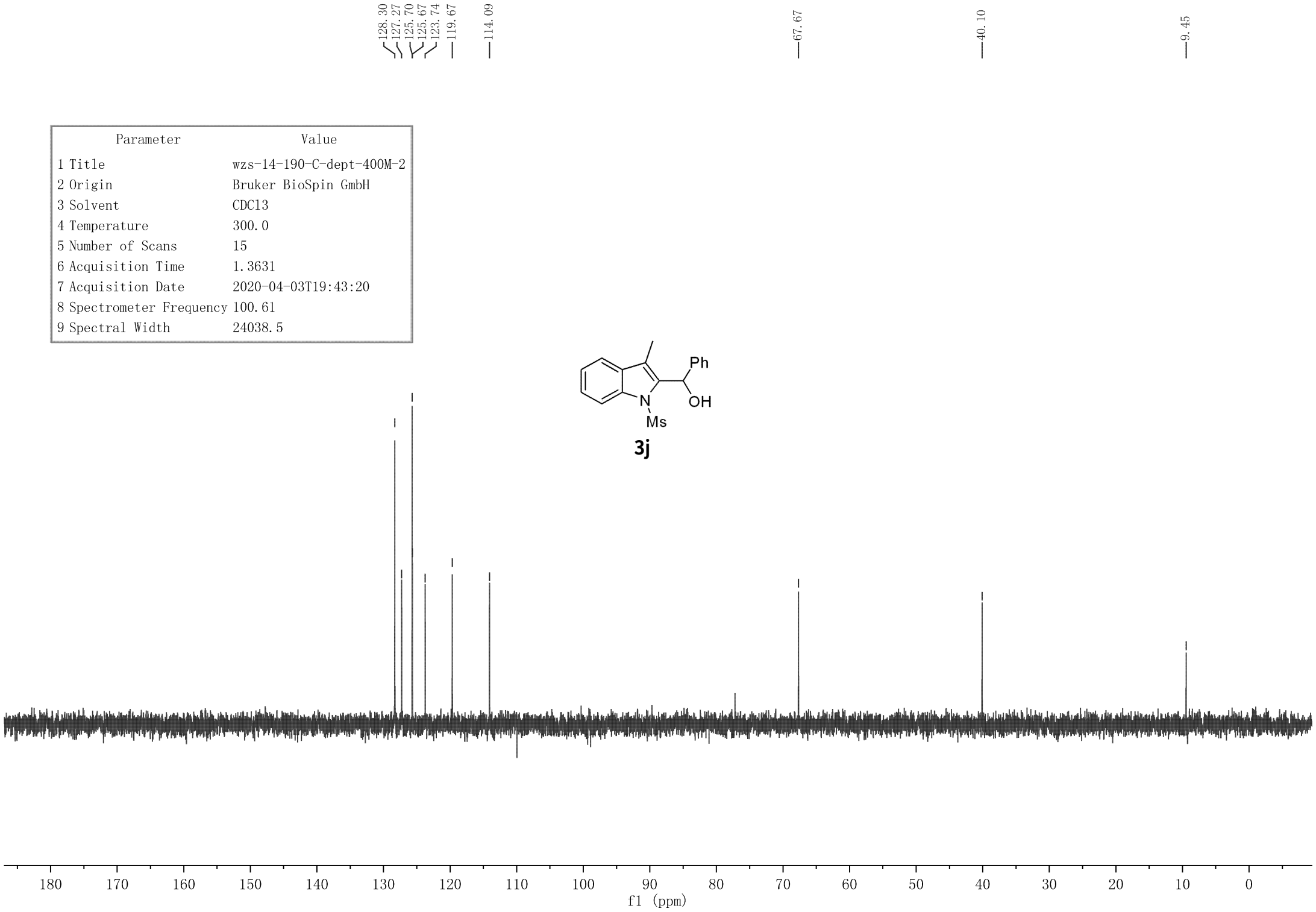



**3i**



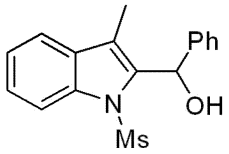

7.979
7.974
7.959
7.957
7.603
7.586
7.381
7.364
7.335
7.324
7.253
7.244
6.420
6.392
4.357
4.329
2.575
2.351
Parameter Value
1 Title wzs-14-190-H-400M-2
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 5
6 Acquisition Time 4.0894
7 Acquisition Date 2020-04-03T19:33:51
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ph
OH
N
Ms
3j
0.98
1.01
6.05
2.30
1.01
1.02
2.99
3.00
f1 (ppm)



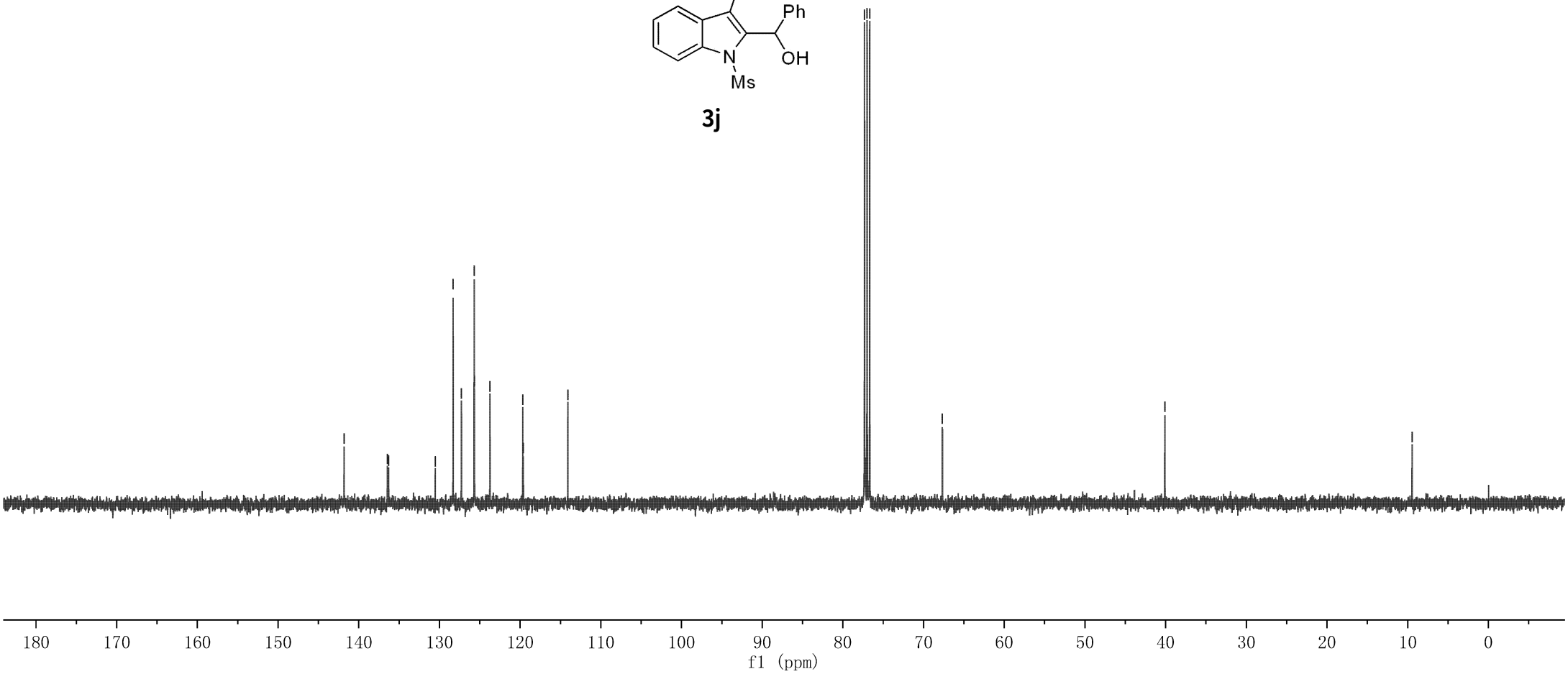

| Parameter | Value |
|---|---|
| 1 Title | wzs-14-190-C-dept-400M-2 |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Number of Scans | 15 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-04-03T19:43:20 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

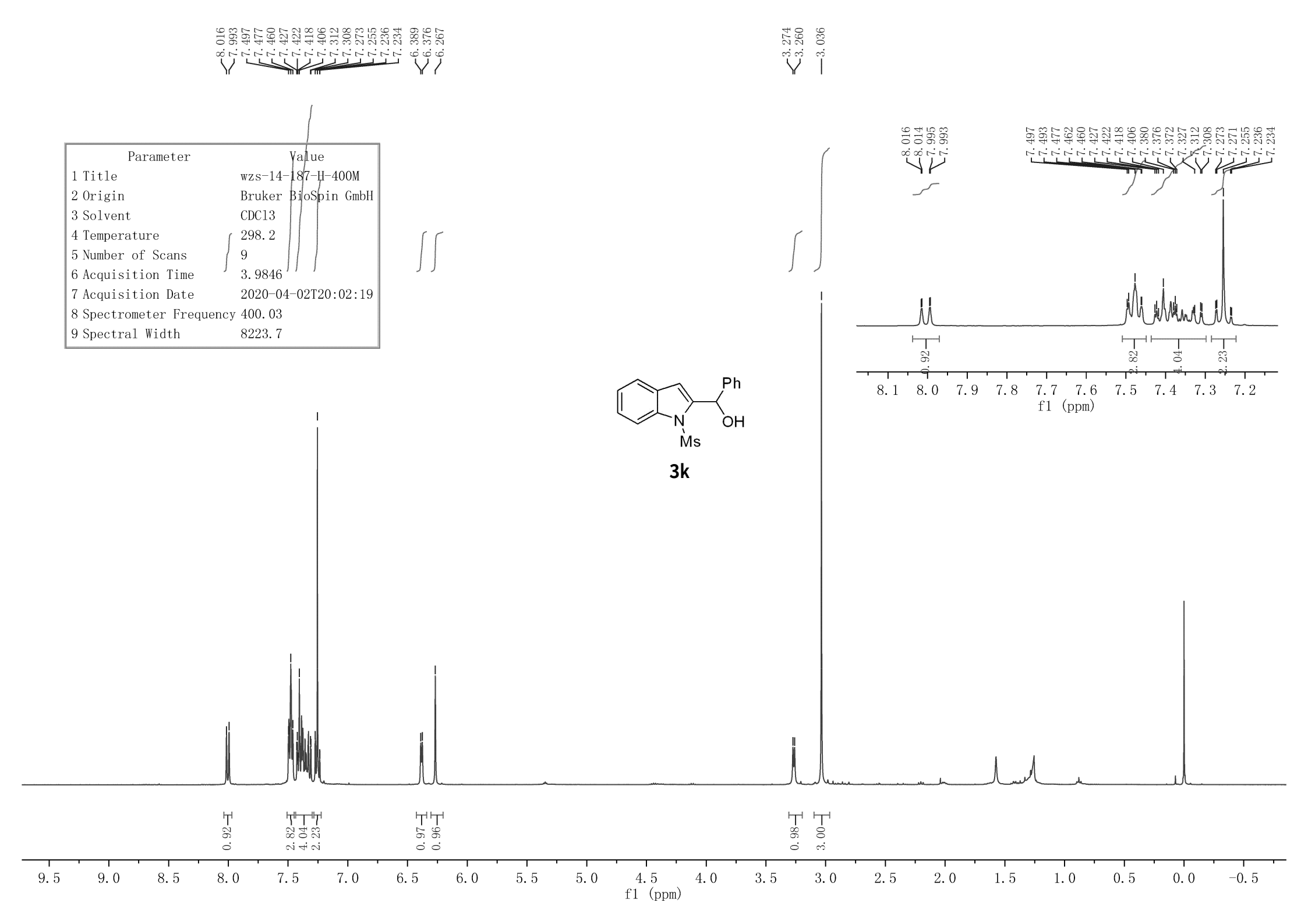
141.82
136.45
136.30
130.52
128.30
127.27
125.70
125.67
123.74
119.67
119.61
114.09
77.32
77.00
76.68
67.67
40.10
9.45

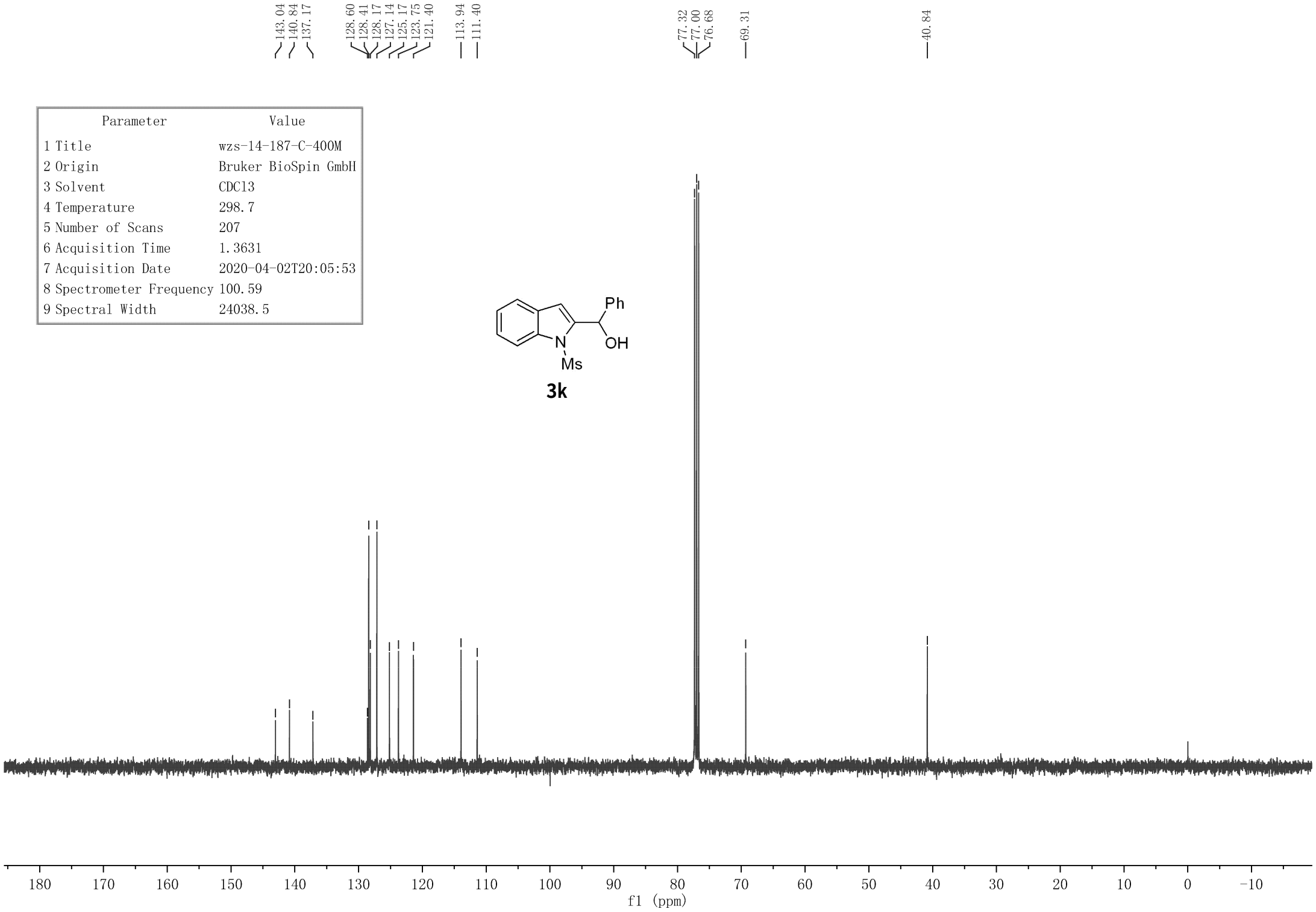
| Parameter | Value |
|---|---|
| 1 Title | wzs-14-190-C-400M-2 |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Number of Scans | 70 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-04-03T19:36:38 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

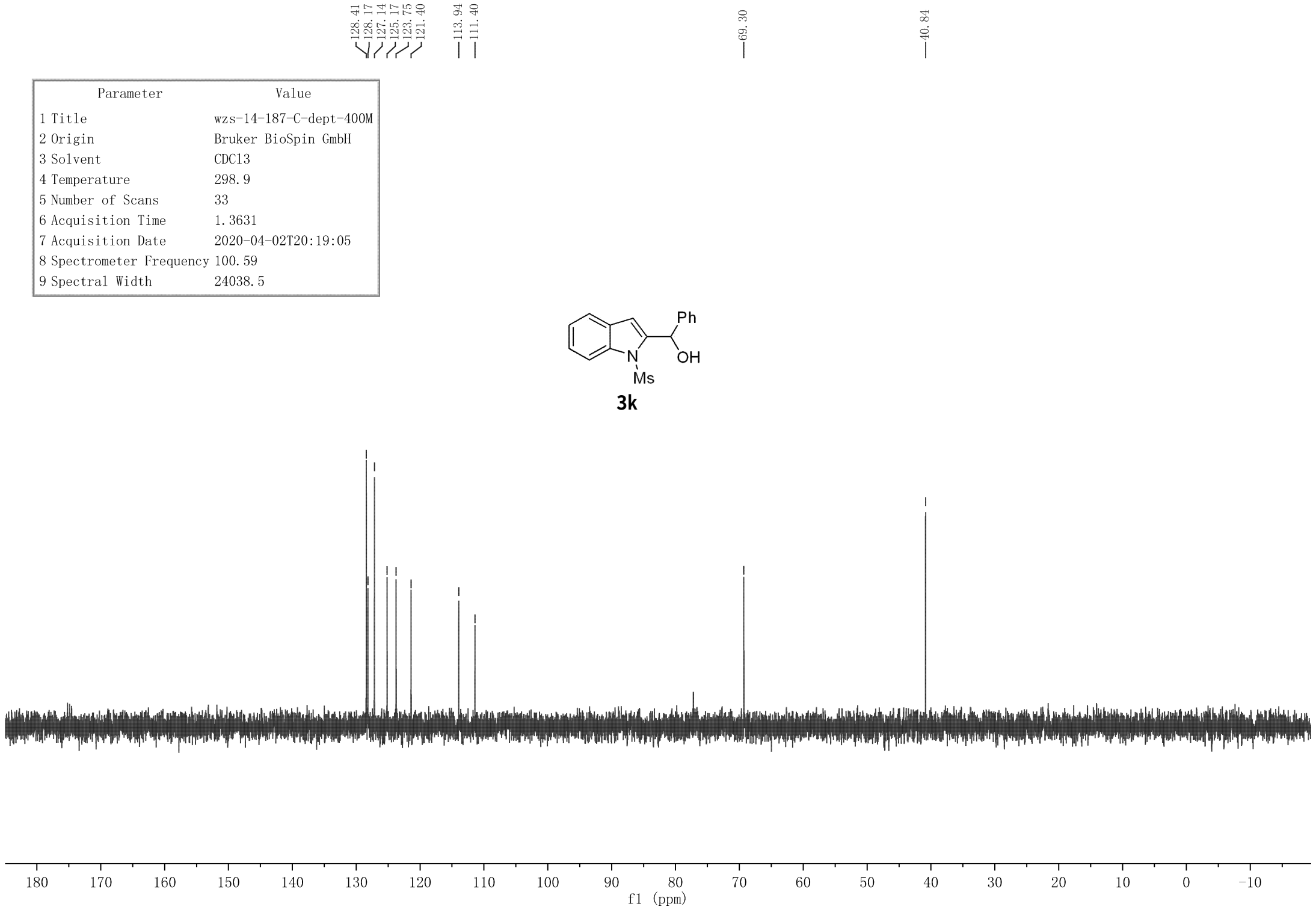


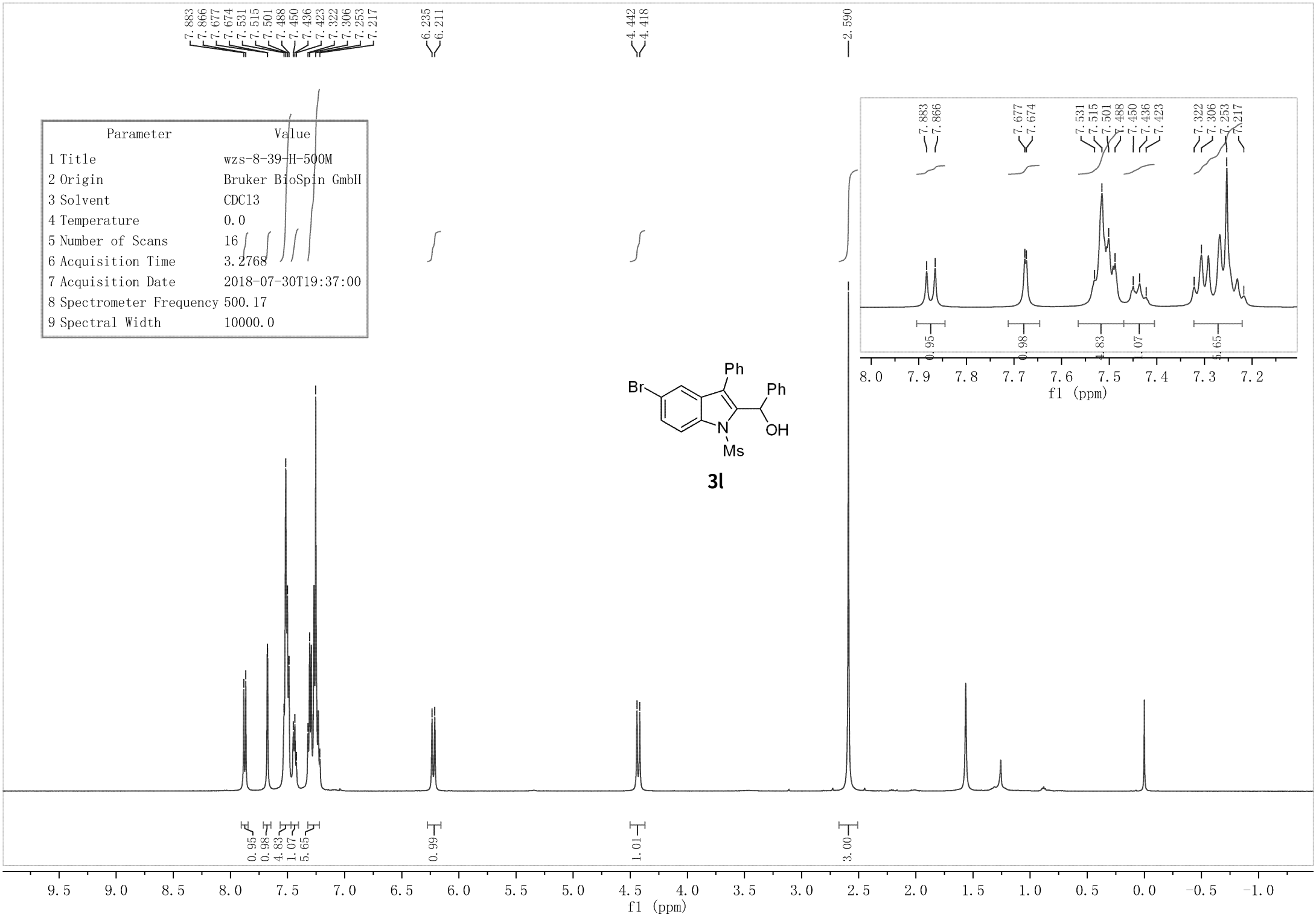

**3j**

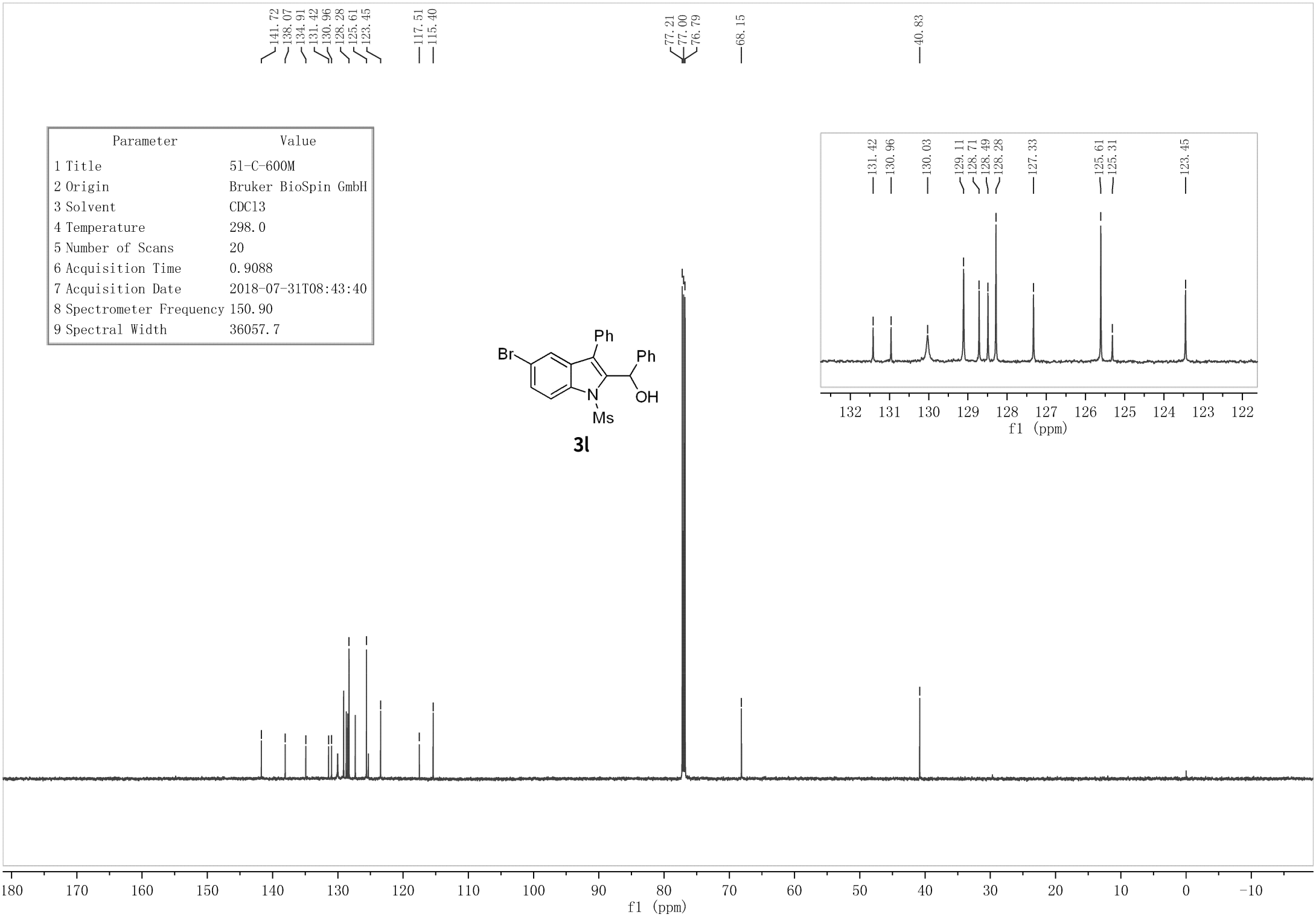


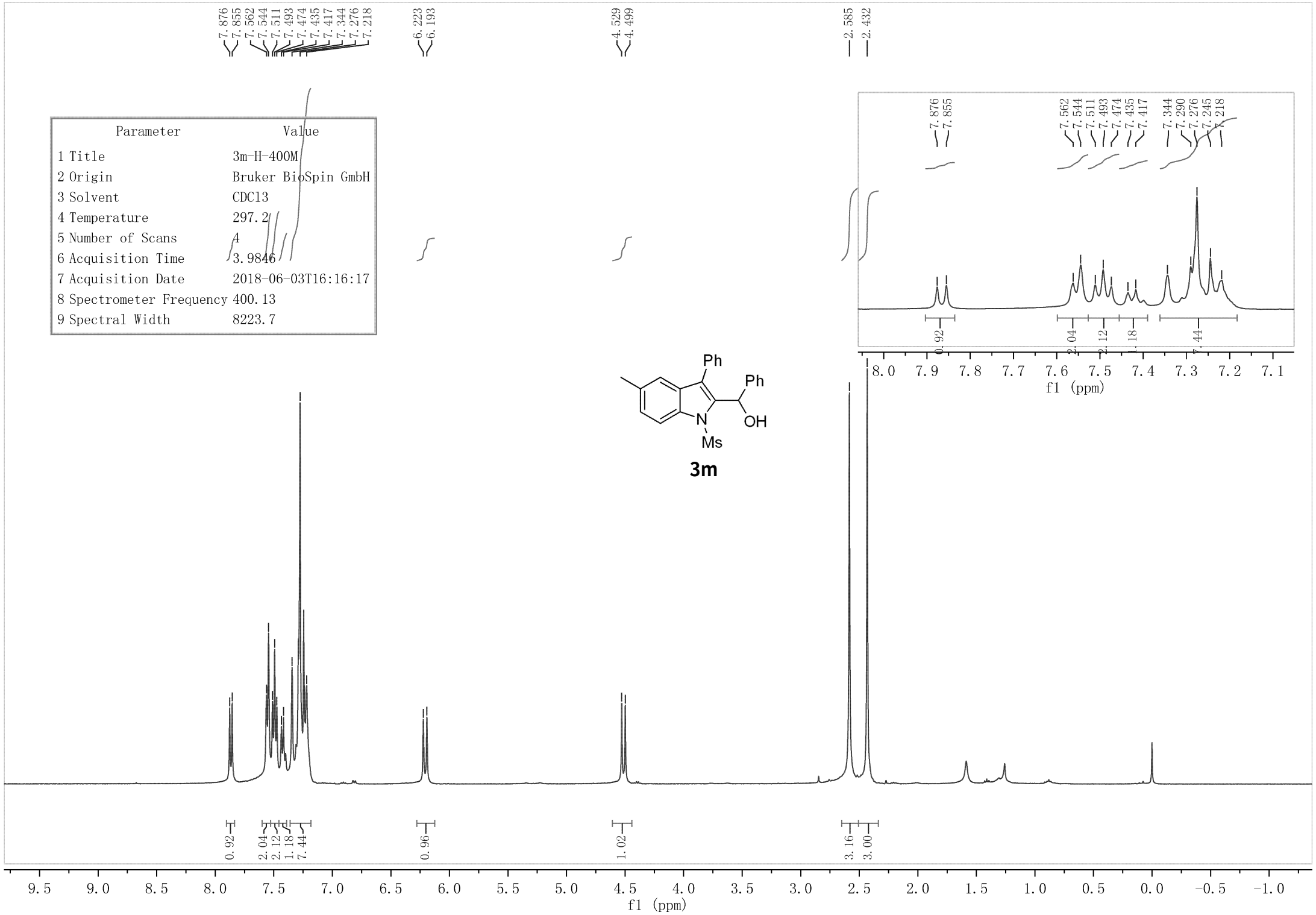

8.016
7.993
7.497
7.477
7.460
7.427
7.422
7.418
7.406
7.312
7.308
7.273
7.255
7.236
7.234
6.389
6.376
6.267
3.274
3.260
3.036
Parameter Value
1 Title wzs-14-187-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 9
6 Acquisition Time 3.9846
7 Acquisition Date 2020-04-02T20:02:19
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
Ph
OH
N
Ms
3k
0.92
2.82
4.04
2.23
0.97
0.96
0.98
3.00
f1 (ppm)

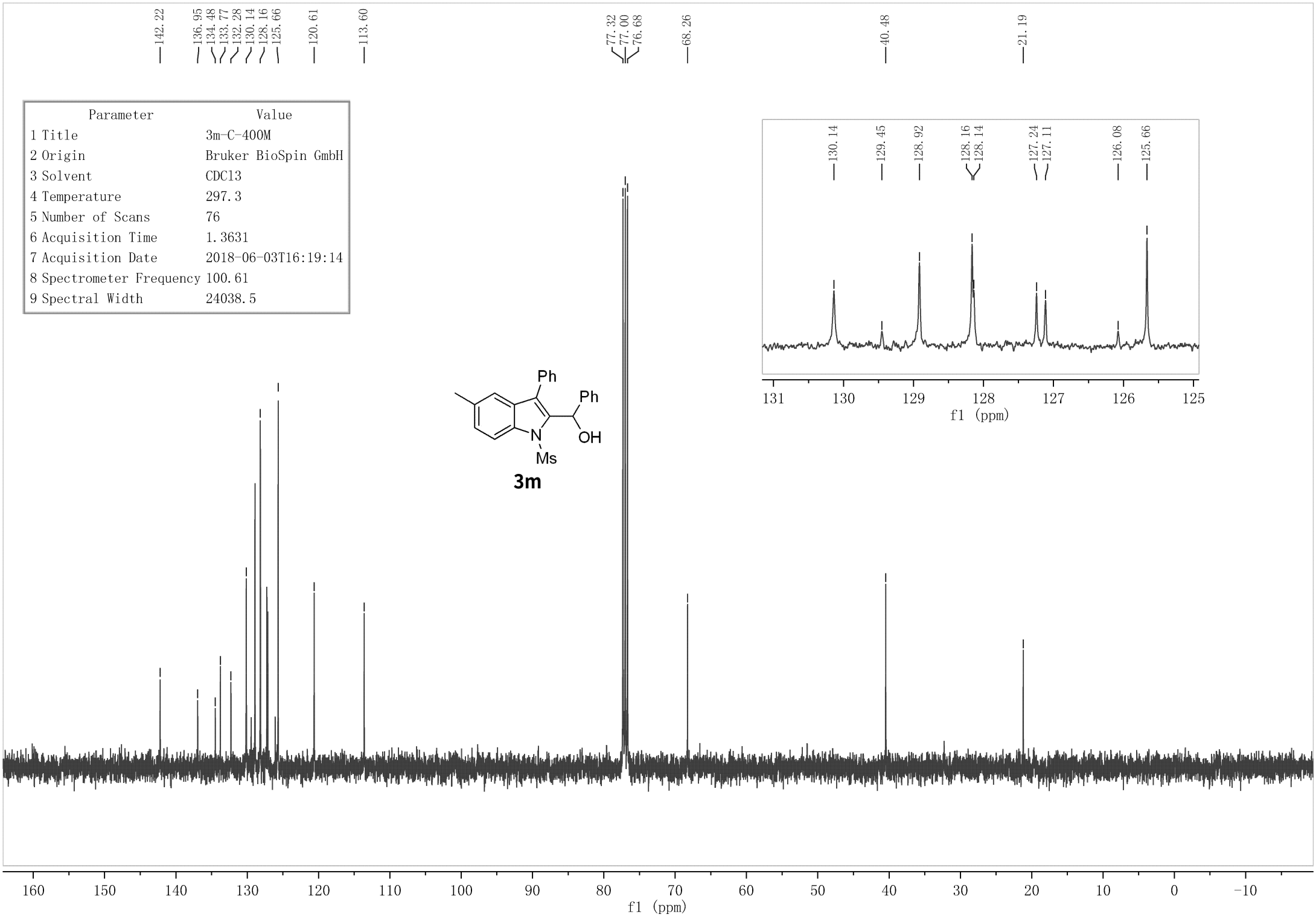

143.04
140.84
137.17
128.60
128.41
128.17
127.14
125.17
123.75
121.40
113.94
111.40
77.32
77.00
76.68
69.31
40.84
Parameter Value
1 Title wzs-14-187-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.7
5 Number of Scans 207
6 Acquisition Time 1.3631
7 Acquisition Date 2020-04-02T20:05:53
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
Ph
OH
N
Ms
3k
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

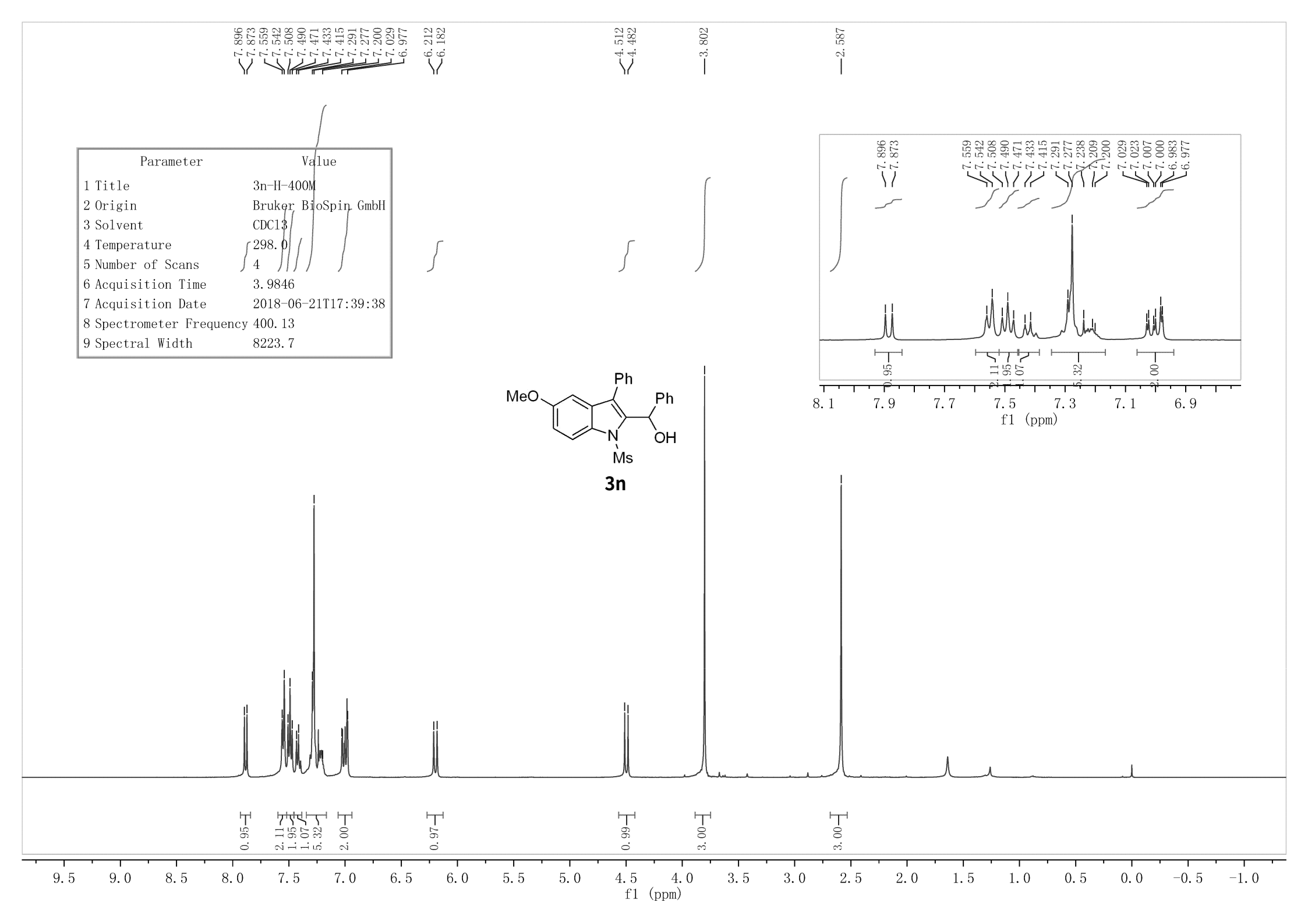

128.41
128.17
127.14
125.17
123.75
121.40
113.94
111.40
69.30
40.84
Parameter Value
1 Title wzs-14-187-C-dept-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 33
6 Acquisition Time 1.3631
7 Acquisition Date 2020-04-02T20:19:05
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
Ph
OH
N
Ms
3k
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

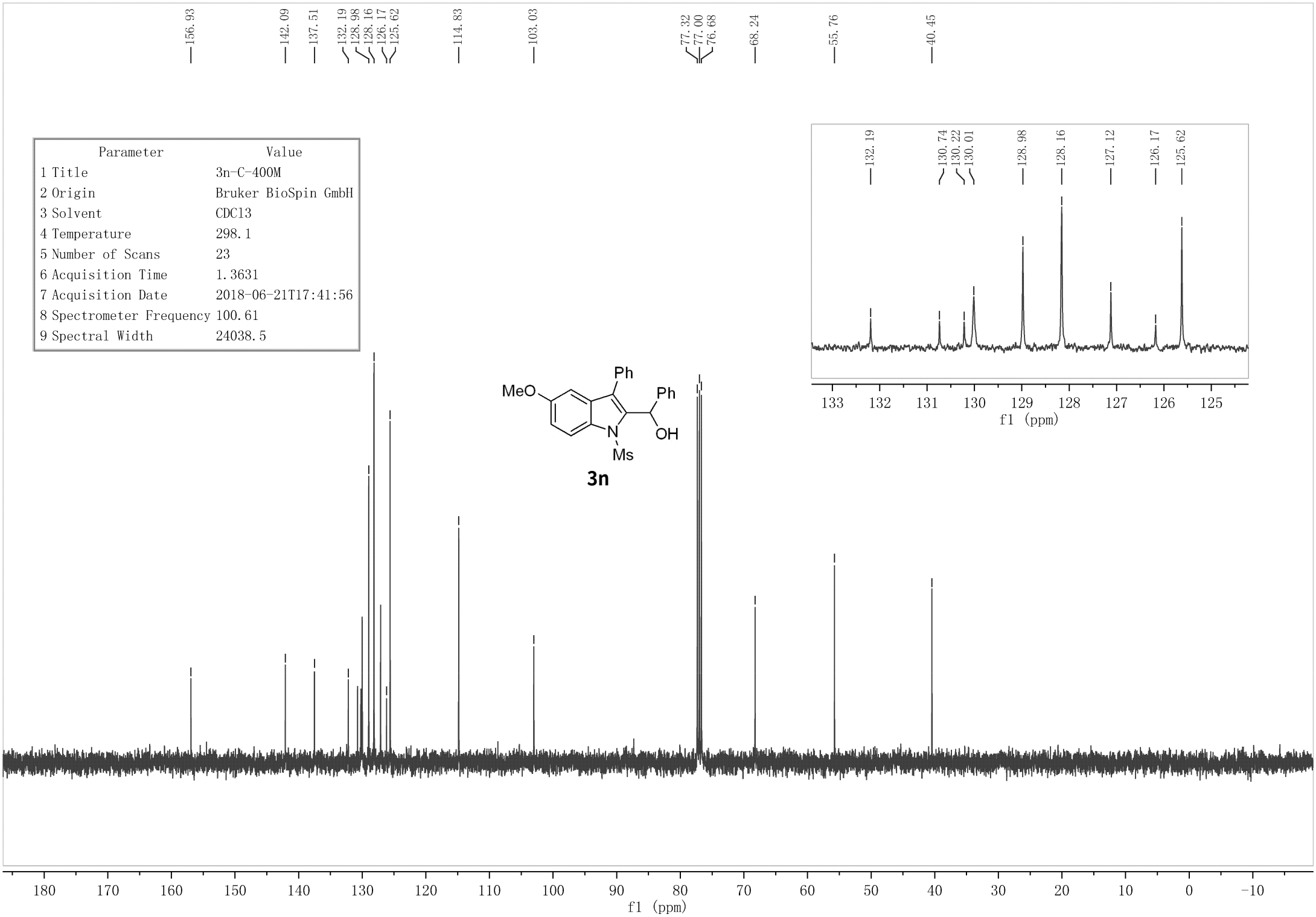

7.883
7.866
7.677
7.674
7.531
7.515
7.501
7.488
7.450
7.436
7.423
7.322
7.306
7.253
7.217
6.235
6.211
4.442
4.418
2.590
Parameter Value
1 Title wzs-8-39-H-500M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 0.0
5 Number of Scans 16
6 Acquisition Time 3.2768
7 Acquisition Date 2018-07-30T19:37:00
8 Spectrometer Frequency 500.17
9 Spectral Width 10000.0
Br
Ph
Ph
OH
N
Ms
3l
0.95
0.98
4.83
1.07
5.65
0.99
1.01
3.00
f1 (ppm)


141.72
138.07
134.91
131.42
130.96
128.28
125.61
123.45
117.51
115.40
77.21
77.00
76.79
68.15
40.83
Parameter Value
1 Title 5l-C-600M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 20
6 Acquisition Time 0.9088
7 Acquisition Date 2018-07-31T08:43:40
8 Spectrometer Frequency 150.90
9 Spectral Width 36057.7
Br
Ph
Ph
OH
N
Ms
3l
131.42
130.96
130.03
129.11
128.71
128.49
128.28
127.33
125.61
125.31
123.45
132 131 130 129 128 127 126 125 124 123 122
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

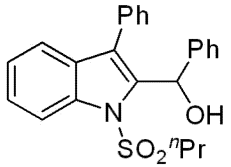

7.876
7.855
7.562
7.544
7.511
7.493
7.474
7.435
7.417
7.344
7.276
7.218
6.223
6.193
4.529
4.499
2.585
2.432
Parameter Value
1 Title 3m-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.2
5 Number of Scans 4
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-03T16:16:17
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Ph
Ph
OH
N
Ms
3m
0.92
2.04
2.12
1.18
7.44
0.96
1.02
3.16
3.00
f1 (ppm)


142.22
136.95
134.48
133.77
132.28
130.14
128.16
125.66
120.61
113.60
77.32
77.00
76.68
68.26
40.48
21.19
Parameter Value
1 Title 3m-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.3
5 Number of Scans 76
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-03T16:19:14
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
130.14
129.45
128.92
128.16
128.14
127.24
127.11
126.08
125.66
131 130 129 128 127 126 125
f1 (ppm)
Ph
Ph
OH
N
Ms
3m
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

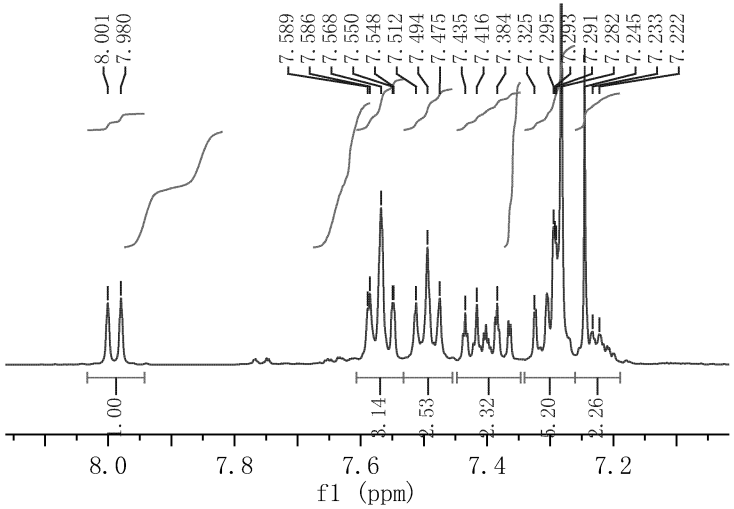

7.896
7.873
7.559
7.542
7.508
7.490
7.471
7.433
7.415
7.291
7.277
7.200
7.029
6.977
6.212
6.182
4.512
4.482
3.802
2.587
Parameter Value
1 Title 3n-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 4
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-21T17:39:38
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
MeO
Ph
Ph
OH
N
Ms
3n
f1 (ppm)

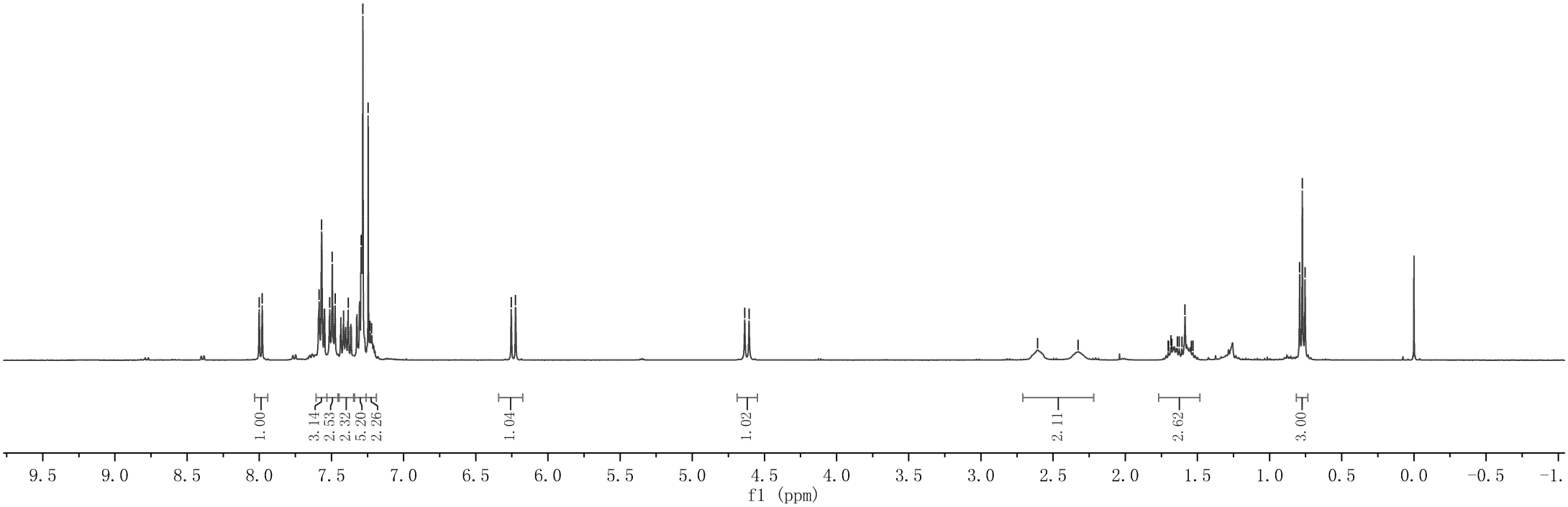

156.93
142.09
137.51
132.19
128.98
128.16
126.17
125.62
114.83
103.03
77.32
77.00
76.68
68.24
55.76
40.45
Parameter Value
1 Title 3n-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.1
5 Number of Scans 23
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-21T17:41:56
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
MeO
Ph
Ph
OH
N
Ms
3n
132.19
130.74
130.22
130.01
128.98
128.16
127.12
126.17
125.62
133 132 131 130 129 128 127 126 125
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

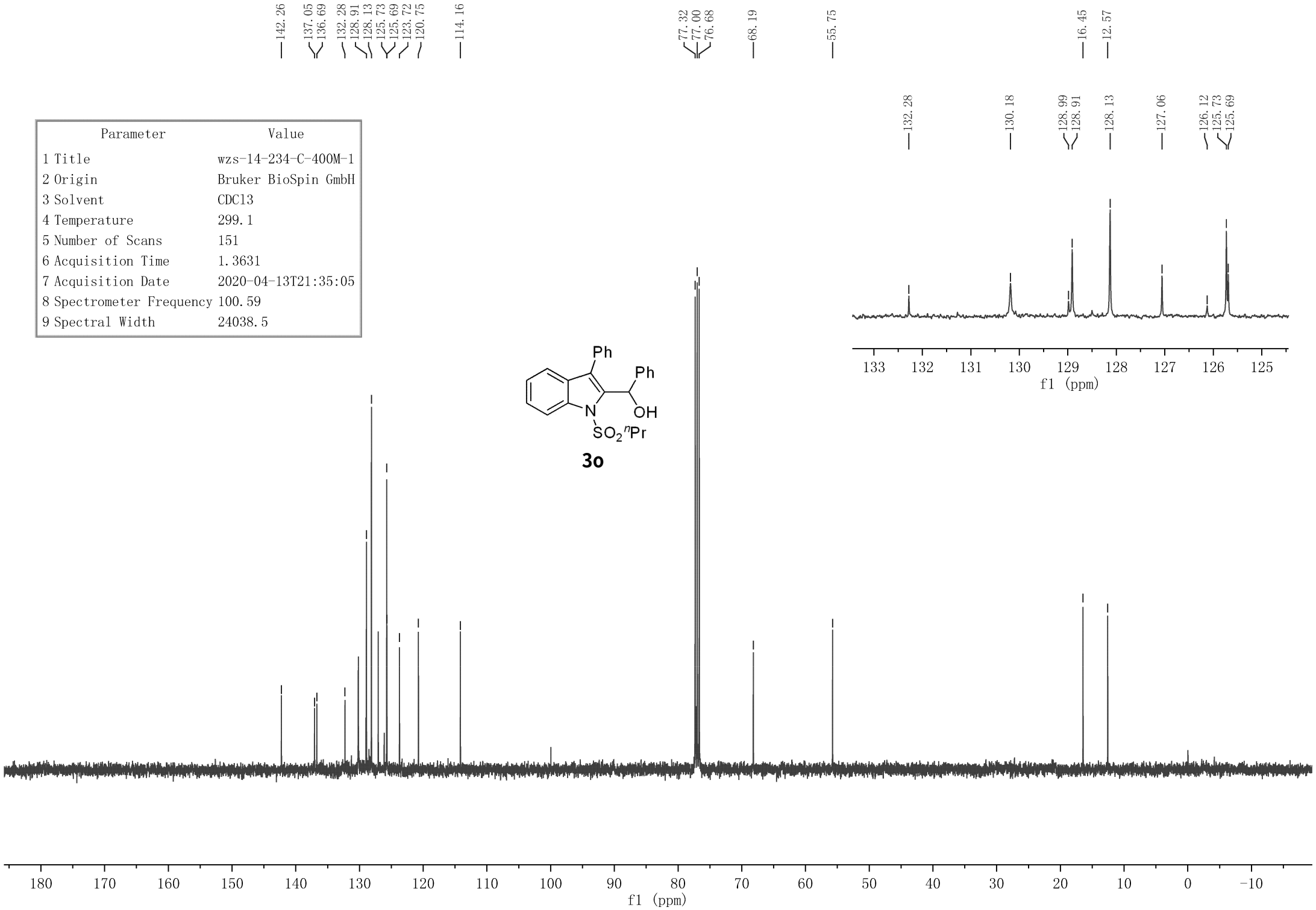
| Parameter | Value |
|---|---|
| 1 Title | wzs-14-234-H-400M-1 |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.3 |
| 5 Number of Scans | 8 |
| 6 Acquisition Time | 3.9846 |
| 7 Acquisition Date | 2020-04-13T21:31:31 |
| 8 Spectrometer Frequency | 400.03 |
| 9 Spectral Width | 8223.7 |

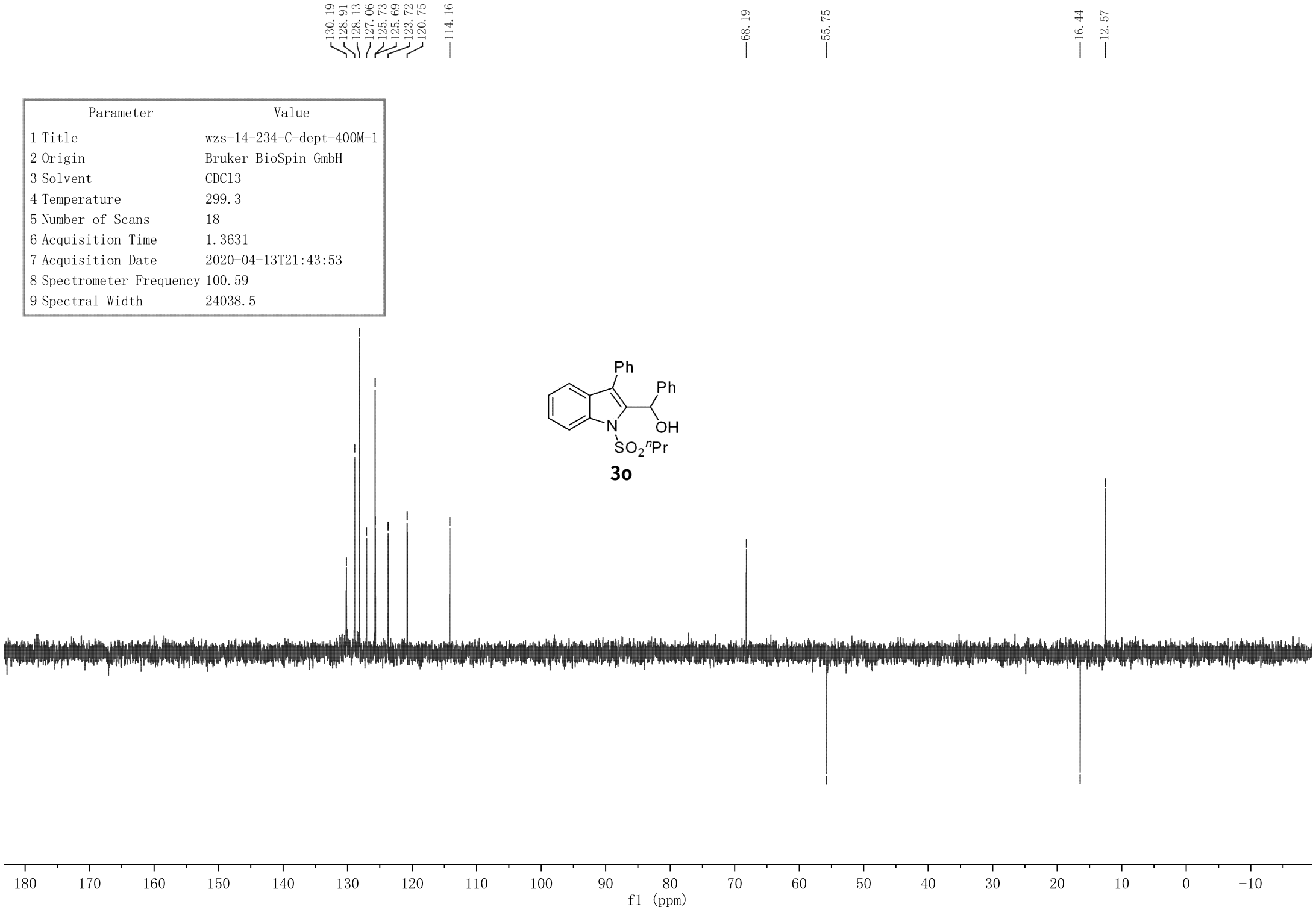



**3o**

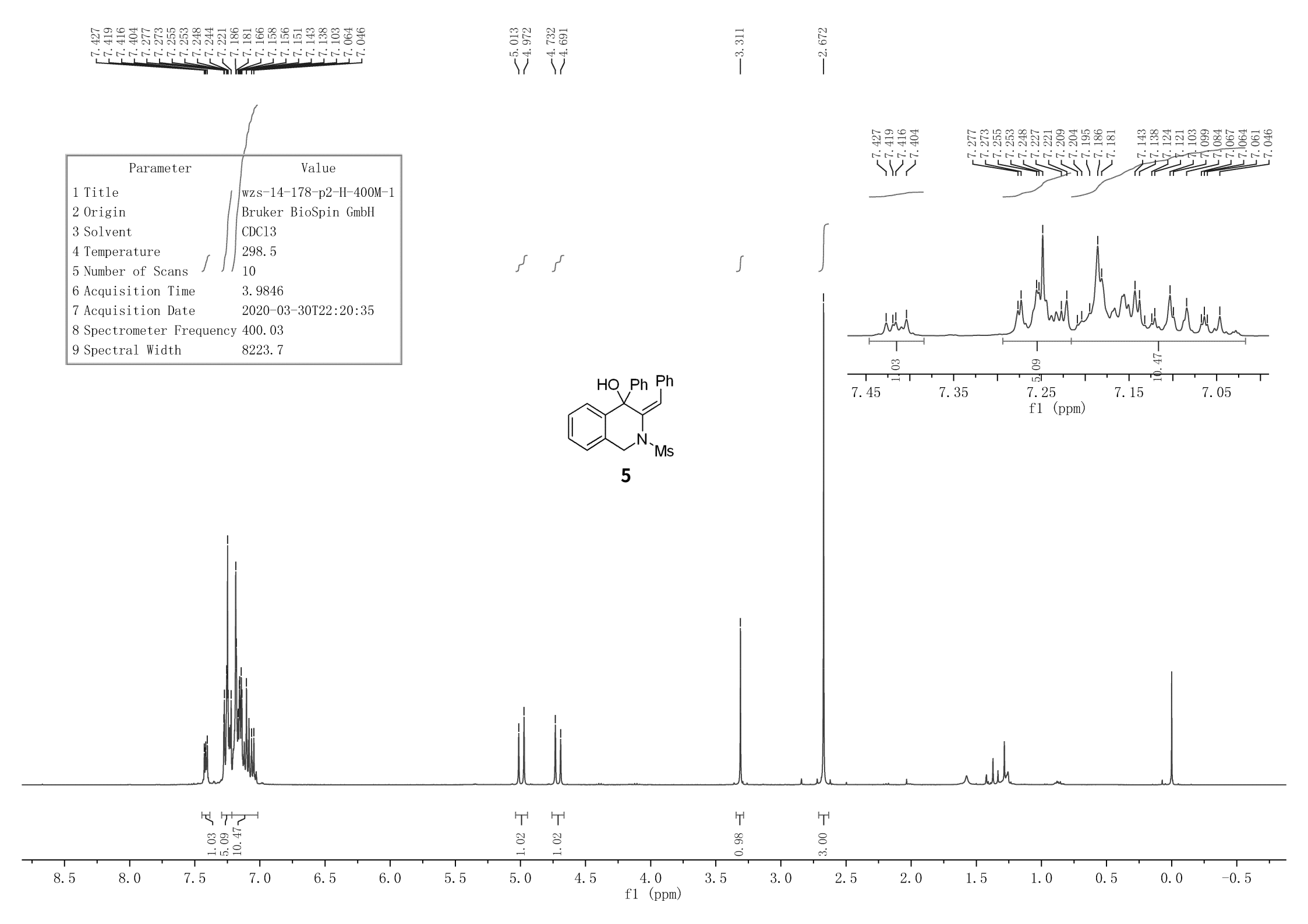



142.26
137.05
136.69
132.28
128.91
128.13
125.73
125.69
123.72
120.75
114.16
77.32
77.00
76.68
68.19
55.75
16.45
12.57
Parameter Value
1 Title wzs-14-234-C-400M-1
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.1
5 Number of Scans 151
6 Acquisition Time 1.3631
7 Acquisition Date 2020-04-13T21:35:05
8 Spectrometer Frequency 100.59
9 Spectral Width 24038.5
Ph
Ph
OH
N
SO2nPr
3o
132.28
130.18
128.99
128.91
128.13
127.06
126.12
125.73
125.69
133 132 131 130 129 128 127 126 125
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)




| Parameter | Value |
|---|---|
| 1 Title | wzs-14-234-C-dept-400M-1 |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.3 |
| 5 Number of Scans | 18 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-04-13T21:43:53 |
| 8 Spectrometer Frequency | 100.59 |
| 9 Spectral Width | 24038.5 |

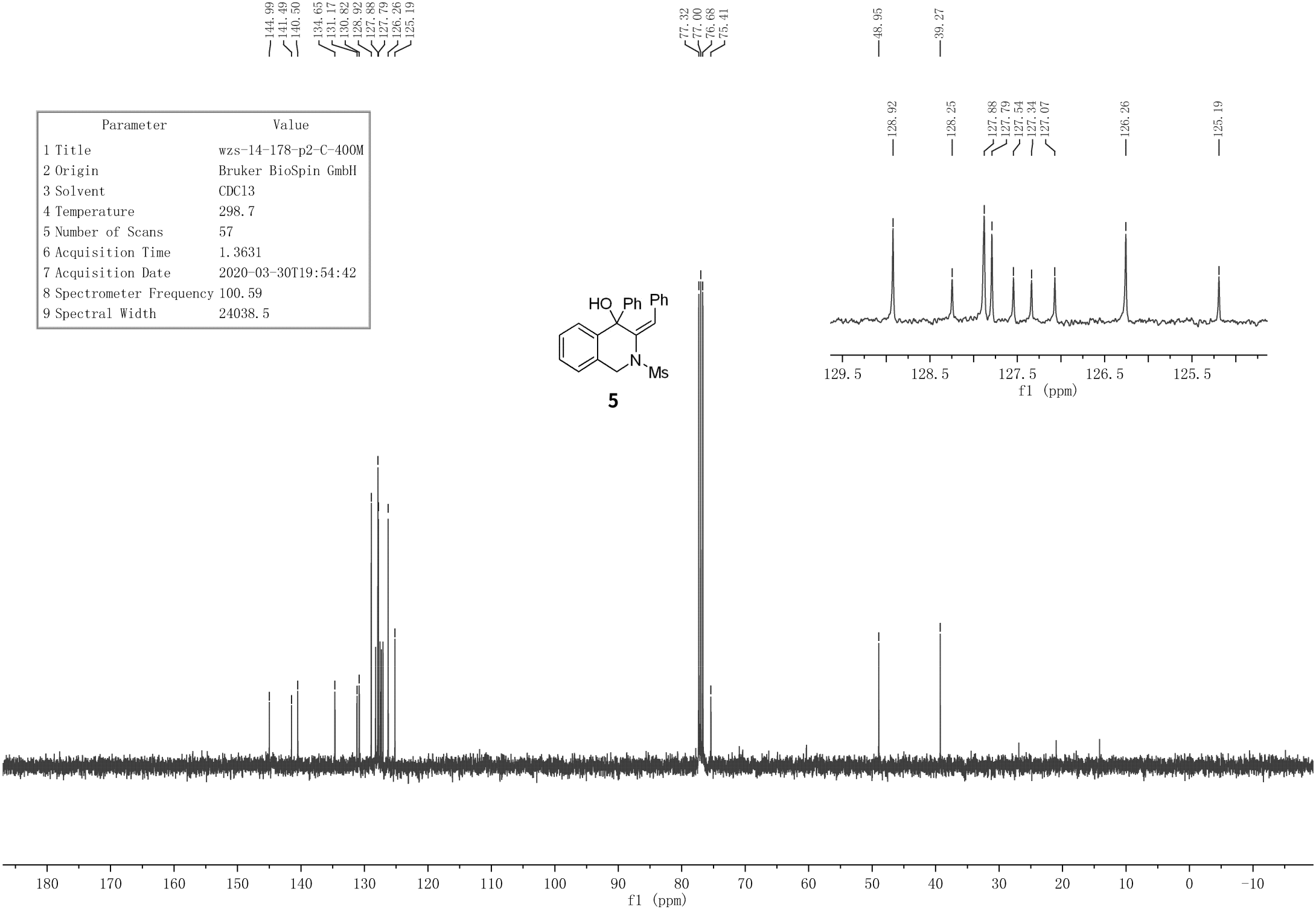

7.427
7.419
7.416
7.404
7.277
7.273
7.255
7.253
7.248
7.244
7.221
7.186
7.181
7.166
7.158
7.156
7.151
7.143
7.138
7.103
7.064
7.046
5.013
4.972
4.732
4.691
3.311
2.672
Parameter Value
1 Title wzs-14-178-p2-H-400M-1
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.5
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2020-03-30T22:20:35
8 Spectrometer Frequency 400.03
9 Spectral Width 8223.7
HO Ph Ph
N
Ms
5
1.03
5.09
10.47
1.02
1.02
0.98
3.00
f1 (ppm)

| Parameter | Value |
|---|---|
| 1 Title | wzs-14-178-p2-C-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.7 |
| 5 Number of Scans | 57 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-03-30T19:54:42 |
| 8 Spectrometer Frequency | 100.59 |
| 9 Spectral Width | 24038.5 |




**5**

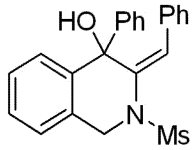


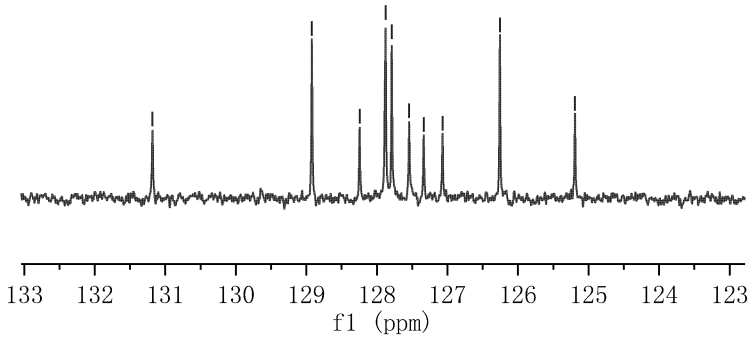
131.18
128.92
128.25
127.88
127.79
127.54
127.34
127.07
126.26
125.19

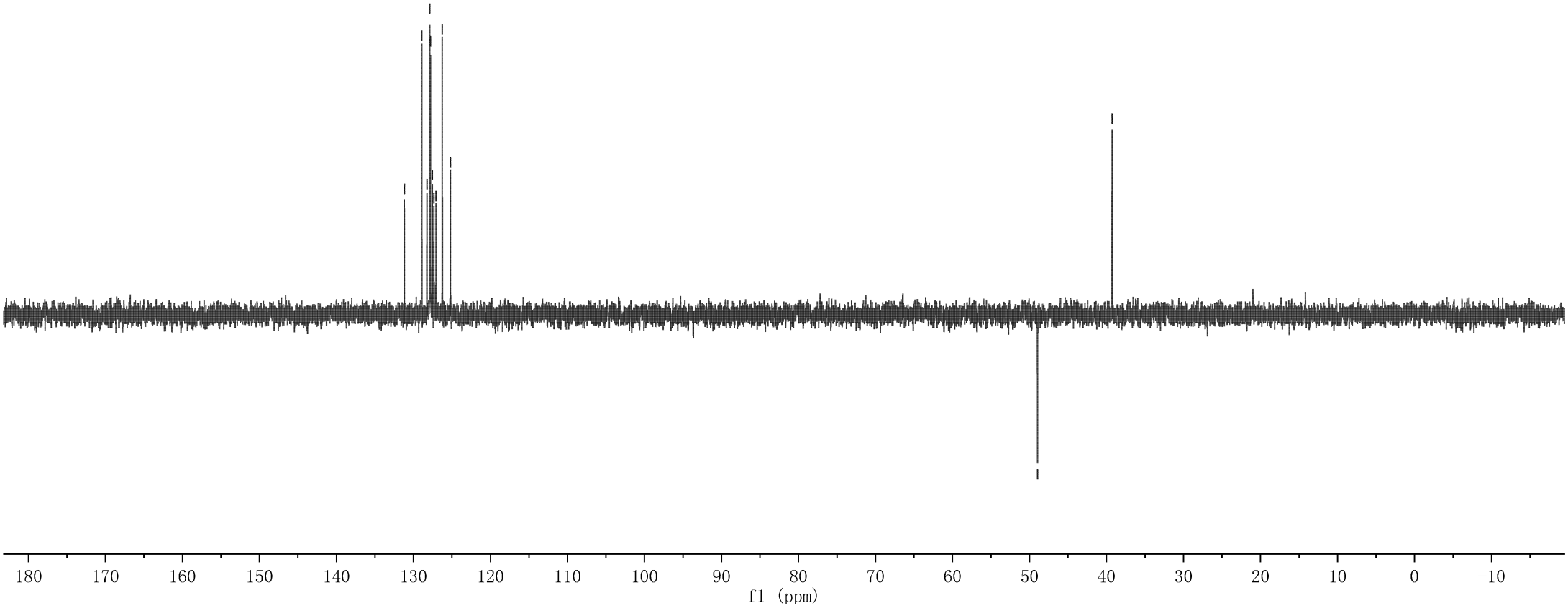
48.96
39.27

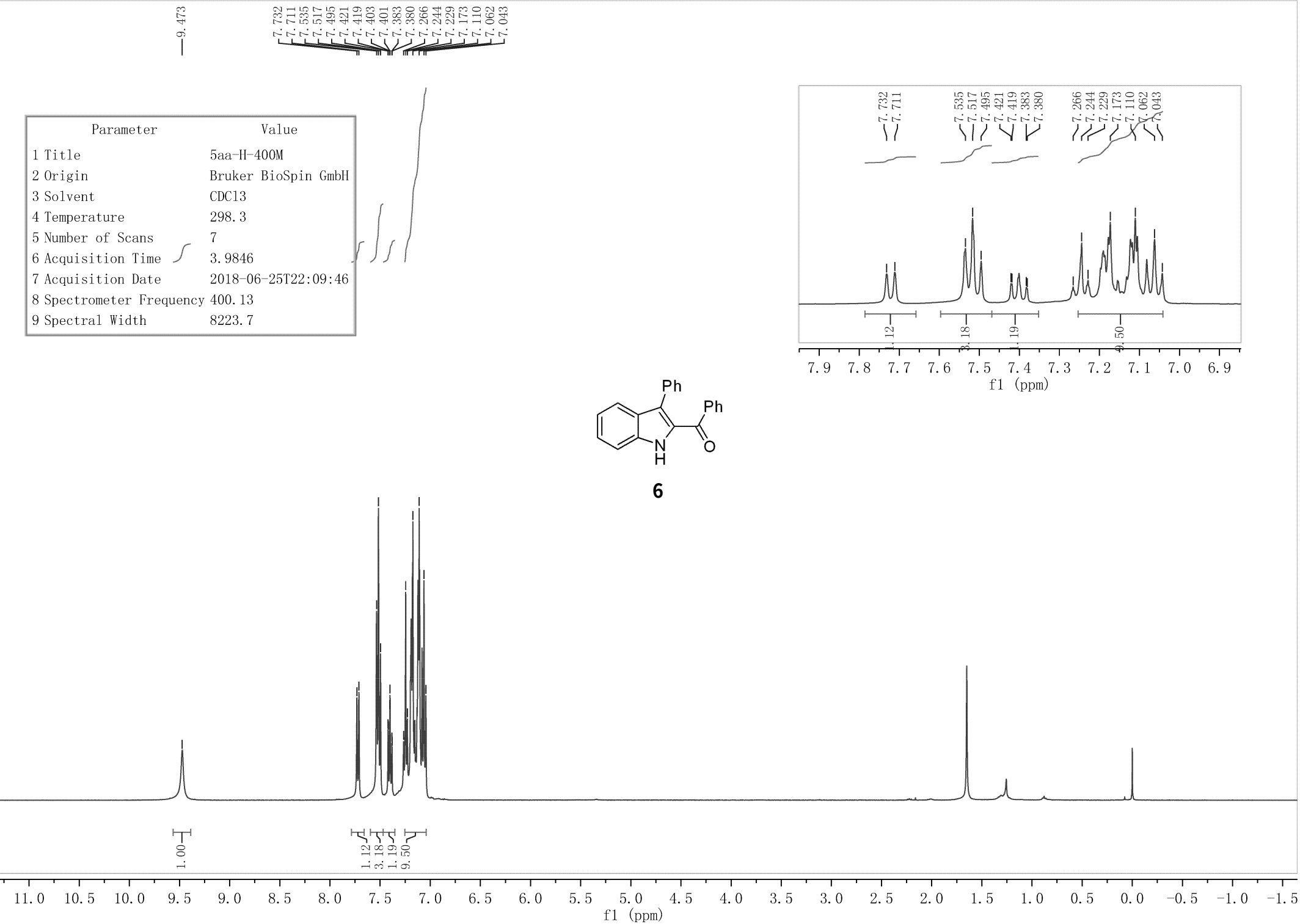
| Parameter | Value |
|---|---|
| 1 Title | wzs-14-178-p2-C-dept-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 298.9 |
| 5 Number of Scans | 16 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2020-03-30T19:59:00 |
| 8 Spectrometer Frequency | 100.59 |
| 9 Spectral Width | 24038.5 |

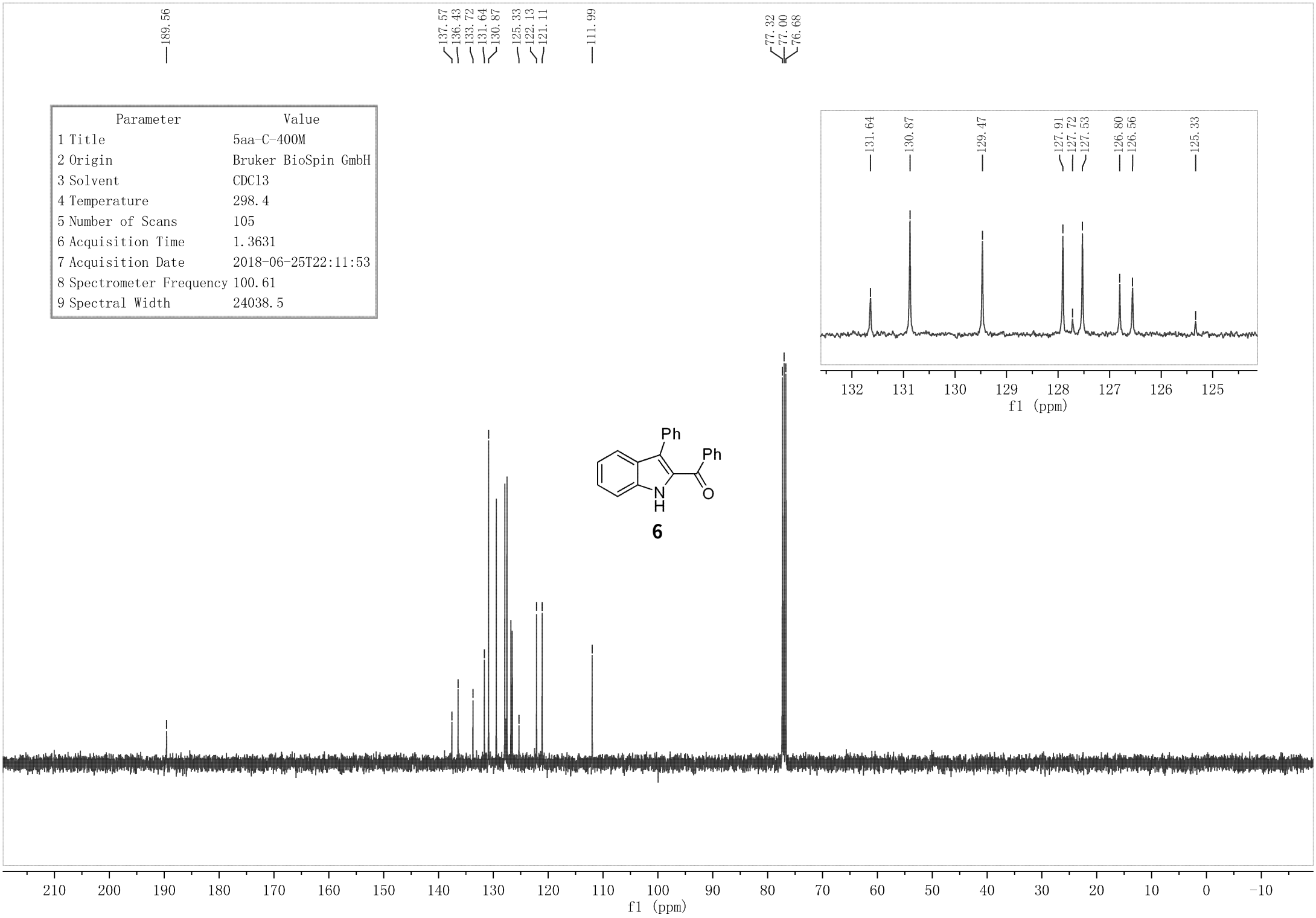



**5**



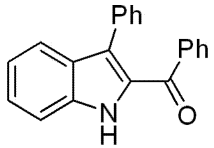




9.473
7.732
7.711
7.535
7.517
7.495
7.421
7.419
7.403
7.401
7.383
7.380
7.266
7.244
7.229
7.173
7.110
7.062
7.043
Parameter Value
1 Title 5aa-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.3
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2018-06-25T22:09:46
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
1.12
3.18
1.19
9.50
f1 (ppm)
Ph
Ph
N
H
O
6
1.00
1.12
3.18
1.19
9.50
f1 (ppm)

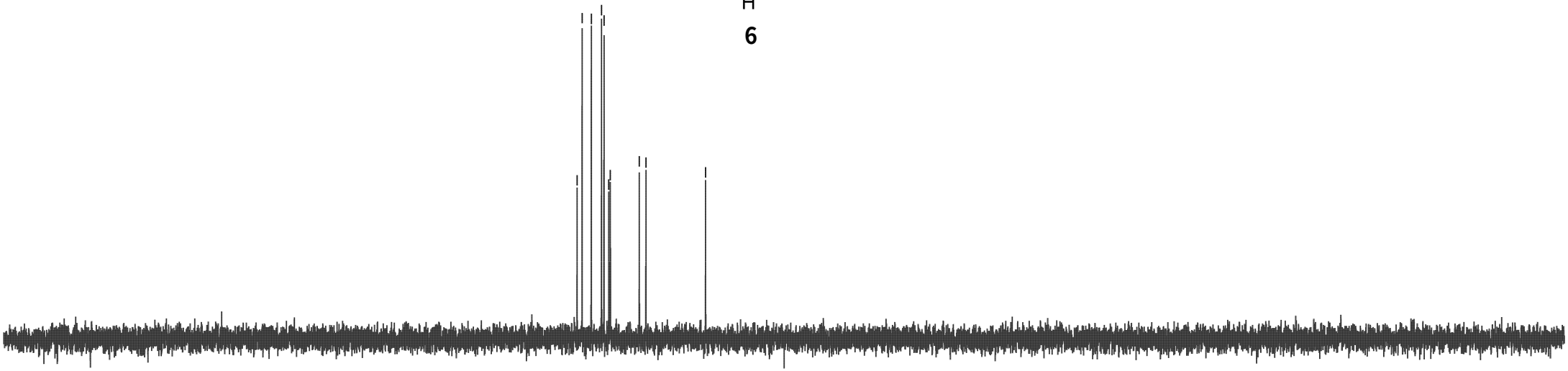

189.56
137.57
136.43
133.72
131.64
130.87
125.33
122.13
121.11
111.99
77.32
77.00
76.68
Parameter Value
1 Title 5aa-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.4
5 Number of Scans 105
6 Acquisition Time 1.3631
7 Acquisition Date 2018-06-25T22:11:53
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
131.64
130.87
129.47
127.91
127.72
127.53
126.80
126.56
125.33
132 131 130 129 128 127 126 125
f1 (ppm)
Ph
Ph
N
H
O
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

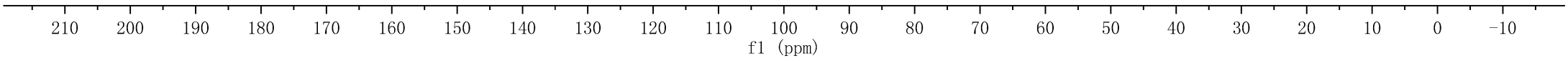
131.64
130.87
129.47
127.91
127.53
126.80
126.55
122.13
121.11
111.99

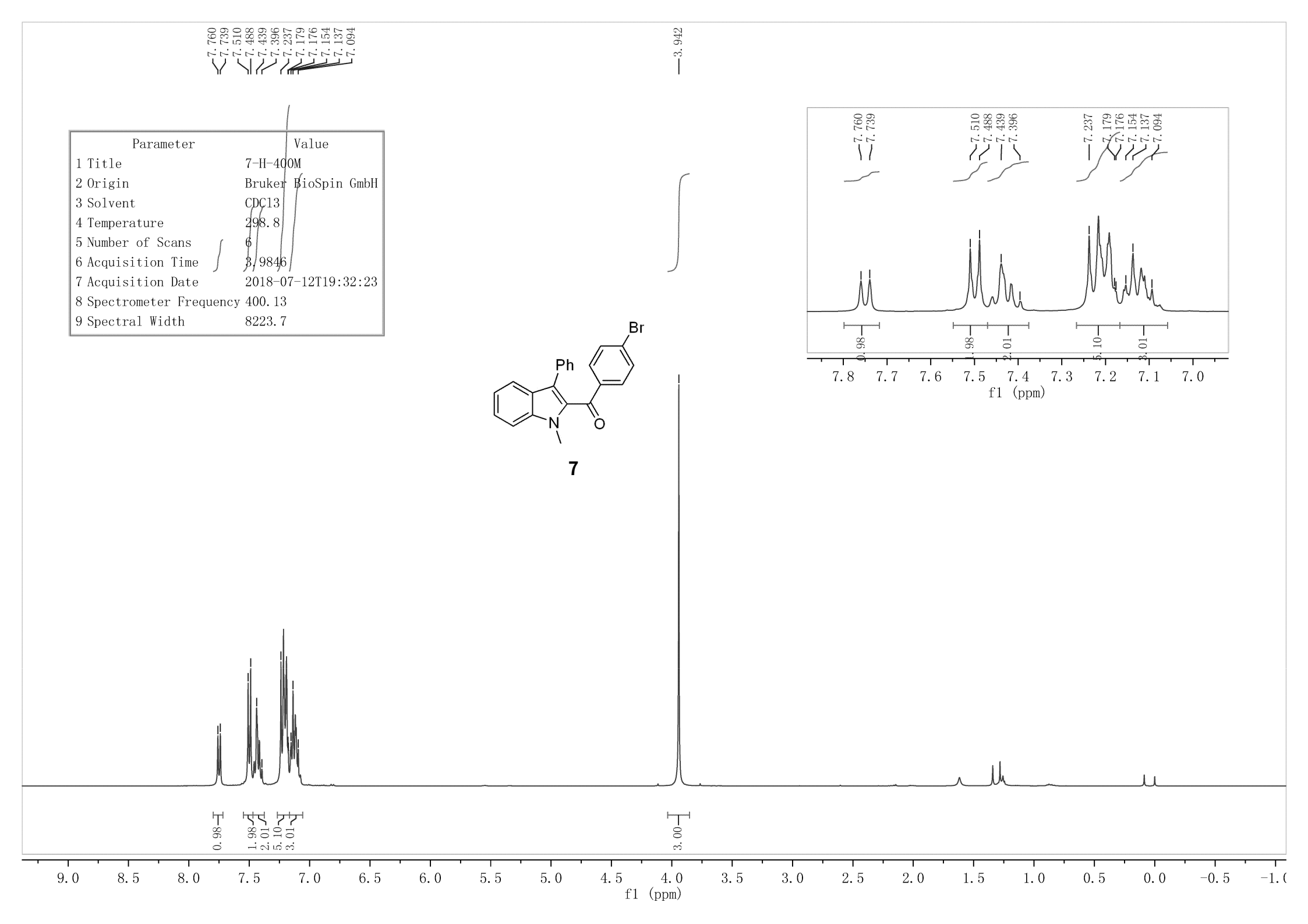
| Parameter | Value |
|---|---|
| 1 Title | 5aa-C-dept-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.1 |
| 5 Number of Scans | 16 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-06-25T22:18:34 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |

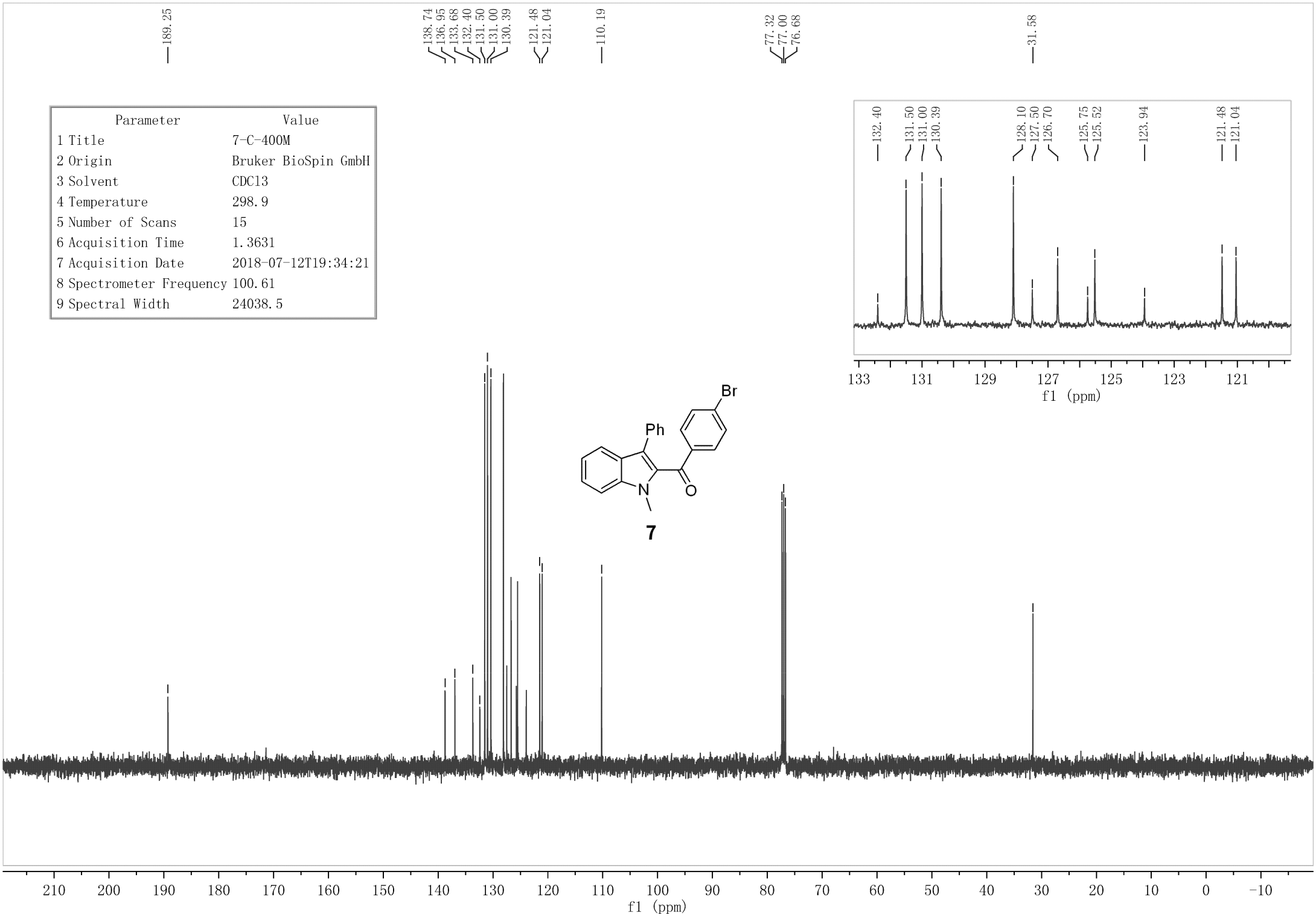


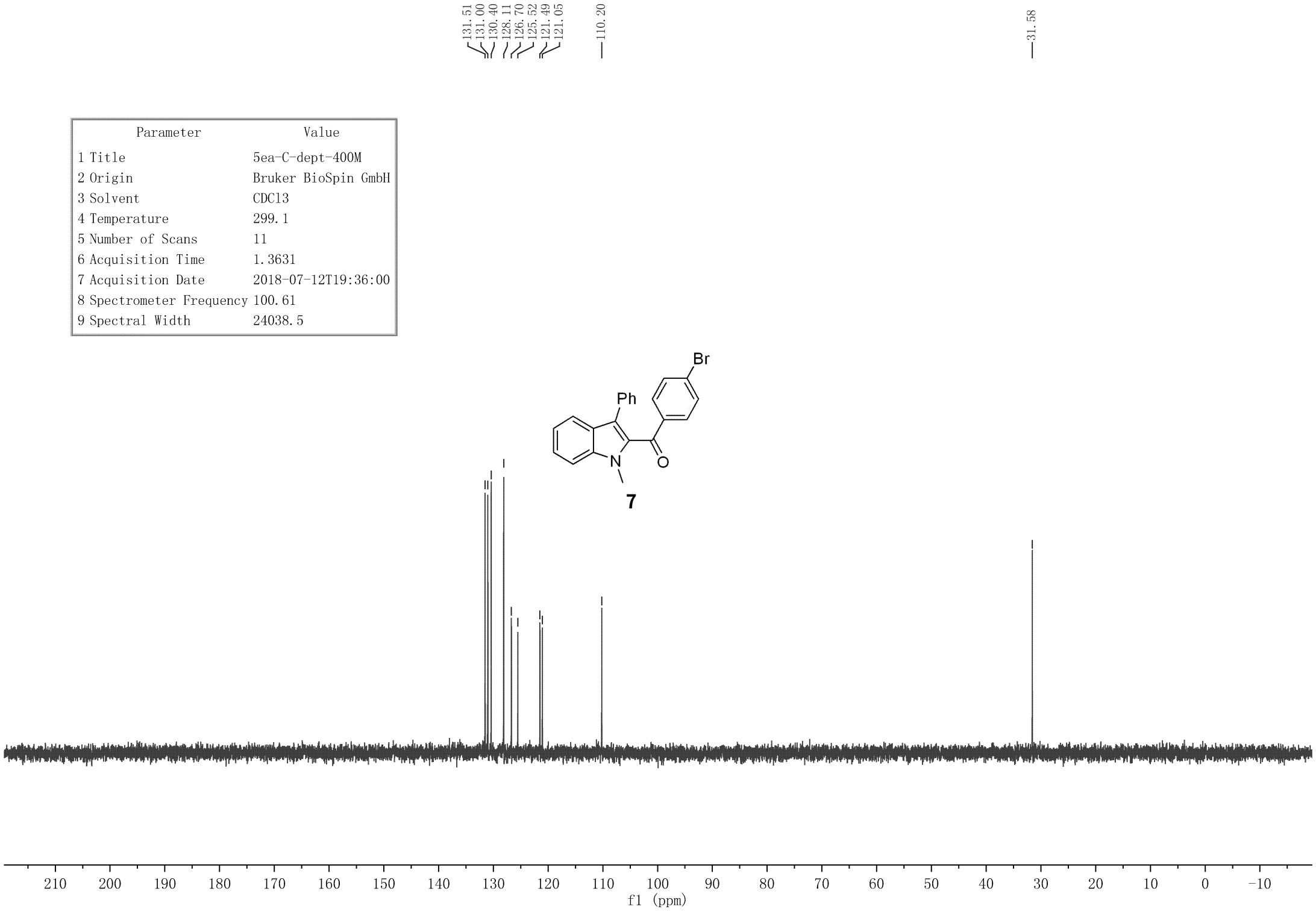

**6**






7.760
7.739
7.510
7.488
7.439
7.396
7.237
7.179
7.176
7.154
7.137
7.094
3.942
Parameter Value
1 Title 7-H-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.8
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2018-07-12T19:32:23
8 Spectrometer Frequency 400.13
9 Spectral Width 8223.7
Br
Ph
N
O
7
0.98
1.98
2.01
5.10
3.01
3.00
f1 (ppm)


189.25
138.74
136.95
133.68
132.40
131.50
131.00
130.39
121.48
121.04
110.19
77.32
77.00
76.68
31.58
Parameter Value
1 Title 7-C-400M
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 15
6 Acquisition Time 1.3631
7 Acquisition Date 2018-07-12T19:34:21
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
132.40
131.50
131.00
130.39
128.10
127.50
126.70
125.75
125.52
123.94
121.48
121.04
133
131
129
127
125
123
121
f1 (ppm)
Br
Ph
N
O
7
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




| Parameter | Value |
|---|---|
| 1 Title | 5ea-C-dept-400M |
| 2 Origin | Bruker BioSpin GmbH |
| 3 Solvent | CDCl3 |
| 4 Temperature | 299.1 |
| 5 Number of Scans | 11 |
| 6 Acquisition Time | 1.3631 |
| 7 Acquisition Date | 2018-07-12T19:36:00 |
| 8 Spectrometer Frequency | 100.61 |
| 9 Spectral Width | 24038.5 |